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IP1

How to Reveal a Matrix's Rank

While at SIAM LA24 you will find a large fraction of the presentations about low-rank approximation and singular value estimation. Low-rank structure appears in Krylov methods, gravity simulations, and large data sets. In this talk, we will discuss analytical and numerical approaches for revealing low-rank structure across diverse scientific applications. We find that one can analytically bound the singular values of a structured matrix if it satisfies a discrete heat-like equation. On the numerical side, we will explore rank-revealers based on QR and Gaussian elimination and show that so-called local maximum volume pivoting is necessary and sufficient for them to estimate a matrix's singular values. Finally, we will see that large data tables are inherently low-rank, underscoring that low-rank structures have a growing and widespread relevance.

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IP2

Conservation Laws for Gradient Flows

Understanding the geometric properties of gradient descent dynamics is a key ingredient in deciphering the recent success of very large machine learning models. A striking observation is that trained over-parameterized models retain some properties of the optimization initialization. This "implicit bias" is believed to be responsible for some favorable properties of the trained models and could explain their good generalization properties. In this talk I will first rigorously expose the definition and basic properties of "conservation laws", which are maximal sets of independent quantities conserved during gradient flows of a given model (e.g. of a ReLU network with a given architecture) with any training data and any loss. Then I will explain how to find the exact number of these quantities by performing finite-dimensional algebraic manipulations on the Lie algebra generated by the Jacobian of the model. In the specific case of linear and ReLu networks, this procedure recovers the conservation laws known in the literature, and prove that there are no other laws. The associated paper can be found here https://arxiv.org/abs/2307.00144 and the open source code is here https://github.com/sibyllema/Conservation_laws. This is a joint work with Sibylle Marcotte and Rmi Gribonval.

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IP3

Randomly Pivoted Cholesky

Andr-Louis Cholesky entered cole Polytechnique as a student in 1895. During his work as a surveyer for the French army, Cholesky invented a technique for solving positive-definite systems of linear equations. Cholesky's method can also be used to approximate a positive-semidefinite (psd) matrix using a small number of columns, called "pivots". A longstanding question is how to choose the pivot columns to achieve the best possible approximation. This talk describes a simple but powerful randomized procedure for adaptively picking the pivot columns. This algorithm, randomly pivoted Cholesky (RPC), provably achieves near-optimal approximation guarantees. Moreover, in experiments, RPC matches or improves on the performance of alternative algorithms for low-rank psd approximation. Cholesky died in 1918 from wounds suffered in battle. In 1924, his colleague, Commandant Benoit, published Cholesky's manuscript. One century later, a modern adaptation of Cholesky's method still yields state-of-the-art performance for problems in scientific machine learning. Joint work with Yifan Chen, Ethan Epperly, and Rob Webber. Available at arXiv:2207.06503.

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IP4

Randomized Orthogonalization Methods

We discuss the potential of randomization as a viable alternative approach towards orthogonalization. Issues include: strategies for sampling and sketching; matrix concentration inequalities for analysing the error due to randomization; numerical conditioning and stability; and the use of mixed precision arithmetic.

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IP5

Superfast Direct Inversion Methods for Highly Structured Matrices

Highly structured matrices, such as Cauchy, Vandermonde, and Toeplitz matrices, arise in all kinds of contexts in computational math. One important example is the nonuniform discrete Fourier transform matrix, which is essential in various image and signal processing tasks. All of these matrices are only a fast transform away from a collection of rank-structured Cauchy-like matrices. We explain in this talk how this fact can be applied to create extremely efficient rank-structured direct solvers for linear systems involving these matrices. In particular, we highlight a new a least-squares method for solving the inverse nonuniform discrete Fourier transform problem.

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IP6

Global Convergence of Hessenberg Shifted QR

The Shifted QR algorithm is the most widely used algorithm for computing the eigenvalues and eigenvectors of a dense matrix. Rapid convergence of the shifted QR algorithm on real symmetric tridiagonal matrices was shown by Wilkinson more than fifty years ago. In contrast, an understanding of the convergence properties of the shifted QR algorithm on nonsymmetric Hessenberg matrices remained elusive. I will present some recent progress on this question. First I will present a new modification of the Wilkinson shift which converges rapidly on every normal Hessenberg matrix, in exact arithmetic. Then I will show how to generalize it to all diagonalizable Hessenberg matrices whose eigenvectors have a controlled condition number. Finally, I will explain how this yields a shifting rule

which converges rapidly on a small random perturbation of every input matrix, with high probability and in finite arithmetic with a polylogarithmic bound on the number of bits of precision. Joint work with Jess Banks and Jorge Garza Vargas.

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IP7

Eigenstructures of Low-rank Matrix Polynomials (Supported in Cooperation with the International Linear Algebra Society)

Challenging and intriguing mathematical problems involving matrix polynomials arise in various applications. These problems often revolve around the eigenstructures of the polynomials, emphasizing the importance of the eigenstructures. In this talk we consider the set of matrix polynomials of bounded rank and degree and describe the eigenstructures that these polynomials typically have, so called generic eigenstructures. We also find such generic eigenstructures for the sets of symmetric and skew-symmetric matrix polynomials. Notably, these symmetries have drastic effect on generic eigenstructures, for example, on whether we can anticipate the appearance of eigenvalues in the eigenstructures or not. This talk is primarily based on joint work with Froiln Dopico and Fernando De Tran.

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IP8

A Journey in the Kemeny Constant: Centrality Measures, Stochastic Complementation and Infinite-dimensional Matrices (supported in cooperation with the International Linear Algebra Society)

In a Markov chain, the Kemeny constant represents the expected time required to reach a random state, sampled from the stationary distribution, starting from a given initial state. Its formulation, expressed as the trace of a suitable matrix, reveals that this quantity is independent of the given initial state. We provide an overview of the main properties of the Kemeny constant, show some recent applications in network analysis and analyze its interplay with stochastic complementation and its extension to infinite-dimensional matrices. More specifically, a measure of centrality of an edge in a graph is introduced, based on the variation of the Kemeny constant after removing the given edge. Applications to real road networks show that this measure is particularly effective in revealing bottleneck roads whose removal would greatly reduce the connectivity of the network. The interplay of the Kemeny constant of a stochastic matrix and of its stochastic complements leads to explicit expressions for the Kemeny constant of Markov chains with special structures, and to bounds in the general case. For Markov chains with denumerable infinite-state space, the Kemeny constant is always infinite. Instead, for continuous-time Markov processes, the Kemeny constant may be finite or infinite. In this regard, sufficient conditions under which birth-and-death processes have finite Kemeny's constant are discussed.

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IP9

Accurate and Verified Computations in Numerical Linear Algebra

Verified numerical computations aim to know accuracy of results obtained by numerical computations. We focus on how to efficiently know and improve accuracy of computed solutions in numerical linear algebra problems, for example, solving linear systems and eigenvalue problems. When obtaining an initial approximate solution with some working precision in floating-point arithmetic, we may refine it by the use of higher precision arithmetic. Therefore, the idea of mixed precision arithmetic is naturally adapted to iterative refinement. For example, when solving linear systems, single precision arithmetic is first used for performing LU factorization and calculating an initial approximate solution, and then double precision arithmetic is used for refining it. If the computational cost for the refinement process is reasonable, such a mixed precision approach works efficiently, especially for large-scale problems. The main question is how accurate computed solutions are. In many cases, that depends on condition number of a given problem. However, condition number is usually not known beforehand. Thus, another question is how long arithmetic precision is sufficient to obtain an initial approximate solution and refine it. In this talk, we discuss how to utilize and combine verified numerical computations with iterative refinement.

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IP10

Coupled Matrix and Tensor Factorizations Improving our Understanding of Complex Systems Through the Analysis of Temporal and Multimodal Data

There is an emerging need to jointly analyze multimodal data sets and capture the underlying patterns in order to extract insights about complex systems. For instance, joint analysis of omics data (e.g., metabolomics, microbiome, genomics) holds the promise to bring together genomics, phenomics and environment in the quest for precision health. Such data sets are heterogeneous they are a collection of static and dynamic data. Dynamic data can often be arranged as a higher-order tensor (e.g., subjects by metabolites by time) while static data can be a matrix (e.g., subjects by genes). Tensor factorizations have been successfully used to reveal the underlying patterns in higher-order data, and extended to joint analysis of multimodal data through coupled matrix and tensor factorizations (CMTF). However, integrating heterogeneous data sets has still many challenges, especially when the goal is to capture interpretable (time-evolving) patterns. In this talk, we discuss CMTF models and algorithms for temporal and multimodal data mining. We focus on a flexible, accurate and computationally efficient framework (based on Alternating Optimization and Alternating Direction Method of Multipliers) that facilitates the use of a variety of constraints, loss functions and couplings with linear transformations when fitting CMTF models. Through various applications, we discuss the advantages and limitations of

available CMTF methods.

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SP1

SIAM Activity Group on Linear Algebra Early Career Prize: The Growth Factor in Gaussian Elimination

The solution of a linear system, i.e., given a matrix A and vector b, finding a vector x satisfying $Ax = b$, is one of the oldest problems in mathematics. Gaussian elimination is one of the most fundamental and well-known techniques for solving linear systems, by factoring a matrix into the product of a lower and upper triangular matrix. Surprisingly, a number of questions regarding the worst-case stability of this algorithm remains. In this talk, we will study the history of this subject, a story that spans over seventy-five years, and discuss some recent progress.

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SP2

SIAG/LA Best Paper Prize: Recovering Green's Functions with Randomized Numerical Linear Algebra

There is a strong connection between the recovery of structured matrices from matrix-vector products in numerical linear algebra and the growing field of operator learning, which aims to discover properties of unknown physical systems from experimental data. The randomized SVD is one of the most popular algorithms for constructing low-rank approximations to matrices using matrix-vector products with standard Gaussian random vectors. In this talk, we will generalize the randomized SVD to random vectors generated from any multivariate Gaussian distribution. Our approach allows us to extend the randomized SVD to infinite dimensions and approximate Hilbert-Schmidt operators, which are continuous analogues of matrices, from integration against random functions sampled from a Gaussian process. Finally, we will construct a randomized algorithm for recovering Green's functions of elliptic partial differential equations and derive a learning rate to characterize the number of input-output pairs needed to learn Green's functions within a prescribed tolerance.

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CP1

Model Order Reduction for Parametric Generalized EVPs

We investigate the resolution of parametric generalized eigenvalue problems in the form

$$A(\sigma)x(\sigma) = \lambda(\sigma)Mx(\sigma) \tag{1}$$

for given $\sigma \in S$ with $(\lambda(\sigma), x(\sigma)) \in (0, \Lambda) \times \mathbb{R}^n$, $A(S) \subset \mathbb{S}_{++}^{n\times n}$ and $M \in \mathbb{S}_{++}^{n\times n}$. We look for a rapid solution to (**??**) using the Ritz method. We first find a basis for the Ritz subspace $V \subset \mathbb{R}^n$ and solve the EVP in this subspace. We built V using an average matrix $\overline{A}$ related to $(0, \rho\Lambda)$ with the help of a correction formula. For this, we use a sparse collocation operator of the correction function to built the lagrange interpolants of the correction. We finally use the average eigenbasis to solve the problem to estimate the approximation error and prove the convergence rate.

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CP1

A Warm-Started Krylov-Schur Eigensolver

Sequences of eigenvalue problems emerge in a range of applications, for instance when computing the eigenvectors for parametrized partial differential equations. Rather than starting the eigensolver with a single initial vector for each matrix, it may be advantageous to warm-start the Krylov-Schur algorithm with the approximate invariant subspace of a previous matrix in the sequence. However, the approximate invariant subspace for another matrix is generally not a Krylov space for the new matrix, even if it is computed using the Krylov-Schur algorithm. To accommodate for this, we make several critical modifications to Krylov-Schur. We first compute the approximate Krylov decomposition with the smallest backward error, which emits a residual matrix. This is followed by a sequence of Arnoldi iterations, then a Krylov-Schur truncation that takes the residual matrix into account. As the standard convergence test for Krylov-Schur can no longer be used, we propose a straightforward replacement test based on the residual of the eigenvalue problem. We analyze how a cycle of our warm-start Krylov-Schur eigensolver reduces the norm of the residual matrix and demonstrate how this relates to the convergence of the standard Krylov-Schur algorithm to an approximate invariant subspace. We provide good results for sequences of eigenvalue problems arising in several applications, including the numerical simulation of brake squeal.

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CP1

Choleskyqr Type Algorithm and Its Development

CholeskyQR algorithm is a popular QR algorithm which is widely used in both academia and industry. In order to improve the orthogonality, CholeskyQR2 is developed. Furthermore, researchers put a shifted item in the Cholesky factorization and for Shifted CholeskyQR to deal with ill-conditioned matrices. We construct a new norm of the matrix based on column properties and find new proper shifted items which avoids the singular value decomposition and could deal with more ill-conditioned matrices. Also, for some sparse matrices, we may have new shifted items based on the sparsity of the gram matrix which is meaningful in the real practice. Moreover, we explore the connection between CholeskyQR type algorithms and random linear algebra, doing probabilistic error analysis for CholeskyQR

type algorithms and give some results.

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CP1

Computing Largest Singular Triplets of Very Large Sparse Matrices and Applications

We have developed a hybrid restarted Golub-Kahan Lanczos Bidiagonalization (GKLB) algorithm that combines restarting with Ritz vectors with restarting with *iterative refined Ritz vectors* to compute the largest singular triplets of large sparse matrices. The iterative refined Ritz vectors is a new strategy based on refined Ritz approximations that has proven via numerical examples to perform very well when using small subspaces. The method uses only matrix-vector products with the large matrix combined with computing the SVD of a 2×2 and a 3×2 matrix which can easily and quickly be handled with simple LAPACK routines. This allows for an overall simple, yet fast software that can easily be implemented in different programming languages. Time permitting, we will discuss the details of explicit deflation for any GKLB based method (e.g., MATLABs svds) to compute the next set of largest singular triplets of a matrix from an already computed partial singular value decomposition.

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CP1

A General Framework for Inverse-Free Spectral Divide-and-Conquer

Recent developments in randomized numerical linear algebra produced the first divide-and-conquer eigensolvers that can diagonalize any matrix or matrix pencil. The key insight of this work is the phenomenon of pseudospectral shattering, which implies a procedure for reliably dividing the spectrum of a perturbed matrix or pencil with high probability. Once a divide is chosen, these algorithms proceed with divide-and-conquer as usual, computing spectral projectors that split the original problem in two. Consequently the methods are flexible, allowing the building blocks of divide-and-conquer to be adjusted without impacting the accuracy of the final result. With this in mind, we present a general framework for developing (and analyzing) routines that compute spectral projectors, for both the standard and generalized eigenvalue problems. We exhibit a number of alternatives to the most popular choice the Newton iteration for the matrix sign function each of which admits an inverse-free implementation using only QR and matrix multiplication. With an eye toward high performance implementations of general, randomized eigensolvers, our goal is to refine this step of divide-and-conquer in terms of complexity and stability.

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CP1

Investigation of the Effects of Initial Guess and Subspace Iteration Acceleration on Feast Solver

Symmetric eigenvalue problems arise from various scientific applications. One of the state-of-the-art solution techniques is the FEAST algorithm, which can be considered as an accelerated subspace iteration that approximates the spectral projector of the desired eigenspace by utilizing contour integration techniques. In this work, we study the effects of the initial guess and various hybrid approaches on the convergence rate of FEAST. Additionally, we study the impact of hybrid approaches for accelerating (and stabilizing) FEAST for different initial guesses. By iterating the inverse subspace method a few times, we create an approximate eigenspace and use it as an initial guess for FEAST. This preprocessing cost can be amortized by the performance improvement of FEAST. Moreover, we observe that enforcing orthogonalization of the eigenspace further accelerates FEAST. Nevertheless, the orthogonalization process is costly; hence, there is also a trade-off between the FEAST iteration count and cost. In the study, we propose several variants of FEAST, including applying QR factorization in each iteration, as well as hybrid methods, such as alternating FEAST and inverse subspace iterations. As an additional benefit, numerical results show that proposed variants decrease the likelihood of the appearance of spurious eigenvalues and make it possible to use a smaller subspace dimension than originally suggested.

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CP2

Geometry of Interval Linear Systems

Linear interval systems are linear systems of equalities and inequalities, where the real coefficients are replaced by intervals. This enables computation that takes into account

rounding errors and limited resolution. The solution sets are generally non-convex since they are composed of exponentially many convex polyhedra, thus many associated problems are NP-hard. On the other hand, the forms the solution sets can take are strongly constrained by clear rules that make them interesting to study. We set out to explore the geometry of these sets. First, we characterize the conditions for convexity and give an intuitive description of the topological boundary and interior. Then, we show that the closure of the convex hull is a convex polyhedron with some additional convenient properties. It is known that for systems of equalities with invertible matrices, the solution set has exponentially many unique vertices, which are also the vertices of the convex hull. We extend this by showing that for the case of inequalities, we simply get an affine cone with a unique vertex and only linearly many spanning rays as a convex hull, with the added caveat that computing these is still hard. Were we to find an efficient description of the convex hull for some special type of interval matrix, we could reduce Interval Linear Programming problems to ordinary Linear Programming.

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CP2

Adaptively Restarted Block Krylov Subspace Methods with Low-Synchronization Skeletons

With the recent realization of exascale performance by Oak Ridge National Laboratorys Frontier supercomputer, reducing communication in kernels like QR factorization has become even more imperative. Low-synchronization Gram-Schmidt methods, first introduced in Swirydowicz et al. (Numer. Lin. Alg. Appl. 28(2):e2343, 2020), have been shown to improve the scalability of the Arnoldi method in highperformance distributed computing. Block versions of low-synchronization GramSchmidt show further potential for speeding up algorithms, as column-batching allows for maximizing cache usage with matrix-matrix operations. In this work, low-synchronization block Gram-Schmidt variants from Carson et al. (Linear Algebra Appl. 638:150195, 2022) are transformed into block Arnoldi variants for use in block full orthogonalization methods (BFOM) and block generalized minimal residual methods (BGMRES). An adaptive restarting heuristic is developed to handle instabilities that arise with the increasing condition number of the Krylov basis. The performance, accuracy, and stability of these methods are assessed via a flexible benchmarking tool written in MATLAB. The modularity of the tool additionally permits generalized block inner products, like the global inner product.

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CP2

Inner-outer Krylov Solvers with Deflated Restarting for High-Fidelity CFD Simulations

In the present work, we evaluate robustness and efficiency of inner-outer Krylov solvers with deflated restarting approaches (FGMRES-DR, FGCRO-DR) to address large, sparse and ill-conditioned linear systems arising from high-fidelity simulations in computational fluid dynamics (CFD). The considered matrices are real, nonsymmetric, not positive definite, with a symmetric sparsity pattern containing dense blocks. The flexible preconditioning operator is defined by an inner GMRES solver that uses the Block-ILU(0) algorithm as a first-level preconditioner and the Restricted Additive Schwarz (RAS) method as a second-level preconditioner. Numerical experiments with the ONERA Aghora code based on high-order discontinuous Galerkin (DG) discretization methods are conducted to assess the performances of these strategies.

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CP2

Comparative Study of Mixed-Precision and Low-Rank Compression Techniques in Sparse Direct Solvers.

Sparse direct solvers play a crucial role in numerical simulation and are one of the most time-consuming steps in many applications. Recently, many efforts have been made to reduce the complexity of dense and sparse direct solvers by introducing low-rank compression techniques. These techniques allow applications to reduce the amount of information stored in the matrix, depending on the quality of the solution being sought, and greatly reduce both memory requirements and computational complexity. Another solution driven by the computational capabilities of the hardware is the use of mixed-precision computations. This has been continuously in vogue with new generations of hardware providing single to double performance ratios of more than two. In our study, we extend the sparse direct solver PaStiX to use reduced-precision factorization and compare it to its low-rank strategy in terms of time to solution, numerical stability, memory consumption, and energy consumption. The goal of this study is to evaluate whether the tradeoff between computational speed and solution accuracy is worthwhile, and if so, which strategy, low-rank or mixed-precision, is better.

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CP2

Accurate Computations with Some Subclasses of Totally Positive Matrices

We say that a matrix is totally positive if all its minors are nonnegative. The bidiagonal decomposition of a nonsingu-

lar totally positive matrix provides a natural parametrization to perform algebraic operations to high relative accuracy. In fact, if the bidiagonal decomposition is known with high relative accuracy, then the computation of the inverse of the matrix, of its eigenvalues or of its singular values can be also performed with high relative accuracy. However, the obtention of the bidiagonal decomposition to high relative accuracy has been got, up to now, only for a few subclasses of nonsingular totally positive matrices. Recent advances on this subject are presented in this talk. In particular, we show new subclasses of nonsingular totally positive matrices, relevant in several fields, for which the bidiagonal decomposition has been obtained with high relative accuracy.

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CP2

Global GMRES Method for Sylvester Quaternion Matrix Equations

We consider the solution of a large-scale and sparse Sylvester matrix equation over the skew-field of quaternions by means of a global GMRES method. The approach that we propose operates on a space of quaternion matrices over real numbers, and is based on a real inner product defined on this space. Orthonormal bases are constructed gradually for quaternion Krylov subspaces of this space by an Arnoldi process and by making use of the associated Sylvester operator. The proposed global GMRES method seeks the best solution of the Sylvester quaternion matrix equation in the constructed quaternion Krylov subspaces. Finally, we illustrate the efficiency and convergence of the proposed approach on several synthetic examples.

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CP3

Kirigami Metamaterial Design Using Linear Algebra

Kirigami, the art of paper cutting, has been widely used for the design of mechanical metamaterials in recent years. However, most prior approaches for kirigami design either focus only on creating simple periodic patterns or require solving complicated optimization problems to generate more complex patterns. Here, we present an efficient method for the inverse design of kirigami-based mechanical metamaterials using linear algebra. Specifically, by considering the negative spaces in a quad kirigami structure as four-bar linkages, we can identify a simple relationship between adjacent linkages and formulate the kirigami design problem as a matrix multiplication, which allows us to easily decouple different fields in the design space of kirigami. By encoding different physical properties such as compatibility, reconfigurability and rigid-deployability into the design matrix in the equation, we can create a wide range of kirigami patterns.

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CP3

A Bayesian Framework for Cryo-Em Heterogeneity Analysis Using Regularized Covariance Estimation

Proteins and the complexes they form are central to nearly all cellular processes. Their flexibility, expressed through a continuum of states, provides a window into their biological functions. Cryogenic-electron microscopy (cryo-EM) is an ideal tool to study these dynamic states as it captures specimens in non-crystalline conditions and enables high-resolution reconstructions. However, analyzing the heterogeneous distribution of conformations from cryo-EM data is challenging. Current methods face issues such as a lack of explainability, overfitting caused by lack of regularization, and a large number of parameters to tune; problems exacerbated by the lack of proper metrics to evaluate or compare heterogeneous reconstructions. To address these challenges, we present RECOVAR, a white-box method based on principal component analysis (PCA) computed via regularized covariance estimation that can resolve intricate heterogeneity with similar expressive power to neural networks with significantly lower computational demands. RECOVAR is rooted in the estimation of the covariance matrix of conformations based on: (1) a particular discretization, under which the covariance estimator reduces to a Hadamard system, (2) an efficient regularization scheme based on dataset partition, (3) a randomized SVD-like method to extract principal components of the massive and implicitly defined covariance matrix.

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CP3

Parallel High-Resolution Compact PFFT-Type Algorithms for 3D Stochastic Subsurface Scattering Problems.

In this talk, we present efficient parallel compact high-resolution algorithms for the solution of a stochastic subsurface electromagnetic scattering problem. The methods are based on a combination of the GMRES method and a partial FFT-type (PFFT) lower-order deterministic preconditioner. The four and six-order compact finite difference schemes and the second-order finite element approach are considered for the solution of the 3D stochastic Helmholtz equation. The PFFT preconditioner utilized the fast implementation of low-dimensional eigenvectors solvers to efficiently implement the developed iterative approach. The convergence analysis of the proposed iterative method for the stochastic scattering problem is analyzed based on an extension of the approaches proposed by authors in previous publications to analyze the deterministic subsurface solvers. The parallel variants of the developed algorithms are implemented in OpenMP, MPI, and hybrid environments. The complexity and scalability of the methods are analyzed on scattering problems with realistic ranges of parameters in soil and mine-like targets.

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CP3

Data Assimilation for Quantum Nv Diamond Spectroscopy

Nitrogen-vacancy (NV) defect centers in diamond have generated much interest for their uses in quantum information and sensing. Negatively charged centers (NV-) are used for high spatial-resolution sensing and for quantum information. In this work we construct a statistical model for NV spectroscopy and use it in synthetic experiments to solve inverse problems. Our principal application is to develop a primary sensor based on the NV diamond quantum optical properties. This is a significant challenge because the NV diamond structure is sensitive to temperature and pressure as well as magnetic and electric fields, including electromagnetic fields of nearby atoms and molecules. First, using the Hamiltonian for the effects of local strain and the environmental variables, we identify the observable components based on the invertibility of various observation systems. Next, we observe the influence of temperature and pressure on the NV center by solving the Schrdinger Equation and computing the theoretical spectroscopy curve. We assume that the observed photon counts are Poisson random variables with rates proportional to the theoretical spectroscopy. Then, using the Maximum Likelihood Estimation we find the parameter values that maximize the likelihood. Last but not the least we determine the robustness of the model using sensitivity analysis.

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CP3

Parallel Coordinate Descent Methods for Full Configuration Interaction

Solving the time-independent Schrdinger equation gives us full access to the chemical properties of molecules. Among all the ab-initio methods, full configuration interaction (FCI) provides the numerically exact solution under a predefined basis set. However, the FCI problem scales exponentially with respect to the number of bases and electrons and suffers from the curse of dimensionality. The FCI problem could be reformulated as an unconstrained minimization problem. This work proposes a novel algorithm to address the minimization problem. The algorithm introduces an extra search dimension to enable the exact line search for the multi-coordinate descent method, which could be fully parallelized. Hence, the proposed algorithm benefits from both exact line search and parallelization. Numerically, we demonstrate the parallel efficiency of the algorithm. The algorithm achieves better energy and parallelism on systems with approximately a hundred electrons than other existing methods.

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CP4

Deflated Gauss-Newton Methods

Objective functions with many local minima are one of the biggest obstacles to finding the global minimum of non linear least squares problems. In this talk we will discuss deflated Gauss-Newton methods designed to systematically find all local minima of a problem, and thus the global minima. We will then cover the application of these methods to inverse eigenvalue problems associated with inelastic neutron scattering. This is joint work with Marcus Webb (University of Manchester) and Mike Baker (Dept Chemistry, University of Manchester).

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CP4

Matrix Balancing Based Interior Point Methods for Point Set Matching Problems

Point sets matching problems can be handled by optimal transport. The mechanism behind it is that optimal transport recovers the point-to-point correspondence associated with the least curl deformation. Optimal transport is a special form of linear programming with dense constraints. Linear programming can be handled by interior point methods, provided that the involved ill-conditioned Hessians can be computed accurately. During the decade, matrix balancing has been employed to compute optimal transport under entropy regularization approaches. The solution quality relies on two factors: the accuracy of matrix balancing and the boundedness of the dual vector. High accurate matrix balancing is achieved by the application of Newton methods on a sequence of matrices along a central path. In this work, we apply sparse support constraints to matrix-balancing based interior point methods, in which the sparse set fulfilling total support is iteratively updated to truncate the domain of the transport plan. Total support condition is one crucial condition, which guarantees the existence of matrix balancing as well as the boundedness of the dual vector.

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CP4

A New Self-adaptive Inertial Algorithm for Solving Variational Inclusion Problems with Applications

Developing iterative schemes to tackle variational inclusion problems (VIP) has been a dynamic research field for several decades. In this presentation, we will provide an overview of the current algorithms designed to solve VIPs within a specific class. Additionally, we will introduce a novel and efficient algorithm based on the Mann method for VIP resolution. This approach incorporates inertial extrapolation terms and self-adaptive step sizes, offering improved convergence properties without the need for stringent conditions. This version is more flexible, featuring easily implementable criteria for the inertial factor and relaxation parameter. Finally, we will present some

numerical experiments to demonstrate the practical implementation and comparative performance of the proposed algorithm.

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CP4

An Efficient and Accurate Iterative Method for Solving Bilevel Variational Inequality Problems with Some Applications

The study of Bilevel Variational Inequality Problems (BVIP) has long been a subject of intense research interest, owing to the diverse applications in various fields such as science, engineering, medicine, cryptography, image and signal processing, and optimal control. In this presentation, we give an overview of some methods proposed over time to solve variational inequality problems including bilevel case. In particular, this talk will introduce our recently proposed iterative scheme for solving BVIP involving monotone operators. The presence of the inertial parameter and more efficient step-size make the proposed algorithm a very robust scheme. Furthermore, our iterative scheme involves a single projection onto half-space which contributes to the reduction in the computational cost compared to some existing related work. Finally, we demonstrate the effectiveness of our proposed algorithm through some numerical experiments, highlighting its efficiency and clear advantages.

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CP4

A Self-Adaptive Iterative Method for Solving Split Variational Inclusion Problem with Applications

In this study, we propose a new inertial viscosity-type method with self- adaptive step sizes for approximating the solution of the problem called Split Hierarchical Monotone Variational Inclusion Problem with multiple output sets in real Hilbert spaces. We propose and analyze a new viscosity-type iterative method for solving this class of problems. The convergence analysis of the proposed iterative method under some suitable conditions is studied. The presence of the inertial parameter and the efficient step size make the proposed method more robust. We show that the sequence of iterates generated by this method converges strongly to a minimum-norm solution of the problem. Finally, we present some numerical experiments to illustrate the practical potential and effectiveness of our proposed method.

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CP5

Preconditioner Design Using the Bregman Log-Determinant Divergence

We present a framework for preconditioning Hermitian positive definite linear systems based on the Bregman log determinant divergence. This divergence provides a measure of discrepancy between a preconditioner and a target matrix, giving rise to the study of preconditioners given as the sum of a Hermitian positive definite matrix plus a low-rank correction. We describe under which conditions the preconditioner minimises the ℓ_2 condition number of the preconditioned matrix, and obtain the low-rank correction via a truncated singular value decomposition (TSVD). Numerical results from variational data assimilation (4D-VAR) support our theory. We also apply the framework to approximate factorisation preconditioners with a low-rank correction (e.g. incomplete Cholesky plus low-rank). In such cases, the approximate factorisation error is typically indefinite, and the low-rank correction described by the Bregman divergence is generally different from one obtained as a TSVD. We compare these two truncations in terms of convergence of the preconditioned conjugate gradient method (PCG) and show numerous examples where PCG converges to a small tolerance using the proposed preconditioner, whereas PCG using a TSVD-based preconditioner fails. We also consider matrices arising from interior point methods for linear programming that do not admit such an incomplete factorisation by default, and present a robust incomplete Cholesky preconditioner based on the proposed methodology.

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CP5

Matrix Nearness Problems with Structure Rank Constraints

We consider the rank-structured matrix nearness problems for symmetric positive definite (SPD) matrix. The problems are motivated by the computational advantage of rank-structured matrix, and the solution of such problems can thus be applied to e.g., Gaussian process regression and for preconditioning. Our focus is on matrices with hierarchical off-diagonal low-rank (HODLR) structure. We formulate some matrix nearness problems with different discrepancy criteria and rank-structure constraints to address different problem assumptions. We derive closed-form solutions for some of the matrix nearness problems, and we use them to construct an efficient, SPD-preserving greedy approximation scheme for computing HODLR approximations that preserve positive definiteness. We then briefly discuss the practical implementations, and we will illustrate the advantages and limitations of the method with some numerical results.

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CP5

Low Rank Method for Multi-Output Gaussian Processes with Structured Data

Gaussian processes offer flexible and sophisticated methods to regress data for interpolation purposes. We consider data consisting of multiple sets of time dependent values and we model each of them as a Gaussian Process. Including the (hidden) connection between these sets leads to a Multi-Output Gaussian Process (MOGP) model giving rise to a graph structure with time dependent values on the nodes. To calculate the mean vector and the covariance matrix including the information encoded in the graph edges we need to solve a linear system with a shifted kernel matrix which leads to fast rising computational costs. We propose the use of an iterative solver utilizing the Kronecker product structure of the Multi-Output covariance matrix. For this a low rank conjugate gradient matrix algorithm will be presented and we will test the performance on different sized datasets.

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CP5

Nonlinear Adm Method for Low Rank Representation of Noisy and Incomplete Data

Sparse representation may not capture the global structures of the data. Low rankness may be a more appropriate criterion. Low rank representation at data aims at finding the lowest rank representation of the observation data X affected by noise/ measurement error E. With the help of an appropriate dictionary (or basis) matrix $A \in \mathbb{R}^{m\times n}$, the underlying row space can be recovered via the lowest rank representation such that the true segmentation of data can be correctly revealed. Thus, the Low-Rank Representation (LRR) method can suitably handle the data extracted from a union of multiple subspaces. In this paper, we propose a nonlinear alternate direction method to solve the LRR problem for incomplete and noisy data. Incompleteness is accounted by linearly projecting the incomplete data matrix, N onto the completion argument of the incomplete data matrix M, i.e., $P_\Omega(N) = M$. This problem can be further generalized to the case where the matrix $N = AZ + E$ is not determined by itself but instead by a more general directionary matrix A. We compare its performance against state-of-the-art methods on various matrix size, noise and percentage of incompleteness.

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CP5

Maximum-Volume Matrix Factorization

Nonnegative matrix factorization with a maximum volume criterion (maxvol NMF) is an identifiable regularized low-rank model that has not been studied as much as its counterpart minimum-volume NMF (minvol NMF). Given a matrix dataset X, maxvol NMF consists in finding two nonnegative low-rank factors, W and H, such that their product approximates X while the volume spanned by the origin and the rows of H is as large as possible. This maxvol criterion, combined with nonnegativity, will incite H to be sparser. In minvol NMF, the volume criterion is on W and should be minimized. In the exact case, that is, $X = WH$, minvol NMF is equivalent to maxvol NMF. Here, we show that maxvol MF behaves rather differently than minvol MF in the presence of noise, especially when the penalty on the volume criterion is increased. We also show how maxvol NMF creates a continuum between NMF and orthogonal NMF which imposes the rows of H to be orthogonal. Finally, we propose several algorithms to solve maxvol NMF, which we apply on real datasets.

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CP5

Truncation Strategy for Truncation Preconditioners for Stochastic Galerkin Finite Element Method with Log-Normal Random Field

Stochastic Galerkin finite element methods (SGFEM) are one of the powerful numerical methods for elliptic partial differential equations with random data. However, applying SGFEM to such a problem results in a very large coupled linear system. Particularly, if the diffusion coefficient is expanded by generalized polynomial chaos (gPC) expansion, then the stochastic Galerkin matrix is block-dense. Therefore, an efficient iterative solver such as Krylov subspace methods is required to solve such problems and preconditioning techniques are crucial to improve the efficiency of the iterative solvers. Recently, the truncation preconditioners with standard truncation or adaptive truncation have been studied and it has been shown that they can improve the rate of convergence of the linear solvers. In this work, we assume the diffusion coefficient in the elliptic problem to be lognormal and we introduce a new truncation strategy for the truncation preconditioner. The diffusion coefficient is represented by a gPC expansion. The new truncation strategy aims to capture the important features of the stochastic Galerkin matrix and preserve some properties of the system matrix such as positivity. We will compare the speed of convergence of our truncation preconditioner with our truncation strategy with other existing preconditioners such as the mean-based and the Kronecker product preconditioners in terms of iteration counts.

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CP6

Inertial Alternating Direction Method of Multipli-

ers for Non-Linear Matrix Decompositions

Low-rank matrix approximations are widely used in many fields such as data analysis and machine learning. Recently, there has been a growing interest in exploring nonlinear matrix decompositions (NMDs): given a matrix X, find low-rank factors W and H such that $X \approx f(WH)$, where f is an element-wise nonlinear function. When dealing with nonnegative and sparse matrices, as commonly encountered in document data sets, it becomes meaningful to consider $f(\cdot) = \max(0, \cdot)$, representing the rectified linear unit (ReLU) activation. This variant is referred to as ReLU-NMD. The talk will provide a brief overview of the existing applications and state-of-the-art algorithms for ReLU-NMD. Notably, existing algorithms do not directly address ReLU-NMD; instead, they tackle a latent-variable model that is not equivalent to the original problem. In response to this gap, our work introduces an inertial alternating direction method of multipliers (iADMM) designed to directly address the ReLU-NMD. Our proposed iADMM provides a better solution than the state of the art. Furthermore, we demonstrate the adaptability of the iADMM algorithm to other nonlinear models, such as $f(WH) = (WH)^{\cdot 2}$ and $f(WH) = \max(a, \min(WH, b))$, which have practical applications in the representation of probabilistic circuits and recommender systems, respectively.

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CP6

Non-Convex Algorithms for the Computation of the Nonnegative Rank

The nonnegative rank of a nonnegative matrix X is the minimum number of nonnegative rank-one factors required for the exact reconstruction of X. It is of significance in diverse fields such as data mining, graph theory, and computational geometry. Its computation, however, remains a challenging task, since (i) it is an NP-hard problem, and (ii) no practical algorithm is known for its computation. In this work, based on non-convex optimization, we propose a first exact algorithm which can be used on matrices of moderate sizes. This novel idea also extends to the computation of the main lower bounds on the nonnegative rank. We demonstrate the efficacy of our proposed methods on synthetic matrices and on slack matrices of polytopes for which the computation of the nonnegative rank is of great importance.

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CP6

The Hypermatrix Factor Model: A Non-Negative Tensor Model for Multi-Omics Integration

Analyzing multi-omic data using tensor methods offers several advantages over matrix-based approaches. Multi-omic data encompasses many biological data types, including methylation, histone modifications and histone variants, three-dimensional genome, and transcriptome, each adding an additional dimension to the dataset. When such data is treated as a collection of matrices, however, critical information is lost. This is analogous to the fact that the eigenvalues of a matrix are lost when the entries of the matrix are reorganized as a vector. Here, we introduce a nonnegative tensor model for multi-omics, called the Hypermatrix Factor Model. This model finds a low rank factorization of a non-negative three-fold tensor with first two components equal. This model is a generalization of both Non-Negative Matrix Factorization (NMF) and Principal Component Analysis (PCA) that is particularly well-suited for Hi-C datasets. We show that Non-Negative Tensor Factorization and Non-Negative Matrix Factorization can equally infer the A and B chromosomal compartments in high resolution and low resolution Hi-C data. This demonstrates that linear relationships among genomic bin interactions alone determine A/B compartments. We further show that the Hypermatrix Factor Model can infer chromosomal subcompartments from multic-omic data and provides a better clustering of chromatin territories than Non-Negative Matrix Factorization and Principle Component Analysis.

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CP6

Using Orthogonally Structured Positive Bases for Constructing Positive k-Spanning Sets with Cosine Measure Guarantees

Positive spanning sets span a given vector space by nonnegative linear combinations of their elements. These have attracted significant attention in recent years, owing to their extensive use in derivative-free optimization. In this setting, the quality of a positive spanning set is assessed through its cosine measure, a geometric quantity that expresses how well such a set covers the space of interest. In this paper, we investigate the construction of positive k-spanning sets with geometrical guarantees. Our results build on recently identified positive spanning sets, called orthogonally structured positive bases. We first describe how to identify such sets and compute their cosine measures efficiently. We then focus our study on positive k-spanning sets, for which we provide a complete description, as well as a new notion of cosine measure that accounts for the resilient nature of such sets. By combining our results, we are able to use orthogonally structured positive bases to create positive k-spanning sets with guarantees on the value of their cosine measures.

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CP6

Algorithms for Nonlinear Matrix Decomposition with the Relu Function

In this talk, I will study the following nonlinear matrix decomposition (NMD) problem: given a matrix X, find a low-rank matrix Θ such that $X \approx f(\Theta)$, where f is an element-wise nonlinear function. I will focus on the so-called ReLu-NMD, where $f(\cdot) = \max(0, \cdot)$, the rectified unit (ReLu) non-linear activation, in which case X should

be sparse and nonnegative. I will review the current existing algorithms developed to tackle ReLu-NMD, and then introduce two new algorithms: (1) aggressive accelerated NMD (A-NMD) which uses an adaptive Nesterov extrapolation to accelerate an existing algorithm by Saul (SIAM J. Math. Data Sci., 2022), and (2) three-block NMD (3B-NMD) which parametrizes $\Theta = WH$ and leads to a significant reduction in the computational cost. I will illustrate the effectiveness of the proposed algorithms on synthetic and real-world data sets, also discussing some applications.

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CP6

Orthogonal Symmetric Nonnegative Matrix Tri-Factorization

Given a nonnegative n-by-n symmetric matrix X and a factorization rank r, Symmetric Nonnegative Matrix Tri-Factorization (SNMTF) looks for a nonnegative n-by-r matrix W and a nonnegative r-by-r symmetric matrix S such that WSW^T is the best possible approximation of X. This model has been used successfully in community detection, topic modeling, and hidden Markov chains. For example, in community detection, X is the adjacency matrix of a graph, and each column of W will correspond to a community while S will indicate the interactions between the communities. Imposing that the columns of W are orthogonal imply that each row of W has at most one positive entry, meaning that each node of the graph can belong to at most one community. In this work, we propose a new coordinate descent method to tackle orthogonal SNMTF. We illustrate its effectiveness compared to the state of the art on synthetic and real-world data sets.

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CP7

Multipreconditioning with Domain Decomposition for High-Frequency Helmholtz Problems

We consider the use of multipreconditioning, which allows for multiple preconditioners to be applied in parallel, on high-frequency Helmholtz problems. Typical applications present challenging sparse linear systems which are complex non-Hermitian and, due to the pollution effect, either very large or else still large but under-resolved in terms of the physics. These factors make finding general purpose, efficient and scalable solvers difficult and no one approach has become the clear method of choice. In this work we take inspiration from domain decomposition strategies and, in particular, sweeping methods which have gained notable interest for their ability to yield nearly-linear asymptotic complexity and which can also be favourable for high-frequency problems. While successful approaches exist, such as those based on higher-order interface conditions, perfectly matched layers (PMLs), or complex tracking of wave fronts, they can often be quite involved or tedious to implement. We investigate the use of simple sweeping techniques applied in different directions which can then be incorporated in parallel into a multipreconditioned GMRES strategy. Each sweep consists of solving smaller Helmholtz problems, which need not be done to high accuracy, for which we can use the same strategy recursively or else any other effective Helmholtz solver; this allows the potential for a matrix-free approach. Numerical results will demonstrate the strengths of our overall solver strategy.

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CP7

A Diagonalization-Based Parallel-in-Time Preconditioner for Instationary Flow Control Problems

PDE-constrained optimization problems arise in various applications in industry and can also be useful in other mathematical fields. Applications can be found in physics, chemistry, biology, medical imaging, optimal transport, and many other areas. Due to the lack of analytical solutions to these problems in general, the fast and robust numerical solution is of utmost importance. However, the discretization of such problems often results in huge-scale systems of linear or possibly also non-linear equations. Black-box solvers, such as direct solvers for linear systems, often fail when applied to these systems. During recent years, preconditioned iterative methods have been successfully applied to a range of PDE-constrained optimization problems, including large-scale flow control problems, on which we focus here. In this talk, we will explore a diagonalization-based approach to create effective preconditioners for a range of problems, including unsteady Stokes and Oseen control. Our methodology involves approximating the original problem by a time-periodic equivalent, allowing us to perform a temporal diagonalization. This results in a parallel-in-time preconditioner tailored for solving complex flow control problems. Our approach demonstrates robustness with respect to model parameters

and the discretization.

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CP7

Multilevel Tau Preconditioners for sSymmetrized Multilevel Toeplitz Systems with Applications to Solving Space Fractional Diffusion Equations

In this work, we propose a novel preconditioner for solving space-fractional diffusion equations. Following standard discretization, the resultant linear system is a non-symmetric, multilevel Toeplitz system. Through a simple symmetrization strategy, we convert the original linear system into a real symmetric multilevel Hankel system. Subsequently, we introduce a symmetric positive definite multilevel Tau preconditioner for this Hankel system, which can be implemented efficiently using discrete sine transforms. We demonstrate that mesh-independent convergence can be achieved using the minimal residual method. Specifically, the eigenvalues of the preconditioned matrix are bounded within intervals containing 1, without extreme outliers. We provide numerical examples that critically discuss the results, showcase the spectral distribution, and support the efficacy of our preconditioning strategy.

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CP7

Cholesky-Like Preconditioner for Hodge Laplacians via Heavy Collapsible Subcomplex

Techniques based on higher-order Hodge Laplacian operators L_k are widely used to describe the topology as well as the governing dynamics of higher-order systems modelled as simplicial complexes and all require the solution of a number of least square problems with L_k as coefficient matrix to e.g. compute some portions of the spectrum or integrate the dynamical system. Based on the notion of optimal collapsible subcomplex, in this work, we present a fast combinatorial algorithm for the computation of a sparse Cholesky-like preconditioner for L_k that directly exploits the topological structure of the simplicial complex. The performance of the developed preconditioner is tested for CGLS on a variety of simplicial complexes with different dimensions and edge densities and it is shown that, for sparse simplicial complexes, it significantly reduces the condition number and performs better than standard incomplete Cholesky.

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CP7

Robust and Efficient Preconditioners for Generalised Double Saddle Point Problems Arising in Stokes-Darcy Systems

Linear systems with generalised double saddle point structure, where the matrix is not necessarily symmetric, arise in discretisations of many applications, e.g. surface/subsurface flow interactions. Such linear systems are often large, sparse, and ill-conditioned, which leads to slow convergence of the GMRES method. To accelerate convergence, efficient and robust preconditioners are required. In this talk, we present several preconditioners for coupled Stokes-Darcy problems and analyse the spectra of the preconditioned systems. Since applying exact preconditioners is computationally expensive, we develop inexact versions that are spectrally equivalent to the exact variants. We demonstrate the effectiveness and robustness of the proposed preconditioners in numerical experiments for modelling Stokes-Darcy problems describing coupled systems of free flow and porous media.

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CP7

Mass Lumping Techniques for Isogeometric Analysis

Explicit time integration schemes coupled with Galerkin discretizations of time dependent PDEs in structural dynamics require solving a linear system with the mass matrix at each time step. The repeated solution of those linear systems has long been acknowledged as one of the most expensive steps in the solution process but is further exacerbated in isogeometric analysis. Moreover, the stringent constraint on the step size stemming from the outlier eigenvalues leads to an increasingly large number of linear systems. Instead of solving those linear systems exactly, practitioners resort to ad hoc approximations, with mass lumping being one of its best known examples. Mass lumping has a long history and consists in replacing the mass matrix in the time integration scheme by some diagonal approximation. Among the scores of methods proposed for classical finite element methods, only a handful are applicable to isogeometric analysis. The row-sum technique is one of them. In this talk, we provide a linear algebra view on mass lumping, identify some of its desirable properties and later extend them to families of non-diagonal matrices, including banded matrices and Kronecker products whose structure allows to solve linear systems very efficiently. These techniques pave the way to an even larger class of methods applicable to nontrivial problems.

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CP8

High-order Ordinary Differential Operators:

Eigenvalues, Eigenpolynomials and Relationships Among Them

Given a finite order differential operator

$$L \equiv \sum_{i=0}^{N} a_i(x)\partial_x^i,$$

we consider the sequence of eigenvalues $\{\lambda_n\}$ and the sequence of polynomials $\{P_n\}$ which are eigenfunctions of L, that is,

$$\sum_{i=1}^{N} a_i(x)\partial_x^i P_n(x) = \lambda_n P_n(x)\,, \quad \forall n \in \mathbb{N}.$$

The first goal of this work is to show that each eigenvalue λ_i with $i > N$ can be expressed as a linear combination of $\{\lambda_1, \ldots, \lambda_N\}$. Additionally, we define a sequence $\{\delta_n^{(k)}\}$ as

$$\delta_n^{(k)} = \sum_{i=k}^{n} \binom{n}{i} i! a_{i,i-k}, \quad k = 0, 1, \ldots, n,$$

where $a_{i,i-k}, i = k, \ldots, n$ are the coefficients of $a_i(x)$, this is,

$$a_i(x) = a_{i,i}x^i + \cdots + a_{i,1}x + a_{i,0}.$$

This sequence plays a pivotal role in obtaining the explicit expression of the eigenvalues and eigenfunctions. Then, our second goal is to show that for a fixed k, each $\delta_n^{(k)}, n > N$, depends linearly on $\delta_k^{(k)}, \ldots, \delta_N^{(k)}$. Finally, we study some particular cases. Acknowledgements: Work partially supported by Agencia Estatal de Investigacin, Ministerio de Ciencia e Innovacin, Spain, under grants PID2019-106362GB-I00 and PID2021-122154NB-I0.

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CP8

A Finite Sample Analysis of the Spiked Covariance Model Using New Eigenvalue Perturbation Inequalities

Principal Component Analysis (PCA) is a very useful standard technique for high dimensional data analysis which is widely used in many fields of experimental science and engineering. PCA has been generalized in various directions, such as Robust PCA [candes2011robust] and Sparse PCA [zhang2012sparse]. The problem of studying the error between the empirical and the theoretical covariance matrices has been the subject of a tremendous research activity in the past years, at the crossroads of Probability Theory and Functional Analysis, as it is related to the Kannan, Lovazs and Simonovits conjecture. Very intriguing stochastic phenomena have also been subject to extensive research for a variant of the PCA problem, named the Spiked Covariance Model, where a signal detection threshold was discovered in [**?**]. When all but finitely many eigenvalues of the expected covariance matrix are sufficiently large, the main theorem of [baik2005phase] characterised a precise asymptotical phase transition providing an explicit level above which these eigenvalues can be detected. The case of real Wishart matrices was studied in [nadler2008finite], [mo2012rank] and [bloemendal2013limits]. The goal of the present work is to propose a refined analysis in the spirit of [nadler2008finite], using novel and more precise eigenvalue perturbation lower and upper bounds that may be of interest to the Linear Algebra community in their own right.

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CP8

A Conjecture on the Eigenvalues of a Class of Mass Action Jacobian Matrices

The eigenvalues of the Jacobian matrix are used to determine the stability of an equilibrium point of a system of differential equations. In this talk, we consider the Jacobian matrices of systems modeled with mass action kinetics, in particular those derived from exactly one chemical reaction of the form $X+Y \to Z$. We present a conjecture that these matrices, which we refer to as matrices with one combining term, cannot have eigenvalues with positive real parts. We show that any real eigenvalue of these matrices must be non-positive, and prove the conjecture for several special cases, including the 3×3 case. We discuss the challenges of making further progress on proving the full conjecture and suggest approaches for future work.

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CP8

Extension of Brauer and Rado Perturbation Theorems for Regular Matrix Pencils

In this work, we propose new results for changing eigenvalues of a regular matrix pencil $A - \lambda B$, which are based on the well-known Brauer's theorem (A. Brauer, Limits for the characteristic roots of a matrix. IV. Applications to stochastic matrices, Duke Math. J., 19(1), 75-91, 1952) and Rado's theorem (H. Perfect, Methods of constructing certain stochastic matrices II, Duke Math. J., 22, 305-311, 1955). These results allow us to change eigenvalues of the original matrix pencil without altering its regularity and in a quite simple way, even allowing to change infinite eigenvalues. We also present an extension of Rado's theorem that allows changing eigenvalues of a regular symmetric matrix pencil without altering its symmetric structure, and we show how to use these results in order to change the eigenvalues of a quadratic polynomial matrix.

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CP8

Polynomial Eigenvalue Exclusion Sectors

Polynomial eigenvalue problems are much harder to solve

than the standard (linear) eigenvalue problem, which makes easily computable eigenvalue inclusion and exclusion regions especially valuable. Such regions can often be obtained from similar scalar polynomial properties. An important subclass of such polynomials are those whose coefficients have sign restrictions, corresponding to positive and negative definite matrices for the polynomial eigenvalue problem, which are often encountered in applications. Examining this subclass more closely, one recalls the classical result that (scalar) polynomials with nonnegative coefficients cannot have zeros in a sector around the positive real axis. However, this single exclusion sector does not capture the behavior of the zeros for, e.g., polynomials with large gaps between their powers or with coefficient signs exhibiting a $+/-/+$ pattern, because it turns out that such zeros are excluded from additional sectors that are not detected by previous results. Here, this shortcoming is addressed using a geometric approach, with the aim to generalize the resulting scalar polynomial zero exclusion regions to polynomial eigenvalue exclusion regions. Additional results include upper and lower bounds on the eigenvalues, and an application to vibrational problems related to aerodynamics is presented.

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CP8

Structured Eigenvalue Backward Errors for Rational Matrix Functions with Symmetry Structures

Let $G(z)$ be an $n \times n$ *rational matrix function* (RMF) of the form

$$G(z) = \sum_{p=0}^{d} z^p A_p + \sum_{j=1}^{k} \frac{s_j(z)}{q_j(z)} E_j,$$

where A_p's and E_j's are $n \times n$ constant matrices, and $s_j(z)$ and $q_j(z)$ are scalar polynomials. $G(z)$ is said to be structured if A_p's, E_j's and functions $\frac{s_j(z)}{q_j(z)}$ follows some symmetry structure. Given a structured RMF $G(z)$ and a scalar $\lambda \in \mathbb{C}$, the problem of computing the nearest (with respect to some norm) structured RMF $\tilde{G}(z)$ of which λ is an exact eigenvalue is called the *structured eigenvalue backward error* of λ with respect to $G(z)$. Although the eigenvalue/eigenpair backward errors have been well studied for matrix polynomials, there is only a little literature that deals with the perturbation analysis of rational or more general nonlinear eigenvalue problems. We derive explicit computable formulas for the structured eigenvalue backward error of RMFs that carry a symmetry structure. These structures include symmetric, skew-symmetric, Hermitian, skew-Hermitian, $*$-palindromic, T-even, T-odd, $*$-even, and $*$-odd structures. We show over various numerical experiments show that the backward errors with respect to structure-preserving and arbitrary perturbations are significantly different. As far as we know, no other work has been done in the literature on the structured eigenvalue backward error of RMF.

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CP9

Communication Lower Bounds and Optimal Algorithms for Multiple Tensor-Times-Matrix Computation

Multiple Tensor-Times-Matrix (Multi-TTM) is a key computation in algorithms for computing and operating with the Tucker tensor decomposition, which is frequently used in multidimensional data analysis. We establish communication lower bounds that determine how much data movement is required (under mild conditions) to perform the Multi-TTM computation in parallel. The crux of the proof relies on analytically solving a constrained, nonlinear optimization problem. We also present a parallel algorithm to perform this computation that organizes the processors into a logical grid with twice as many modes as the input tensor. We show that with correct choices of grid dimensions, the communication cost of the algorithm attains the lower bounds and is therefore communication optimal. Finally, we show that our algorithm can significantly reduce communication compared to the straightforward approach of expressing the computation as a sequence of tensor-times-matrix operations when the input and output tensors vary greatly in size.

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CP9

Multiword Matrix Multiplication over Large Prime Fields on GPUs

This work deals with the efficient matrix multiplication over large prime fields on GPU architectures, a key kernel in computational linear algebra, particularly for the solution of polynomial systems. Existing methods based on double precision floating-point arithmetic cannot handle primes larger than 26 bits and are limited to CPU libraries. We propose a new multiword approach that efficiently manages prime numbers up to 50 bits. The number of words used by each of the matrices is an adjustable parameter that determines the maximum size of the prime that the algorithm can handle. Our implementation of this multiword approach harnesses the power of GPUs to surpass existing open-source CPU implementations like FFLAS, FLINT, and NTL.

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CP9

Low-Rank Tensor Approximation of Linear Quadratic Hamilton-Jacobi-Bellman Equation.

Solving high-dimensional PDEs, such as the Hamilton-Jacobi-Bellman (HJB) equation, requires a large-scale time-space discretization in numerical simulations. As the dimensionality increases, the number of grid points grows exponentially, leading to a significant increase in storage requirements, which results in severe computational difficulties, often called the curse of dimensionality. Recently, the use of low-rank tensor techniques has been acknowledged as a class method to mitigate the curse of dimensionality. These techniques benefit from the idea that certain high-dimensional tensors, may have a low-rank structure. We propose to assess the computational efficiency or the potential limitations of low-rank tensor techniques for a specific form of the HJB equation, that arises within the framework of linear quadratic optimal control problems, where both the system dynamics and the cost functions are characterized by linear and quadratic dependencies, respectively.

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CP9

Low-Rank Tensor Decomposition for Motion Capture Data Recovery

Motion Capture (MoCap) is an essential technology for capturing and analyzing complex human and object movements. However, MoCap systems frequently encounter the challenge of missing data, stemming from occlusion or equipment limitations. Precise recovery of these missing data is imperative to maintain the reliability and integrity of MoCap data. In this study, we tackle this challenge by using the tensor completion approach. We model the MoCap data as a 3rd-order tensor to effectively capture the inherent correlation within the skeleton data. We explore the low-rank tensor recovery framework using the Canonical Polyadic (CP) tensor decomposition for filling the gaps in skeleton sequences. Specifically, we introduce two tensor completion algorithms, based on the CP and the sparse CP decompositions, respectively. Numerically, we perform experimental tests on diverse MoCap sequences from the CMU motion capture dataset. This work is in collaboration with Andri Dmytryshyn

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CP9

Alternative Basis Matrix Multiplication is Fast and Stable

Alternative basis matrix multiplication algorithms are the fastest matrix multiplication algorithms in practice to date. However, are they numerically stable? We obtain the first numerical error bound for alternative basis matrix multiplication algorithms, demonstrating that their error bounds are asymptotically identical to the standard fast matrix multiplication algorithms, such as Strassen's. We further show that arithmetic costs and error bounds of alternative basis algorithms can be simultaneously and independently optimized. Particularly, we obtain the first fast matrix multiplication algorithm with a 2-by-2 base case that simultaneously attains the optimal leading coefficient for arithmetic costs and optimal asymptotic error bound, effectively beating the Bini and Lotti (1980) speed-stability trade-off for fast matrix multiplication. We provide high-performance parallel implementations of our algorithms with benchmarks that show our algorithm is on par with the best in class for speed and with the best in class for stability. Finally, we show that diagonal scaling stability improvement techniques for fast matrix multiplication are as effective for the alternative basis algorithms, both theoretically and empirically. These findings promote the use of alternative basis matrix multiplication algorithms in practical applications.

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CP10

Structured Approximation from Matrix-Vector Products: Two New Upper Bounds

We study the query complexity of structured matrix approximation. That is, we are given a matrix that is accessible only through matrix-vector product queries. We wish to find the best approximation to it from some family of structured matrices using as few of these queries as possible. For the case of low rank approximation, this problem has been extensively studied in the randomized numerical linear algebra community. More recent work considers ex-

act recovery when the input matrix comes from a variety of other structured families, such as hierarchical (HODLR, HSS) and Toeplitz-like matrices. We generalize the problem to approximating an arbitrary input matrix by a structured one, starting with two important structured classes – low rank plus diagonal matrices and sparse matrices with known sparsity pattern. We prove new upper bounds for this problem by using tools from communication complexity and NP-Hard heuristics in a novel way. Applications of our work include operator learning, trace estimation, compression, and denoising.

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CP10

Adaptive Mesh Deformation Based on Randomized RBF Solvers

Mesh deformation methods have been widely used for the past decades in various fields such as fluid-structure interaction and aerodynamic shape optimization. Among the existing methods, radial basis functions interpolation (RBF) is particularly suitable for unstructured mesh applications due to its simplicity and the high quality of the resulting mesh. Such approach requires solving dense linear systems, generally symmetric positive definite (SPD), which tends to be computationally expensive and memory demanding, which is a major drawback when dealing with large-scale meshes. In this work, we aim to speed-up RBF mesh deformation procedure using methods coming from probabilistic linear algebra to solve the associated dense linear system. We will explore the adaptive creation of an approximation to the RBF matrix by projecting the initial large-scale operator onto a smaller subspace. This subspace will that exhibits specific properties such as a better sparsity, while taking into account diverse solving strategies. Utilizing the spectral properties of RBF matrices, we will introduce a novel adaptive strategy to determine the projection dimension at each factorization step. Additionally, we will present a new randomized variant of the traditional linear solver for SPD matrices and conduct a comparative analysis with the existing randomized strategy. Our proposed approach will be thoroughly examined through practical applications in both 2D and 3D contexts.

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CP10

Computing the Hierarchical Semi-Seperable Representation of a Matrix with a Subsampled Randomized Hadamard Transform Sketching Operator

We present an algorithm for computing the hierarchical semi-separable representation of a matrix A where the sketch of Col A is attained via a subsampled randomized Hadamard transform. The algorithm is implemented in STRUMPACK C++ library. We report on the accuracy and storage requirements of the algorithm compared to the version that employs a Gaussian sketching operator for Col A.

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CP10

RTSMS: Randomized Tucker Via Single-Mode-Sketching

We propose RTSMS (Randomized Tucker via Single-Mode-Sketching), a randomized algorithm designed to compute a low-rank Tucker decomposition of a given tensor. RTSMS employs sketching and least-squares to compute the Tucker decomposition in a sequentially truncated manner [N. Vannieuwenhoven, R. Vandebril, and K. Meerbergen, A new truncation strategy for the higher-order singular value decomposition, SIAM J. Sci. Comput. 34 (2012) A1027-A1052.]. It is based on sketching the tensor from just one side at a time, not two or more. As a result, the sketch matrices are significantly smaller than alternative methods thus avoiding operations that can slow down the computation. This is achieved by finding a low-rank approximation of unfoldings based on generalized Nystrm, instead of the randomized SVD [N. Halko, P. G. Martinsson, and J. A. Tropp, Finding structure with randomness: probabilistic algorithms for constructing approximate matrix decompositions, SIAM Rev. 53 (2011) 217-288] but replacing the second sketch with a subsampling matrix chosen via the leverage scores of the first sketch. In addition, we employ regularization and iterative refinement techniques to improve the numerical stability. RTSMS is demonstrated to be competitive with existing methods, sometimes outperforming them by a large margin.

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CP10

Computing Nearest Singularities and Solutions of Polynomial Systems

A polynomial homotopy is a family of polynomial systems, typically in one parameter. Given a polynomial homotopy and an isolated solution, the nearest singular solution in this homotopy can be computed via application of the ratio theorem of Fabry. This application requires the computation of power series and the solution of a lower triangular block Toeplitz system. The first block in this Toeplitz system is the Jacobian matrix while the other blocks collect the information of the higher-order derivatives with respect to the parameter in the homotopy. For Newton's method to converge to accurate values of the higher-order coefficients of the series, multiprecision arithmetic is needed. As multiprecision arithmetic leads to a significant overhead in the computational cost, deciding the right level of precision depends on the computed number of terms in the series and the proximity to the nearest singular solution. For higher precision, multiple double arithmetic is applied. A multiple double is an unevaluated sum of hardware doubles. If the result can be represented exactly by the leading double(s), then the trailing double represents the error on the result. This property of multiple doubles, combined with the freedom to multiply the parameter in the homotopy with a nonzero constant, leads to an adaptive Newton method to accurately compute the coefficients of power series solutions of polynomial homotopies.

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CP11

Ergodic Estimations for Toeplitz Sequences Generated by a Symbol

We analyse the convergence of the ergodic formula for Toeplitz matrix-sequences generated by a symbol and we produce explicit bounds depending on the size of the matrix, the regularity of the symbol and the regularity of the test function.

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CP11

Spectrum of Certain Special Matrices

We prove that if $g : \mathbb{R} \to [0, \infty)$ is a conditionally negative definite function and $f : [0, \infty) \to [0, \infty)$ is a Bernstein function, then the function $f \circ g$ is conditionally negative definite. The inertia of the matrix $[f(g(p_i - p_j))]$ is $(1, 0, n - 1)$ if $g(x) = 0$ only for $x = 0$ and f is non-linear. A new and easy proof is also presented to demonstrate that the matrix $[\log(1 - p_i p_j)]$ is negative definite for n distinct positive real numbers $p_i < 1$, $\forall\ i$. Numerous more relevant results are discussed. These results supplements and unifies previous findings for operator monotone functions demonstrated by several authors, including Dyn, Goodman and Michelli, Bhatia and Jain, Garg and Aujla, and Garg and Agarwal.

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CP11

Recent Applications of the Theory of Glt Sequences

We present various examples of applications of the theory of generalized locally Toeplitz (GLT) sequences. In particular we discuss recent results on the spectral distribution of non-Hermitian matrix sequences, eigenvalue orderings for matrices generated by non-monotone symbols, and analysis PDE discretizations.

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CP11

Eigenvalue Analysis in Pde Approximation and Imaging

New results on eigenvalue distribution and localization are presented in the non-normal case. Several applications to preconditioned and nonpreconditioned matrix-sequences ranging from Imaging, to Number Theory, to numerical approximations of PDEs are presented.

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CP11

Joint Spacetime Multigrid Method for Solving Mean Field Games Arising from Economics

Dynamic Bertrand oligopolies are competitive markets in which a small number of firms producing similar goods use price as their strategic variable. In a two-person cooperative game, it can be modelled as a zero-sum game which can be formulated as a Hamilton-Jacobi-Bellman (HJB) PDE. If they compete non-cooperatively, it will then give rise to a nonzero-sum game, which leads to a system of HJB equations. For multi-person competition, they are often modelled as mean field games in which each firm competes with the rest as a group. In this talk, we will present numerical methods for solving systems of HJB and Kolmogorov-Fokkar-Planck (KFP) equations arising from mean field games. We propose an efficient multigrid method based on the idea of the joint spacetime, utilizing techniques of semi-coarsening, kernel preserving biased restriction, and artificial viscosity modified coarse grid correction. Finally, we will present numerical results for a number of application problems.

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CP12

Algebraic Connectivity of Kronecker Products of

Line Graphs

Let X be a tree with n vertices and $L(X)$ be its line graph. In this work, we completely characterize the trees for which the algebraic connectivity of $L(X) \times K_m$ is equal to $m-1$, where $\times$ denotes the Kronecker product. We provide a few necessary and sufficient conditions for $L(X) \times K_m$ to be Laplacian integral. The algebraic connectivity of $L(X) \times K_m$, where X is a tree of diameter 4 and k-book graph is discussed.

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CP12

The Graphs of Pyramids Are Determined by Their Spectrum

For natural numbers $k \leq n$ we study the graphs $T_{n,k} := K_k \vee \overline{K_{n-k}}$. For $k = 1$, $T_{n,1}$ is the star S_{n-1}. For $k > 1$ we refer to $T_{n,k}$ as a graph of pyramids. We prove that the graphs of pyramids are determined by their spectrum, and that a star S_n is determined by its spectrum iff n is prime. We also show that the graphs $T_{n,k}$ are completely positive iff $k \leq 2$.

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CP12

From Linear Algebra to Graph Theory: Minimum Rank of Regular Bipartite Graphs

How can we use linear algebra in fields like combinatorics and graph theory? In this lecture, we will introduce essential tools such as the zero-forcing set and how it relates to the minimum rank of a matrix. More specifically, we will study a family of matrices called Hankel matrices to give rise to computing the minimum rank for regular bipartite graphs.

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CP12

Cayley-Menger Extension of Metrics on Affine Spaces.

As soon as 1841 Cayley noted that squared distances between pairs of points (and also its generalization, the power associated to pairs of hyperspheres or hyperplanes) show a particular predilection to satisfy certain algebraic relations. Menger, Lachlan, Darboux, Cox, Mbius and Lie, among others, extended Cayley's results both from the affine or projective perspective. Due to its relevance for technological applications the branch of distance geometry has attracted renewed interest and these euclidean squared-distances relations are still explored from the perspective of positive-definite or Cayley-Menger matrices. Associated to any affine space A endowed with a metric structure of arbitrary signature we consider the space of affine functionals operating on the space of quadratic functions of A. On this functional space we characterize a symmetric bilinear form derived from the metric structure in a functorial way. We explore the geometrical relations of the relevant objects in this new metric space. Their properties encode all characteristics known in the literature for euclidean squared distance matrices, Cayley-Menger matrices and determinants, squared distance coordinate systems, and Lie and Mbius sphere geometries. Birthing this form as Cayley-Menger product, it represents a geometrical foundation unifying results in all these areas, bringing new light to non-trivial relations concerning euclidean squared distances and its non-euclidean analogues.

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CP12

Detection of Change Points in a Non-Stationary Time Series via the Fiedler Vectors of the Graph Laplacian

There are many opportunities to involve applied linear algebra in mass production systems. In this study, we focused on predictive maintenance, which is real-time data monitoring/processing of production systems to ensure the equipment safety. Equipment conditions may change, leading to non-stationary patterns in sensor readings. On the other hand, to build a proper machine learning model, segmenting the time series data into almost stationary parts is crucial. The selection of those change points, defined as the transition points from one working regime to another, is computationally expensive. Beyond many methods and algorithms, some linear algebraic applications can detect change points in a multivariate time series. We proposed a novel approach based on the neighborhood graph of a given time series data empowered with proper detection metrics derived from the Fiedler values and vectors of the graph Laplacian. Those metrics represent the connectivity of time series segments and enable us to understand the segments behavior, thus predicting the change points that are out of the thresholds. The main challenge of this work is making the most precise measurement based on graph Laplacian properties while reducing the overall computational cost of the proposed detection mechanism. Efficient computation of Fiedler values is well-studied in the literature, and we combine those computational approaches with the stationarity assumption of time series in a defined segment.

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CP13

Generalized Mittag-Leffler Functions and Its Ra-

tional Approximations with Real Distinct Poles

Mittag-Leffler functions are indispensable in the theory of fractional calculus and many other applications in engineering. However, their computational complexities have made them difficult to deal with numerically. A real distinct pole rational approximation of the two-parameter Mittag-Leffler function is proposed. Under some mild conditions, this approximation is proven and empirically shown to be L-Acceptable. These approximations are especially useful in developing efficient and accurate numerical schemes for partial differential equations of fractional order. Some applications are presented, such as complementary error function and solution of fractional differential equations.

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CP13

Immanent Functions and Mates

The set of all matrices with row and colum sums are 1 is called doubly stochastic matrices and it is denoted by Ω_n. Two unequal matrices $A, B \in \Omega_n$ doubly stochastic matrices A and B, are said to be $g-$mates if the function $g(\alpha A + (1-\alpha)B)$ is a constant, $0 \leq t \leq 1$. In this paper, we have shown conditions for two matrices are g_χ-mates, where g_χ is the generalized matrix function.

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CP14

Quantum Krylov Methods for Computing Hamiltonian Properties

One of the most promising expected applications of near-term quantum computers lies in the study of static and dynamical properties of quantum many-body systems. Many quantum computing algorithms have been proposed with this goal in mind, with a focus on Hamiltonian eigenvalue extraction, a problem central to chemistry, physics, and materials science. However, the majority of established quantum algorithms require a prohibitively large number of resources for near-term hardware. Here we discuss a number of quantum algorithms relying on real-time evolution for energy eigenvalue determination such as quantum Krylov methods and the recently introduced observable-Dynamic Mode Decomposition. Real-time evolution is native to quantum hardware, making these algorithms particularly suited for the near term. We provide strong theoretical and numerical evidence that these methods can converge rapidly even in the presence of noise and demonstrate their efficacies numerically on a range of chemically relevant Hamiltonians.

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CP14

Robust Diffusive Stability and Common Lyapunov Functions

We present some results on robust diffusive stability (RDS) for pairs of matrices modelling two coupled linear time-invariant systems. Sufficient conditions are derived for RDS for several matrix classes, in the Hurwitz and Schur cases. We also discuss how the existence of various types of common Lyapunov functions relate to RDS. We discuss some necessary conditions for RDS involving the convex hull and present results on RDS for the special case where each system is modelled by a Leslie matrix.

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CP14

Parametric Model Order Reduction Using Pod-Deim and Machine Learning Techniques

In this work, we present a framework for parametric model order reduction. The proposed methodology called POD-DEIM-GrROM is based on using machine learning techniques to build a classifier that automatically selects the best local reduced-order basis in a dictionary for a given parameter value. The dictionary is constructed by clustering the solution manifold enabling the identification of reduced-order bases which are computed from proper orthogonal decomposition (POD). For the reduced-order modeling task, the selected POD basis for the state variable is employed with the Galerkin projection. To further reduce the complexity on nonlinear term, the selected POD basis for systems nonlinearity is applied with the discrete empirical interpolation method (DEIM). The resulting reduced-order model (POD-DEIM-GrROM) are demonstrated to be efficient in reducing simulation time while preserving accuracy compared to the POD-DEIM-ROM in general setting.

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CP15

An Accelerated Denoising Approach Based on Singular Value Decomposition of a Modified Hankel Matrix

A denoising process based on using Hankel matrix with its truncated singular value decomposition (HSVD) has been successfully applied to many applications in signal processing for eliminating the background noise and improving the reliability of the fault detection process. In general, the HSVD approach becomes time consuming as the dimension of signal increases. This work aims to provide a new strategy for constructing a modified Hankel matrix to reduce the computational time of the HSVD denoising process. Instead of using a traditional way of constructing Hankel matrix, the proposed strategy introduces an operator that modifies Hankel matrix to have much smaller dimension and therefore this can significantly decrease the computational time for denoising signals. The proposed approach is tested on different kinds of signals, including synthetic periodic and aperiodic signals, as well as signals describing natural sound. This approach is shown to give the same level of accuracy as the standard HSVD approach while using substantially less computational time. Some theoretical

insights of the proposed approach are also discussed.

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CP15

Solution of Linear Ill-Posed Problems by Modified Truncated Singular Value Expansion

The numerical solution of linear ill-posed problems generally requires incorporation of regularization to yield a meaningful approximate solution. A common approach to compute a regularized approximate solution is to apply the truncated singular value expansion of the operator. A modification of the truncated singular value expansion for linear discrete ill-posed problems in finite dimensions has been described earlier and was shown to furnish approximate solutions of higher quality than the standard truncated singular value expansion. This research extends the modified singular value expansion to ill-posed problems in a Hilbert space setting.

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CP15

Adaptive Bregman-Kaczmarz: An Approach to Solve Linear Inverse Problems with Independent Noise Exactly

We consider the block Bregman-Kaczmarz method for finite dimensional linear inverse problems. The block Bregman-Kaczmarz method uses blocks of the linear system and performs iterative steps with these blocks only. We assume a noise model that we call *independent noise*, i.e. each time the method performs a step for some block, one obtains a noisy sample of the respective part of the right-hand side which is contaminated with new noise that is independent of all previous steps of the method. One can view these noise models as making a fresh noisy measurement of the respective block each time it is used. In this framework, we are able to show that a well-chosen adaptive stepsize of the block Bergman-Kaczmarz method is able to converge to the exact solution of the linear inverse problem. The plain form of this adaptive stepsize relies on unknown quantities (like the Bregman distance to the solution), but we show a way how these quantities can be estimated purely from given data. We illustrate the finding in numerical experiments and confirm that these heuristic estimates lead to effective stepsizes.

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CP16

More on Almost Semimonotone Matrices and the Linear Complementarity Problem

The linear complementarity problem (LCP) is the problem of finding a complementary pair of nonnegative vectors in a finite dimensional real vector space that satisfies a given system of inequalities. LCP is well studied in the literature on mathematical programming and a number of applications are reported in operations research, mathematical economics, geometry and engineering. Much of the theory of the LCP and its solutions are intimately linked, in various ways, to specific matrix classes. In this paper, we explore the connection between an almost semimonotone matrix and a real square matrix whose off-diagonal entries are nonpositive and some interesting matrix theoretic properties of this class. We also discuss the number of solutions of the associated linear complementarity problems.

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CP16

Unique Solvability and the Solution Set Properties for Interval Absolute Value Equations

The absolute value equations is a feasibility algebraic problem in the form $Ax+|x| = b$; its slightly generalized version reads as $Ax + B|x| = b$. Many questions related to this problem are NP-hard, for instance to find a solution, or to check for unique solvability. Since real-life problems are often subject to diverse types of uncertainties, the input data can hardly be considered to be exact. That is why we focus on the problem with uncertain coefficients. We model uncertainty by the interval range of possible values, so that the input matrix A and vector b become interval-valued. For this interval-valued problem, we investigate the basic problems regarding solvability and the solution set. In particular, we first state several ways to characterize unique solvability for every realization of interval values. To this end, we can utilize regularity of a certain set of matrices, or an algebraic system of nonlinear inequalities; in any case, the property is co-NP-hard to check. Then we describe the solution set, which forms a union of convex polyhedral sets, and discuss a characterization of its convex hull. In view of the intractability of the problems, we consider also certain polynomially solvable subclasses of the interval problems; one such class consists of inverse nonnegative matrices.

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CP16

Spectral Inequalities for Means of Matrices

Some spectral inequalities, involving Kubo-Ando operator connections and means of positive semidefinite matrices, are surveyed. As a result, some log-majorization type inequalities are obtained. Singular values inequalities, concerning the Heinz mean of matrices and its 'harmonic' variant, are also derived.

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CP16

Eigenvalue Properties of Positive Interval Matrices

This paper focuses on the eigenvalue properties of positive interval matrices. Some new results concerning the bounds for the Perron root of positive interval matrices are studied. The Perron-Frobenius theory for the generalized interval eigenvalue problem is explored. The study offers a comprehensive examination of the eigenvalue properties of positive interval matrices, establishing multiple novel findings and

refining existing bounds. This analysis highlights the fundamental properties of positive interval matrices and contributes to the development of new tools and techniques for analyzing and manipulating interval matrices. Keywords: Perron root, Generalized eigenvalue problem, Irreducible matrix, Perron-Frobenius theory, Interval matrix.

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MS0

Nicholas J. Higham Memorial Session - Speaker 7

This is a special session to celebrate the life and work of Nicholas J. Higham (1961-2024).

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Nicholas J. Higham Memorial Session - Speaker 6

This is a special session to celebrate the life and work of Nicholas J. Higham (1961-2024).

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This is a special session to celebrate the life and work of Nicholas J. Higham (1961-2024).

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Nicholas J. Higham Memorial Session - Speaker 2

This is a special session to celebrate the life and work of Nicholas J. Higham (1961-2024).

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Nicholas J. Higham Memorial Session - Speaker 1

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Nicholas J. Higham Memorial Session - Speaker 5

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Nicholas J. Higham Memorial Session - Speaker 9

This is a special session to celebrate the life and work of Nicholas J. Higham (1961-2024).

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MS1

Representation Equivalent Neural Operators: a Framework for Alias-free Operator Learning

Recently, operator learning, or learning mappings between infinite-dimensional function spaces, has garnered significant attention, notably in relation to learning partial differential equations from data. Conceptually clear when outlined on paper, neural operators necessitate discretization in the transition to computer implementations. This step can compromise their integrity, often causing them to deviate from the underlying operators. This research offers a fresh take on neural operators with a framework Representation equivalent Neural Operators (ReNO) designed to address these issues. At its core is the concept of operator aliasing, which measures inconsistency between neural operators and their discrete representations. We explore this for widely-used operator learning techniques. Our findings detail how aliasing introduces errors when handling different discretizations and grids and loss of crucial continuous structures. More generally, this framework not only sheds light on existing challenges but, given its constructive and

broad nature, also potentially offers tools for developing new neural operators.

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MS1

An Overview of Operator Learning

Operator learning, a prominent field of machine learning, has gained significant momentum in recent years. It offers novel approaches to data-driven approximation of operators associated with partial differential equations and dynamical systems. This talk will provide a high-level overview of operator learning and Koopman operator theory, and their connections with linear algebra. We will start the minisymposium with a survey of the latest advances in the field and a roadmap of the minisymposium.

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MS1

Learning Dynamical Systems with the Spectral Exterior Calculus

We present a framework for learning dynamical systems based on the exterior calculus on manifolds. Our approach employs the Spectral Exterior Calculus (SEC) technique that represents vector fields in frames (overcomplete bases) for L^2 and Sobolev spaces. Using the eigenvalues and eigenfunctions of the Laplacian on functions, the SEC approximates vector fields as linear combinations of frame elements, which act as generators of dynamical systems. In addition, the scheme admits a data-driven formulation utilizing Monte Carlo approximation from data sampled on manifolds. We solve initial-value prediction problems using the learned vector fields and compare the behavior of the solutions with those of the true system.

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MS1

On Consistent Spectral Approximation of Koopman Operators Using Resolvent Compactification

Koopman operators and transfer operators represent dynamical systems through their induced linear action on vector spaces of observables, enabling the use of operator-theoretic techniques to analyze nonlinear dynamics in state space. The extraction of approximate Koopman or transfer operator eigenfunctions (and the associated eigenvalues) from an unknown system is nontrivial, particularly if the system has mixed or continuous spectrum. We discuss a spectrally-accurate approach to approximate the skew-adjoint Koopman generator via a compactification of the resolvent of the generator. This approach employs kernel integral operators to approximate the skew-adjoint Koopman generator by a family of skew-adjoint operators with compact resolvent, whose spectral measures converge in a suitable asymptotic limit, and whose eigenfunctions are approximately periodic. We also discuss a data-driven formulation of our approach, which converges in the limit of large training data under natural assumptions on the dynamical system and observation modality. We explore implementations of this technique using data from several different example systems including Lorenz 63.

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MS2

Updating the Bidiagonalization with Low-Rank Corrections

A bidiagonal factorization of a possibly sparse matrix is the essential first reduction for computing the SVD. Similarly, the bidiagonalization can be used to find an effective low rank approximation to a given matrix or to efficiently solve with a sequence of shifted linear systems. When low-rank corrections are added to an existing factorization it is important to incorporate the new information economically, without having to refactor the matrix from scratch. Methods for updating a singular value decomposition exist, however they typically don't use the bidiagonal factors and they often solve for the zeros of a nonlinear scalar secular equation, instead. This work exploits the available sparsity when a Lanczos Golub-Kahan process is used to restore bidiagonal form after low rank updates. Because the bidiagonalization is upadated directly, new methods for revising an SVD can be developed that don't need to find the zeros of a scalar equation.

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MS2

Advancements in libHSL: Enhancing HSL_MA57 Solver for Quasi-Definite Structures and GPU Acceleration

We present the latest developments in libHSL, with a focus on significant enhancements to the HSL_MA57 solver—particularly the challenges posed by quasi-definite structures that commonly arise in the linear systems within interior-point methods. We also shed light on the initial stages of integrating GPU acceleration to empower HSL_MA57, ensuring efficient and scalable solutions for symmetric indefinite linear systems.

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MS2

Linear Systems Arising in Interior Methods for Convex Optimization: A Symmetric Formulation with Bounded Condition Number

We provide eigenvalues bounds for a new formulation of the step equations in interior methods for convex quadratic optimization. The matrix of our formulation, named $K2.5$, has bounded condition number, converges to a well-defined limit under strict complementarity, and has the same size as the traditional, ill-conditioned, saddle-point formulation. We evaluate the performance in the context of a Matlab object-oriented implementation of PDCO, an interior-point solver for minimizing a smooth convex function subject to linear constraints. The main benefit of our implementation, named PDCOO, is to separate the logic of the interior-point method from the formulation of the system used to compute a step at each iteration and the method used to solve the system. Thus, PDCOO allows easy addition of a new system formulation and/or solution method for experimentation. Our numerical experiments indicate that the $K2.5$ formulation has the same storage requirements as the traditional ill-conditioned saddle-point formulation, and its condition is often more favourable than the unsymmetric block 33 formulation.

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MS2

Algorithm NCL for Constrained Optimization and its use of SQD Systems

Algorithm NCL was devised to solve large optimization problems whose constraints do not satisfy LICQ at a solution. It emulates the augmented Lagrangian algorithm LANCELOT, which solves a short sequence of bound-constrained subproblems and has no LICQ difficulties. NCLs subproblems are much bigger and need to be solved by a nonlinear interior method (ideally using first and second derivatives). We study the linear systems arising within nonlinear interior methods. For convex problems the linear systems are SQD (symmetric quasi-definite) and hence solvable by sparse Cholesky-type methods.

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MS3

Batched Iterative Solvers for Memory Constrained Problems

Many applications rely on solving many, small linear systems. Each individual linear system is usually cheap to solve, but the sheer number, often in the millions or more, of systems make this a difficult task to solve. One of the prevailing method to accelerate the solution time is to employ batched direct solvers, which are even provided by hardware vendor libraries. But recently, batched iterative solvers have shown to be competitive, if not faster, than direct solvers. Additionally, many problems, especially in the exascale regime, are memory constrained and cant afford to store all matrices explicitly. One example of this case are high-order FEMs, where the storage requirements of the matrix grows rapidly with the chosen order. As a consequence, these applications use matrix-free methods. The batched iterative methods are thus a natural choice for the batched parts of the solution process, e.g. in a preconditioner for the global system. This talk aims to evaluate using matrix-free representations in batched iterative methods, and present preliminary results on artificial problems arising from high-order discretization.

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MS4

Geodesic Convexity Structures of Eigenvalue Problems and an Application to High-dimensional

Canonical Correlation Analysis

We discuss important geodesic convexity structures for the problem of computing a subspace spanned by a block of leading eigenvectors of a symmetric matrix. This problem is posed naturally on the Grassmann manifold. We will also show how this theory can be extended to a preconditioned algorithm for the generalized eigenvalue problem in a high dimensional regime, which avoids computing costly inverses of large matrices. The most prominent application of this breakthrough is high-dimensional canonical correlation analysis.

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MS4

How to Estimate Covariance Matrices from One-Bit Samples

We consider covariance estimation of any subgaussian distribution from finitely many i.i.d. samples that are quantized to one bit of information per entry. We show how reliable estimators can be constructed for one-bit quantizers with and without dithering. The latter uses uniformly distributed dithers on $[-\lambda, \lambda]$ but enjoys near-minimax optimal, non-asymptotic error estimates in the operator and Frobenius norms only if λ is chosen proportional to the largest variance of the distribution. However, this quantity is not known a-priori, and in practice λ needs to be carefully tuned to achieve good performance. To resolve this problem we further introduce a tuning-free variant of this estimator, which replaces λ by a data-driven quantity. We prove that this estimator satisfies the same non-asymptotic error estimates - up to small (logarithmic) losses and a slightly worse probability estimate.

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MS4

Gauss-Southwell Type Descent Methods for Low-rank Matrix Optimization

We consider gradient-related methods for low-rank matrix optimization with a smooth strongly convex cost function. The methods operate on single factors and share aspects of both alternating and Riemannian optimization. We compare two possible choices for the search directions based on Gauss-Southwell type selection rules: one using the gradient of a factorized non-convex formulation, the other using the Riemannian gradient. Both methods provide convergence guarantees for the gradient that are analogous to the unconstrained case.

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MS4

Breaking the Cone : Averaging SPD Matrices with Missing Information

Symmetric positive definite (SPD) matrices permeates numerous scientific disciplines, including machine learning, optimization, and signal processing. Equipped with a Riemannian geometry, the space of SPD matrices benefits from compelling properties and its derived Riemannian mean is now the gold standard in some applications, eg brain-computer interfaces (BCI). In this presentation, we address the problem of averaging covariance matrices with missing variables and generalize the problem to missing subspaces. This situation often occurs with inexpensive or unreliable sensors, or when artifact-suppression techniques remove corrupted sensors or sources leading to rank deficient matrices, hindering the use of the Riemannian geometry in covariance-based approaches. An alternate but questionable method consists in removing the rank-deficient matrices (with either missing variables or sources), thus reducing the training set size. We address those limitations and propose a new formulation grounded in geodesic convexity. Our approach is evaluated on synthetic datasets with a controlled number of missing variables/subspaces and a known baseline, demonstrating the robustness of the proposed estimator. The practical interest of this approach is assessed on real BCI datasets. This presentation extends the work of Yger et al. 2018 and entitled "Geodesically-convex optimization for averaging partially observed covariance matrices"

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MS5

A Dynamical Low-rank Collocation Method for Nonlinear Tensor Differential Equations

We present a new method for computing the solution to a nonlinear tensor differential equation with dynamical low-rank approximation. The idea of dynamical low-rank approximation is to project the differential equation onto the tangent space of a low-rank tensor manifold at each time. Traditionally, an orthogonal projection onto the tangent space is employed, which is challenging to compute for nonlinear differential equations. In this talk, we introduce a novel interpolatory projection onto the tangent space that

satisfies the differential equation at a set of carefully selected indices and is easily computed for many nonlinear differential equations.

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MS5

Low-Rank Tensor Frames

Low-rank tensor decompositions are particularly useful for the numerical solution of PDEs, as a technique for the adaptive low-parametric approximation of solutions in vast discretization spaces. The conventional approach consists in the low-rank approximation of function coefficients with respect to a fixed discretization basis. The coefficients are either long vectors or high-dimensional tensors, depending on whether the Kronecker product or the tensor product is used in the definition of the decomposition. Particularly suited for solving PDEs is the tensor decomposition known as matrix product states (MPS) in computational quantum physics and as tensor train (TT) in computational mathematics. In this talk, we present a generalization of the MPS-TT decomposition from the case of a vector coefficient (w.r.t a basis) to that of a frame coefficient (w.r.t. a redundant frame). In the multilevel setting, corresponding to the Kronecker product, this construction covers the standard multilevel frames developed in the context of finite-element methods. Our construction comes with a notion of decomposition orthogonality and with a quasi-optimal low-rank approximation algorithm based on the matrix SVD, analogous to those of the original, vector setting. We demonstrate the significance of this contribution with the numerical solution of PDEs with singular and highly oscillatory solutions in three physical dimensions using up to 2^{80} degrees of freedom in each dimension.

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MS5

A Hierarchical Low-Rank Complexity Reduction Algorithm for the Kinetic Chemical Master Equation

The stochastic description of chemical reaction networks with the kinetic chemical master equation (CME) is important for studying biological cells, but it suffers from the curse of dimensionality: the amount of data to be stored grows exponentially with the number of chemical species and thus exceeds the capacity of common computational devices for realistic problems. Therefore, time-dependent model order reduction techniques such as the dynamical low-rank approximation are desirable. In this talk, a dynamical low-rank algorithm for the kinetic CME is presented. The dimensionality of the problem is reduced in this approach by dividing the reaction network into two partitions. Only reactions that cross partitions are subject to an approximation error. The dynamical low-rank approximation, compared to the commonly used Monte Carlo methods such as the stochastic simulation algorithm (SSA), has the advantage that it is completely noise-free. Moreover, we demonstrate that in some cases the proposed method can drastically reduce memory consumption and run time and provide even a better accuracy than SSA. Finally, the extension of this algorithm to tree-tensor networks will be addressed.

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MS6

A Block Preconditioner Approach for Incompressible Navier-Stokes Equations

We consider linear systems that arise from the discretization of Navier-Stokes equations by the so-called PolyMAC method (1). This finite volume method generalizes the MAC scheme to general meshes and presents the advantage to strictly conserve mass, momentum and kinetic energy (2). One specificity of the approach is to use the vorticity to express the diffusion term. The resulting linear system is then a 3 x 3 block matrix, with three types of unknowns: velocity, pressure and vorticity. Such a system forms a double saddle-point system and is quite challenging to solve. In this presentation, we study the structure of the system and define ideal preconditioners. Following this analysis, we consider practical approximations of the preconditioners and test their robustness to the Reynolds number Re on a Cartesian test case. However, on complex geometries, deformed meshes are common in practice. Hence, in a second time, we look at a broad benchmark of challenging meshes in 2D and 3D and evaluate the robustness of the different preconditioners. References: (1) P.-L. Bacq, A. Gerschenfeld, M. Ndjinga, PolyMAC: Staggered Finite Volume Methods on General Meshes for Incompressible Navier-Stokes Problems, Finite Volume for Complex Applications X, 2023. (2) R. Beltman, M. Anthonissen, B. Koren, Conservative Polytopal Mimetic Discretization of the Incompressible Navier-Stokes Equations, Journal of Computational and Applied Mathematics, 340, 2018, pp. 443-473.

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MS6

Numerical Solution of the Stokes-Darcy Equations

In this talk, we discuss multigrid methods for the numerical solution of the Stokes-Darcy equations discretized by the Marker and Cell (MAC) scheme, a finite difference method. The resulting discretization leads to a double saddle-point system, and the design of fast solvers poses several challenges. We propose two block smoothers based on a block LDL decomposition of the matrix. To make them more computationally practical, we develop inexact versions based on damped Jacobi. Numerical experiences show that our approach is robust with respect to the mesh-size and the physical parameters.

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MS6

Achieving h and p-Robust Monolithic Multigrid Solvers for Saddle-Point System

Recent years have seen substantial interest in the development of high-order spatial discretizations for many saddle-point systems, including the Stokes and Navier-Stokes equations. While monolithic multigrid is well-known to be an h-robust preconditioner for corresponding low-order discretizations, its extension to higher-order discretizations has not been well-studied. In this work, we consider the extension of monolithic multigrid with Vanka (overlapping Schwarz) relaxation to this setting, considering how the relaxation schemes should change to achieve both h- and p-robustness of the resulting solver.

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MS6

A Block-Acoustic Preconditioner for the Elastic Helmholtz Equation

The Helmholtz equation models wave propagation in the frequency domain. The acoustic Helmholtz equation models acoustics and electromagnetics, while the elastic one models wave propagation in elastic media, such as the earths sub-surface. Both versions are difficult to solve numerically, as the discrete linear system is large, indefinite, and ill-conditioned. The elastic version amplifies these difficulties both because of its larger size, as a system of PDEs, and its more complicated physics. We suggest a reduction-based approach for the solution of the elastic Helmholtz equation: bearing in mind that the elastic equation can be reformulated as a generalized saddle-point system, and using a simple block elimination, we introduce a block-acoustic preconditioner. That is, a preconditioner comprised of acoustic Helmholtz blocks, applied on each of the components of the elastic Helmholtz equation. Thus, we enable the solution of the elastic version by the use of any existing solver for the acoustic Helmholtz equation as a black-box. We give numerical results, comparing our approach to monolithic multigrid applied on the elastic Helmholtz equation in mixed formulation, and demonstrate that our solver is scalable both with respect to the Poisson ratio, and with respect to the grid size.

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MS7

Using the Fast Multipole Method to Accelerate Matrix-Vector Products - Application to the Magnetostatic Moment Method.

In electrical engineering, solving low-frequency Maxwell's equations is crucial for modeling devices with ferromagnetic materials and large air volumes, typically due to voids and gaps. In such cases, the Magnetostatic Moment Method (MMM), based on volume integral equations, offers an efficient alternative to the Finite Element Method (FEM). The MMM's advantage lies in not requiring air region meshing, thus significantly reducing unknowns. However, the MMM leads to linear systems with dense matrices, resulting in computational challenges in memory and execution time for large problems. To address this issue, we consider a low-rank approximation of the matrix using the Fast Multipole Method (FMM). This hierarchical algorithm, which uses tree-based domain partitioning, can reduce the complexity of matrix-vector product calculations from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$. Our work focused on adapting a black-box FMM variant, available in the C++ ScalFMM library, to accelerate matrix-vector products within the MMM framework. Additionally, we also worked on a parallel, shared memory-based version to further improve computational efficiency. This enhanced FMM-based matrix-vector product, integrated with a GMRES algorithm, efficiently solves dense linear systems. Our numerical results demonstrate the efficiency of the new FMM-based GMRES solver in a simplified application modeling a low-frequency antenna.

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MS7

Algebraic Multigrid Solver for Nonlocal Equations

The naive discretization of nonlocal operators leads to matrices with significant density, as compared to classical PDE equations. This makes the efficient solution of nonlocal models a challenging task. In this presentation, we will discuss on-going research into hierarchical assembly and algebraic multigrid solution techniques that are suitable for nonlocal models.

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MS7

Overlapping Schwarz Preconditioner with Geneo Coarse Space for Nonlocal Equations

Domain Decomposition Methods, such as Additive Schwarz, can be used to precondition linear systems, and they usually rely on an additional coarse space to scale with the number of subdomains. The Generalized Eigenproblems in the Overlaps (GenEO) has emerged as one of the most promising coarse space for sparse symmetric positive definite problems, see Spillane et al. (2014). Ge-

nEO takes eigenvectors of well-chosen local eigenproblems as a basis for the coarse space. As one of its interesting features, GenEO is only based on the knowledge of the stiffness matrix elements and discretization agnostic, left apart a few reasonable assumptions. Recently, the GenEO approach has been extended to Boundary Integral Equations (BIEs) for the hypersingular operator in Marchand et al. (2020). In this context, the discretized operator is nonlocal so that the resulting linear system is dense. Thus, the local eigenproblems used to build the GenEO coarse space are adapted to the non-local nature of the problem and its $\|\cdot\|_{\widetilde{H}^{1/2}}$ energy norm. In this talk, we will present theoretical and numerical results aiming at adapting GenEO to the integral fractional Laplacian of order $s \in (0,1)$. It shares many similarities with BIEs, e.g. its non-local nature and the energy norm $\|\cdot\|_{\widetilde{H}^s}$, that will be used to introduce a new distributed solver using the libraries PyNucleus, Htool-DDM and HPDDM.

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MS7

Block and Hierarchical Low Rank Solvers for Fractional Diffusion Equations

The discretization of multidimensional fractional diffusion integral equations results in formally dense matrices, with polynomial growth in memory footprint and arithmetic operations. For special cases, including infinite spatial domains with spatially homogeneous properties and fractional order, the fractional diffusion operator reduces to the classical fractional Laplacian and the growth in computational complexity can be reduced via suitable well-understood transforms. However, these methods do not apply for general finite domains or for spatially varying diffusivity and fractional order. Hence, there is a need for the development of representations and solvers that do suffer from the undesirable growth in memory and arithmetic operations in order to make fractional diffusion models, and nonlocal models generally, practical for applications. In this talk, we present such methods based on block low rank and hierarchically low rank approximations of the discretized operators. The methods tame the computational complexity of constructing the discrete operator and of solving the resulting system of equations. The block low rank methods are simpler in structure and easily map onto GPUs. The hierarchically low rank representation and preconditioners have optimal $O(N)$ complexity and comfortably scale to very large problem sizes in 2D and 3D.

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MS8

A Nested PrimalDual Iterated Tikhonov Method for Regularized Convex Optimization

In practical applications, we often need to minimize a convex functional given by

$$\underset{u\in\mathbb{R}^d}{\operatorname{argmin}}\ f(u) + h(Wu), \tag{2}$$

where $f : \mathbb{R}^d \to \mathbb{R}$ is convex and smooth, $h : \mathbb{R}^{d'} \to \mathbb{R}\cup\{\infty\}$ is convex and possibly nonsmooth, and $W \in \mathbb{R}^{d'\times d}$ is a linear operator. In this talk, we explore a modified version of a Nested Primal-Dual algorithm. The core idea of our method is to use a preconditioning matrix P_n at each iteration and incorporate the induced metric in the definition of the proximity operator. We prove the convergence to the solution of the initial problem. To achieve this, we just assume that the sequence of preconditioning matrices $\{P_n\}$ satisfies the condition

$$P_n \preceq (1+\zeta_{n-1})P_{n-1}, \quad \forall\ n \geq 0 \tag{3}$$

where $\{\zeta_n\} \in \mathbb{R}^+$ is a summable sequence. Focusing on the image deblurring problem with Gaussian noise, we define the preconditioning matrices as $P_n = A^TA + \nu_n I$, where A represents the blur operator, and $\{\nu_n\}$ satisfy condition (3). With a proper choice of ν_n, this strategy accelerates convergence as confirmed in the numerical results.

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MS8

Limited Memory Restarted Lp-Lq Minimization Methods Using Generalized Krylov Subspaces

Regularization of certain linear discrete ill-posed problems, as well as of certain regression problems, can be formulated as large-scale, possibly nonconvex, minimization problems, whose objective function is the sum of the p^{th} power of the ℓ^p-norm of a fidelity term and the q^{th} power of the ℓ^q-norm of a regularization term, with $0 < p, q \leq 2$. We describe new restarted iterative solution methods that require less computer storage and execution time than the methods described by [Huang et al., Majorization-minimization generalized Krylov subspace methods for $\ell_p - \ell_q$ optimization applied to image restoration. BIT (2017)]. The reduction in computer storage and execution time is achieved by periodic restarts of the method. Computed examples illustrate that restarting does not reduce the quality of the computed solutions.

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MS8

Flipped Structured Matrix Sequences in Image Deblurring with General Boundary Conditions

In this talk, we explore advanced preconditioning techniques aimed at optimizing iterative regularization methods for image deblurring challenges. We introduce the anti-identity preconditioner to symmetrize the coefficient matrix for zero boundary conditions, enabling the use of MINRES as an effective regularization approach. This preconditioner also enhances GMRES performance when dealing with more complex boundary conditions such as reflective and anti-reflective options and strongly nonsymmetric point spread functions (PSFs). Further, we show the effectiveness of both stationary and iteration-dependent regularizing circulant preconditioners combined with the anti-identity matrix and utilized with standard and flexible Krylov subspace methods. The efficacy of our proposed preconditioning strategies is evidenced through extensive numerical experiments. The results show the improved performance in terms of iteration speed and also highlight the regularization properties of the preconditioned methods. Furthermore, we discuss the advantages of using more precise boundary conditions. The talk concludes with a discussion of the outcomes and suggests directions for future research.

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MS9

A Data Driven Koopman-Schur Decomposition for Computational Analysis of Nonlinear Dynamics

We introduce a new theoretical and computational framework for a data driven Koopman mode analysis of nonlinear dynamics. To alleviate the potential problem of ill-conditioned eigenvectors in the existing implementations of the Dynamic Mode Decomposition (DMD) and the Extended Dynamic Mode Decomposition (EDMD), the new method introduces a Koopman-Schur decomposition that is entirely based on unitary transformations. The analysis in terms of the eigenvectors as modes of a Koopman operator compression is replaced with a modal decomposition in terms of a flag of invariant subspaces that correspond to selected eigenvalues. The main computational tool from the numerical linear algebra is the partial ordered Schur decomposition that provides convenient orthonormal bases for these subspaces. In the case of real data, a real Schur form is used and the computation is based on real orthogonal transformations. The new computational scheme is presented in the framework of the Extended DMD, with the same functionalities (snapshot reconstruction and forecasting) and the kernel trick is used.

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MS9

Elliptic PDE Learning Is Provably Data-Efficient

Can one learn a partial differential equation (PDE) from only input-output function pairs? If so, how many are needed? We provide theoretical guarantees on the number of input-output training pairs required to learn a 3D uniformly elliptic PDE. In particular, we exploit randomized numerical linear algebra and PDE theory to derive a provably data-efficient algorithm that recovers the corresponding Green's function and achieves an exponential convergence rate of the error with respect to the size of the training dataset with an exceptionally high probability of success. This work provides a theoretical explanation for the observed strong performance of recent deep learning techniques in PDE learning, even when there is limited data availability.

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MS9

Low-Rank Approximation of the Koopman Operator

Since the work of Schmid [J. Fluid Mech., 2010], there has been a surge of interest in data-driven approximation of the Koopman operator with *Dynamic Mode Decomposition* (DMD) and its variants establishing themselves as the go-to algorithms. For high-dimensional problems, regularization is mandatory to get stable estimators of this infinite-dimensional linear operator. By reframing the inference problem as a multivariate reduced-rank regression problem, we will illustrate how a rigorous data-driven low-rank approximation of the Koopman operator can be computed. Despite being non-convex, the reduced-rank regression problem admits a closed-form solution. This reframing of the problem also has the added benefit of highlighting the connection between *Proper Orthogonal Decomposition* (POD) and DMD. Furthermore, it enables us to put under the limelight the equivalence between DMD and many linear system identification techniques (e.g. ERA, N4SID, etc). The resulting algorithm requires only two singular value decompositions of data matrices and is thus computationally efficient and tractable. Its performances are evaluated on standard examples, from low-dimensional chaotic systems to linear control theory and reduced-order modelling for fluid dynamics applications. In all cases, it outperforms the golden standards (vanilla DMD, Exact DMD, DMD with control, etc) currently used in the community while benefitting from *a priori* prediction error estimates.

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MS10

Randomized Generalized Eigenvalue Problems

We present a randomized, inverse-free algorithm for producing an approximate diagonalization of any $n \times n$ matrix pencil (A, B). The bulk of the algorithm rests on a randomized divide-and-conquer eigensolver for the generalized eigenvalue problem originally proposed by [Ballard, Demmel, and Dumitriu, Technical Report, 2010]. We demonstrate that this divide-and-conquer approach can be formulated to succeed with high probability provided the input pencil is sufficiently well-behaved, which is accomplished by generalizing the recent pseudospectral shattering work of [Banks, Garza-Vargas, Kulkarni, and Srivastava, Foundations of Computational Mathematics 2022].

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MS10

Scalable Gaussian Process Regression via Iterative Numerical Methods

Gaussian processes are a powerful Bayesian method commonly used to achieve uncertainty quantification in regression, with applications including Bayesian optimization, regression on spatiotemporal data, calibrating deep neural networks for regression, and more. However, using GPs on more than a few thousand training examples has historically been challenging due to the need to the cubic complexity of computing linear solves and log determinants with an n x n covariance matrix. Historically, this cost has been most commonly mitigated by introducing conditional independencies via so-called inducing point methods. In this talk, I discuss an alternative approach to scalability by using iterative numerical tools. I'll first discuss how Krylov subspace methods like conjugate gradients can be used to estimate linear solves and log determinants of kernel matrices with strong application specific guarantees. Then, motivated by the empirical lack of need for highly precise solves during training, I discuss more recent work based on an alternating projection iteration. This method coonverges to exact solutions no slower than gradient descent, but has only linear time and space complexity per iteration, dramatically improving over the cubic time and quadratic space complexity of direct methods.

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MS10

Efficient Parallel Implementation of the Multiplicative Weight Update Method for Graph-Based Linear Programs

Positive linear programs (LPs) model many graph and operations research problems. One can solve for a $(1 + \epsilon)$-approximation for positive LPs, for any selected ϵ, in polylogarithmic depth and near-linear work via variations of the multiplicative weight update (MWU) method. Despite extensive theoretical work on these algorithms through the decades, their empirical performance is not well understood. In this work, we implement and test an efficient parallel algorithm for solving positive LP relaxations, and apply it to graph problems such as densest subgraph, bipartite matching, vertex cover and dominating set. We accelerate the algorithm via a new step size search heuristic. Our implementation uses sparse linear algebra optimization techniques such as fusion of vector operations and use of sparse format. Furthermore, we devise an implicit representation for graph incidence constraints. We demonstrate the parallel scalability with the use of threading OpenMP and MPI on the Stampede2 supercomputer. We compare this implementation with exact libraries and specialized libraries for the above problems in order to evaluate MWUs practical standing for both accuracy and performance among other methods. Our results show this implementation is faster than general purpose LP solvers (IBM CPLEX, Gurobi) in all of our experiments, and in some instances, is faster than state-of-the-art specialized parallel graph algorithms.

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MS10

Inverse Eigenvalue Problems for Quantum Sensing

A system of tunnel-coupled quantum dots is considered in the presence of an applied electric field. Given the measurements of differences between ground state and excited state energy levels as the electric field is varied, we seek to recover the quantum Hamiltonians that describe this system. We formulate this as a parameterized inverse eigenvalue problem and develop algebraic and computational methods for solving for parameters to represent these Hamiltonians. The results demonstrate that this approach is highly precise even when there is error present within the measurements. This theory could aid in the design of high resolution tunable quantum sensors.

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MS11

Optimization on Product Manifolds: Preconditioned Methods and Applications

Since optimization on Riemannian manifolds relies on the chosen metric, it is appealing to know that how the performance of a Riemannian optimization method varies with different metrics and how to exquisitely construct a metric such that a method can be accelerated. To this end, we propose a general framework for optimization problems on product manifolds where the search space is endowed with a preconditioned metric, and we develop the Riemannian gradient descent and Riemannian conjugate gradient methods under this metric. Specifically, the metric is constructed by an operator that aims to approximate the diagonal blocks of the Riemannian Hessian of the cost function, which has a preconditioning effect. We explain the relationship between the proposed methods and the variable metric methods, and show that various existing methods, e.g., the Riemannian GaussNewton method, can be interpreted by the proposed framework with specific metrics. In addition, we tailor new preconditioned metrics and adapt the proposed Riemannian methods to the canonical correlation analysis and the truncated singular value decomposition problems, and we propose the GaussNewton method to solve the tensor ring completion problem. Numerical results among these applications verify that a delicate metric does accelerate the Riemannian optimization methods.

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MS11

Approximating Maps into Manifolds

Many functions that are worth approximating map into Riemannian manifolds. The distance between two points on a manifold depends on the intrinsic geometry of that manifold. For example, the distance between two orthogonal matrices A and B in the space of orthogonal matrices will always be greater than or equal to the distance between A and B in the space of matrices. Hence, when approximating functions that map into manifolds, it is natural to measure the error on the manifold. Especially, for embedded manifolds, when the dimension of the ambient space is much larger than the dimension of the manifold, such as for low rank tensors, it becomes unfeasible to measure the error in the ambient space. In this presentation, we present a scheme to approximate maps into manifolds by first pulling back the problem to the tangent space and then applying a scheme for approximating maps into vector spaces. Our main result is a theorem that bounds the approximation error on the manifold, given that the error on the tangent space is bounded.

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MS11

GR-RTRMC: Graph-Regularized Riemannian Trust-Region Matrix Completion, with an Application to Air Temperature Data Completion

We address the problem of low-rank matrix completion by incorporating graph regularization into the existing Riemannian Trust-Region Matrix Completion (RTRMC) framework. The latter uses the geometry of the low-rank constraint to rephrase the problem as an unconstrained optimization problem on a Grassmann manifold. Our approach, named Graph-Regularized RTRMC (GR-RTRMC), exploits the inherent relationships between rows, resp. columns, of the matrix. By using these relationships, we aim to improve the accuracy and robustness of matrix completion, particularly in scenarios where the underlying data exhibits strong correlations between rows or columns. As an application, we tackle the problem of missing entries in the air temperature data recorded by meteorological stations operated by the Royal Meteorological Institute (RMI) in Belgium. Preliminary results demonstrate the performance of GR-RTRMC in comparison to the original RTRMC and the state of the art, showcasing the benefits of using graph regularization for matrix completion tasks.

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MS11

Riemannian Acceleration with Preconditioning for symmetric eigenvalue problems

In this talk, we introduce a Riemannian Acceleration with Preconditioning (RAP) for solving symmetric eigenvalue problems and provide a rigorous analysis of its acceleration. To ensure the local geodesic convexity, we devise a new measurement called leading angle, tailored specifically for assessing the quality of preconditioners in symmetric eigenvalue problems. In our pursuit of improved performance and faster convergence, we propose the Locally Optimal Riemannian Accelerated Gradient (LORAG) method, meticulously designed to address local geodesic convexity issues. The comprehensive theoretical proof of LORAG's convergence and acceleration properties are given. By integrating the concept of local geodesic con-

vexity for preconditioned eigensystems into LORAG, we propose RAP, promising significant acceleration in solving symmetric eigenvalue problems. Furthermore, we rigorously analyze the asymptotic convergence rate when employing the Schwarz preconditioner for elliptic eigenvalue problems. RAP achieves an impressive asymptotic rate of convergence as $1-C\kappa^{-1/2}$, where C is a universal constant, $\kappa = \kappa_\nu \lambda_2/(\lambda_2 - \lambda_1)$, κ_ν is from the stable decomposition, λ_1 and λ_2 are the smallest two eigenvalues. This performance significantly outperforms the preconditioned steepest descent method, whose convergence rate is limited to $1 - C\kappa^{-1}$.

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MS12

Leverage-Based Sampling at Scale for Sparse Tensor CP Decomposition

Sparse tensor Candecomp / PARAFAC (CP) decomposition is a useful tool for analyzing datasets as diverse as social network data, packet trace, and knowledge graphs, but its computation is demanding. In the first part of this talk, introduce a new randomized sampling algorithm based on statistical leverage scores to accelerate the linear least-squares problems involved in CP decomposition. We demonstrate that this new algorithm, STS-CP, achieves asymptotic and practical runtime lower than existing state-of-the-art methods. In the second part of this talk, we extend two randomized CP algorithms to the distributed-memory setting, showing that they can compete on the scale of thousands of CPU cores with well-optimized packages for non-randomized CP decomposition. Experiments demonstrate an 11x speedup for our algorithm over the well-known SPLATT package to decompose a tensor with 4.7 billion nonzeros.

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MS12

Riemannian Optimization on Low Rank Tensor Manifolds

Tensor completion is a technique to fill in missing entries in multi-dimensional data using decomposition methods like Tucker, CP, or Tensor-train. Recent works have proposed Riemannian optimization algorithms for this problem and have shown that these algorithms perform better than traditional optimization methods like alternating minimization. We analyze the computations involved in Riemannian optimization algorithms and improve upon the asymptotic computational complexity in the existing algorithms. We leverage the sparse tensor contraction primitives to implement these algorithms and compare Riemannian optimization with alternating minimization in distributed-memory setting for practical applications.

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MS13

Multigrid for Block Toeplitz Matrices Arising in the Discretization of PDEs

Multigrid methods are known to be optimal solvers for large classes of PDEs, most notable elliptic ones. They also work well for systems of PDEs, e.g., elasticity or Stokes. In the case of geometric multigrid methods the analysis is usually carried out using Fourier analysis. This does not allow for an asymptotic multilevel analysis. Instead, we use structured matrices, i.e., Toeplitz matrices or circulant matrices, and traditional multilevel theory to analyze the properties of the multigrid methods. While this approach is similar to Fourier analysis, an estimate of the convergence rate is also possible for the multilevel case. For scalar problems, including those arising from the discretization of PDEs, this technique has been studied intensively. Recently, we started transfering these results to the systems case that results in block-Toeplitz matrices or block-circulant matrices [Bolten, Donatelli, Ferrari and Furci, SIMAX 2022]. Besides studying higher-order discretizations of scalar PDEs, systems of PDEs also fit in this framework. Additionally, we considered systems with saddle point structure, applying recent results for multigrid for such systems [Notay, Numer. Math. 2016] to the structured matrix case [Bolten, Donatelli, Ferrari and Furci, LAA 2023; Bolten, Donatelli, Ferrari and Furci, APNUM 2023]. In the talk the analysis technique, the derived sufficient conditions for optimal convergence and numerical results will be presented.

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MS13

Block-Preconditioning Techniques for Fully Implicit Runge-Kutta Methods

Fully implicit RungeKutta methods offer the possibility to use high-order-accurate time discretization with desir-

able stability properties. For general implicit RungeKutta methods all stages are coupled leading to a potentially costly and involved solution procedure which has been a major barrier to their widespread use. We present a stage-parallel block preconditioner for the class of L-stable Radau IIA RungeKutta methods. The preconditioner exploits a property of the coefficient matrices to construct a block lower-triangular preconditioner. During the application of the preconditioner, a basis change can be applied to obtain a block-diagonal form, in this way allowing us to decouple the stages when solving for the blocks. In the linear case this basis change can be applied directly for non-linear equations further approximations are needed to achieve this decoupling. For the linear case, we discuss the analysis of the preconditioned matrices which are non-symmetric and in tensor form. We give eigenvalue bounds for the two- and three-stage methods under symmetric positive definite assumptions. We illustrate the performance by numerical examples, including also applications to non-linear problems. Finally the parallel behavior is demonstrated, comparing space-parallel but serial in stages against fully stage-parallel implementations on HPC platforms.

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MS13

Algebraic Multigrid Methods for Simulation of Single Phase Flow in Fractured Media

The interaction between fluid and fractured porous media is a complex and multifaceted phenomenon that plays a pivotal role in different engineered systems. From the modelling of the subsurface flow of hydrocarbons in fractured reservoirs to the transport of contaminants in fractured geological formations or the optimization of geothermal energy extraction from fractured rock, fast and accurate simulations of fluid behaviour in fractured porous media are of interest. The presence of an intricate network of fractures, joints, and pores in the media presents a set of challenges both for the modelling and the simulation. Such systems are naturally multiscale and bring the necessity of formulating mixed-dimensional models, that is, finding approaches for treating together differential problems on coupled domains of different dimensionalities, e.g., 1D/2D, 2D/3D fracture/rock domains. Challenges for the solution of the related linear systems thus stem from the inherent heterogeneity, anisotropy, and nature of fractured systems. In this contribution, we will focus on the applicability study and performance analysis of some of the preconditioners available in PSCToolkit [DAmbra Durastante Filippone, Parallel Sparse Computation Toolkit, Software Impacts 15 (2023): 100463] for the solution of these linear systems on heterogeneous hardware architectures.

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MS13

Multilevel Methods for Isogeometric Analysis

Isogeometric analysis (IGA) is a computational technique for the numerical solution of partial differential equations (PDEs). It is based on the idea of using spline-type functions, which are exploited in computer aided design (CAD) software for the parametrization of the computational domain, in order to approximate the unknown solution of the PDE. There are several issues that make this approach advantageous over classical finite element methods (FEM). The design of fast solvers for isogeometric analysis is receiving a lot of attention due to the challenge that offers to find an algorithm with a robust convergence with respect to the spline degree. Multilevel methods seem to be a good choice, given that they are among the fastest solvers for FEM discretizations. Here, we analyze the application of multigrid methods to this type of discretizations. This will be done with the help of a local Fourier analysis (LFA).

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MS14

Multi-Step One-Shot Iterative Methods for Linear Inverse Problems

When an inverse problem is solved by a gradient-based optimization algorithm, the corresponding forward and adjoint problems, which are introduced to compute the gradient, can be also solved iteratively. In this framework, one-shot inversion methods iterate at the same time on the inverse problem unknown and on the forward and adjoint problem solutions. We are especially interested in the case where the inner iterations for the direct and adjoint problems are incomplete, that is, stopped before achieving a high accuracy on their solutions. If two or more inner iterations are performed on the state and adjoint state be-

fore updating the parameter, by starting from the previous iterates as initial guess for the state and adjoint state, we speak of multi-step one-shot methods. For general linear inverse problems and fixed-point iterations for the associated forward/adjoint problems, we analyze several variants of multi-step one-shot methods, in particular semi-implicit schemes with a regularization parameter. We establish sufficient conditions on the descent step for convergence which are explicit in the number of inner iterations. We provide numerical experiments to illustrate the convergence of these methods in comparison with the classical gradient descent, where the forward and adjoint problems are solved exactly by a direct solver instead.

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MS14

Efficient Solvers for the Sparse Systems That Arise from Three-Dimensional Hps Discretizations

Numerical results indicated that the Hierarchical Poincare-Steklov (HPS) discretization is effective at solving two-dimensional Helmholtz problems even in the high frequency regime. The efficiency of the method is thanks to its nested dissection inspired direct solver. Unfortunately, while it is straight forward to extend the discretization to three-dimensional problems, the natural extension of the direct solver is not efficient. This talk presents alternative methods for solving the linear system that arises from the discretization. The methods utilize both sparse direct solver and iterative solver techniques. This combination allows them to easily parallelized. Preliminary numerical results will be presented.

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MS14

Efficient Handling of Multiple Sources and Operators in Domain Decomposition Methods for Full Waveform Inversion

Full Waveform Inversion in the frequency domain requires the resolution of sequences of Helmholtz-like problems, each one of them with many right-hand sides (i.e. many sources). For large-scale 3D problems, Domain Decomposition Methods are a popular choice, but usual Krylov methods do not handle multiple right-hand sides efficiently. Coupling Optimized Restrictive Additive Schwarz with Block Krylov Methods (e.g. Block GMRES) has proven to significantly reduce the iteration count [P. Jolivet and P.-H. Tournier, "Block Iterative Methods and Recycling for Improved Scalability of Linear Solvers", 2016], but with an overhead that mitigates these benefits for large blocks. In this work, we investigate similar ideas for non-overlapping methods that solve a substructured problem, i.e. with unknowns on the subdomain interfaces. We show that this approach has comparable convergence properties, but can handle larger blocks due to the reduced size of the vectors managed by the Krylov method. This property makes substructured non-overlapping methods particularly attractive when many sources are involved. We also explore the problem of subspace recycling for a changing operator (i.e. different iterations in the inversion process): Once the problem has been solved for a given model, can we efficiently reuse information to accelerate the solution of the next one, again for all sources ? We compare three approaches involving deflation and preconditionners for the new problem.

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MS14

Iterative Solvers Based on Hybridizable Discontinuous Galerkin Methods for Time-Harmonic Problems

We consider the iterative solution of time-harmonic wave propagation problems discretized with finite element methods. These problems are notoriously difficult to solve iteratively because the matrice of the resulting discrete systems is sparse, complex, and indefinite. We have recently proposed a discontinuous Galerkin (DG) scheme with a new hybridization procedure [https://hal.science/hal-03909368]. In contrast to standard hybridizable discontinuous Galerkin (HDG) schemes, which use numerical traces as Lagrange multipliers, this new approach, called CHDG, uses characteristic variables. This choice changes the properties of the reduced system. Numerical results will be presented to compare the iterative solution of the DG, HDG and CHDG systems with different iterative procedures on 2D benchmarks. On all the considered test cases, the number of iterations is reduced for CHDG as compared to DG and HDG, often by a large amount. Interestingly, the CGNR iteration converges almost as fast as the GMRES iteration for the CHDG system.

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MS15

Linear Algebra Revisited: An Intermediate Course for Students Interested in Data Science

With the increase in popularity in data science, an opportunity exists for us to expose students a second time to some ideas from linear algebra and to introduce them to some more advanced topic than are typically seen in an introductory class. In this talk, I will discuss two classes developed at Brigham Young University for students interested in data science (one for math majors and one for non-majors) that dig deeper into the relevant linear alge-

bra. I will also discuss how to balance the need for rigor, computational projects, and real-world applications while maintaining student interest.

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MS15

Applied Linear Algebra Projects with MATLAB

In this talk, we will present interactive MATLAB live scripts that apply fundamental concepts and basic terminology related to linear algebra. We will focus on identifying applications of linear algebra to academic disciplines and fields beyond mathematics. Based on topics from a first course in linear algebra such as vector and matrix arithmetic, solving matrix equations, null spaces, eigenvalues, and eigenvectors, we will cover applications including balancing chemical reactions, solving static force scenarios, encryption, systems modeling, and explainable machine learning. These interactive notebooks can be used as demonstrations in lectures, class activities, or interactive assignments outside class.

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MS15

Teaching and Learning Linear Algebra with Matlab

Linear algebra is a vital topic in mathematics and has many applications in other disciplines. Technology can play an important role in understanding linear algebra concepts, applications, and helping with immediate and accurate computations. The Linear Algebra Curriculum Study Group 2.0 recommended that technology be included in the curriculum (Stewart et al., 2022). In this talk, I will describe the integration of Matlab in a second course in linear algebra. The aim of this course is to equip students with linear algebra concepts, learn computational skills, validate proofs, and work with applications. The course (Abstract Linear Algebra) is proof-based. It covers topics including vector spaces, finite-dimensional vector spaces, linear maps, polynomials, inner product spaces, operators on inner product spaces, eigenvalues, and eigenvectors. Students are also introduced to some applications, such as Markov Chains and Singular Value Decomposition (SVD).

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MS15

Linear Algebra Education for the Modern World of 2024 and beyond

Currently our first Linear Algebra courses task seems to be teaching incoming students how to prove classical math statements from Linear Algebras history. But we should teach modern Matrix Theory and applied topics instead. How can this be solved? Modern Linear Algebra has been crucial for all STEM fields for more than five decades now. Driven by rapid advances in science and technologies, the significance of Linear Algebra has increased by its need in computations and by its ubiquitous use there. Now Linear Algebra classes must be fundamentally restructured on the College level. This talk presents a vision for our future teaching of Linear Algebra. It offers Math Educational ways to increase the awareness of faculty and the knowledge of students in our modern subject. I focus on the demands from technology on teaching and on learning the subject today. In modern early Linear Algebra courses, teachers need to pay attention and re-consider students struggles with fundamental Linear Algebra con- cepts. And we must find alternate modern ways to present our ancient subject anew. My approach to this rebirth of Linear Algebra courses connects students early on with modern Industrial Applications and it requires us to bring modern Matrix Theoretic and Computational ways of thinking into our College Math Curricula. Linear Algebra teaching can be transformed by using a set of seven Lesson Plans for a complete and fully coherent first modern introductory Linear Algebra course, available on the ILAS educational website at url https://la-education. //oucreate.com/teaching-resources/lesson-plans/.

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MS16

Hybrid Iterative Solvers for Inverse Problems

Inverse problems arise in a variety of applications: machine learning, image processing, finance, mathematical biology, and more. Solution schemes are formulated by applying algorithms that incorporate regularization techniques and/or statistical approaches. In most cases these solution schemes involve the need to solve large-scale ill-conditioned linear systems that are corrupted by noise and other errors. In this talk we consider new hybrid Krylov subspace methods to solve these linear systems, including how to choose regularization parameters.

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MS16

Iterated Arnoldi-Tikhonov method

The Arnoldi-Tikhonov method is a well-established regularization technique for solving large-scale ill-posed linear inverse problems. This method leverages the Arnoldi decomposition to reduce computational complexity by projecting the discretized problem into a lower-dimensional Krylov subspace, in which it is solved. Our study considers the iterated Arnoldi-Tikhonov method and provides a thorough analysis that considers all approximation errors. Additionally, we propose a new strategy for choosing the regularization parameter. This choice yields more accurate approximate solutions than the standard Arnoldi-Tikhonov method. Moreover, the proposed method is robust with respect to the regularization parameter as con-

firmed in the numerical results.

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MS16

A Tensor Bidiagonalization Method for Higher-Order Singular Value Decomposition With Applications

The need to know a few singular triplets associated with the largest singular values of a third-order tensor arises in data compression and extraction. We describe a new method for their computation using the t-product. Methods for determining a couple of singular triplets associated with the smallest singular values also are discussed. The proposed methods generalize available restarted Lanczos bidiagonalization methods for computing a few of the largest or smallest singular triplets of a matrix. The methods use Ritz and harmonic Ritz lateral slices to determine accurate approximations of the largest and smallest singular triplets, respectively. Applications include data compression, the solution of ill-posed problems, and face recognition.

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MS17

Rigged DMD: Data-Driven Koopman Decompositions via Generalized Eigenfunctions

Koopman operators globally linearize nonlinear dynamical systems, and their spectral information serves as a powerful tool for analysing and decomposing nonlinear dynamics. However, Koopman operators are inherently infinite-dimensional, posing a significant challenge in computing their spectral information, especially in the presence of continuous spectra. We can often access this spectral information by considering a rigged-Hilbert space structure that allows us to diagonalise the operator. In the rigged Hilbert space setting, there is a smaller topological space which contains some structure corresponding to the operator, and the dual of this space where the generalised eigenvectors live. We have developed an algorithm capable of computing these generalized eigenfunctions for Koopman operators associated with general measure-preserving systems. This algorithm leverages the resolvent to compute smoothed approximations of generalized eigenfunctions. We demonstrate explicit high-order convergence theorems for our algorithm, termed RiggedDMD. These generalized eigenfunctions enable a rigorous approach to Koopman mode decomposition. We demonstrate the algorithm on several examples, include systems with Lebesgue spectrum, integrable systems, the Lorenz system and a turbulent boundary layer flow with Reynolds number 6×10^4 and state-space dimension $> 10^5$.

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MS17

Operator Is the Model

Modeling of complex physical, biological, social, cyber systems entered a new phase with the age of machine learning. Koopman operator theory (KOT) emerged as the leading candidate for modeling of such dynamical systems. I propose that the operator itself can be thought as the model, and the key question is that of existence of its finite-dimensional (linear or nonlinear) representations. This turns on its head the usual approach, which considers the Koopman operator a (linear) representation of the underlying, possibly nonlinear dynamics. In other words, "Ask not what the operator can do for you, but what you can do for the operator."

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MS17

Rigorous Adjoint-Free Approximation of Nonnormal Pde Solution Operators Using Fourier Bases

Existing methods for low-rank approximation of nonnormal matrices and solution operators of linear partial differential equations (PDEs) rely on queries to both the forward and adjoint actions of the operator. While it is possible to efficiently estimate the range of a low-rank nonnormal operator using generic queries, without additional side-information the adjoint must be queried to obtain efficient estimates of the co-range. For elliptic PDEs, we show that the regularity property of the adjoint solution operator provides useful side information about the co-range that can be used to construct low-rank approximations with guaranteed accuracy based on querying the forward solution operator only. The queries are constructed using eigenfunctions of the Laplace-Beltrami operator (LBO), which are shown to have guaranteed approximation power for func-

tions in Sobolev spaces. If solutions of the adjoint equation have k weak derivatives in L^2 and the spatial domain has dimension d, then our approximation of the solution operator based on queries using the leading n eigenfunctions of the LBO has asymptotic error $\mathcal{O}(n^{-k/d})$ with respect to the operator norm. We demonstrate this approach numerically by constructing low-rank approximations for solution operators of an advection-diffusion equation with space dimension $d = 1$ and for linear elasticity problems with space dimensions $d = 2$ and $d = 3$.

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MS17

Operator Learning for Multiscale Elliptic PDEs with History Dependence

Multiscale partial differential equations (PDEs) may be approached via homogenization theory, which averages out dependence on finer scales to obtain macroscopic response. For PDEs describing constitutive equations, homogenization allows for computational efficiency but introduces additional complexities to the system such as dependence on system history. In a simple theoretical setting, the decay modes of history dependence relate to the solutions of a Sturm-Liouville problem. Additionally in this setting, it is known that there exists an operator learning architecture that reduces the history dependence to a Markovian form and can provably approximate the true dynamics. In more complex settings, such as in higher dimensional systems, the viability of operator learning is less justified theoretically. In this talk, we discuss these connections between theory and operator learning architecture.

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MS18

Quantum advantage in linear algebra and its applications

The advent of error-corrected quantum computers is anticipated to usher in a new era in computing. So which scientific computing, and in particular, linear algebra challenges are likely to benefit from quantum computers? I will first discuss some essential criteria and considerations towards realizing quantum advantages in these problems. I will then introduce some recent advancements in quantum algorithms, especially for matrix exponentials of relevance to open quantum system dynamics.

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MS18

Topological Data Analysis on Noisy Quantum Computers

Topological data analysis (TDA) is a powerful technique for extracting complex and valuable shape-related summaries of high-dimensional data. However, the computational demands of classical algorithms for computing TDA are exorbitant, and quickly become impractical for high-order characteristics. Quantum computers offer the potential of achieving significant speedup for certain computational problems. Indeed, TDA has been purported to be one such problem, yet, quantum computing algorithms proposed for the problem, such as the original Quantum TDA (QTDA) formulation by Lloyd, Garnerone and Zanardi, require fault-tolerance qualifications that are currently unavailable. In this talk, we present NISQTDA, a fully implemented end-to-end quantum machine learning algorithm needing only a short circuit-depth, that is applicable to high-dimensional classical data, and with provable asymptotic speedup for certain classes of problems. The algorithm neither suffers from the data-loading problem nor does it need to store the input data on the quantum computer explicitly. The algorithm was successfully executed on quantum computing devices, as well as on noisy quantum simulators, applied to small datasets. Preliminary empirical results suggest that the algorithm is robust to noise.

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MS18

Quantum Krylov Methods for Eigenvalue Estimation

Classical algorithms based on Krylov subspaces are among the most successful tools in the field of numerical linear algebra. More recently, the emergence of quantum subspace methods has resulted in a promising class of hybrid quantum-classical algorithms for eigenvalue approximation, e.g., in the fields of condensed matter physics and electronic structure theory. These quantum Krylov methods harness quantum computers to generate the subspace basis states and retrieve the projected problem through quantum measurement. However, the classical computation of the Ritz values often poses challenges due to the ill-conditioning of the associated generalized eigenvalue problem. In this talk, we present an overview of quantum subspace algorithms from a numerical linear algebra perspective. We discuss strategies to avoid solving an ill-conditioned eigenvalue problem, explain their implemen-

tation on quantum computers, and provide numerical and theoretical evidence of their convergence. Furthermore, we present strategies to improve the robustness, especially in the presence of noise.

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MS19

Algebraic Methods for Graph Signal Processing

We study graphs signals that are sparse in either spatial or frequency domain. In both cases the results will depend on nonvanishing of minors of the eigenvector matrix. We will study a sufficient algebraic condition that implies nonvanishing of these minors. We end by giving probabilistic results.

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MS19

Approximation of Graph Signals with Positive Definite Graph Basis Functions

We show how the concept of positive definite functions can be transfered to a graph setting in order to approximate graph signals with generalized shifts of a graph basis function (GBF). This concept merges kernel-based approximation with spectral theory on graphs and can be regarded as a graph analog of radial basis function approximation in euclidean spaces or on the sphere. We provide several descriptions of positive definite functions on graphs, the most relevant one is a Bochner-type characterization in terms of positive Fourier coefficients. These descriptions allow us to design GBFs and to study GBF approximation in more detail: we are able to characterize the native spaces of the interpolants, we give explicit estimates for the approximation error and provide efficient ways (based on Krylov subspace methods) to calculate the GBF approximants. As an application, we show how GBFs can be used for classification tasks on graphs.

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MS19

On Graph Uncertainty Principle and Eigenvector Delocalization

Uncertainty principles present an important theoretical tool in signal processing, as they provide limits on the time-frequency concentration of a signal. In many real-world applications the signal domain has a complicated irregular structure that can be described by a graph. Therefore, generalization of uncertainty principles to the graph setup is a crucial task in graph signal processing. In this talk, we will focus on the global uncertainty principle on graphs and propose new connections between the uncertainty bound for graph signals and graph eigenvectors delocalization. We will also derive uncertainty bounds for random d-regular graphs and provide numerically efficient upper and lower approximations for the uncertainty bound on an arbitrary graph.

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MS19

Hodge Laplacians and Signal Processing on Complexes

The analysis of networks by means of the graph Laplacian has been a staple to analysis graphs and signals defined on graphs. Typically, this involves leveraging the structure of the graph as encoded in the spectral properties of the graph Laplacian. However, the typically considered variants of the graph Laplacian may not suitable when dealing with signals that encode flows on the edges or data associated to multiple nodes. To overcome this limitation, we devise signal processing tools based on the Hodge-Laplacian and the associated discrete Hodge Theory for simplicial (and cellular) complexes. We discuss applications of these ideas for signal processing on discrete or discretized spaces.

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MS20

Nonbacktracking Centralities for Temporal Networks

Though seemingly they belong to two different worlds, matrix functions and network science have some degree of overlap thanks to a very simple fact; powers of the adjacency matrix count traversals in the underlying network. This concept in turn allows for the definition of centrality measures in terms of entries (or sums thereof) of functions of the adjacency matrix. In this talk, we will focus on discrete temporal networks, where edges appear and disappear over time, and on walks that are not allowed to revisit the node that they just left. We will present theory and results, as well as discuss challenges of such an approach.

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MS20

Is the Lanczos-Method for Matrix Functions Nearly Optimal?

The Lanczos method for matrix function approximation (Lanczos-FA) is one of the most widely used algorithms approximating f(A)b, when A is a symmetric matrix. In the case $f(x) = 1/x$ and A is positive definite, Lanczos-FA is mathematically equivalent to the well-known Conjugate Gradient method, and therefore optimal (in a certain norm) among all Krylov subspace methods. Is Lanczos-FA nearly optimal in other cases? We discuss some recent work on near-optimality guarantees for rational functions and the square root and inverse square root.

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MS20

A Posteriori Bounds for the Computation of the Action of Matrix Exponential and its Moments via Lanczos Algorithm

We compute $\exp(A)b$ and $b^* \exp(A)b$ with real symmetric matrix A via Lanczos algorithm. The problem is reformulated as diffusion on the graph-Laplacian corresponding to the Lanczos tridiagonal matrix. This allows us to obtain easily computable a posteriori bounds on the Lanczos approximation error, including sharp two-sided bound for $b^* \exp(A)b$. The bounds are extendable for the Stieltjes matrix functions.

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MS20

Algorithm-Agnostic Low-Rank Approximation of Operator Monotone Matrix Functions

Computing low-rank approximations of matrix functions $f(A)$ is an important task in many areas of computational mathematics. Most methods to compute low-rank approximations to $f(A)$ require access to the matrix $f(A)$. This is often considerably more expensive than directly accessing A. Persson and Kressner (SIMAX 2023) proposed fun-Nystrm, which constructs a low-rank Nystrm approximation to A using subspace iteration, and then uses this approximation to directly obtain a low-rank approximation to $f(A)$ for any continuous operator monotone function satisfying $f(0) = 0$. In this work, we significantly generalize the results of Persson and Kressner beyond subspace iteration. We show that if $\widehat{A}$ is a near-optimal low-rank Nystrm approximation to A then $f(\widehat{A})$ is a near-optimal low-rank approximation to $f(A)$, *independently of how* $\widehat{A}$ *is obtained*. Further, we show sufficient conditions for a basis Q to produce a near-optimal Nystrm approximation $\widehat{A} = AQ(Q^TAQ)^\dagger Q^TA$. We use these results to establish that many ubiquitous low-rank approximation methods produce near-optimal Nystrm approximations to A and therefore near-optimal low-rank approximations to $f(A)$.

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MS21

Fast Multiplication of Random Dense Matrices with Sparse Matrices

This work focuses on accelerating the multiplication of a dense random matrix with a (fixed) sparse matrix, which is frequently used in sketching algorithms. We develop a novel scheme that takes advantage of blocking and recomputation (on-the-fly random number generation) to accelerate this operation. The techniques we propose decrease memory movement, thereby increasing the algorithm's parallel scalability in shared memory architectures. On the Intel Frontera architecture, our algorithm can achieve 2x speedups over libraries such as Eigen and Intel MKL on some examples. In addition, with 32 threads, we can obtain a parallel efficiency of up to approximately 45%. We also present a theoretical analysis for the memory movement lower bound of our algorithm, showing that under mild assumptions, it's possible to beat the data movement lower bound of general matrix-matrix multiply (GEMM) by a factor of $\sqrt{M}$, where M is the cache size. Finally, we incorporate our sketching algorithm into a randomized least squares solver. For extremely over-determined sparse input matrices, we show that our results are competitive with SuiteSparse; in some cases, we obtain a speedup of 10x over SuiteSparse.

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MS21

Symmetries and Sparsity in Tensor Trains: Application to Quantum Chemistry

Conservation of symmetries is key in many fields. It usually involves figuring out the right sparsity pattern. In quantum chemistry, the most important symmetries are the particle number conservation and the total spin symmetry. The first is abelian whereas the other is not. This talk will discuss how these symmetries, are preserved within the tensor train format which is central in DMRG (Density Matrix Renormalisation Group). This is a joint work with Siwar

Badreddine, Eric Cances and Laura Grigori.

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MS21

Leveraging Sparsity in High-Dimensional Bayesian Modeling

This talk delves into high-dimensional Bayesian inference tasks whose underlying latent parameter spaces are represented by sparse Gaussian Markov random fields (GMRFs). GMRFs belong to a widely used class of undirected probabilistic graphical models, and have been shown to efficiently encode dependency structures between random variables, making them popular in the field of spatial and spatio-temporal statistics. Frequently arising computational bottleneck operations in Bayesian modeling include the repeated factorization and selected matrix inversion of the precision (inverse covariance) matrices of the GMRF. These precision matrices are usually high-dimensional, sparse and exhibit a recurring sparsity pattern. We discuss and present different solution methods and linear solvers to tackle the predominant operations. Our case studies focus on parameter estimation and prediction for large-scale spatio-temporal climate datasets.

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MS21

Nonblocking Execution for Iterative Solvers

We investigate the use of nonblocking execution for sparse iterative solvers executed on multi-core architectures. Nonblocking execution enables optimizations performed by delaying the execution of operations. The presented design employs lazy evaluation and performs the loop fusion and loop tiling optimizations at run-time. The design is fully dynamic as it handles algorithms with arbitrary control-flow and benefits from an analytic model that automatically selects suitable performance parameters for the parallel execution of the optimized code. Conjugate Gradient is one of the most used iterative solvers and is a valuable target for nonblocking execution. Its loop is composed of a relatively long chain of linear algebraic operations that benefit from memory optimizations. In particular, the operations are memory bound, and reusing data in cache can speed up the overall performance. Our evaluation on Conjugate Gradient shows that the nonblocking execution achieves between 0.9x and 2.2x speedup over the corresponding blocking execution for various matrices selected from the SuiteSparse Matrix Collection and the Stanford Network Analysis Project. The evaluation of the analytic model shows that the automatically selected parameters lead to almost the same performance with the best manual configuration. Therefore, the evaluation shows that the nonblocking execution makes the performance improvement possible in a fully automatic way, without any user intervention.

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MS22

Substructuration of the Hiptmair-Xu Preconditioner for Positive Maxwell Problems

Considering positive Maxwell problems in 3D discretized by low order Ndlec edge elements, we propose a substructured variant of the Hiptmair-Xu preconditioner based on a new formula that expresses the inverse of Schur systems in terms of the inverse matrix of the global volume problem. We obtain condition number estimates stemming from those available for the original Hiptmair-Xu preconditioner. Besides theory, we shall present numerical results confirming stabilisation of the condition number with respect to the meshwidth.

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MS22

A Robust and Adaptive GenEO-Type Domain Decomposition Preconditioner for H(curl) Problems in General Non-Convex Three-Dimensional Geometries

In this work we develop and analyse domain decomposition methods for linear systems of equations arising from conforming finite element discretisations of positive Maxwell-type equations, namely for **H**(**curl**) problems. It is well known that convergence of domain decomposition methods rely heavily on the efficiency of the coarse space used in the second level. We design adaptive coarse spaces that complement a near-kernel space made from the gradient of scalar functions. The new class of preconditioner is inspired by the idea of subspace decomposition, but based on spectral coarse spaces, and is specially designed for curl-conforming discretisations of Maxwell's equations in heterogeneous media on general domains which may have holes. Our approach has wider applicability and theoretical justification than that in [R. Hiptmair and J. Xu, Nodal auxiliary space preconditioning in **H**(**curl**) and **H**(div)

spaces, SIAM J. Numer. Anal. 45 (2007)], with results extending to the variable coefficient case and non-convex domains at the expense of a larger coarse space.

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MS22

Using Spectral Coarse Spaces of the H-Geneo Type for Efficient Solutions of the Helmholtz Equation

The Helmholtz equation is a widely used model in wave propagation and scattering problems. However, its numerical solution can be computationally expensive in high-frequency regime due to the oscillatory solution and the potential contrasts in coefficients. Parallel domain decomposition methods have been identified as promising solvers for such problems, but they often require a suitable coarse space to achieve robust behaviour. In this talk, we present the H-GenEO coarse space, which constructs an effective coarse space using localized eigenvectors of the Helmholtz operator. While the GenEO coarse space is designed for symmetric positive definite problems, the theory cannot be extended directly to the H-GenEO coarse space due to the indefinite nature of the underlying problem. During this talk it will be shown what the H-GenEO coarse space is capable of providing the required robust behaviour when used with a suitable domain decomposition method. Numerical experiments for increasing wave numbers demonstrate the efficiency of the method in solving complex Helmholtz problems, with potential applications in various scientific and engineering domains.

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MS23

Motivating Linear Algebra Concepts and Computations with Network Science

Representations of social network data with adjacency matrices and graph Laplacians provide a natural connection between network science and common topics from introductory linear algebra classes, including eigenvalues and matrix factorizations. Similarly, many commonly studied metrics and dynamical processes on networks have natural interpretations in terms of linear algebraic concepts. In this talk I will present several examples of these relationships and use them to motivate learning activities for linear algebra courses that help students explore and extend standard topics with an emphasis on applied network modeling. Finally, I will discuss how to incorporate modern software libraries into these exercises and address some common challenges with classroom implementations of technology.

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MS23

Teachings on Reflections and Generalized Rotations

One standard algorithm for computing the QR decomposition of a matrix is based on Householder transformations. This type of orthogonal matrix, which maps between two vectors x and y is a reflection, which we can derive using elementary geometric concepts. The product of multiple Householder transformations may thus result either in a reflection or a rotation. If the orthogonal matrix Q in the QR decomposition is supposed to be a rotation we can replace the Householder reflections with a set of Givens rotations. The product of rotations will always produce a rotation as a result. However, computing a QR decomposition using Householder transformations is computationally twice as efficient as a corresponding algorithm using Givens rotations. This raises the question if there exists an alternative orthogonal transformation with computational properties similar to a Householder transformation, but which is a rotation. For this type of orthogonal transformation, I will use the term generalized rotation. This contribution presents an algebraic derivation of such a generalized rotation to be used for computing a QR decomposition. Interestingly, this class of generalized rotations is practically never mentioned in standard textbooks on Linear Algebra. The derivation is based on elementary algebraic properties of orthogonal matrices and matrix algebra. Exceptions exist in the domain of robotics or computer vision, where the dimension of the corresponding vector spaces is constrained to be $n = 3$. There, rotations are realized via the exponential map of a skew-symmetric matrix, which contains the information about rotation axis and rotation angle. However, the associated computational scheme doesnt generalize directly into dimensions higher than 3. I will further discuss a few properties of such generalized rotations.

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MS23

Teaching Linear Algebra with Applications

Linear Algebra has many rich and beautiful applications which can be used to inspire the development of its central concepts. In this talk, we will share an application approach to designing a first-semester linear algebra course where applications are used to motivate and inform the development of central concepts including span, linear transformations, eigenvectors and eigenvalues, and the invertible matrix theorem. We will discuss our use of labs and other activities which connect linear algebra concepts with applications in computer graphics, predictive modeling, radiography/tomography, and more. These activities enhance students' experiences by providing them with clear applications of linear algebra concepts and the opportunity to learn accessible modeling techniques used by researchers. We will also discuss how technology can be used for both the implementation of applications as well as its pedagogical use in enhancing the learning experience.

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MS23

Linear Algebra, Statistics, and R

Linear algebra is a pervasive topic in statistics. In this talk, we will explore some ways in which linear algebra can be used to make statistical estimates and show how utilizing matrix representations will help make R functions more concise and efficient.

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MS24

Minimal Degenerations of Eigenstructure for Skew-Symmetric Matrix Polynomials

In this presentation, we describe qualitatively how eigenstructure of skew-symmetric matrix polynomials of odd degree changes under small perturbations in the matrix coefficients. Using strong linearization we prove a necessary and sufficient condition for one orbit of the linearization of a matrix polynomial to be a proper subset of the closure of the orbit of linearization of another polynomial. To achieve this, we introduce a set of rules describing structure transitions of the canonical blocks of the polynomial's linearization. These rules facilitate the construction of the stratification graphs of linearization of the polynomials. Finally, we state a method that allows us to sketch the entire or a part of the stratification graph of one matrix polynomial's linearization in relation to another matrix polynomial's linearization, provided both polynomials share the same degree but have different dimensions.

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MS24

Solving Parametric Eigenvalue Problems by Taylor Series and Chebyshev Expansion

We discuss two approaches to solving the parametric (or stochastic) eigenvalue problem. One of them uses a Taylor expansion and the other a Chebyshev expansion. The parametric eigenvalue problem assumes that the matrix A depends on a parameter μ, where μ might be a random variable. Consequently, the eigenvalues and eigenvectors are also functions of μ. We compute a Taylor approximation of these functions about μ_0 by iteratively computing the Taylor coefficients. The complexity of this approach is $O(n^3)$ for all eigenpairs, if the derivatives of $A(\mu)$ at μ_0 are given. The Chebyshev expansion works similarly. We first find an initial approximation iteratively which we then refine with Newtons method. This second method is more expensive but provides a good approximation over the whole interval of the expansion instead around a single point. We present numerical experiments confirming the complexity and demonstrating that the approaches are capable of tracking eigenvalues at intersection points. Further experiments shed light on the limitations of the Taylor expansion approach with respect to the distance from the expansion point μ_0. Finally, we present a dynamical system depending on a parameter μ. We estimate μ based on a recorded trajectory of the system using a kernel density estimator. This box is for abstract text content only.

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MS24

Minimization of the Pseudospectral Abscissa of a Matrix Polynomial

We consider a matrix polynomial dependent on several parameters. The minimization of its spectral abscissa, real part of its rightmost eigenvalue, over the parameters is motivated by stability considerations on the associated higher-order linear control system, yet comes with computational challenges especially due to the non-Lipschitz nature of the spectral abscissa. We instead propose to minimize the pseudospectral abscissa, the real part of the rightmost eigenvalue attainable over all perturbations of the matrix polynomial of prescribed norm. The pseudospectral abscissa is not only locally Lipschitz, but can also be used to ensure the stability of all nearby systems. We describe an approach to minimize the pseudospectral abscissa of a matrix polynomial over parameters. Especially, the larger matrix polynomials are nearly as easy to deal with as the smaller problems, as we also introduce a framework that converts larger problems to a sequence of smaller problems by means of one-sided subspace restrictions. We formally argue that the framework converges globally and at a superlinear rate. The efficiency and applicability of the proposed approach are illustrated numerically on several large matrix polynomials dependent on parameters.

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MS24

High Order Perturbation Methods for Multi-Parametric Quadratic and Generalized Eigenvalue Problems. Application to Duct Acoustics and the Importance of the Exceptional Points.

This work reviews the state of the art for high order perturbation methods for parametric eigenvalue problems. An extension of the method to the multi-parametric case for which the occurrence of spectral degeneracies like exceptional points (EPs) is known to increase is also proposed. An EP corresponds to specific value of the parameters, where the eigenvalues and the associated eigenvectors coalesce at a branch point singularity. These non-Hermitian degeneracies have raised considerable attention in the Physics community as these can have a great impact in a variety of problems (PT-symmetry, stability analysis...) but also because these spectral singularities limit the convergence of perturbation methods. The proposed approach is based on the computation of the successive derivatives of some selected eigenpairs with respect to the parameters so that, after a recombination step, part of characteristic polynomial coefficients can be approximated. This algebraic manipulation smoothers the problem allowing i) to quickly solve the eigenvalue problem in the parameter space, ii) to track modal branches, iii) to locate higher order EPs. The approach can be applied for the analysis of large sparse matrices. Illustrative applications

are presented in order to locate high order EPs in acoustic waveguides. The role of EPs on modal attenuation is demonstrated.

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MS25

A Nonlinear Spectral Core-Periphery Detection Method for Multiplex Networks

Core-periphery detection aims to separate the nodes of a complex network into two subsets: a core that is densely connected to the entire network and a periphery that is densely connected to the core but sparsely connected internally. The definition of core-periphery structure in multiplex networks that record different types of interactions between the same set of nodes but on different layers is nontrivial since a node may belong to the core in some layers and to the periphery in others. We propose a nonlinear spectral method for multiplex networks that simultaneously optimizes a node and a layer coreness vector by maximizing a suitable nonconvex homogeneous objective function by an alternating fixed point iteration. We prove global optimality and convergence guarantees for admissible hyper-parameter choices and convergence to local optima for the remaining cases. We derive a quantitative measure for the quality of a given multiplex core-periphery structure that allows the determination of the optimal core size. Numerical experiments on synthetic and real-world networks illustrate that our approach is robust against noisy layers and outperforms baseline methods with respect to a variety of core-periphery quality measures. In particular, all methods based on layer aggregation are improved when used in combination with the novel optimized layer coreness vector weights.

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MS25

Topological Duality in Multilayer Networks

Multilayer network science has revolutionized the study of complex systems characterized by nodes interacting across different layers. However, multilayer networks can be equivalently represented in terms of layers connected across different nodes. Surprisingly, the properties of such layerwise representation, as well as its relationship with the standard nodewise one, have been systematically overlooked and poorly investigated. Here, we provided a first characterization of the "dark" side of multilayer networks, where nodes become layers and layers become nodes, and unveiled their topological duality. We showed analytically and confirmed with extensive simulations that both sides are necessary to capture the network structure in terms of local connectivity. By providing complementary information, node-layer duality allows to better characterize different real-world multilayer networks, including social, infrastructure and biological systems. Notably, we found that neurodegeneration in Alzheimer's disease is more accurately reflected by connectivity changes across different frequencies of brain activity, rather than changes in connectivity among different brain regions. Taken together, these results unveil previously unappreciated hidden properties of multilayer networks that can be further developed to study the structure and dynamics of complex interconnected systems

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MS25

Learning the Right Layers of a Multilayer Network in Semi-Supervised Learning

Multilayer graphs can have a large number of layers describing a variety of different properties; however, it is a-priori not clear whether all the layers are actually useful to classify the nodes. Layers may carry the same or complementary clustering information, some layers may be more informative than others, and certain layers can potentially be just noise (i.e., they carry no information about the node clusters). Deciding which of these situations better describes a given dataset and identifying which are the most (and the least) informative layers is both very useful and highly challenging. We propose a new approach to semi-supervised community detection on multiplex networks. It is a Laplacian-regularized model that learns an optimal combination of the different layers from the available input labels. In our model, the layers are combined via nonlinear generalized mean functions which include as special cases several aggregation functions previously used in the literature. We formulate the problem as a bilevel optimization problem which we solve using an inexact Frank-Wolfe algorithm combined with a parametric Label Propagation scheme. We tested our methods over various synthetic and real multiplex networks, showing its effectiveness in dealing with diverse clustering scenarios, especially when certain layers are dominated by noise.

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MS26

Quantum Matrix State Linear Algebra

Quantum circuits inherently perform linear algebra operations on quantum states, suggesting the potential for executing numerical linear algebra computations on quantum computers. However, state-of-the-art quantum algorithms often rely on specific quantum access assumptions for data loading, limiting practicality. Common assumptions involve QRAM or quantum matrix oracles; yet QRAM's fea-

sibility is uncertain. In this talk, we propose an approach that assumes quantum access through state preparation circuits. We present qMSLA, a framework for operating on classical descriptions matrix state preparation circuits, using natural numerical linear algebra primitives. Each operation within qMSLA takes classical descriptions of matrix state preparation circuits as input and generates classical descriptions of new state preparation circuits, implementing matrix algebra between input matrices. Although the algorithms are classical to classical, they produce circuits intended for execution on a quantum computer. The framework streamlines quantum algorithm construction. Instead of intricate, problem-specific designs, mathematical solutions can be translated into qMSLA operations, yielding runnable quantum circuits. This simplifies implementation, enabling straightforward quantum algorithm development. We demonstrate the power of qMSLA via reimplementation of classic quantum algorithms (Hadamard Test, QFT, Phase Estimation, Qubitization, Block Encoding, etc.), and innovative algorithms (e.g. computing the trace matrix) product.

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MS27

Efficient Block Preconditioners for the Interior Point Solution of Convex Constrained Optimization

We address the preconditioned iterative solution of the saddle-point linear systems arising from the (regularized) Interior Point method applied to linear and quadratic convex programming problems, typically of large scale. Starting from the well-studied Constraint Preconditioner [L. Bergamaschi, J. Gondzio, and G. Zilli, *Preconditioning indefinite systems in interior point methods for optimization*, Comput. Optim. and Appl., 28 (2004)], we review a number of inexact variants with the aim to reduce the computational cost of the preconditioner application within the Krylov subspace solver of choice. In all cases we illustrate a spectral analysis showing the conditions under which a good clustering of the eigenvalues of the preconditioned matrix can be obtained, which foreshadows (at least in case PCG/MINRES Krylov solvers are used), a fast convergence of the iterative method. Results on a set of large size optimization problems [*A new preconditioning approach for an interior point-proximal method of multipliers for linear and convex quadratic programming*, Numer. Lin. Alg. Appl., 28 (2021)] [G. Zilli and L. Bergamaschi, *Block preconditioners for linear systems in interior point methods for convex constrained optimization*, Annali dell'Università di Ferrara, 68 (2022)]. confirm that the Inexact variants of the Constraint Preconditioner can yield efficient solution methods.

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MS27

Preconditioners for Interior Point Methods

We address the use of Interior Point Methods for optimization of problems in which direct solution techniques are too expensive and appropriately preconditioned iterative methods should be used. We briefly discuss the handling of inexactness caused by the use of iterative schemes and then focus on preconditioners well-suited to specific applications.

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MS27

Parameter-Robust Preconditioning for Oseen Iteration Applied to Navier-Stokes Control Problems

Optimal control problems with PDEs as constraints arise very often in scientific and industrial problems. Due to the difficulties arising in their numerical solution, researchers have put a great effort into devising robust solvers for this class of problems. An example of a highly challenging problem attracting significant attention is the distributed control of incompressible viscous fluid flow problems. In this case, the physics is described by the incompressible NavierStokes equations. Since the PDEs given in the constraints are non-linear, in order to obtain a solution of Navier-Stokes control problems one has to iteratively solve linearizations of the problems until a prescribed tolerance on the non-linear residual is achieved. In this talk, we present efficient and robust preconditioned iterative methods for the solution of the time-dependent incompressible NavierStokes control problems, with backward Euler discretization in time. The proposed preconditioner is based on a saddle-point type of approximation. We employ an inner iteration for the (1, 1)-block accelerated by a preconditioner for convectiondiffusion control problems when employing backward Euler in time. In addition, in order to derive an approximation for the Schur complement we employ a potent and flexible commutator argument applied to an appropriate block matrix. We show the effectiveness and robustness of our approach through a range of numerical experiments.

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MS28

Deep Learning-Guided Linear Algebra: Results and Challenges

This talk presents two results of the attempt to bridge the gap between deep learning and classical linear algebra. One the one hand, we will show how to generate sparsity patterns for effective block-Jacobi preconditioners with convolutional neural networks. On the other hand, we will demonstrate the effectiveness of using deep multi-layer perceptrons to predict optimal iterative Krylov solver for a

given sparse linear problem. The talk is concluded with a perspective on challenges hindering deep-learning research in numerical linear algebra, such as data availability and formatting, as well as opportunities, for example system generation and self-supervised training.

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MS28

Deeponet for Matrix-Free Preconditioners Construction

Preconditioning of linear systems is an essential element for guaranteeing a fast convergence of Krylov subspace methods and a very mature field of research. However, severe difficulties may still arise when dealing with matrix-free environments, where the system matrix is too big or too dense for being explicitly computed and stored. In this study, we propose a novel approach to approximate the application of a matrix inverse by utilizing a supervised deep learning framework called DeepONet that can learn nonlinear operators through a training process on input-output vector pairs. Specifically, we implement DeepONets to approximate the action of the inverse of the Schur Complement arising in saddle-point problems, the use of which can be very effective to precondition indefinite block systems in many applications. We test the proposed approach on some preliminary case problems to investigate its potential as a valid and innovative alternative to compute preconditioners for matrix-free iterative methods.

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MS28

Training Robust Low-Rank Neural Networks

As model and data sizes increase, interest is growing in parameter reduction techniques for neural networks. A prominent approach uses a memory-saving low-rank matrix factorization of the layers and trains directly over the low-rank manifold. Although able to retain accuracy, we observe that low-rank methods tend to compromise model robustness against adversarial perturbations. By modeling robustness in terms of the condition number of the neural network, we argue that this loss of robustness is due to the exploding singular values of the low-rank weight matrices. Thus, we introduce a robust low-rank training algorithm that simultaneously enforces low-rank and approximate orthonormal constraints. We present a variety of experimental tests showing that the resulting model reduces both training and inference costs while ensuring well-conditioning and thus better adversarial robustness, without compromising model accuracy.

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MS29

Stabilization of a Matrix Via a Low Rank-Adaptive Matrix Ode

Let A be a square matrix with a given structure (e.g. real matrix, sparsity pattern, Toeplitz structure, etc.) and assume that it is unstable, i.e. at least one of its eigenvalues lies in the complex right half-plane. The problem of stabilizing A consists in the computation of a matrix B, whose eigenvalues have negative real part and such that the perturbation $\Delta = B - A$ has minimal norm. The structured stabilization further requires that the perturbation preserves the structural pattern of A. We solve this nonconvex problem by a two-level procedure which involves the computation of the stationary points of a matrix ODE. We exploit the low rank underlying features of the problem by using an adaptive-rank integrator that follows slavishly the rank of the solution. We show the benefits derived from the low rank setting in several numerical examples, which also allow to deal with high dimensional problems.

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MS29

From Non-Autonomous Linear Odes to a Matrix Equation and Its Efficient Approximation

In many quantum mechanics problems one encounters a non-autonomous linear system of ODEs of the form

$$\frac{d}{dt}U(t) = H(t)U(t), \qquad U(-1) = I, \qquad t \in [0, T]\,.$$

The Hamiltonian $H(t)$ is an $N \times N$ matrix valued function. For many-body problems, this Hamiltonian grows exponentially in size with the number of, e.g., spins in nuclear magnetic resonance spectroscopy. This growth makes solving such a system of ODEs challenging, even for a moderate amount of spins. By starting from a new analytical expression for the solution $U(t)$ and expanding the resulting function in a basis of Legendre polynomials, we can reformulate this problem into finding the solution to an infinite system of linear equations. In this talk we propose a numerical solver based on solving a finite system of linear equations obtained by truncating the infinite system. Since

the Hamiltonians appearing in quantum mechanics problems are highly structured, the system of linear equations can be recast into a matrix equation. One such problem is described by the generalized Rosen-Zener model, for which we show that our solver, based on solving a matrix equation combined with low-rank truncation, outperforms the current state-of-the-art for large N.

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MS30

A Geometric Objective for Graph Coarsening with Machine Learning Applications

Graph coarsening is a technique for solving large-scale graph problems by working on a smaller version of the original graph, and possibly interpolating the results back to the original graph. Popularized by algebraic multigrid methods applied to solving linear systems of equations, graph coarsening finds a new chapter in machine learning, particularly graph-based learning models. However, it is challenging to naively apply existing coarsening methods, because it is unclear how the multigrid intuition matches the machine learning problem at hand. We develop an objective-driven approach by explicitly defining the coarsening objective, which admits a geometric interpretation-maintaining the pairwise distance of graphs. We derive the objective function by bounding the change of the distance and show its relationship with weighted kernel k-means clustering, which subsequently defines the coarsening method. We demonstrate its effective use in graph regression and classification tasks.

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MS30

Register Tiling for Sparse Neural Network Inference

The unstructured sparsity pattern of matrices in pruned machine learning models along with their sparsity ratio has rendered useless the large class of libraries and systems that optimize sparse matrix multiplications. Reusing registers is particularly difficult because accesses to memory locations should be known statically. In this talk I will discuss our work Sparse Register Tiling, a new technique composed of an unroll-and-sparse-jam transformation followed by data compression that is specifically tailored to sparsity patterns in ML matrices.

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MS30

S-Step Dual Coordinate Descent Methods for Kernel Problems

This talk will present s-step derivations of dual coordinate descent (DCD) methods for solving the kernelized ridge regression and support vector machines problems. We show that the new s-step methods reduce latency cost by a tunable factor of s at the expense of a factor of s additional computation. We show theoretical analysis which shows the computation, bandwidth and latency tradeoffs of the newly designed algorithms and numerical experiments which highlight the stability of the s-step DCD methods. Finally, we implement these methods in C using Intel MKL SparseBLAS for linear algebra subroutines and MPI for distributed-memory parallelism. Our preliminary results illustrate that the new s-step DCD methods are 2 - 5x faster than the classical methods on a contemporary parallel cluster without altering convergence rate or solution accuracy.

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MS31

The Moore-Penrose Inverse of a Laplacian Matrix of a Threshold Graph

Different methods for the calculation of the Moore-Penrose inverse of a Laplacian matrix of a connected threshold graph G will be presented. Combinatorial formula for $L(G)^\dagger$ depends on the number of spanning trees of a threshold graph G, which can be significantly large. Therefore, this formula can be inconvenient for use in computations, and some different approaches should be investigated. We will derive three algebraic methods for computation the Moore-Penrose inverse of $L(G)$ which are based on recovering the form of $L(G)^\dagger$ from matrices of smaller sizes. One method reduces the problem of determining $L(G)^\dagger$ to the problem of computing the ordinary inverse of a smaller matrix, while the second applies the singular value decomposition of an associated matrix of reduced size. Third method reconstruct $L(G)^\dagger$ from its divisor matrix. From a computational point of view, all methods have their benefits. The computations in first method are realized on the matrices of the smallest size among matrices used in second two methods. The advantage of second method is usage of singular value decomposition of a matrix, while the third approach reduce the determining of $L(G)^\dagger$ to the computation of Moore-Penrose inverse of smaller symmetric matrix.

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MS31

The (b,c)-Core Inverse and Its Applications

Given $a, b, c \in S$, we say that a is (b, c)-*core invertible* if there exists an $x \in S$ such that $caxc = c$, $xS = bS$ and $Sx = Sc^*$. It is proved that such an x is unique whenever it exists. In this case, x is called the (b, c)-core inverse of a. This provides a unified framework for the Moore–Penrose inverse, core inverse and w-core inverse, where $w \in S$. Sev-

eral characterizations of the (b, c)-core inverse are derived. For instance, it is proved that a is (b, c)-core invertible if and only if a is (b, c)-invertible and c is $\{1, 3\}$-invertible. Also, we introduce the dual (b, c)-core inverse and obtain some results dual to those on the (b, c)-core inverse. An element $y \in S$ is called the dual (b, c)-core inverse of a if $byab = b$, $yS = b^*S$ and $Sy = Sc$. We show that a is both (b, c)-core and dual (b, c)-core invertible if and only if a is (b, c)-invertible and cab is Moore–Penrose invertible. Finally, (b, c)-core inverses and dual (b, c)-core inverses are investigated in a ring with an involution.

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MS32

Improved Perturbation Bounds for Eigenvalues in the Parameter-Dependent Quadratic Eigenvalue Problem Enabling Efficient Damping Optimization

Quadratic eigenvalue problems (QEPs) with parameters, denoted as parameter-dependent quadratic eigenvalue problems (PQEPs), are expressed by the equation:

$$(\lambda^2(\mathbf{v})M + \lambda(\mathbf{v})D(\mathbf{v}) + K)x(\mathbf{v}) = 0,$$

where M and K are Hermitian positive definite matrices of size $n \times n$, and $D(\mathbf{v})$ is an $n \times n$ Hermitian positive semidefinite matrix dependent on a vector of damping (viscosity) parameters $\mathbf{v} \in \mathbb{R}^k_+$. These problems find applications in various fields. A prior study [Truhar, Tomljanovic, and Puvaca, Approximation of damped quadratic eigenvalue problem by dimension reduction, Appl. Math. Comput., 347: 40-53 (2019)] established a perturbation bound for approximating the eigenvalues of the PQEP through dimension reduction and leveraging the Gerschgorin theorem. Expanding upon the findings of the paper mentioned above, by using Cassini ovals, we present perturbation bounds applicable to the eigenvalues of the PQEP, particularly beneficial for damping optimization. These bounds are anticipated to enhance the efficiency in determining optimal eigenvalue positions, thus contributing to improved solutions in practical applications.

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MS32

Fast Optimization of Viscosities for Frequency-Weighted Damping of Second-Order Systems

We consider frequency-weighted damping optimization for vibrating systems described by a second-order differential equation. The goal is to determine viscosity values such that eigenvalues are kept away from certain undesirable areas on the imaginary axis. We present two complementary techniques. First, we propose new frameworks using nonsmooth constrained optimization problems, whose solutions both damp undesirable frequency bands and maintain stability of the system. These frameworks also allow us to weight which frequency bands are the most important to damp. Second, we also propose a fast new eigensolver for the structured quadratic eigenvalue problems that appear in such vibrating systems. In order to be efficient, our new eigensolver exploits special properties of diagonal-plus-rank-one complex symmetric matrices, which we leverage by showing how each quadratic eigenvalue problem can be transformed into a short sequence of such linear eigenvalue problems. The result is an eigensolver that is substantially faster than existing techniques. By combining this new solver with our new optimization frameworks, we obtain our overall algorithm for fast computation of optimal viscosities. The efficiency and performance of our new methods are verified and illustrated on several numerical examples.

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MS33

Diagnosing Local Minima and Accelerating Convergence of Variational Quantum Eigensolvers with Quantum Subspace Techniques

Recent research has shown that wavefunction evolution in real- and imaginary-time can generate quantum subspaces with significant utility for obtaining accurate ground state energies. Inspired by these methods, we propose combining quantum subspace techniques with the variational quantum eigensolver (VQE). In our approach, the parameterized quantum circuit is divided into a series of smaller subcircuits. The sequential application of these subcircuits to an initial state generates a quantum subspace that we use to obtain high-accuracy groundstate energies. We dub this technique the circuit subspace variational quantum eigensolver (CSVQE) algorithm. By benchmarking CSVQE on a range of quantum chemistry problems, we show that it can achieve significant error reduction compared to conventional VQE, particularly for poorly optimized circuits, which greatly improves convergence rates. Furthermore, we demonstrate that when applied to circuits trapped at a local minima, CSVQE can still produce energies close to the global minimum of the energy landscape, making it a promising tool for diagnosing local minima and addressing barren plateaus.

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MS33

Error Analysis in Quantum Krylov Algorithms

We present a nonasymptotic error analysis of quantum Krylov algorithms based on real-time evolutions, subject to generic errors in the outputs of the quantum circuits. We prove upper and lower bounds on the resulting ground state energy estimates, and the error in the upper bound is linear in the input error rates. This resolves a misalignment between known numerics, which exhibit approximately linear error scaling, and prior theoretical analysis, which only provably obtained square-root scaling. Our main technique is expressing generic errors in terms of an effective target Hamiltonian studied in an effective Krylov space, which may be of independent interest.

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MS33

Hybrid Quantum Algorithms for Finding Low-Energy Eigenstates in Condensed Matter Physics

In this talk, we show a proof-of-principle demonstration of two medium-term hybrid quantum algorithms for finding low-energy eigenstates, unitary variational quantum phase estimation (UVQPE) and observable dynamical mode decomposition (ODMD). Both algorithms use the native capability of quantum devices for unitary evolution to generate a small linear algebra problem that is solved classically to find an approximate ground state and corresponding energy. We demonstrate both algorithms on a model from condensed matter physics that has competing, or "frustrated,' interactions between particles that make scaled-up versions of the system difficult to study with a classical computer. We run simulations on the Quantinuum H1 processor and the corresponding noisy emulator. Even in the presence of noise, both algorithms rapidly converge, giving good approximations to the lowest eigenvalue of the model and the corresponding eigenstate. We furthermore show how, using the block-diagonal structure of the Hamiltonian matrix describing the system, the same algorithms can be used to find further eigenstates, giving access to important physical properties such as the magnetization curve.

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MS34

A Posteriori Error Estimation for Randomized Low-Rank Approximation

A number of algorithms are now available—including Halko-Martinsson-Tropp, interpolative decomposition, CUR, generalized Nystrom, and QR with column pivoting—for computing a low-rank approximation of matrices. Some methods come with extremely strong guarantees, while others may fail with nonnegligible probability. We present methods for efficiently estimating the error of the approximation for a specific instantiation of the methods. Such certificate allows us to execute "responsibly reckless" algorithms, wherein one tries a fast, but potentially unstable, algorithm, to obtain a potential solution; the quality of the solution is then assessed in a reliable fashion, and remedied if necessary.

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MS34

Computationally Efficient Tracking for Iterative Random Sketching

Iterative randomized linear algebra techniques have become increasingly popular for large-scale problems because they can quickly generate updates to a solution by solving small, approximate sub-problems. Unsurprisingly, the main computational cost with these methods is the cost of solving these sub-problems. If the sub-problems were unrelated, there would be no obvious way to reduce these costs; however, since the sub-problems are approximations of the same problem, they are similar in a statistical sense. This talk will use relatively weak distributional assumptions on the randomness of sub-problems to quantify this statistical similarity. Then, it will combine this quantification with the robust literature on deflation methods, which accelerate Krylov solvers applied to similar linear systems, to develop a technique that accelerates randomized block coordinate descent least-squares solvers. As part of this presentation, we will present rigorous theoretical bounds and numerical experiments to demonstrate our technique's substantial improvements over standard methods for efficiently solving randomized sub-problems.

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MS35

Efficient Arithmetic Operations for $\mathcal{H}^2$-Matrices

$\mathcal{H}^2$-matrices can be used to represent large dense matrices with linear complexity both in storage requirements and computational work. While the nested low-rank factorizations underlying this representation are crucial for efficient storage and matrix-vector multiplication, preserving this structure during arithmetic operations poses a signficiant challenge. This talk presents an algorithm for approximating the matrix multiplication of $\mathcal{H}^2$-matrices, a crucial building block for more advanced algorithms. The new algorithm has linear complexity and uses adaptively chosen bases to guarantee a prescribed accuracy of the result.

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MS35

Coupled Clustering Strategies for Hierarchical Matrices in Saddle Point Problems

Fluid flow problems can be modeled by the Navier-Stokes or, after linearization, by the Oseen equations. Their discretization results in discrete saddle point problems. These systems of equations are typically very large and need to be solved iteratively. Standard (block) precondition-

ing techniques rely on an approximation of the (inverse) Schur complement which may be obtained by a hierarchical LU decomposition. Its computational complexity depends, among other things, on the hierarchical block structures of the involved matrices. Widely used techniques do not consider the connection between the discretization grids for the velocity field and the pressure, respectively. Here, we present a hierarchical block structure for the finite element discretization of the gradient operator that is improved by considering the connection between the two involved grids. Numerical results imply that this new structure allows for a faster computation of the Schur complement which often is the bottleneck for the setup of the (hierarchical) block LU factorization of the entire saddle point matrix to be used as a preconditioner.

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MS35

A Boundary Integral Scheme for an Acoustic Scattering Problem

One way to solve the acoustic wave equation is by transforming the problem into one posed in frequency space. This then requires one to solve the exterior Helmholtz problem over a band of frequencies, and to then transform the solution back into the time domain. At each frequency, this can be efficient since fast direct solvers for the Helmholtz equation exist. We discuss some of the challenges that arise in this setting, and how they can be overcome.

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MS36

Fast Computation of Functions of Hierarchical Semiseparable Matrices

Introducing a general definition of telescopic decomposition, we link different representations of Hierarchical Semiseparable (HSS) matrices already proposed in the literature and we show how to convert them into a standard one. We also present an algorithm that, taking as input a telescopic decomposition of an HSS matrix A, computes a telescopic decomposition of $f(A)$. Combining this technique with the randomized procedure presented in [J. Levitt and P.G. Martinsson, Linear-complexity black-box randomized compression of hierarchically block separable matrices, arXiv:2205.02990, 2022] we are able to compute a compressed representation of $f(A)$ just by performing a small number of matrix-vector products involving A.

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MS36

Backward Errors for Nonlinear Eigenvalue Problems

The backward error analysis is an important part of the perturbation theory and it is particularly useful for the study of the reliability of the numerical methods. Given an approximate eigenpair $(\hat{\lambda}, \hat{v})$ of the nonlinear eigenvalue problem $\mathcal{F}(\lambda) = \sum_{i=1}^{k} f_i(\lambda) F_i$, with $F_i \in \mathbb{C}^{n\times n}$, the backward error can be defined as the smallest perturbations ΔF_i such that $(\hat{\lambda}, \hat{v})$ is an exact eigenpair of $\sum_{i=1}^{k} f_i(\lambda)\,(F_i + \Delta F_i)$. We provide theoretical results about the combined backward error of a set of approximate eigenpairs $(\hat{\lambda}_1, \hat{v}_1), \ldots, (\hat{\lambda}_p, \hat{v}_p)$, that is finding a set of matrices ΔF_i such that $\sum_{i=1}^{k} f_i(\hat{\lambda}_j)(F_i + \Delta F_i)\hat{v}_j = 0$, for each $j = 1, \ldots, p$. Indeed, small backward errors for separate eigenpairs do not imply small combined backward errors for a set of approximate eigenpairs. In this talk, we propose a characterization of the combined backward error for a set of eigenvalues of nonlinear matrix-valued functions using an a-posteriori quantity and introduce a computable upper bound. Time permitting, we discuss imposing additional structures on the coefficients of the matrix-valued function (for instance Hermitian matrices) and derive a few results for the structured backward errors in this setting.

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MS36

Numerical Solution of a Class of Quasi-Linear Matrix Equations and Applications

Given the matrix equation $\mathbf{AX} + \mathbf{XB} + \mathbf{f}(\mathbf{X})\mathbf{C} = \mathbf{D}$ in the unknown $n \times m$ matrix $\mathbf{X}$, we analyze existence and uniqueness conditions, together with computational solution strategies for $f : \mathbb{R}^{n\times m} \to \mathbb{R}$ being a linear or nonlinear function. We characterize different properties of the matrix equation and of its solution, depending on the considered classes of functions f. Our analysis mainly concerns small dimensional problems, though several considerations also apply to large scale matrix equations.

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MS37

Learning Low-Dimensional Models of Microscopes

Linear operators appear in microscopy as a model for the spatially varying blurs an acquisition device impairs images with. In real-world applications, the operators are very large objects thus computationally intensive to deal with. To bypass this burden, state-of-the-art methods rely on the coarse approximation of the operators by convolutions. In this talk we will first investigate some tools to efficiently represent and estimate these operators. Then, we will present a method to learn a low dimensional subset of operators from the observation of the action of a few of them on micro-beads images. This computationally efficient procedure allows to accurately calibrate microscopes whose physics of degradation relies on a small number of parameters (even though the physics might seem complex at first). This approach is an essential step towards the effective resolution of blind (or semi-) blind inverse problems.

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MS37

How Many Neurons do we Need? A Refined Analysis for Shallow Networks Trained with Gradient Descent

We analyze the generalization properties of two-layer neural networks in the neural tangent kernel (NTK) regime, trained with gradient descent (GD). For early stopped GD we derive fast rates of convergence that are known to be minimax optimal in the framework of non-parametric regression in reproducing kernel Hilbert spaces. On our way, we precisely keep track of the number of hidden neurons required for generalization and improve over existing results. We further show that the weights during training remain in a vicinity around initialization, the radius being dependent on structural assumptions such as degree of smoothness of the regression function and eigenvalue decay of the integral operator associated to the NTK. This is a joint work with Mike Nguyen (TU Braunschweig)

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MS37

Conservation Laws for Gradient Flows

Understanding the geometric properties of gradient descent dynamics is a key ingredient in deciphering the recent success of very large machine learning models. A striking observation is that trained over-parameterized models retain some properties of the optimization initialization. This "implicit bias" is believed to be responsible for some favorable properties of the trained models and could explain their good generalization properties. In this talk I will first rigorously expose the definition and basic properties of "conservation laws", which are maximal sets of independent quantities conserved during gradient flows of a given model (e.g. of a ReLU network with a given architecture) with any training data and any loss. Then I will explain how to find the exact number of these quantities by performing finite-dimensional algebraic manipulations on the Lie algebra generated by the Jacobian of the model. In the specific case of linear and ReLu networks, this procedure recovers the conservation laws known in the literature, and prove that there are no other laws. The associated paper can be found here https://arxiv.org/abs/2307.00144and the open source code is here https://github.com/sibyllema/Conservation_laws. This is a joint work with Sibylle Marcotte and Rmi Gribonval.

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MS37

Fast Multipole Attention: A Divide-and-Conquer Attention Mechanism for Long Sequences

Transformer-based models have achieved state-of-the-art performance in many areas. However, the quadratic complexity of self-attention with respect to the input length hinders the applicability of Transformer-based models to long sequences. To address this, we present Fast Multipole Attention (FMA), a new attention mechanism that uses a divide-and-conquer strategy to reduce the time and memory complexity of attention for sequences of length n from $\mathcal{O}(n^2)$ to $\mathcal{O}(n) \log n$ or $\mathcal{O}(n)$ while retaining a global receptive field. The hierarchical approach groups queries, keys, and values into levels of resolution, where groups at greater distances are increasingly larger in size and the weights to compute group quantities are learned. As such, the interaction between tokens far from each other is considered in lower resolution in an efficient hierarchical manner. This multi-level divide-and-conquer strategy is inspired by fast summation methods from n-body physics and the Fast Multipole Method. We find empirically that the Fast Multipole Transformer performs much better than other efficient transformers on autoregressive and bidirectional language modeling tasks in terms of memory size and accuracy. The FMA mechanism has the potential to empower large language models with much greater sequence lengths, taking the full context into account in an efficient, naturally hierarchical manner during training and when generating long sequences.

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MS38

Low Rank Methods for Parametric Partial Differ-

ential Equations

We consider systems of parametric Partial Differential Equations (PDEs), and we look for an approximation of the solution as function of the space-time coordinates and the parameters. This is beneficial when dealing with Uncertainty quantification and parameter estimation tasks. In this work, we investigate a low-rank tensor approximation of the solution, in which we separate the dependence on space-time and parameters. The rank is not fixed a priori, instead, it is determined based on error criteria. A tensor GMRES solver is presented. In view of improving the convergence of the iterations we introduce several possible preconditioners and compare their performances in terms of accuracy, ability to preserve the structure of the solution (conserved quantities) and computational cost. Several numerical experiments are shown.

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MS38

Low-Rank Tree Tensor Network Operators for Quantum Spin Systems

Recently, tree tensor networks (TTNs) turned out to be a promising ansatz to overcome the so-called "curse of dimensionality', as they are an efficient hierarchical data sparse format to approximate tensors. Based on dynamical low-rank approximation, several time-integration schemes for TTNs have been proposed. All integration schemes require several applications of the right-hand side of the differential equation per time-step, such that a compact representation of the underlying operator in the same TTN format is crucial. The compactness of this so-called tree tensor network operator (TTNO) depends on the needed ranks to represent the Hamiltonian in a tree format. A novel low-rank tree tensor network representation for long-range Hamiltonians is introduced. The construction is based on a hierarchical semi-separable (HSS) matrix decomposition of the interaction matrix. In a HSS decomposition all off-diagonal blocks of the interaction matrix are represented by a low-rank factorization of at most rank k, called HSS-rank. It is shown that if the interaction matrix admits a HSS decomposition of HSS-rank k, then the Hamiltonian can be exactly represented by a TTNO of maximal rank $k+2$. ϵ-HSS approximations of the interaction matrix can be used to approximate the corresponding Hamiltonian. Numerical experiments validate the theoretical results and show that small HSS ranks are indeed encountered for many relevant Hamiltonians of interest.

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MS38

Approximation to Multivariate Functions in the Extended Tensor Train Format

This talk introduces the extended functional tensor train (EFTT) format for compressing and working with multivariate functions on tensor product domains. Our compression algorithm combines tensorized Chebyshev interpolation with a low-rank approximation algorithm that is entirely based on function evaluations. Compared to existing methods based on the functional tensor train format, our approach often reduces the required storage, sometimes considerably, while achieving the same accuracy. In particular, we reduce the number of function evaluations required to achieve a prescribed accuracy by up to over 96% compared to the algorithm from [Gorodetsky, Karaman and Marzouk, Comput. Methods Appl. Mech. Eng., 347 (2019)].

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MS39

Some Quaternion Tensor Decompositions with Applications to Signal Processing

In this talk, we establish some simultaneous decomposition for tensors via different tensor products. These simultaneous decompositions trans- forms the tensors into some nice forms. We conclude with applications in the color video signal processing and color watermark processing.

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MS39

Solvability of Some Systems of Operator Equations in Hilbert C^*-Modules

We will consider the system of equations $AX = C$, $XB = D$ in the framework of Hilbert C^*-modules. This system has been widely studied for matrices, Hilbert space operators, and closed range operators on Hilbert C^*-modules. The previous results are mainly focused on the regular case, that is, the ranges of the associated operators are assumed to be closed (which always holds for matrices) and the main tool in dealing with such kind of operators are the bounded generalized inverses. In this talk, we will consider the solvability of this system and related equations under less restrictive conditions. We will present necessary and sufficient conditions for the existence of Hermitian and positive solutions of this system and the general form of such solutions.

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MS39

Low Rank Pure Quaternion Approximation for Pure Quaternion Matrices

Quaternion matrices are employed successfully in many color image processing applications. In particular, a pure quaternion matrix can be used to represent red, green, and blue channels of color images. A low-rank approximation for a pure quaternion matrix can be obtained by using the quaternion singular value decomposition. However, this approximation is not optimal in the sense that the resulting low-rank approximation matrix may not be pure quaternion, i.e., the low-rank matrix contains a real component which is not useful for the representation of a color image. The main contribution of this paper is to find an optimal rank-r pure quaternion matrix approximation for a pure quaternion matrix (a color image). Our idea is to use a projection on a low-rank quaternion matrix manifold and a projection on a quaternion matrix with zero real component, and develop an alternating projections algorithm to find such optimal low-rank pure quaternion matrix approximation. The convergence of the projection algorithm can be established by showing that the low-rank quaternion matrix manifold and the zero real component quaternion matrix manifold has a nontrivial intersection point. Numerical examples on synthetic pure quaternion matrices and color images are presented to illustrate the projection algorithm can find optimal low-rank pure quaternion approximation for pure quaternion matrices or color images.

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MS39

Some Novel Results on Quaternion Matrix Equations

In this talk, I will give a brief introduction to the new developments on Sylvester-type matrix equations over the quaternion algebra.

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MS40

Nonsmooth Optimization on Manifolds

Within the context of optimization on manifolds, a research direction of particular interest is the investigation of algorithms fit to optimize non-smooth objectives. This research area is relevant since the need for optimizing nonsmooth objective functions arises in many real-world problems and applications such as image and signal restoration, denoising, inpainting, etc. In this talk, we discuss optimization techniques for real-valued, lower-semicontinuous, and geodesically convex functions defined on Riemannian manifolds, as many of the applications mentioned previously can be studied as minimization tasks where the objective function has this type of structure. We showcase a novel algorithm as well as numerical examples.

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MS40

Bounding Geometric Penalties in First-Order Riemannian Optimization

Convergence rates of Riemannian optimization algorithms often depend on geometric quantities depending on the sectional curvature and the distance between iterates and an optimizer. Numerous previous works bound these distances only by assumption, leading to an incomplete analysis and unquantified rates. I will talk about different first-order algorithms and techniques that remove this limitation in different geodesically-convex or convex-concave problems. There are two ways of avoiding these problems: (A) constraining the iterates, making the algorithm deal with those constraints (which presents its challenges, even for projected gradient descent) or (B) showing that your algorithm naturally stays in some bounded set that you can quantify. As a result, different geometric penalties appear in the convergence rates, which I will summarize.

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MS40

Introduction to Manifold Methods in Numerical Linear Algebra

Riemannian geometry led to major breakthroughs in various numerical linear algebra problems such as matrix/tensor factorization and completion, or optimal rotation computation. This talk will provide an overview of recent applications of Riemannian geometry to numerical linear algebra, connections with optimization theory and numerical analysis, and will introduce the key geometric notions and fundamental results needed by the contributed talks of this minisymposium.

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MS40

Analysis of CG on Indefinite Matrices with Application to Local Convergence of Trust-Regions

The core theory of conjugate gradient (CG) assumes a positive definite operator. We develop new tools to analyze the dynamics of CG in the presence of small eigenvalues of any sign carrying little weight. In substance, we relate the iterates that CG produces to the ones stemming from an associated well-behaved positive definite instance. The main application of interest is the analysis of trust-region methods (TR) around minimizers where the Polyak–Lojasiewicz condition holds. In this setting, the Hessian can have vanishingly small, possibly negative eigenvalues at points arbi-

trarily close to minimizers. We prove super-linear convergence for a specific subproblem solver based on CG, known as the truncated conjugate gradient method.

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MS41

Strategies for Simulating Time Evolution of Hamiltonian Lattice Field Theories

Simulating the time evolution of quantum field theories given some Hamiltonian H requires developing algorithms for implementing the unitary operator e^{-iHt}. A variety of techniques exist that accomplish this task, with the most common technique used in this field so far being Trotterization, which is a special case of the application of a product formula. However, other techniques exist that promise better asymptotic scaling in certain parameters of the theory being simulated, the most efficient of which are based on the concept of block encoding. In this work we derive and compare the asymptotic complexities of several commonly used simulation techniques in application to Hamiltonian Lattice Field Theories (HLFTs). As an illustration, we apply them to the case of a scalar field theory discretized on a spatial lattice. We also propose two new types of block encodings for bosonic degrees of freedom. The first improves the approach based on the Linear Combination of Unitaries (LCU), while the second is based on the Quantum Eigenvalue Transformation for Unitary Matrices (QETU). The paper includes a pedagogical review of utilized techniques, in particular Product Formulas, LCU, Qubitization, QSP, QETU, as well as a technique we call HHKL based on its inventors.

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MS42

On the Concentration and Variance of the Error of Randomized Iterative Methods

Stochastic iterative methods are useful in a variety of large-scale numerical linear algebraic, machine learning, and statistical problems, in part due to their low-memory footprint. They are frequently used in a variety of applications, and thus it is imperative to have a thorough theoretical understanding of their behavior. For stochastic methods, this motivates providing bounds on the variance and concentration of their error, which can be used to generate confidence intervals around the bounds on their expected error. In this talk, we provide both upper and lower bounds for the concentration of the error and an upper bound on the variance of the error of a general class of stochastic iterative methods, including the randomized Kaczmarz method and the randomized Gauss-Seidel method. This is joint work with Dr. Jamie Haddock (HMC) and Toby Anderson (HMC).

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MS42

Novel Randomized Algorithms for QR with Column Pivoting and Their Implementations in RandLAPACK

We present a pair of novel algorithms for QR decomposition with column pivoting. These algorithms use methods from RandNLA, in particular carefully using randomized sketching to accelerate both pivot decisions for the input matrix and the process of decomposing the pivoted matrix via Cholesky QR. The original algorithm, CQRRPT (pronounced "see-crypt"), is designed specifically for tall data matrices, while its successor, CQRRP, is applicable for matrices of any aspect ratio. We implement the algorithms in RandLAPACK by calling into RandBLAS and vendor-provided BLAS/LAPACK libraries. Experiments with these implementations were performed on an Intel Xeon Gold 6248R CPU and demonstrated order-of-magnitude speedups relative to LAPACKs standard function for QRCP, significant speedups over existing algorithms for QRCP and, in the case with CQRRPT, comparable performance to a specialized algorithm for unpivoted QR of tall matrices.

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MS42

Efficient Randomization Techniques for Data Assimilation

Strong Constraint 4D Variational (SC-4DVAR) is a data assimilation method that is widely used in climate and weather. Computing the maximum a posteriori estimate in SC-4DVAR involves solving a minimization problem. We use the Gauss-Newton Method. The computation of the descent direction is expensive since it involves a large linear solve of an ill-conditioned linear system. To address this, we efficiently construct scalable preconditioners using three different randomization techniques. The randomized techniques rely on a certain low-rank structure involving the Gauss-Newton Hessian. We also develop an adaptive approach to estimate the rank and to determine when to recompute the preconditioner. The proposed techniques are amenable to parallelization and drastically reduce the number of (Gauss-Newton) Hessian products. The proposed techniques also come with theoretical guarantees on the condition number. We demonstrate the performance and effectiveness of our methodology on various problems such as Burgers and barotropic vorticity equation.

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MS42

On Sketches and Corruptions: Devising Adaptive

Randomized Iterative Methods for Large Linear Systems

When the data is large or comes in a streaming way, randomized iterative methods provide an efficient way to solve a variety of problems, including solving linear systems, finding least square solutions, solving feasibility problems, and beyond. Randomized Kaczmarz algorithm for solving overdetermined linear systems is one of the popular choices due to its efficiency and its simple, geometrically intuitive iterative steps. In challenging cases, for example, when the condition number of the system is bad, or some of the equations contain large corruptions, the geometry can be also helpful to augment the solver in the right way. For example, it can inform an exploration stage that helps avoid corrupted equations, as we have recently proposed in the Quantile Randomized Kaczmarz method. I will explain this idea and then talk about our recent work that proposes the Kaczmarz-based algorithms that use external knowledge about the linear system to (a) accelerate the convergence of iterative solvers, and (b) enable convergence in the highly corrupted regime.

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MS43

Construction of Hierarchically Semi-Separable Matrix Using Faster Randomized Sketching

We extend our early work on an adaptive partially matrix-free Hierarchically Semi-Separable (HSS) matrix construction algorithm using Gaussian sketching operators to a broader class of Johnson-Lindenstrauss (JL) sketching operators. We present theoretical work which justifies this extension. In particular, we extend the earlier concentration bounds to all JL sketching operators and examine this bound for specific classes of such operators including the original Gaussian sketching operators, subsampled randomized Hadamard transform (SRHT) and the sparse Johnson-Lindenstrauss transform (SJLT). We demonstrate experimentally that using SJLT instead of Gaussian sketching operators leads to 1.5-2.5x speedups of the HSS construction implementation in the STRUMPACK C++ library. The generalized algorithm allows users to select their own JL sketching operators with theoretical lower bounds on the size of the operators which may lead to faster runtime with similar HSS construction accuracy.

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MS43

Fast Randomized Algorithms for Rank Structured Matrices

The talk describes a set of recently developed randomized algorithms for computing a data sparse representation of a rank structured matrix (such as an $\mathcal{H}$-matrix, or an HBS/HSS matrix). The algorithms are black box in the sense that they interact with the matrix to be compressed only through its action on vectors, making them ideal for tasks such as forming Schur complements in sparse direct solvers, or for matrix matrix multiplication. In situations where the operator to be compressed (and its transpose) can be applied in $O(N)$ operations, the compression as a whole has linear complexity as well, in many environments. Of particular interest is a recent technique ("Randomized Strong Recursive Skeletonization", or RSRS) that simultaneously both compresses and factorizes an $\mathcal{H}^2$-matrix with a strong admissibility criterion.

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MS43

Leveraging Low-Rank Updates and Interpolation in Parallel-in-Time Algorithms Based on the Diagonalization Technique

This work is concerned with linear matrix equations that arise from the space-time discretization of time-dependent linear partial differential equations (PDEs). Such matrix equations have been considered, for example, in the context of parallel-in-time integration leading to a class of algorithms called ParaDiag. We develop and analyze two novel approaches for the numerical solution of such equations. Our first approach is based on the observation that the modification of these equations performed by ParaDiag in order to solve them in parallel has low rank. Building upon previous work on low-rank updates of matrix equations, this allows us to make use of tensorized Krylov subspace methods to account for the modification. Our second approach is based on interpolating the solution of the matrix equation from the solutions of several modifications. Both approaches avoid the use of iterative refinement needed by ParaDiag and related space-time approaches in order to attain good accuracy. In turn, our new algorithms have the potential to outperform, sometimes significantly, existing methods. This potential is demonstrated for several different types of PDEs.

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MS43

A Stable Matrix Version of the 2D Fast Multipole Method

The fast multipole method (FMM) is important in accelerating some kernel matrix-vector multiplications. One of the goals of this talk is to show an intuitive matrix version of the FMM in 2D. Additionally, we give a strategy to efficiently construct FMM matrices satisfying certain norm bounds to ensure stable operations. To illustrate our ideas, we focus our discussion on the generalized Cauchy kernel, the Poisson kernel, and the 2D Helmholtz kernel. It is worth noting that these ideas can in fact be applied to other kernels. Some numerical results are provided to validate our strategy. Finally, we provide the long overdue backward stability result for the FMM. Our analysis shows that the entrywise backward error only depends logarithmically on the matrix size, which is better than the standard dense matrix-vector multiplication, whose entrywise backward error depends linearly on the matrix size. This is joint work with Xiaofeng Ou and Jianlin Xia.

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MS44

Advanced Balancing-Based Model Reduction for Data Assimilation

Solving Bayesian inverse problems quickly becomes infeasible in high dimensions. This is where numerical linear algebra methods come in, especially model order reduction. Balanced truncation is a well-established model order reduction method that has proven useful in linear Gaussian Bayesian inference and especially for the Bayesian smoothing problem. While classical balanced truncation preserves states of a system that are both easily reachable and easily observable, Bayesian inference requires a balance between prior knowledge and information from (error-prone) observations. In both cases, the solution of the Lyapunov equations must be determined to obtain the two system Gramians, and then a generalized eigenvalue problem with these two matrices must be solved. In this talk we will present extensions of this concept beyond linear Gaussian smoothing problems. In particular, we will study modified Gramians: While fixed Gramians have been considered for the linear smoothing problem, evolving Gramians and thus matrix updates are necessary to enable Bayesian filtering. Quadratic nonlinearities also lead to changing Gramians and thus to more involved numerical methods.

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MS44

Iterative Approaches for Tensor Inverse Problems

In applications involving inverse problems, large-scale data is a common challenge. In this presentation, we introduce an iterative method for approximating the solution of large-scale multi-linear systems, represented in the form A*X=B under the tensor t-product. Unlike previously proposed randomized iterative strategies, such as the tensor randomized Kaczmarz method (row slice sketching) or the tensor Gauss-Seidel method (column slice sketching), which are natural extensions of their matrix counterparts, our approach delves into a distinct scenario utilizing frontal slice sketching. In particular, we explore a context where frontal slices, such as video frames, arrive sequentially over time, and access to only one frontal slice at any given moment is available. This talk will present our novel approach, shedding light on its applicability and potential benefits in approximating solutions to large-scale multi-linear systems.

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MS44

Mixed Precision Arithmetic for Large Scale Linear Inverse Problems

Recently a lot of attention has been focused on developing methods that can exploit capabilities of modern GPU architectures, and particular mixed precision arithmetic, for solving linear systems. However, very little work has been done for ill-conditioned problems that arise from large-scale inverse problems. Special considerations, which normally do not arise when solving well-conditioned problems, such as incorporating regularization into the developed methods, need to be considered. In this talk we consider iterative refinement methods for least squares problems, and show the connection to iterated Tikhonov regularization and the preconditioned Landweber method.

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MS44

Undersampling Raster Scans in Spectromicroscopy Using Higher Order Data Completion for Reduced Dose and Faster Measurements

X-ray spectromicroscopy is a powerful tool for studying material distributions, which is extracted from the data using a combination of PCA and cluster analysis. However, the traditional data collection setting has some significant weaknesses (e.g., long scanning times and material degradation due to x-ray radiation). It has been demonstrated

[O Townsend, Undersampling Raster Scans in Spectromicrsocopy for reduced dose and faster measurements, 2022] that iterative methods based on low-rank matrix completion are well suited for recovery of near identical results from undersampled data, greatly reducing the experimental time. However, the data sets formed through spectromicroscopy experiments are naturally 3D tensors, allowing for further improvement in data recovery. In this talk, we present a novel iterative algorithm for low rank tensor completion, recovering the missing entries in the datas native space. The new method allows the selection of robust sampling patterns, tensor multi-rank and undersampling ratio, while minimising the impact of undersampling on the cluster analysis. Results obtained on real data will be illustrated.

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MS45

Adaptive Approximation and Generalization of Deep Neural Network with Intrinsic Dimensionality

In this talk, we show that an intrinsic low dimensionality of covariates is the main factor that determines the performance of deep neural networks (DNNs). DNNs generally provide outstanding empirical performance. Hence, numerous studies have actively investigated the theoretical properties of DNNs to understand their underlying mechanisms. In particular, the behavior of DNNs in terms of high-dimensional data is one of the most critical questions. However, this issue has not been sufficiently investigated from the aspect of covariates, although high-dimensional data have practically low intrinsic dimensionality. In this study, we derive bounds for an approximation error and a generalization error regarding DNNs with intrinsically low dimensional covariates. We apply the notion of the Minkowski dimension and develop a novel proof technique. Consequently, we show that convergence rates of the errors by DNNs do not depend on the nominal high dimensionality of data, but on its lower intrinsic dimension. We further prove that the rate is optimal in the minimax sense. We identify an advantage of DNNs by showing that DNNs can handle a broader class of intrinsic low dimensional data than other adaptive estimators. Finally, we conduct a numerical simulation to validate the theoretical results.

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MS45

Deep Learning Theories for Problems with LowDimensional Structures

Deep neural networks have demonstrated a great success on many applications, especially on problems with high-dimensional data sets. In spite of that, most existing statistical theories are cursed by data dimension and cannot explain such a success. To bridge the gap between theories and practice, we exploit the low-dimensional structures of data set and establish theoretical guarantees with a fast rate that is only cursed by the intrinsic dimension of the data set. This presentation addresses our recent works on theories of deep neural networks that exploits low-dimensional data structures including autoencoders and operator learning.

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MS45

Hypergraph Neural Diffusion Networks

We present the Hypergraph Neural Diffusion Networks (HNDiffN) for learning node embedding and hyperedge embedding in hypergraphs. The main novelty lies in developing a continuous-time diffusion equation defined on nodes and hyperedges in hypergraphs suitably. With the resulting system of well-posed differential equations, well-established numerical differential equation schemes can be employed to devise various families of neural networks with desirable stability properties. We also point out some similarities between diffusion on hypergraphs and staggered grids in computational fluid dynamics to provide an alternative interpretation of the proposed hypergraph model. Experimental results fully demonstrate that HNDiffN performs consistently better than all baseline methods on specific evaluation indicators when solving numerous semi-supervised classification problems. Moreover, the experiments show that the prediction accuracy remains steady as the network depth increases, whereas other graph-based and hypergraph-based baseline models deteriorate. This is attributed to the fact that differential equation approach yields much better controlled network gradients, which helps to overcome the depth dilemma and retain rather decent stability.

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MS45

Manifold Fitting: An Invitation to Data Science

This manifold fitting problem can go back to H. Whitneys work in the early 1930s (Whitney (1992)). The solution to the Whitney extension problem leads to new insights for data interpolation and inspires the formulation of the Geometric Whitney Problems (Fefferman et al. (2020, 2021a)). Assume that we are given a set $Y \subset \mathbb{R}^D$. When can we construct a smooth d-dimensional submanifold $\widehat{M} \subset \mathbb{R}^D$ to approximate Y, and how well can $\widehat{M}$ estimate Y in terms of distance and smoothness? To address these problems, various mathematical approaches have been proposed (see Fefferman et al. (2016, 2018, 2021b)). However, many of these methods rely on restrictive assumptions, making extending them to efficient and workable algorithms challenging. As the manifold hypothesis (non-Euclidean structure exploration) continues to be a foundational element in statistics, the manifold fitting Problem, merits further exploration and discussion within the modern statistical community. The talk will be partially based on recent works of Yao and Xia (2019) and Yao, Su, Li and Yau (2022) and

Yao, Su and Yau (2023)

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MS46

Randomized Householder-Cholesky QR Factorization with Multisketching

CholeskyQR2 and shifted CholeskyQR3 are two state-of-the-art algorithms for computing tall-and-skinny QR factorizations since they attain high performance on current computer architectures. However, to guarantee stability, for some applications, CholeskyQR2 faces a prohibitive restriction on the condition number of the underlying matrix to factorize. Shifted CholeskyQR3 is stable but has 50% more computational and communication costs than CholeskyQR2. In this talk, a randomized QR algorithm called Randomized Householder-Cholesky (`rand_cholQR`) is proposed and analyzed. Using one or two random sketch matrices, it is proved that with high probability, its orthogonality error is bounded by a constant of the order of unit roundoff for any numerically full-rank matrix, and hence it is as stable as shifted CholeskyQR3. An evaluation of the performance of `rand_cholQR` on a NVIDIA A100 GPU demonstrates that for tall-and-skinny matrices, `rand_cholQR` with multiple sketch matrices is nearly as fast as, or in some cases faster than, CholeskyQR2. Hence, compared to CholeskyQR2, `rand_cholQR` is more stable with almost no extra computational or memory cost, and therefore a superior algorithm both in theory and practice.

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MS46

Orthogonalization Schemes in Tensor-Train Format

In the framework of tensor spaces, we consider orthogonalization kernels to generate an orthogonal basis of a tensor subspace from a set of linearly independent tensors. In particular, we investigate numerically the loss of orthogonality of six orthogonalization methods, namely Classical and Modified Gram-Schmidt with (CGS2, MGS2) and without (CGS, MGS) re-orthogonalization, the Gram approach, and the Householder transformation. To tackle the curse of dimensionality, we represent tensor with low-rank approximation using the Tensor Train (TT) formalism, and we introduce recompression steps in the standard algorithm outline through the TT-rounding method at a prescribed accuracy. After describing the algorithm structure and properties, we illustrate numerically that the theoretical bounds for the loss of orthogonality in the classical matrix computation round-off analysis results are maintained, with the unit round-off replaced by the TT-rounding accuracy. The computational analysis for each orthogonalization kernel in terms of the memory requirement and the computational complexity measured as a function of the number of TT-rounding, which happens to be the most computationally expensive operation, completes the study.

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MS46

Fast Low-Rank QRCP of Sparse Matrices with RandBLAS

It is well-known randomized sketching is a simple and effective tool for low-rank matrix approximation. This is especially true for sparse matrices, since the randomized algorithms can often make due with nothing more than access to the sparse matrix as a linear operator. This talk concerns low-rank approximations of such matrices obtained by randomized truncated QRCP. It focuses on high-performance implementations of the aforementioned randomized algorithms using new features of the C++ RandBLAS library. The bulk of the talk demonstrates these implementations as subroutines in a recently proposed nested-dissection approach to solving large-scale positive definite linear systems. We end the talk with a brief but general overview of RandBLAS' support for sketching sparse matrices.

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MS46

A General Framework for the Stable Rounding of Low-Rank Tensors with Error Analysis

Tensor computations are essential in algorithms from various domains like AI, signal processing and quantum simulation. However, the size of a tensor is exponential in its number of dimensions, which is referred to as the "curse of dimensionality". A standard approach to address this problem is to use low-rank approximations, which can reduce the size from exponential to polynomial in the number of dimensions using a tensor decomposition. Crucially, the ranks obtained by this tensor decomposition might be non-optimal after some operations (e.g., low-rank arithmetic). This requires a rounding step that tightens the ranks to the optimal, satisfying an error tolerance. In this talk, we present a general framework for the stable rounding of low-rank tensors. The method is based on a tree topology of tensors that can be applied to Tucker, Tensor-Train, and Hierarchical Tucker decompositions. We provide a detailed error analysis and experimental results to demonstrate the

reliability of this approach.

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MS47

Multi-Linear PageRank: Theory and Algorithm

Multi-linear PageRank is a generalization of PageRank, which can be applied to Data clustering, Hypergraph partitioning et al.. In this talk we focus on theoretical analysis and numerical algorithms for solving multi-linear PageRank in recent years. Numerical examples are given to illustrate the efficiency of the proposed algorithms.

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MS47

Block Diagonalization of Quaternion Circulant Matrices with Applications to Quaternion Tensor Singular Value Decomposition

It is well known that a complex circulant matrix can be diagonalized by a discrete Fourier matrix with imaginary unit `i`. The main aim of this talk is to demonstrate that a quaternion circulant matrix cannot be diagonalized by a discrete quaternion Fourier matrix with three imaginary units `i`, `j` and `k`. Instead, a quaternion circulant matrix can be block-diagonalized into 1-by-1 block and 2-by-2 block matrices by permuted discrete quaternion Fourier transform matrix. With such a block-diagonalized form, the inverse of a quaternion circulant matrix can be determined efficiently similar to the inverse of a complex circulant matrix. We make use of this block-diagonalized form to study quaternion tensor singular value decomposition of quaternion tensors where the entries are quaternion numbers. A numerical example of color video as a third-order quaternion tensor is adopted to verify the efficiency of our proposed diagonalized method.

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MS48

Curvature Corrected Semi-Nonnegative Matrix Factorization of Manifold-Valued Data

The manifold of symmetric positive definite matrices of fixed dimension is home to data arising from many scientific applications. Low-dimensional representations of such data are useful for data analysis, and algorithms for computing these representations need to account for the geometry of the underlying manifold. In this talk, I will first present a general framework for curvature-corrected low rank factorizations of manifold-valued data. Using this framework, we develop a scheme for curvature corrected semi-nonnegative matrix factorization of manifold-valued data. As a case study, we apply our method to data collected via diffusion tensor magnetic resonance imaging, which take on values in $\mathcal{P}(3)$, the manifold of 3×3 symmetric positive definite matrices.

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MS48

Using the Nystrm Method for Faster Manifold Learning in Wasserstein Space

We will discuss the use of the Nystrm method, which is a low-rank kernel matrix approximation technique, in approximating distance matrices that give rise to nonlinear dimensionality reduction algorithms. We consider the data to be embedded to consist of probability measures in Wasserstein space, and the distance matrix to be approximated to consist of pairwise Wasserstein distances between the data. Computing the full distance matrix is impractical, and the Nystrm method allows us to approximate it by computing only a small number of columns of the matrix. Procrustes type error bounds on embeddings will be discussed as well as some numerical examples illustrating the speed-up of the technique.

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MS48

Gradient-Type Subspace Iteration Methods for the Symmetric Eigenvalue Problem

We explore variants of the subspace iteration algorithm for computing approximate invariant subspaces that exploit gradient-type techniques combined with a Grassmann manifold viewpoint. Convergence of this gradient-based algorithm is analyzed and a few numerical experiments are reported, indicating that the proposed algorithms are sometimes superior to a standard Chebyshev-based subspace iteration when compared in terms of number of matrix vector products, but do not require estimating optimal parameters. An important contribution to achieve this good performance is the accurate and efficient implementation of an exact line search. In addition, new convergence proofs are presented for a non-accelerated gradient method that includes a locally exponential convergence if started in a $\sqrt{\delta}$ neighbourhood of the dominant subspace with spectral gap δ.

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MS48

Multivariate Hermite Interpolation on Matrix Manifolds

We consider two methods for multivariate Hermite interpolation of manifold-valued functions. On the one hand, we approach the problem via computing weighted Riemannian barycenters. This approach is intrinsic in the sense that it does not depend on local coordinates. As an alternative, we consider straightforward Hermite interpolation in a tangent space. Here, the actual interpolation is conducted via classical vector space operations. Both approaches are illustrated by means of numerical examples.

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MS49

Accelerating Quantum Algorithms with Parallelism and Precomputation

Real-world applications of computing can be extremely time-sensitive. It would be valuable if we could accelerate such tasks by performing some of the work ahead of time. Motivated by this, we propose a cost model for quantum algorithms that allows quantum precomputation; i.e., for a polynomial amount of "free" computation before the input to an algorithm is fully specified, and methods for taking advantage of it. We analyze two families of unitaries that are asymptotically more efficient to implement in this cost model than in the standard one. The first example of quantum precomputation, based on density matrix exponentiation, could offer an exponential advantage under certain conditions. The second example uses a variant of gate teleportation to achieve a quadratic advantage when compared with implementing the unitaries directly. These examples hint that quantum precomputation may offer a new arena in which to seek quantum advantage.

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MS49

Evaluating Sums of Non-Commuting Pauli Terms Using Diagonalization and Extrapolation

Calculating expectation values on near-term quantum computers often requires a very large number of measurements. One strategy to mitigate this problem has been to partition an operators Pauli terms into sets of commuting operators. Here, we introduce methods that do not require non-commuting terms to be measured in separate batches, which in turn lowers the total number of measurements required for calculating expectation values. The first method is based on a simple function extrapolation procedure. The second method is based on a string-matching and diagonalization procedure that has not been previously introduced. Both methods have tailorable circuit depth, i.e. they allow for a trade-off between circuit depth and total measurements.

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MS49

Quantum Computing and the Boltzmann Method

The unparalleled strengths of quantum computers is their ability to work efficiently in an exponentially large space, at least theoretically. This has been the starting point for research into how this feature can be exploited to solve practical problems on (future) quantum computers that will have a sufficient number of qubits with sufficiently long decoherence time. Recently there has been a boom of research in computational fluid dynamics as a potential application area for quantum computers. As for any other problem that will be ran on a quantum computer, the first challenge to overcome is to cast the problem at hand into a form that fits onto a quantum computer. This basically means to linearise the problem and represent the algorithm as a sequence of unitary operations. Subsequently the problem needs to be loaded into a quantum computer and finally we need to be able to efficiently read out the resulting quantities of interest. In this talk we will consider the lattice Boltzmann method and propose quantum primitives for the streaming, collision and reflection step. The focus of our talk will be on how to efficiently encode the problem such that we can solve it on a quantum computer, as well as how the resulting quantum state can be efficiently read out to retrieve relevant quantities of interest.

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MS50

Solving Polynomial Systems Using Determinantal Formulas

In the context of polynomial system solving, symbolic-numeric algorithms use techniques from algebraic geometry to symbolically reduce the problem to a linear algebra one, subsequently solving it approximately using numerical linear algebra. The objective of this talk is to delve into the first step of this approach in detail and demonstrate how different methods of computing the resultant lead to new and faster algorithms for solving structured polynomial systems. Our focus will be on constructing determinantal formulas, which serve as the algebraic counterparts of the smallest matrices that can be constructed to linearize our problems.

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MS50

Solving Equations Using Khovanskii Bases

We will introduce a new eigenvalue method for solving structured polynomial equations over any field. The equations are defined on a projective algebraic variety which admits a rational parameterization by a Khovanskii basis, e.g., a Grassmannian in its Plcker embedding. This generalizes established algorithms for toric varieties, and introduces the effective use of Khovanskii bases in computer algebra. We investigate regularity questions and discuss several applications.

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MS50

Back to the Roots of Multivariate Polynomial Systems

In this presentation, we survey the problem of rooting a set of multivariate polynomial equations from the points of view of algebraic geometry, system theory, operator theory and numerical linear algebra.

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MS50

Block Krylov Methods from the Perspective of Orthogonal Matrix Polynomials

The profound link between standard Krylov methods, scalar orthogonal polynomials, and moment matrices is well known, especially for Hermitian and unitary matrices. Here, we illustrate this connection for block Krylov methods and orthogonal matrix polynomials. By representing the elements of a block Krylov subspace via matrix polynomials, we consider a matrix-valued inner product defined over the latter. This, in the non-degenerate case, induces a linear isometry. Hence, any set of orthonormal matrix polynomials corresponds to an orthonormal basis of the block Krylov subspace. For normal matrices, we show that the inner product admits an integral representation that is well known in the literature of orthogonal matrix polynomials. This implies that, in the unitary case, we get a Szeg recurrence in the block Arnoldi procedure. For non-normal matrices, we still get a representation with a double integral. Furthermore, we consider the block moment matrix and discuss its structure. We show the relation between any Cholesky-like decomposition of the block moment matrix, orthogonal matrix polynomials, and recurrence coefficients.

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MS51

Regularized Methods via Cubic Subspace Minimization for Nonconvex Optimization

At the heart of adaptive cubic regularization methods for solving nonconvex problems lies the need to efficiently compute the trial step, which requires an approximate minimizer of the cubic model. We propose a new approach in which the cubic model is minimized in a low dimensional subspace that, in contrast to classic approaches, is reused for a number of iterations. In case the trial step produced by this low-dimensional minimization process is unsatisfactory, a regularized Newton step is employed. In our novel framework, the regularization term is a by-product of the low-dimensional subspace minimization process. We show that the worst-case complexity of classic cubic regularized methods is preserved, although a regularized Newton step can be possibly used. While polynomial Krylov subspaces often achieve very good computational performance, we also explore the use of rational Krylov subspaces as an alternative option for the low-dimensional subspace construction. We provide several experimental results illustrating the gains of our new approach when compared to classic implementations.

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MS51

Matrix Free Parameter Learning for Nonlocal Image Denoising

This work considers the numerical solution of a bilevel optimisation problem for the estimation of parameters in nonlocal image denoising models. We use an extended Gaussian ANOVA kernel as a nonlocal operator for denoising, in which the relevant parameters are the fidelity weight and a weight within the kernel. Under a suitable discretisation of the first order optimality conditions, we use a nonequispaced fast Fourier transform [J. Keiner, S. Kunis, D. Potts. "Using NNFT 3 - a software library for various nonequispaced fast Fourier transforms". ACM Transactions on Mathematical Software 36, 130, 2009] to efficiently compute the action of the nonlocal kernel as in [F. Nestler, M. Stoll, T. Wagner. "Learning in high-dimensional feature spaces using ANOVA-based fast matrix-vector multiplication". Foundations of Data Science 4(3), 423- 440, 2022]. As the conditioning of the optimality system depends crucially on the fidelity parameter, we present a family of matrix-free preconditioners based on the nonlocal operator

to accelerate the convergence of a Krylov method. Several experiments are provided to illustrate the efficiency of the method and contrast them against the dense-matrix approximation showcased in the previous work [M. DElia, J. C. De Los Reyes, A. Miniguano-Trujillo. Bilevel parameter learning for nonlocal image denoising models. Journal of Mathematical Imaging and Vision 63, 753775, 2021].

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MS51

Approximating Large-Scale Hessian Matrices Using Secant Equations

Large-scale optimization algorithms frequently require sparse Hessian matrices that are not readily available. Existing methods for approximating such matrices either do not impose sparsity or are computationally prohibitive. To overcome these limitations, we propose a novel approach that seeks to satisfy as many componentwise secant equations as necessary to define each row of the Hessian matrix. A naive application of this idea is prohibitively expensive when the Hessian has some relatively dense rows but by carefully taking into account the symmetry and connectivity of the Hessian matrix, we are able devise an approximation algorithm that is fast and efficient with scope for parallelism. Sparse Hessian matrices taken from the CUTEst test problem collection for optimization illustrate the effectiveness and robustness of the new method.

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MS52

Solving Linear Systems on a GPU with Hierarchically Off-Diagonal Low-Rank Approximations

We are interested in solving linear systems arising from three types of applications: (1) kernel methods in machine learning, (2) discretization of boundary integral equations from mathematical physics, and (3) Schur complements formed in the factorization of large sparse matrices. The coefficient matrices are often data-sparse in the sense that their off-diagonal blocks have low numerical ranks; specifically, we focus on hierarchically off-diagonal low-rank (HODLR) matrices. We introduce algorithms for factorizing HODLR matrices and for applying the factorizations on a GPU. The algorithms leverage the efficiency of batched dense linear algebra, and they scale nearly linearly with the matrix size when the numerical ranks are fixed. The accuracy of the HODLR-matrix approximation is a tunable parameter, so we can construct high-accuracy fast direct solvers or low-accuracy robust preconditioners. Numerical results show that we can solve problems with several millions of unknowns in a couple of seconds on a single GPU.

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MS52

Formats of Structured Matrices and the Quest for Memory Minimization

Many different structured lowrank formats have been implemented since the introduction of general hierarchical matrices more than 20 years ago, e.g., Uniform-H, H, HSS, HODLR or BLR. Each of these formats has different structural and arithmetic advantages (and disadvantages). We will look into the memory consumption of these formats for different applications. A special focus will be on the applicability of additional storage compression, e.g., via mixed/adaptive precision, which further reduces storage costs. While storage reduction will have priority, basic matrix arithmetic will also be of interest.

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MS52

Optimal Quantization of Rank-One Matrices for Butterfly Factorization

What is the optimal quantization of a rank-one matrix xy^T on t bits of precision? To our surprise, the natural approach of separately quantizing x and y is far from optimal: we prove the existence of an optimal quantization that can achieve an almost *doubled* precision (as if using $2t$ bits). Moreover, we characterize this optimal quantization as suitably scaled x and y vectors, and present an algorithm of tractable complexity to find the optimal scaling parameters. We apply this discovery to the factorization of butterfly matrices and obtain storage savings up to 30% with no loss of accuracy.

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MS52

Iterative Refinement With Hierarchical Low-Rank Preconditioners Using Mixed Precision

Green's function matrices in boundary integral problems, covariance matrices in statistics, and Hessian matrices in

inverse problems are often dense matrices of full rank, but have a particular structure that results in low-rank off-diagonal blocks. $\mathcal{H}$-matrices exploit this low-rank structure to reduce the cost of matrix-matrix multiplication and Cholesky/LU factorization to $\mathcal{O}(N \log^2 N)$, while being able to control the low-rank approximation error through the rank. When using such approximate dense linear algebra methods, it is wasteful to use double precision since the final accuracy is already limited by the prescribed rank. In this work, we investigate the optimal use of mixed precision for various $\mathcal{H}$-matrix operations. We consider the use of $\mathcal{H}$-matrix LU factorization as a preconditioner within a mixed precision iterative refinement. We evaluate the performance in terms of the execution time, comparing it to a general dense solver from LAPACK and a preconditioned GMRES. On large matrices, we are able to achieve a speedup of more than 16 times when compared to a dense solver.

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MS53

Linear Algebra Perspectives on Inducing Point Selection.

In kernel-based regression methods such as Gaussian process regression and RBF interpolation, the cost of dense linear algebra becomes a bottleneck for data sets involving more than a couple thousand data points. One way to address this scaling problem is to via a smaller or more structured set of points (inducing points) that serve as the basis for a new problem. In this talk, we discuss methods for selecting and using inducing points, their connection to pivoted matrix factorizations, and connections between linear algebraic, statistical, and approximation theoretic perspectives on their use.

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MS53

Mixed Precision Training of Gaussian Processes

Gaussian processes are one of the most popular tools in scientific computing. Depending on the application, different kernel functions and their gradients can be used. Computing the gradient of the kernel matrix can be computationally very expensive and may exceed the memory limit. Due to matrix and vector operations, gradient calculation dominates the cost of the whole algorithm depending on the size of the dataset. There are various techniques currently being used in Gaussian processes to avoid memory and cost-related problems, such as low-rank approximation and using matrix determinant lemma. Another technique can be using multiple precisions in the training algorithm. When the data is large, one may not need a high accuracy for training. Low precision is thus commonly used in data science applications. However, using lower precision can introduce stability issues in direct or iterative solvers used in the training algorithm. Thus, one must use a higher precision in such parts of the algorithm without sacrificing the performance. In this talk, we introduce a new mixed-precision approach to train Gaussian processes using several techniques. Motivated by the recent emergence of commercially available low-precision hardware, we propose to use multiple precisions during training, low-rank approximation, and a stable direct solver to have a cheap, fast, and stable algorithm.

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MS53

NFFT-Based Additive Hyperparameter Optimization for Gaussian Processes

Gaussian processes (GPs) are a crucial tool in machine learning given their ability to quantify the uncertainty in the model. The covariance matrices of GPs arise from kernel functions and are typically dense and large-scale. Depending on their dimension even computing all their entries is challenging and the cost of matrix-vector products scales quadratically with the dimension, if no customized methods are applied. We present a matrix-free approach that exploits the computational power of the non-equispaced fast Fourier transform (NFFT) and is of linear complexity for fixed accuracy. With this, we cannot only speed up multiplications with the covariance matrix but also take care of the derivatives needed for the gradient method avoiding the costly Hadamard products of the Euclidean distance matrix and the kernel matrix. Our method utilizes a derivative kernel which is then well suited for multiplying with the Hadamard product. We propose to work with an additive kernel where each one captures lower order feature interactions only. This potentially provides better accuracy for many real-world datasets and employs the full efficiency of the NFFT approach that pays off most for small input dimensions. Accordingly we introduce a preconditioner for this additive procedure. By applying our preconditioned NFFT-accelerated multiplication technique, fitting the kernel and the derivative kernel will allow for fast tuning of the hyperparameters.

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MS53

Hpytorch: A High Performance Preconditioned Gaussian Process Package

Gaussian processes (GPs) are a powerful tool for many applications, however, their performance heavily relies on selecting suitable hyperparameters. In this talk, we introduce HPyTorch, a scalable preconditioned GP package that addresses the hyperparameter selection problem while harnessing hardware acceleration capabilities through OpenMP and CUDA. HPyTorch is designed to exhibit robust performance across a wide range of hyperparameters, owing to its utilization of data-driven matrix routines that dynamically adjust components in response to the spectrum decay of the kernel matrices. Moreover, when employing gradient-based optimization methods, our package eliminates the need for auto-differentiation, further enhancing its computational efficiency. We evaluate the performance of HPyTorch on several real-world datasets, demonstrating that it outperforms state-of-the-art packages in terms of both accuracy and efficiency. This is joint work with Hua Huang, Edmond Chow, Tianshi Xu and Yuanzhe Xi.

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MS54

Streaming Methods for Very Large Linear and Nonlinear Systems

As big data applications become ever more prominent, in many applications we need to solve problems such as linear or nonlinear inversion, handling only a relatively small amount of data at a time. This may happen because the volume of data is massive, or that data comes in at a rate that only sampled data can be used, or because the data comes in continually, so the data set is never complete. In such cases, we need to design solvers and regression methods that can perform partial solves on limited data, store a very limited selection of the data or information derived from the data, and combine this with incoming data or data read from secondary memory to incrementally further improve the solution/make the solution more accurate. In addition, if necessary, regularization may need to be applied consistently to the overall problem. We discuss several techniques to store and combine intermediate/selected information and methods to incrementally or iteratively improve the solution. This is joint work with Mirjeta Pasha and Misha Kilmer

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MS54

A Review of Quadrature-Based Error Bounds in the Conjugate Gradient Algorithm

The preconditioned conjugate gradient (PCG) algorithm is quite often the method of choice for solving linear systems $Ax = b$ with a symmetric positive definite matrix. As it was already known from the early days of the algorithm, using the residual norm to stop the iterations is not always reliable. Since PCG minimizes the A-norm of the error a more robust stopping criterion can be based on estimates or preferably bounds on that norm. In this talk we will review how to obtain bounds on the A-norm of the error using quadrature-based formulas. More precisely, we could use Gauss and Gauss-Radau quadrature rules to cheaply compute lower and upper bounds d iterations back from the current one. We will discuss heuristic techniques to adaptively compute the delay d and also explain why we may sometimes have a loss of accuracy of the upper bound given by the Gauss-Radau quadrature rule. This talk is based on papers published with Petr Tichý and Jan Papež.

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MS54

Role of *hp*-Robust Iterative Solvers in Adaptive Finite Element Algorithms for Optimal Complexity

Adaptive finite element methods (AFEM) have been successfully used in numerical solutions of partial differential equations (PDEs) yielding optimal convergence rates with respect to degrees of freedom. However, due to the nature of AFEM, each refinement step requires a new set of computations leading to cumulated work. One then strives to achieve optimality with respect to overall cost, i.e. total elapsed time. The core question becomes to design contractive algebraic iterative solvers used within AFEM. In the context of symmetric linear elliptic second order PDEs, we propose a local adaptive multigrid solver, where the linear system stems from a finite element discretization with polynomial degree p and bisection-generated meshes with local size h. The proposed solver contracts the algebraic error hp-robustly and comes with a built-in a posteriori error estimator. This estimator provides a two-sided bound of the algebraic error. More precisely, proving the hp-robust contraction of the solver is in fact equivalent to showing that the built-in estimator provides an hp-robust upper bound on the algebraic error. Moreover, the error-equivalent estimator and its localized decomposition leads to the development of an extension of the solver with an adaptive number of additional local smoothing steps assuring further error contraction. Presented numerical results highlight the performance of the solver, its adaptive version, and optimality of the full algorithm.

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MS54

A Randomly Sketched Minimal Residual Linear

Solver with Subspace Recycling

The techniques of random sketching has been increasingly adopted in numerical linear algebra in recent years, showing significant potential to reduce the orthogonalization cost for developing the basis vectors of Krylov subspace methods. We show that it works well with the minimum-residual linear solvers based on subspace recycling, namely, GCRO-DR. We provide some insight into the convergence behavior of randomly sketched GCRO-DR, showing that it can largely maintain the advantage of shrinking the numerical range by subspace recycling, which is crucial for avoiding slow convergence typically caused by a few small eigenvalues of the original linear operator. Numerical experiments are provided to demonstrate the separate and combined benefits of subspace recycling and random sketching.

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MS55

Constrained Pressure-Temperature Residual (cptr) Preconditioner Performance for Thermal Co2 Injection Simulation

This work studies the performance of a novel preconditioner, designed for thermal reservoir simulation cases and recently introduced in Roy et al., 2019 and Cremon et al., 2020 on large-scale thermal CO2 injection cases. Thermal effects in CCS cold supercritical CO2 injection impact both the simulation results and the solvers performances. Specifically, the usual combination of CPR-GMRES using the physics-based block-preconditioner is known to perform rather poorly or fail to converge when thermal effects are significant. The Constrained Pressure-Temperature Residual (CPTR) preconditioner retains the 2 x 2 block structure (elliptic/hyperbolic) of CPR but includes the temperature in the elliptic subsystem. It allows the solver to appropriately handle the long-range, elliptic part of the parabolic energy equation. The two-equations elliptic subsystem is then dealt with by the system-solver of BoomerAMG. Then a global smoother, ILU(0), is applied to the full system to handle the local, hyperbolic temperature fronts. We implemented CPTR in the multi-physics solver GEOS and present results on various large-scale thermal CCS simulation cases. The CPTR preconditioner severely reduces the number of GMRES iterations and the runtime, shortening day-long simulations with CPR to a few hours. The strong scaling results using hundreds of CPU cores show close to linear scaling. CPTR is also virtually insensitive to the thermal Pclet number hence suitable to any thermal regime.

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MS55

Block Preconditioners for Coupled Flow-Deformation in Fractured Porous Media

This work is focused on the development of efficient and scalable linear preconditioners for the solution of the block linear systems arising from the discretization of coupled fluid-deformation in fractured porous media. There can be two or three blocks, according to the number of fields, i.e., displacement, traction (and pressure). In case of pure contact mechanics, a constraint preconditioner is designed for the 2x2 block linear system, with the primal Schur complement obtained by eliminating the Lagrange multipliers. This Schur complement is an updated stiffness matrix and can be efficiently solved by a multigrid method. Finally, starting from an eigenvalue analysis, a suitable augmentation is presented for the intrinsically stable case. Adding the pressure, the Jacobian matrix has 3 blocks. For this case, we present two scalable preconditioning strategies, based on the physically-informed block partitioning of the unknowns and multigrid preconditioners. The key idea is to restrict the system to a single-physics problem, approximately solve it by an inner algebraic multigrid approach, and finally prolong it back to the fully-coupled problem. Two different techniques are presented, analyzed and compared by changing the ordering of the restrictions. Numerical results mainly illustrate the performance on real-world problems in terms of robustness and efficiency, but also the algorithmic scalability and the impact of the relative number of fracture-based unknowns.

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MS55

Preconditioned Iterative Solvers for Multiple Saddle-Point Systems Arising from Pde-Constrained Optimization

Optimization problems subject to PDE constraints form a mathematical tool that can be applied to a wide range of scientific processes, including fluid flow control, medical imaging, biological and chemical processes, and many others. These problems involve minimizing some function arising from a physical objective, while obeying a system of PDEs which describe the process. Of key interest is the numerical solution of the discretized linear systems arising from such problems, and in this talk we focus on preconditioned iterative methods for these systems. In particular, we describe recent advances in the preconditioning of multiple saddle-point systems, with a focus on positive definite preconditioners which can be applied within MINRES, which may find considerable utility for solving these optimization problems as well as other applications. In particular, these preconditioners lead to a guaranteed convergence rate for MINRES, and often demonstrate superior convergence as opposed to widely-used block diagonal preconditioners. Time permitting, we may also discuss an inexact active-set method for large-scale nonlinear PDE-constrained optimization problems, coupled with block diagonal and block triangular preconditioners for multiple saddle-point systems which utilize suitable approximations

for the relevant Schur complements.

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MS55

Geometric Multigrid Space-Time Finite Element Methods for Dynamic Poroelasticity

Space-time finite element methods (STFEMs) allow the construction of higher order discretizations of systems of multi-physics and offer the potential to achieve accurate results on computationally feasible grids with a minimum of numerical costs. However, the block structure and solution of the resulting algebraic systems become increasingly complex for higher polynomial degrees in space and time. We analyze STFEMs for solutions to the coupled hyperbolic-parabolic problem

$$\rho\partial_t^2\boldsymbol{u} - \nabla\cdot(\boldsymbol{C}\boldsymbol{\varepsilon}(\boldsymbol{u})) + \alpha\nabla p = \rho\boldsymbol{f},$$

$$c_0\partial_t p + \alpha\nabla\cdot\partial_t\boldsymbol{u} - \nabla\cdot(\boldsymbol{K}\nabla p) = g,$$

modeling fluid flow in deformable porous media. Recently, such type of models have attracted researchers' interest in several branches of natural sciences and technology, for instance, to elucidate circulatory diseases in the human brain. For the solving the algebraic systems, we present a robust geometric multigrid (GMG) preconditioner for GMRES iterations. The GMG method uses a local Vanka-type smoother. Due to nonlocal coupling mechanisms of unknowns, the smoother is applied on patches of elements. The parallel implementation of the solver for arbitrary polynomial degrees in space and time in the deal.ii library is addressed briefly. Numerical performance studies for challenging two- and three-dimensional benchmark settings are discussed.

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MS56

A Kronecker Product Structure Preserving Preconditioner for Linear Systems Arising from Multi-Dimension Fractional Diffusion Equations

In this talk, a sine transform based Kronnecker product structure preserving preconditioner is introduced for a non-symmetric multilevel Toeplitz system arising from fractional diffusion equation. By investigating the bounds of spectrum of Hermitian and skew-Hermitian parts of the preconditioned matrix, we show that the GMRES solver has a linear convergence rate independent of the size of the linear system. To the best of our knowledge, this is the first iterative solver with optimal convergence rate for the non-symmetric linear system. The proposed preconditioner is diagonalizable by the sine transform matrix, thanks to which the matrix-vector multiplication in each iteration step can be fast implemented by the fast sine transform (FST). Hence, the total operation cost of the proposed solver for the non-symmetric problem is linearithmic, which is nearly optimal. Numerical results are reported to show the efficiency of the proposed preconditioner.

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MS56

Low-Rank Tensor Regression for Selection of Grouped Variables

Low-rank tensor regression (LRTR) problems are widely studied in statistics and machine learning, in which regressor variables generally have strong correlations in many practical applications. By virtue of the idea of group selection to deal with correlated variables in the classical linear regression framework, we propose an LRTR method for adaptive selection of grouped variables, which is formulated as a group SLOPE penalized low-rank, orthogonally decomposable tensor optimization problem. Moreover, we introduce the notion of tensor group false discovery rate (TgFDR) to measure the group selection performance. The proposed regression method provably controls TgFDR and achieves the asymptotically minimax estimate under the assumption that variable groups are orthogonal to each other. Finally, an alternating minimization algorithm is developed for efficient problem resolution. We demonstrate the performance of our proposed method in group selection and low-rank estimation through simulation studies and real human brain connection data analysis.

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MS56

Complex Matrix Inversion Via Real Matrix Inversions

We study the inversion analog of the well-known Gauss algorithm for multiplying complex matrices. A simple version is $(A+iB)^{-1} = (A+BA^{-1}B)^{-1} - iA^{-1}B(A+BA^{-1}B)^{-1}$ when A is invertible, which may be traced back to Frobenius but has received scant attention. We prove that it is optimal, requiring fewest matrix multiplications and inversions over the base field, and we extend it in three ways: (i) to any invertible $A+iB$ without requiring A or B be invertible; (ii) to any iterated quadratic extension fields, with $\mathbb{C}$ over $\mathbb{R}$ a special case; (iii) to Hermitian positive definite matrices $A+iB$ by exploiting symmetric positive definiteness of A and $A+BA^{-1}B$. We show that a complex matrix with well-conditioned real and imaginary parts can be arbitrarily ill-conditioned, a situation tailor-made for Frobenius inversion. We prove that Frobenius

inversion for complex matrices is faster than standard inversion by LU decomposition and Frobenius inversion for Hermitian positive definite matrices is faster than standard inversion by Cholesky decomposition. We provide extensive numerical experiments, applying Frobenius inversion to solve linear systems, evaluate matrix sign function, solve Sylvester equation, and compute polar decomposition, showing that Frobenius inversion can be more efficient than LU/Cholesky decomposition with negligible loss in accuracy.

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MS56

Tensor Eigenvalue, Singular Value and Decomposition: New Perspectives with Applications

In this talk, I will present some new results on comprehensive study on tensor eigenvalue, singular value and decomposition. A generalize form of tensor eigenvalue and corresponding eigen-tensor is defined, it takes many existing eigenvalue/eigenvector as special examples. Similarly, generalized form of tensor singular value and corresponding singular tensor is also defined, based on which more flexible tensor decomposition and more powerful tensor approximation can be done. Algorithms for computing them and related convergence results will also be given. We have also tried to apply the above results in dimension reduction, denoising and tensor completion. The research is done jointly with Bo Dong, Xinzhu Zhao, Hang Wang and Lulu Pei.

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MS57

Reach of Segre-Veronese Manifolds

We compute the reach and the the second fundamental form of the (spherical) real Segre-Veronese variety; i.e., the manifold of rank-one partially symmetric tensors in $\mathbb{R}^{n_1} \times \cdots \mathbb{R}^{n_d}$ of norm one. In particular, we show that the reach only depends on the dimension d of the tensor, but not on the size of its modes $n_1, \ldots, n_d$. This is joint work with Sarah Eggleston.

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MS57

Strict Saddle Optimization on Manifolds

For functions with strict saddle points, we show that the classical Riemannian trust-region algorithm with exact subproblem minimization finds approximate minimizers in a worst-case number of iterations that improves over known results for nonconvex optimization. The desired accuracy only impacts the last few iterations of the algorithm, which benefit from the local quadratic convergence of Newton's method. Our complexity bound depends polynomially on landscape parameters which represent negative curvature and strong (geodesic) convexity constants. In that sense, we can say that the worst-case complexity is essentially independent of the user-prescribed accuracy. We also present an algorithm with similar complexity guarantees which minimizes the trust-region subproblems approximately with a truncated conjugate gradient scheme.

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MS57

An algorithm for the Riemannian logarithm on the Stiefel manifold designed for a family of metrics

Since its popularization in 1998 in a seminal paper by Edelman et al., the Stiefel manifold has been exhibited to be a key to solve many problems from optimization, statistics and machine learning. In 2021, Huper et al. proposed a one-parameter family of Riemannian metrics on the Stiefel manifold, including the well-known Euclidean and canonical metrics. Since then, several methods have been proposed to obtain a candidate for the Riemannian logarithm given any metric from the family. Most of these methods are based on the shooting method or optimization. For the canonical metric, Zimmermann proposed in 2017 a particularly efficient method based on a pure matrix-algebraic approach. In this work, we derive a generalization of Zimmermann's algorithm, working for the one-parameter family of Riemannian metrics. The algorithm is proposed in two versions, backward and forward, for which we prove that it retains the local linear convergence previously exhibited for the canonical metric.

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MS57

Computing Bouligand Stationary Points Efficiently in Low-Rank Optimization

We consider the problem of minimizing a differentiable function with locally Lipschitz continuous gradient on the set of all m-by-n real matrices of rank at most r, where m, n, and r are positive integers such that $r < \min\{m, n\}$, and present a first-order algorithm designed to find a sta-

tionary point of that problem. This algorithm extends the RFDR algorithm proposed by Olikier and Absil (2023), and is therefore called ERFDR. Like RFDR, ERFDR produces a sequence of iterates whose accumulation points are stationary, and therefore does not follow the so-called apocalypses described by Levin, Kileel, and Boumal (2023). Moreover, the rate at which the stationarity measure converges to zero along this sequence is similar to those of the methods proposed by Olikier, Uschmajew, and Vandereycken (2023). We also introduce a particular case of ERFDR, called CRFDR because it can be thought of as a cheap version of RFDR. Indeed, while RFDR can require the computation of a truncated SVD of a matrix of rank $\min\{m,n\}-r+1$, the most expensive operation required by CRFDR is an SVD of a matrix whose smallest dimension is at most r, which is much cheaper in the frequently encountered case where $r \ll \min\{m,n\}$. Furthermore, we propose a general rank-increasing algorithm based on ERFDR.

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MS58

Tensor Network-Accelerated Solutions for Partial Differential Equations

We present a Finite Element Method (FEM) solver that utilizes a tensor network representation to expedite linear algebra operations. The discrete solution, along with the discrete Galerkin operators, is expressed in the Tensor Train (TT) format. Efficient linear algebra operations in the Tensor Train format are employed to assemble the operators and address the resulting linear systems. The process of tensorizing the data exhibits noteworthy parallels with quantum algorithms, marking a significant stride in the advancement of a quantum FEM solver. To preserve the tensor product structure of the solution while addressing nontrivial domains, we employ Isogeometric Analysis as a discretization technique. The presented solver undergoes benchmarking against several test cases to demonstrate its efficiency in solving problems requiring fine meshes.

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MS58

Quantized Tensor Networks for Solving the Vlasov-Maxwell Equations

We recently showed that the Vlasov-Maxwell equations can be solved with reduced cost using quantized tensor networks (QTNs) for a few standard test problems. One particularly interesting observation was that one often is able to take larger time steps with QTN-based time-stepping schemes as opposed to traditional grid-based methods, which are limited by the CFL condition. Here, we investigate different QTN time evolution schemes in the context of the Vlasov-Maxwell equations, and compare their performance for simple test problems with respect to time step and grid resolution. In particular, we focus on quantifying errors in observables and the amount of numerical noise that is introduced.

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MS59

Tensor Decomposition Using Numerical (Non)Linear Algebra

In (symmetric) tensor decomposition one asks about expressing a given tensor as a sum of simple (symmetric) tensors. These simple tensors, considered as points in projective space, are solutions to a system of homogeneous polynomial equations obtained from flattenings. We propose solving these systems, usually heavily overdetermined, using numerical normal form methods. This method transforms the nonlinear equations into an eigenvalue problem. The complexity of this algorithmic approach is governed by the Hilbert function and regularity of the polynomial system. We propose values for these invariants for generic input and prove several cases and bounds. This question is related to several long-standing conjectures in commutative algebra.

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MS59

Solving Applications from Systems Theory Via Efficient Numerical Linear Algebra Root-Finding Algorithms

We consider the (block) Macaulay matrix framework for solving systems of multivariate polynomial equations and multiparameter eigenvalue problems. The solutions of both problems are retrieved via a multidimensional realization problem in the null space of these (large) structured coefficient matrices. We briefly highlight our recent work in which a recursive/sparse technique to compute the null space of the (block) Macaulay matrices of growing sizes has been proposed, thereby addressing the computational bottleneck of the numerical linear algebra technique. In the second part of the presentation, we apply the solver to tackle several numerical examples originating from system theoretic applications: e.g., H2-norm model reduction and least squares realization of autonomous LTI models, thereby illustrating the relevance and direct impact of numerical linear algebra techniques for solving multiparameter eigenvalue problems in the context of (electrical) engineering. We demonstrate that, when one is interested

in the globally optimal solution(s), both applications are essentially a multivariate root finding problem, or equivalently, when exploiting the linear structure of the problem, a multiparameter eigenvalue problem. The presented numerical examples offer insights into the practical benefits and limitations of the approach.

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MS59

Direct Numerical Computation of Polynomial Multiplication Maps

We present a novel linear algebra-based methodology for numerically finding the common roots of a set of multivariate polynomials. Starting from the Macaulay framework, we show that objects similar to multiplication matrices, which contain the necessary information about the set of common solutions, can be computed and iteratively updated until convergence, without the need to set up a Macaulay matrix or its null space. This allows one to perform monomial substitutions in intermediate steps, reducing the total number of monomials involved and the subproblem sizes compared to the Macaulay matrix approach. Lastly, we compare this novel approach to the state-of-the-art linear-algebra-based rootfinding techniques through numerical examples and discuss the open problems.

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MS60

Preconditioners for the Continuous Optimal Transport Problem with Linear Cost

The Optimal Transport theory studies the problem of moving one nonnegative density into another, minimizing the total cost of displacement. In recent years, numerous authors have contributed to the study of this problem, both on the theoretical and computational level. Thanks to these advances, Optimal Transport is nowadays an established tool for many applications including, for example, the analysis of partial differential equations (PDE), physical modeling, data science and machine learning, economics, and inverse problems. However, the wide-spread usage of optimal transport tools is still hindered by the high computational cost of solving it. When the cost of moving one unit of mass is proportional to the distance covered, the Optimal Transport problem can be reformulated in the form of different (but equivalent) PDE-constrained optimization problems. In this talk, we present the linear algebra challenges involved in solving these optimization problems using Newton-based methods, how different forms share similar computational bottlenecks, and our strategies to cope with them.

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MS60

Efficient Block Preconditioners for Double Saddle Point Linear Systems

Given positive integer dimensions $n \geq m \geq p$, consider the $(n+m+p) \times (n+m+p)$ double saddle point linear system of the form

$$\mathbf{A}w \equiv \begin{bmatrix} A & B^T & 0 & B & -D & C^T & 0 & C & E \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} f \\ g \\ h \end{bmatrix} \equiv b,$$

where A is a symmetric positive definite (SPD) matrix, B and C have full row rank, D and E are square positive semidefinite matrices. Such linear systems arise in a number of scientific applications including constrained least squares problems, constrained quadratic programming, magma-mantle dynamics, to mention a few. Similar block structures arise e.g. in liquid crystal director modeling or in the coupled Stokes-Darcy problem. This work we consider an SPD block preconditioner proposed in [J. W. Pearson and A. Potschka. *On symmetric positive definite preconditioners for multiple saddle-point systems. arXiv preprint*, 2023] in the framework of multiple saddle point linear systems, and we analyze the eigenvalue distribution of the preconditioned matrix. We show that the eigenvalues of the preconditioned matrix are described in terms of the roots of a cubic polynomial with real coefficients. We illustrate the efficiency of the proposed preconditioner, and verify the theoretical bounds, in solving large scale PDE-constrained optimization problems.

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MS60

Generalized Second-Order Adjoints in Optimization

Second-order or Newton-like algorithms exhibit conver-

gence properties superior to gradient-based or derivative-free optimization algorithms. However, deriving and computing second-order derivatives needed for the Hessian-vector product in a Krylov iteration for the Newton step often is not trivial. Second-order adjoints provide a systematic and efficient tool to access second derivative information. In this talk we consider equality constrained optimization problems in an infinite-dimensional setting. We phrase the optimization problem in a general Banach space framework and derive second-order sensitivities and second-order adjoints in a rigorous and general way. We apply the developed framework to a PDE-constrained optimization problem and to machine learning for the training of neural networks.

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MS61

A Deep Learning Algorithm to Accelerate Algebraic Multigrid Methods in Finite Element Solvers

Algebraic multigrid (AMG) methods are among the most efficient solvers for linear systems of equations and they are widely used for the solution of problems stemming from the discretization of Partial Differential Equations (PDEs). A severe limitation of AMG methods is the dependence on parameters that require to be optimized. In particular, the strong threshold parameter is the most relevant since it stands at the basis of the construction of successively coarser grids needed by the AMG methods. This study introduces an innovative deep-learning algorithm designed to minimize the computational cost of the AMG method. The proposed neural network fine-tunes the strong threshold parameter value by interpreting the sparse matrix of the linear system as a grayscale image and subsequently utilizing a pooling operator to transform it into a small multi-channel image. Empirical evidence demonstrates that pooling reduces the cost of processing large sparse matrices, while also preserving the features necessary for the regression task at hand. We train the algorithm on an extensive dataset comprising problems characterized by highly heterogeneous diffusion coefficients defined in different three-dimensional geometries and discretized with unstructured grids and linear elasticity problems with a highly heterogeneous Young's modulus. When evaluated on problems with coefficients or geometries absent from the training data, our algorithm reduces the computational time by up to 30%.

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MS61

Optimal Solver Prediction Via Sparsity-Aware Transformers

Simulations of physical processes provide an integral part of scientific computing. Many of these applications are formulated in form of sparse linear systems of equations. In recent years, deep learning (DL) approaches have emerged as a useful tool to predict matrix properties and speed up computations. However, existing approaches focus either on abstract descriptive parameters or rely on dense representations for utilizing convolutional neural networks, rendering them computationally inefficient. Transformer-based architectures are able to process sequential data, thereby providing the opportunity to efficiently and expressively model sparse matrices, e.g. in COOrdinate (COO) format, without the need for dense conversions. Additionally, the attention-mechanism allows for direct interpretation and analysis of the relative importance of input elements with respect to one another and excels in capturing long-range dependencies. Hence, we hypothesise that Transformer-based models are particularly advantageous when dealing with irregularly structured sparse matrices. In this talk I will introduce the usage of Transformers for the prediction of suitable solvers and preconditioners for large sparse matrices, a precursor task in many applications. I will demonstrate feasibility of the approach on examples from the SuiteSparse matrix collection and compare the predictive performance of the learned representation with hand-engineered features derived by experts.

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MS62

Efficient Uncertainty Quantification with Low-Rank Approximations

Kernel methods are a broad class of powerful non-parametric algorithms in machine learning, which usually come with heavy computational costs. Uncertainty Quantification (UQ) is a crucial aspect of kernel methods in machine learning, especially when dealing with large datasets. In this talk, we will focus on methods in which uncertainty is present and stress out the computational challenges that arise in the learning process. We will discuss ways to scale up such models, where we specifically will explore the integration of random features into them.

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MS62

Iterative Method for Approximating Covariance Matrices from Large Sparse Precision Matrices

Gaussian processes regression is a crucial Bayesian tool for modelling complex data, providing probabilistic function predictions. The drawback of GP regression lies in the computational complexity, which can scale like $\mathcal{O}(n^3)$, where n is the number of training points, due to requiring the inverse of the covariance matrix. Here, we present a novel iterative algorithm to approximate the covariance matrix from the precision matrix, which can re-

duce the overall computational complexity. The method involves partitioning the precision matrix and iteratively using block matrix inversion until the covariance matrix approximation reaches a satisfactory level of accuracy. This iterative approach has the potential to allow problems with more training data to be modelled with GP regression by reducing the overall computational complexity.

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MS63

Recycling and Initial Guess Strategies for Iterative Solvers for High Order Finite Elements

In this talk, we introduce strategies for minimizing the number of iterations when solving a sequence of linear systems. We consider two approaches to reduce the number of iterations: deriving an effective initial guess from historical solutions, and accelerating the convergence of the linear system through subspace recycling iterative methods. The central question we address is how to optimally allocate fixed memory capacity between the initial guess and the recycling subspace for optimal convergence. We propose an algorithm to dynamically determine this optimal allocation. The efficacy of these strategies is demonstrated through various numerical experiments.

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MS63

Multigrid Multilevel Monte Carlo with Orthogonal Projectors

Estimating the trace of the inverse of the discretized Dirac operator, $\mathrm{tr}(D^{-1})$, poses a challenge in lattice QCD simulations. The Hutchinson method's accuracy depends quadratically on the sample size, limiting its precision and making high-accuracy estimation costly. A way to reduce the variance of the estimator is to deflate the lowest eigen or singular vectors of the matrix. This work focuses on reducing the computational cost for constructing the deflation subspace while keeping the application of the deflation projectors cheap and at the same time improving the variance reduction. Using the Multigrid Multilevel Monte Carlo method [Frommer et al., SISC, Vol. 44, Iss. 4 (2022)], we deflate the spectrum through the application of an orthogonal projector derived from the prolongator P used to construct the multigrid methods to solve linear systems with D, effectively reducing computational and memory requirements compared to other deflation techniques. Our approach takes advantage of the rich low-mode spectral information contained in the multigrid prolongator, achieving a variance reduction up to three-fold compared to inexact deflation, which relies on a few iterations of the inverse block power method to obtain the deflation subspace.

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MS63

Deflated PCG in problems of incompressible flows

When solving unsteady problems of incompressible flows by an operator-splitting approach such as the pressure-correction scheme, one gets a sequence of Poisson problems for pressure with a fixed system matrix and varying right-hand side corresponding to different time steps. The problem for each time step is typically solved by the preconditioned conjugate gradient (PCG). In our work, we consider the preconditioner given by one step of Balancing Domain Decomposition based on Constraints (BDDC). The BDDC method provides a powerful preconditioner significantly reducing the number of PCG iterations. The setup of the preconditioner is relatively expensive, however, it is performed just in the first time step. It can be shown that the eigenvalues of the preconditioned problem are larger or equal to one and typically not larger than $O(1)$. In the talk, we discuss setting stopping criteria for PCG and show that the deflation can be successfully used for the sequence of problems. In particular, and in contrast to the typical use of the deflation, we build the deflation space to reduce the effect of large, outlying eigenvalues. Numerical experiments confirm that one can get significant reduction (up to 25%) both in number of PCG iterations and overall time.

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MS64

Block Preconditioners for the Implicit-in-Time Immersed Boundary Method

The Immersed Boundary (IB) method is a popular method for simulating fluid-solid interactions. The IB method was initially designed by Charles S. Peskin to simulate fibrous heart valves, and has since evolved into a general-purpose method for simulating various types of solid dynamics immersed within a fluid. The key idea, and the reason for its popularity, is to keep the solid and fluid variables on two separate, Lagrangian and Eulerian, domains. The two grids communicate forces and velocities via integral operators with Dirac Delta kernels. This allows for simplicity in the code as well as avoids the problem of regeneration of the mesh resulting from deformations and movements of the solid structure. Implicit schemes for the IB method have been around for a while but the real challenge has been to develop a scheme that is computationally competitive with the explicit schemes. The usual approach for the implicit IB method is to either eliminate the Lagrangian variables and solve the fully Eulerian system or vice versa. The first approach leads to a familiar 2×2 block Saddle-Point system that is difficult to solve efficiently due to the

structural force term. We propose an alternative approach of solving the full 3×3 block system and present efficient approximations for the resulting Schur Complements.

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MS64

Approximate Block Factorization Based Preconditioners for Magnetic Confinement Fusion Relevant Resistive Mhd Simulations

A base-level mathematical basis for the continuum fluid modeling of dissipative plasma system is the resistive magnetohydrodynamic model. This model requires the solution of the governing partial differential equations (PDEs) describing conservation of mass, momentum, and thermal energy, along with various reduced forms of Maxwells equations for the electromagnetic fields. The resulting systems are characterized by strong nonlinear and nonsymmetric coupling of fluid and electromagnetic phenomena, as well as the significant range of time- and length-scales that these interactions produce. These characteristics make scalable and efficient iterative solution, of the resulting poorly-conditioned discrete systems, extremely difficult. In this talk we consider the use of block preconditioners for solving the coupled physics block systems. The block preconditioner considered here is based on an approximate factorization and is used to isolate two problematic 2x2 block systems, a magnetics-flow system and a magnetics-constraint system, allowing them to be handled independently. We demonstrate this approach for various resistive MHD problems that are relevant to magnetic confinement fusion applications. Time permitting, we investigate the performance on ARM architectures, and in particular, the performance on the Fugaku Supercomputer.

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MS65

Limit of Iteration of the Induced Aluthge Transformations

Aluthge transform is a well-known mapping defined on bounded linear operators. Especially, convergence property of its iteration has been studied by a lot of authors. In this paper, we shall discuss the problem for the induced Aluthge transforms which is a generalization of the Aluthge transform defined in 2021. We shall give the polar decomposition of the induced Althuge transformations of centered operators and show its iteration converges to a normal operator. In particular, if T is an invertible centered matrix, then iteration of any induced Althuge transformations converges. Using the canonical standard form of matrix algebras we show that the iteration of any induced Althuge transformations with respect to the weighted arithmetic mean and the power mean converge. Those observation are extended to the C^*-algebra of compact operators on an infinite dimensional Hilbert space, and as an application we show the stability of $\mathcal{AN}$ and $\mathcal{AM}$ properties under iteration of the induced Althuge transformations. We also give concrete forms of its limit point for centered matrices and several examples. Moreover, we discuss limit point of the induced Aluthge transformation with respect to the power mean in the injective II_1-factor $\mathcal{M}$ and determine the form of its limit of some centered operators in $\mathcal{M}$. This is a joint work with Professor Takeaki Yamazaki.

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MS65

Drazin Inverses of Matrices Associated to Certain Classes of Digraphs

We obtain formula for the Drazin inverse of matrices associated to certain classes of digraphs, primarily using the characterisation of the Drazin index by the minimal polynomial of the graph matrix.

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MS65

Some Canonical Forms of Tensors and Applications

Canonical forms of matrices are one of fundamental research areas in matrix theory. During the past decade, some canonical forms of tensors have been defined and discussed. In this talk, we will introduce Jordan and Smith forms over some non-commutative rings like quaternions. We also explore some efficient algorithms and applications.

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MS66

Exploiting Linear Algebra to Lower Computational Complexity in Underdetermined Bayesian Inverse

Problems

Many inverse problems are characterized by a large mismatch between the scarce data and the large number of unknown parameters. In the Bayesian framework, all unknowns are modeled as random variables and the solution is in the form of a probability density function, known as the posterior density. Drawing samples from the posterior can be very computationally demanding, effectively limiting the size of the sample. In this talk, we illustrate how to use linear algebra to design effective samplers of reduced computational complexity. The complexity reduction is particularly striking when the data are much fewer than the unknowns. The performance of the proposed method will be illustrated with a few computed examples.

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MS66

A Low-Complexity Explainable ML Algorithm to Realize Multibeam Beamforming

Beamforming is a signal processing technique utilized in fields such as imaging, MIMO wireless communication, and radar applications. With the increasing interest in wireless communication and the use of ML models, there is a need for an efficient and high-performing signal processing technique to address the computational challenges in implementing multi-beam beamforming, without relying on data-heavy network training. This talk presents an ML model to realize multi-beam beamforming by imposing structured weight matrices on a neural network. By using structured and sparse weight matrices, we show that we can reduce the space and computational complexities of the neural network. Finally, we show that the proposed structure-imposed neural network leads to a low-complexity and accurate ML algorithm in realizing multi-beam beamforming. This is a joint work with Hansaka Aluvihare and Arjuna Madanayake. This work was supported by the National Science Foundation award numbers 2229473 and 2229471.

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MS66

Computational Aspects of Simultaneous Gaussian Quadrature Rules

The computation of simultaneous Gaussian quadrature rules associated with multiple orthogonal polynomials (MOP) is considered in this talk. Suppose r weight functions $w^{(i)}(x) \geq 0$, with support Δ_i, $i = 1, \ldots, r$, on the real line are given. The MOP $\{p_n(x)\}_{n=0}^{\infty}$ satisfy the following orthogonality conditions:

$$\int_{\Delta_i} p_n(x) x^k w^{(i)}(x) dx = 0, \quad 0 \leq k \leq n_{i-1},$$

with $n = \sum_{i=1}^{r} n_i$. We focus on the computation of the nodes x_j and weights $\omega_j^{(i)}$ of a simultaneous Gaussian quadrature rule

$$\sum_{j=1}^{n} f(x_j)\omega_j^{(i)} \approx \int_{\Delta_i} f(x) w^{(i)}(x) dx, \quad 1 \leq i \leq r.$$

They can be computed via the eigendecomposition of a banded lower Hessenberg matrix H_n, built on the coefficients of recurrence relations associated with the corresponding MOP. The Golub-Welsch algorithm can be adapted to compute the eigendecomposition of H_n, but it suffers from tremendous instability due to the high non-normality characterizing the latter matrix. Here, we propose a new balancing procedure that drastically reduces the condition of the Hessenberg eigenvalue problem, allowing to computing of the simultaneous Gaussian quadrature rule, in floating point arithmetic, in a reliable way for different kinds of MOP, requiring $O(n^2)$ computational complexity and $O(n)$ memory.

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MS67

Higher Order Generalized Nystrom Approximation

The growing abundance of data that is naturally represented in a multi-way format, such as high-dimensional arrays of numbers, has become a common occurrence in various fields such as computer vision, natural language processing, and bioinformatics. These types of data often poses a computational challenge as they can be too large to store in memory. To effectively analyze and extract insights from such data, efficient low-rank tensor approximation methods are needed. In this paper, we introduce a higher-order Generalized Nystrom approximation method for low-rank Tucker approximations of tensors. We provide theoretical guarantees for the expected approximation error and computational complexity of our approach, establishing it as promising solution for working with large, multi-dimensional datasets.

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MS67

A Fast Randomized Algorithm for Column/row Selection with Strong Rank-Revealing QR

In this talk, we analyze a sublinear-time algorithm for selecting a few rows and columns of a matrix for low-rank approximation purposes. The algorithm is based on an initial uniformly random selection of rows and columns, followed by a refinement of this choice using a strong rank-revealing QR factorization. We prove bounds on the error of the corresponding low-rank approximation (more precisely, the CUR approximation error) when the matrix is a perturbation of a low-rank matrix that can be factorized into the product of matrices with suitable incoherence and/or sparsity assumptions.

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MS67

Small Singular Values can Increase in Lower Precision

We perturb a real matrix of full column rank, and derive lower bounds for the smallest singular values of the perturbed matrix, in terms of normwise absolute perturbations. Our bounds extend existing lower-order expressions, demonstrate the potential increase in the smallest singular values, and represent a qualitative model for the increase in the small singular values after a matrix has been downcast to a lower arithmetic precision. We will also discuss how stochastic rounding to a lower arithmetic precision affects the smallest singular value of tall-and-thin matrices. This is joint work with Christos Boutsikas (Purdue), Gregory Dexter (Purdue), and Ilse Ipsen (NCSU).

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MS67

Efficient Randomized Sampling for Rank-Structured Matrix Compression

Many applications in scientific computing involve matrices that are dense but "data-sparse," having some exploitable low-rank structure that enables compression without loss of information. Rank-structured matrices are data-sparse matrices that can be tessellated into subblocks, which are either small enough to apply deterministic algorithms or else well-approximated by matrices of low rank. For large problem sizes, randomized sampling of the input matrix by a structured random test matrix has proven to be effective for rank-structured matrix compression. We introduce a new sampling technique that we call tagging, suitable for large black-box applications in which the entries of the input matrix are not accessed directly, but rather through fast matrix-vector or matrix-matrix multiplication. We discuss the improved efficiency of randomized sampling with tagging, as well as the accuracy of the overall compression scheme for strongly admissible block low-rank (BLR) matrices with uniform bases for admissible blocks within the same row or column block, termed BLR2.

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MS68

Canonical Polyadic Decomposition, Matrix Pencils and Sets of Polynomial Equations: Inspiring Connections

Solving systems of polynomial equations is important in engineering practice. In this talk, we present a novel strategy to find all (approximate) common roots of an overdetermined polynomial system corrupted by noise (e.g., caused by measurement error). In comparison to earlier frameworks that reduce the problem to a generalized eigenvalue problem, we introduce a multi-pencil approach that reduces the problem to the computation of a canonical polyadic decomposition (CPD) of a tensor (or a block term decomposition (BTD) in the case of coinciding roots [Vanderstukken et al., *Systems of polynomial equations, higher-order tensor decompositions and multidimensional harmonic retrieval: A unifying framework*, SIAM J. Matrix Anal. Appl., 42 (2), 2021, pp. 883-953]. The tensor is obtained from the null space of a Macaulay matrix. For high polynomial degrees, the Macaulay matrix suffers from the curse of dimensionality. However, its algebraic structure can be exploited for efficiency [Govindarajan et al., *A fast algorithm for computing Macaulay nullspaces of bivariate polynomial systems*, SIAM J. Matrix Anal. Appl., 45 (1), 2024, pp. 368-396]. The benefits of this approach, both from a conceptual and numerical standpoint, are analyzed. The technique is illustrated with an application involving the localization of two transmitters from the power received in arbitrary antenna configurations.

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MS68

Tensor Singular Spectrum Decomposition

Signal decomposition tools are important for interpreting complex data and as preprocessing for downstream analysis.Existing methods include Fourier analysis and wavelets and extend to tools like empirical mode decomposition and variational mode decomposition, among others. In this context, singular spectrum analysis (SSA) is a linear algebra-based method that works by performing a low-rank decomposition (SVD) of a Hankel matrix built from a given signal. Singular spectrum decomposition (SSD) automates SSA by extracting a set of band-limited components iteratively in a number of consecutive steps. Tensor decompositions have only been considered to a limited extent for SSD, while they fit naturally in the framework and may provide advantages with respect to matrix methods: tensors naturally extend the existing decomposition methods to a multi-channel context; tensors may allow for combining multiple embedding dimensions simultaneously; tensor decompositions may provide unique (and interpretable) decompositions; and certain decompositions can incorporate the iterative nature of SSD into an up-front multilinear rank estimation step. We will give an overview of our current results, including results on tensorization methods on single-channel signals, as well as examples where tensor decompositions improve multi-channel SSD results. Joint work with Amanda Kane, Spriha Joshi, Martijn Bouss, Jol Karel, Pietro Bonizzi and Ralf Peeters.

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MS68

Extensor and Decomposition

Tensor decomposition is a challenging problem from a computational and numerical point of view. When the rank of a tensor is low, the problem can be reduced to direct eigenvalues and eigenvector computations, but when the rank is higher, the complexity is much higher. In this talk, we will review algebraic geometric approaches, which transform the high rank tensor decomposition problem into a simultaneous diagonalization problem of extended tensors. We will analyse the properties of these varieties of extended tensors or extensors and illustrate the computational approach on some examples.

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MS68

On the Minimal Algebraic Complexity of the Rank-One Approximation Problem for General Inner Products

In this talk, we study the algebraic complexity of the Euclidean distance minimization problem from a generic tensor to the variety of rank-one tensors. More precisely, the Euclidean Distance (ED) degree of the Segre-Veronese variety counts the number of complex critical points of this optimization problem, and hence measures its algebraic complexity. Regarding this invariant as a function of inner products, we prove that this function achieves its minimal value at Frobenius inner product in the case of matrices. Moreover, we will discuss the above optimization problem for other algebraic varieties, which also serves as a description of the corresponding landscape of the above polynomial optimization problem.

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MS69

Impact of Covariance Weighting Matrices on the Convergence of the Conjugate Gradient Algorithm in Variational Data Assimilation

An important class of nonlinear weighted least-squares problems arises from the assimilation of observations in atmospheric and ocean models. In variational data assimilation, inverse error covariance matrices define the weighting matrices of the least-squares problem. For observation errors, a diagonal matrix (*i.e.*, uncorrelated errors) is often assumed for simplicity even when observation errors are suspected to be correlated. While accounting for observation-error correlations should improve the quality of the solution, it also affects the convergence rate of the minimization algorithms used to iterate to the solution. If the minimization process is stopped before reaching full convergence, which is usually the case in operational applications, the solution may be degraded even if the observation-error correlations are correctly accounted for. We explore the influence of the observation-error correlation matrix ($\mathbf{R}$) on the convergence rate of a conjugate gradient algorithm preconditioned by the background error covariance matrix ($\mathbf{B}$). Analytical and numerical results show a strong sensitivity of its convergence rate to the parameters of the observation error correlation models. In practice, a compromise may be required in the parameter specifications of $\mathbf{B}$ and $\mathbf{R}$ between staying close to the best available estimates on the one hand and ensuring an adequate convergence rate of the minimization algorithm on the other.

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MS69

Treating Different Timescales in Variational Data Assimilation for Coupled Systems

Four-dimensional data assimilation (4D-Var) aims to find the best state of a dynamical system by minimizing an objective function that measures the distance of a model trajectory to observations over a given time window, while remaining close to a prior forecast. The time window over which the minimization is performed is limited by the error growth rate of the model. A difficulty arises when applying 4D-Var to a coupled dynamical system with different timescales, as the time window must be chosen based on the fastest error growth. We consider this problem in the context of coupled atmosphere-ocean prediction, now used at operational weather forecasting centres. For this problem the chosen time window must reflect the fast error growth in the atmosphere, which limits the information that can be extracted from observations of the slower ocean. Here, a new method is proposed to address this issue. After running the standard coupled assimilation for several short windows, a new 'smoother' procedure is performed to find an ocean trajectory that best fits all ocean observations over these windows. This allows observations at later assimilation windows to update the state at earlier windows. Furthermore, it permits the use of late-arriving observations that were not available to the short-window assimilations. Using an idealized model with two timescales we

illustrate how the new method is able to improve the estimate of the state and the subsequent coupled model forecast.

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MS69

Stein-Based Preconditioners for Weak-Constraint 4D-Var

State-of-the-art algorithms for data assimilation are very sophisticated schemes which try to predict the most likely state of a dynamical system by combining information from observations and prior models. The linearized weak-constraint four-dimensional variational assimilation problem (4D-Var) can be reformulated as a saddle point problem that needs to be preconditioned to ensure fast convergence in terms of number of iterations. In this talk we illustrate novel preconditioning operators which involve the solution of certain Stein matrix equations. In addition to achieving better computational performance, the latter machinery allows us to derive tighter bounds for the eigenvalue distribution of the preconditioned problem. A panel of diverse numerical results displays the effectiveness of the proposed methodology compared to current state-of-the-art algorithms. This is a joint work with J. M. Tabeart.

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MS69

Preconditioners for Weak-Constraint Four-Dimensional Variational Data Assimilation

Data assimilation algorithms combine information from observations and prior forecasts in order to obtain an improved estimate of the state of a dynamical system at a given time. These updated initial conditions are often used to initialise a forecast, for example in the context of numerical weather prediction. Within the variational data assimilation setting, a number of linearised least squares problems are solved via iterative methods. The arising matrix is very high-dimensional and often ill-conditioned. In this talk we will discuss the role of preconditioning for the weak-constraint 4D-Var problem. In particular we will present novel preconditioners which take the form of low-rank corrections to a commonly-used first-level preconditioner, and show how they can be extended to the case where the first-level preconditioner is itself approximated. We will present theoretical and numerical comparisons of an additive and a multiplicative approach.

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MS70

Principal Pivot Transform: Variational Principles and Relation to the Cherkaev-Gibiansky-Milton Method

Motivated by the celebrated Loewner's theorem, we present our results on the (symmetric) principal pivot transform (PPT) which improve upon the results of J. Pascoe and R. Tully-Doyle. In particular, we supply the minimum hypotheses such that the PPT is matrix monotonic under the Loewner partial order on Hermitian matrices. In addition, we give a new variational principle for the PPT and elaborate on its connection to the Legendre-Fenchel transform from convex analysis and the Cherkaev-Gibiansky-Milton method in the theory of composites. From this minimization principle, we establish concavity of the PPT for kernel equivalent positive semi-definite matrices. Throughout we utilize the fundamental properties of Schur complements and the Moore-Penrose pseudoinverse under the Loewner ordering. This is joint work with Aaron Welters (Florida Institute of Technology).

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MS70

Exact Relations for Effective Tensors of Composites: Laminates Vs. Arbitrary Microstructures

Since the work of Milton it is known that there are elastic composites, whose effective tensors cannot be achieved by laminates that use the same set of materials. However, this is not the case when we restrict our attention to polycrystalline exact relations for conducting, elastic, piezoelectric or thermoelectric composites. In this talk I will describe the minimal example in the context of multi-field physics coupling 4 curl-free and 4 divergence-free fields in two space dimensions. The example is related to the problem in matrix algebra of characterizing all subspaces of real symmetric nxn matrices closed under the symmetrized product AB+BA, which, in turn, is related to formally real Jordan algebras characterized by Jordan, von-Neuman and Wigner in an attempt to build an axiomatic foundation of quantum mechanics. The example can be used, in particular, to build a very symmetric rank-one convex function, which is not quasiconvex.

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MS70

On the Extreme Rays of the Cone of 3 by 3 Quasi-

convex Quadratic Forms

This talk is concerned with the study of the extreme rays (strong extremals) of the convex cone of 3 times 3 quasiconvex quadratic forms. Those are interesting from both quasiconvex analysis and theory of composites perspective. We characterize the forms, the acoustic tensor of which is an extremal polynomial, proving that the extremality of the determinant implies either strong extremality or polyconvexity of the form. By providing counterexamples, we show that similar results do not hold in higher dimensions. Some questions on weak extremals will also be addressed. This is joint work with N. Hovsepyan (Rutgers University)

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MS70

Bessmertnyi Realizations of Effective Tensors for Metamaterial Synthesis: Conjectures and Counterexamples

Effective tensors of isotropic n-phase composites are known to be homogeneous degree-1 functions of n-variables which also belong to the special class known as Herglotz-Nevanlinna functions. Recently, M. Bessmertnyi claimed to characterize any such rational matrix function as being in the Bessmertnyi class because each partial Wronskian associated with it has a polynomial sum-of-squares representation. We disprove this claim by providing a counterexample derived from the basis generating polynomial for the Vamos matroid and give a conjecture on the realizability of effective tensors. Joint work with Aaron Welters.

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MS71

A Path-Following Method for Low-Rank Optimization

We present an online procedure for time-varying matrix optimization, based on the tracking of the solution trajectory of a low-rank matrix factorization in a path-following procedure. There, a path-following predictor-corrector algorithm solves a sequence of linearized systems. This requires the introduction of a horizontal space constraint to ensure the local injectivity of the low-rank factorization. The method produces a sequence of approximate solutions for the original problem. We use this method for solving time-varying semidefinite optimization and we further investigate the application of this idea to quadratic matrix problems with low-rank constraints.

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MS71

A Retraction Perspective on Dynamical Low-Rank Approximation

Retractions play a crucial role in algorithms designed to tackle optimization problems on smooth manifolds, ensuring that the iterates consistently remain within the manifold. In this contribution, we investigate the use of retractions in the numerical integration of differential equations on fixed-rank matrix manifolds, a domain closely associated with Dynamical Low-Rank (DLR) approximation techniques. We demonstrate how retractions can be employed to explore well-known DLR techniques, such as the KSL and KLS algorithms, and to devise novel approaches. In particular, we demonstrate that these retractions are well-suited for constructing curve approximations on manifolds, with a local truncation error of order three. This showcases new perspectives on addressing current time-accuracy constraints in recent robust DLR algorithms. As a result, we introduce two innovative numerical integration schemes applicable to differential equations on general manifolds: the accelerated forward Euler (AFE) method and the Ralston-Hermite (RH) method. The latter extends the use of retractions beyond optimization, covering other computational tasks on manifolds, such as interpolation.

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MS71

Structure Regularization for X-Ray Spectroscopy

X-ray sources continue to improve and new low-emittance sources, promise gains in coherent flux of up to two orders of magnitude which is potentially transformative for high-resolution. A basic form of compressed sensing has been deployed as a proof-of-concept on a single beamline at Diamond (Townsend et al., 2022), exploiting the fact that as there are only a small number of actual chemical states in a system a low-rank description can be formed, and matrix completion methods can be employed to allow us to fill in missing gaps in the measurement from between a fifth and sixth of dose otherwise needed. In this talk, we will extend this initial proof of concept using the low-rank and sparse structure to include additional structure that the chemical states are often spatially structured in a known representation.

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MS72

Mathematical Analysis and Numerical Approxi-

mations of Density Functional Theory Models for Metallic Systems

In this talk, we will introduce our study on the energy minimization model arising in the ensemble Kohn-Sham density functional theory for metallic systems, in which a pseudo-eigenvalue matrix and a general smearing approach are involved. We investigate the invariance of the energy functional and the existence of the minimizer of the ensemble Kohn-Sham model. We propose an adaptive two-parameter step size strategy and the corresponding preconditioned conjugate gradient methods to solve the energy minimization model. Under some mild but reasonable assumptions, we prove the global convergence for the gradients of the energy functional produced by our algorithms. Numerical experiments show that our algorithms are efficient, especially for large scale metallic systems. In particular, our algorithms produce convergent numerical approximations for some metallic systems, for which the traditional self-consistent field iterations fail to converge. This is a joint work with Professor Stefano de Gironcoli, Dr. Bin Yang and Prof. Aihui Zhou.

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MS72

On Inverse Iterations for the Gross-Pitaevskii Eigenvalue Problem

In this talk we discuss the computation of ground states of Bose-Einstein condensates by solving the Gross-Pitaevskii equation (GPE), which is an eigenvalue problem with a nonlinearity in the eigenfunction. For solving it we propose an energy-adaptive Riemannian gradient method with provable global convergence. Furthermore, we show how the method can be interpreted as a generalized inverse iteration with damping and how we can recover explicit convergence rates depending on spectral gaps of a linearized Gross-Pitaevskii operator. We also discuss the implications of our findings on the usage of spectral shifting strategies in such nonlinear settings.

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MS72

An Adaptive Line Search for Self-Consistent Field Problems of Electronic Structure Theory

I will discuss recent joint work with Antoine Levitt in which we developed an adaptive damping algorithm for the self-consistent field (SCF) iterations of Kohn-Sham density-functional theory [M. F. Herbst, A. Levitt, A robust and efficient line search for self-consistent field iterations. J. Comput. Phys., 459, 111127 (2022)]. In our approach we automatically adjust the damping in each SCF step based on a backtracking line search employing a theoretically sound, accurate and inexpensive model for the energy as a function of the damping parameter. In contrast to usual SCF schemes in DFT, the resulting algorithm is fully automatic and does not require the user to select a damping. We are able to prove convergence of our scheme under realistic assumptions for the setting of practical materials simulations, which is further demonstrated by performing numerical experiments on a wide range of challenging materials systems (elongated supercells, surfaces and transition-metal alloys).

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MS72

Optimize the Self-Consistent Field Iteration for Nonlinear Eigenvalue Problems

The nonlinear eigenvalue problem arising from the Kohn-Sham density functional theory is often solved by a nonlinear iterative method called the self-consistent field (SCF) iteration. The method contains several parameters such as the convergence tolerance for the solution of the linear eigenvalue problem in each SCF iteration, the number of previous charge density vectors to be mixed with the charge density approximation obtained in the current iteration, and the mixing ratio. The choice of these parameters can affect the performance of SCF significantly. In most existing solvers, these parameters are often set in advance based on some heuristics. In this talk, I will discuss the possibility of using machine learning techniques to optimize the selection of these parameter dynamically.

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MS73

Real Skew-symmetric and Periodic Skew-symmetric Tridiagonal Matrices with Prescribed Spectral Data

Skew-symmetric matrices have various applications in Physics, one of which is in the gyroscopic system. In this talk, we retrieve a unique real skew-symmetric tridiagonal matrix from the maximal and minimal imaginary parts of the eigenvalues of all its leading principal submatrices, and then we reconstruct a real periodic skew-symmetric tridiagonal matrix from these prescribed spectral data. The necessary and sufficient conditions for the existence of such matrices are given, and we obtain the total number of possible n-by-n periodic skew-symmetric tridiagonal matrices. The proofs of the obtained results provide algorithmic procedures for the aimed reconstructions, which are supported by some illustrative numerical experiments. This is a joint work with Wei-Ru Xu and Yu Zeng.

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MS73

A Quasiseparable Approach to Off-diagonal Decay

of Inverses of Banded Matrices

It has been known for a long time that the inverse of a banded matrix, while generally not banded itself, exhibits an off-diagonal decay behavior, under suitable hypotheses on its spectrum. Starting from the seminal paper by Demko, Moss, and Smith (1984), several authors have studied this property and its generalizations, often relying on techniques such as polynomial approximation. In this work we explore an alternative approach based on quasiseparable matrix structure, that is, the property that off-diagonal blocks have low rank. Since banded matrices exhibit a quasiseparable structure, and quasiseparable theory gives us a characterization of their inverses, it is natural to ask whether we can use such results to investigate decay behavior. We develop explicit inversion formulas that rely on structured versions of classical factorizations such as LU and QR, and derive computable a priori bounds for the off-diagonal decay of inverses of band matrices. Theoretical results are illustrated via numerical experiments and compared to bounds already present in the literature. This is joint work with Y. Eidelman (Tel Aviv University).

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MS73

An Efficient Iterative Solution of M-Matrix Linear Systems in Block-Hessenberg Form

M-matrices and non-negative matrices are intimately related to Markov chains and transition probabilities. Many models in queueing theory lead to Markov processes (or Markov chains) for which the infinitesimal generator (respectively the transition probability matrix) is a (possibly infinite) block-Hessenberg matrix. In this talk, we consider the solution of M-matrix linear systems in (block) Hessenberg form by stationary iterative methods, and we show new comparison results between matrix splittings that hold for this special structure [L. Gemignani and F. Poloni, Comparison theorems for splittings of M-matrices in (block) Hessenberg form, BIT, 62(3):849–867, 2022]. From a more general perspective, these results highlight that the convergence rates of some stationary iterative methods applied for the solution of M-matrix linear systems in (block) Hessenberg form depend on the probabilities of observing certain walks in the Markov chain associated with the input coefficient matrix. A key observation is that these probabilities rely only on the nonzero structure of the matrix, not on the value of its entries. This is a remarkable difference from the classical theory of preconditioners and splitting methods and it promotes the search for preconditioning techniques based on the exploitation of the unweighted graph associated with the input coefficient matrix. This is a joint work with F. Poloni.

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MS73

Randomized Eigenvalue Estimation of Kernel Matrices

In this work, we focus on kernel matrices that arise from a kernel applied to a known distribution of points, and we wish to find out if the given matrix or its sub-blocks have a low numerical rank. This is because, in such cases, it is possible to greatly speed up various matrix computations by applying structured matrix algorithms. In particular, we want to estimate the full spectrum of the kernel matrix without explicitly forming the matrix, since such matrices are often so large that it is infeasible to store them in memory. We propose a randomized algorithm to do just that for certain kernels and distributions of points, and we perform an analysis that makes clear when the use of this algorithm is justified. As input, the algorithm takes the full set of points from which the kernel matrix is formed; and as output, it gives values that describe the spectrum of the matrix in a precise sense. Since we avoid explicit matrix construction with this algorithm, we achieve time and storage costs that are subquadratic in the size of the original matrix. This is a joint work with Yuanzhe Xi.

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MS74

Putting Randomness into LAPACK and Next Generation RandNLA Theory

LAPACK (Linear Algebra PACKage) is a widely-used high-quality software library for numerical linear algebra that provides routines for solving systems of linear equations, linear least squares, eigenvalue problems, singular value decomposition, and matrix factorizations such as LU, QR, Cholesky and Schur decomposition. Randomized Numerical Linear Algebra (RandNLA) is an interdisciplinary research area that exploits randomization as a computational resource to develop improved algorithms for large-scale linear algebra problems. In addition to providing some of the best linear algebra algorithms (in worst-case theory, numerical implementations, and non-trivial implicit statistical properties and machine learning implementations), RandNLA techniques are the basis for best-in-class stochastic second-order optimization algorithms (such as SubSampled Newton's methods, Iterative Hessian Sketch, and Newton-LESS). The time has come to put RandNLA methods into the next generation of LAPACK, and we have begun to do that, developing RandBLAS and RandLAPACK. We will present our high level plan for RandBLAS and RandLAPACK. RandBLAS concerns basic sketching, and our hope is that RandBLAS will grow to become a community standard for RandNLA. RandLAPACK concerns algorithms for solving traditional linear algebra problems (least-squares and optimization, low-rank approximation, etc.) as well as advanced sketching functionality, but its full scope will be larger than linear algebra per se, including certain higher-level primitives in optimization and machine learning that require judicious use of RandNLA. All this motivates new theory, going beyond traditional theoretical computer science and numerical linear algebra approaches to RandNLA. We will give several examples of this new theory, including scalable methods for algorithmic Gaussianization and structured sparse embeddings (such as leverage score sparsified, or LESS, embeddings). These methods significantly reduce the computational cost of sketching, while at the same time providing quantitative performance for a much broader range of sketching algorithms and their use in downstream linear algebra and optimization algorithms. Joint work with Riley Murray, Jim Demmel, Michael Derezinski, and others.

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MS74

Are Sketch-and-Precondition Least Squares Solvers Numerically Stable?

Sketch-and-precondition techniques are efficient and popular for solving large least squares (LS) problems of the form $Ax = b$ with $A \in \mathbb{R}^{m\times n}$ and $m \gg n$. This is where A is "sketched" to a smaller matrix SA with $S \in \mathbb{R}^{\lceil cn\rceil\times m}$ for some constant $c > 1$ before an iterative LS solver computes the solution to $Ax = b$ with a right preconditioner P, where P is constructed from SA. Popular sketch-and-precondition LS solvers are Blendenpik and LSRN. We show that the sketch-and-precondition technique in its most commonly used form is not numerically stable for ill-conditioned LS problems. For provable and practical backward stability and optimal residuals, we suggest using an unpreconditioned iterative LS solver on $(AP)z = b$ with $x = Pz$. Provided the condition number of A is smaller than the reciprocal of the unit round-off, we show that this modification ensures that the computed solution has a backward error comparable to the iterative LS solver applied to a well-conditioned matrix. Additionally, we provide experimental evidence that using the sketch-and-solve solution as a starting vector in sketch-and-precondition algorithms (as suggested in Rokhlin and Tygert (2008)) is preferable to the standard algorithm. This approach often results in much more accuracy—albeit not always backward stable solutions.

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MS74

Randomized low-rank approximations beyond Gaussian random matrices

This paper expands the analysis of randomized low-rank approximation beyond the Gaussian distribution to four classes of random matrices: (1) independent sub-Gaussian entries, (2) independent sub-Gaussian columns, (3) independent bounded columns, and (4) independent columns with bounded second moment. The analysis offers some details on the minimal number of samples and the error in the resulting low-rank approximation. We illustrate our analysis in the context of the randomized subspace iteration method as a representative algorithm for low-rank approximation.

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MS74

High-Accuracy Nystrom Low-Rank Approximations of Kernel Matrices

The Nystrm method is a convenient randomized method to quickly obtain low-rank approximations to kernel matrices. We propose a series of heuristic strategies to make the Nystrm method reach high accuracies (nearly SVD quality) for nonsymmetric kernel matrices. The resulting methods (called high-accuracy Nystrm methods) treat the Nystrm method and a skinny rank-revealing factorization as a fast pivoting strategy in a progressive alternating direction refinement process. Two refinement mechanisms are used: alternating the row and column pivoting starting from a small set of randomly chosen columns, and adaptively increasing the number of samples until a desired rank or accuracy is reached. A fast subset update strategy based on the progressive sampling of Schur complements is further proposed to accelerate the refinement process. Efficient randomized accuracy control is also provided. Relevant accuracy and singular value analysis is given to support some of the heuristics.

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MS75

Tensor Decomposition Meets Reproducing Kernel Hilbert Spaces (RKHS)

Tensor decompositions require that the data maps to a regular d-way grid, but many real-world datasets do not have this property. For example, time-evolving data may be measured at different intervals for different subjects. We can handle irregular grids by treating some modes as continuous rather than discrete, meaning that we expect that resulting factors to be smooth. We develop a generic framework for incorporating continuous modes into the CP tensor decomposition. We approximate the continuous modes in a reproducing kernel Hilbert space (RKHS). We present an alternating least squares algorithm that is computationally efficient. This continuous mode (1) enables practitioners to enforce common structural assumptions about data such as smoothness, (2) extends to situations in where the measurement times do not align by utilizing the framework of missing data, and (3) provides a more principled way to interpolate between observed points. We end by considering how the structure of the resulting least squares updates may be amenable to speed up through randomized algorithms.

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MS75

From Static to Dynamic Biomarkers: Analysis of Time-Resolved Metabolomics Data Using (coupled) Tensor Decompositions

Analysis of time-resolved metabolomics data holds promise

to enhance our comprehension of metabolic mechanisms, thereby advancing precision nutrition and medicine. However, analyzing such longitudinal data is challenging, hampered by the complexities of temporal dynamics, high dimensionality and high biological variability. Conventional analysis methods have limitations in providing a compact summary in terms of groups of subjects, clusters of metabolites, and their temporal profiles simultaneously. In this talk, we arrange time-resolved metabolomics data as a third-order tensor with subjects by metabolites by time modes, and discuss new approaches based on (coupled) matrix and tensor factorizations to extract the underlying patterns in the data and reveal both static and dynamic biomarkers of phenotypes. We analyze simulated data generated from a well-established metabolic model as well as data collected during a meal challenge test from the COPSAC2000 cohort. The results show that our methods can reveal static and dynamic metabolic biomarkers from both simulated and real meal challenge test data. Furthermore, we demonstrate that integrating prior information from mechanistic models into real-world analysis significantly enhances the effectiveness of extracting meaningful patterns.

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MS75

Optimal Sampling for Tensor Learning

We consider the approximation of high-dimensional functions in L^2 from point evaluations. For linear approximation, recent results show that weighted least-squares projections allow to obtain quasi-optimal approximations with near to optimal sampling budget. This can be achieved by drawing from suitable distributions and subsampling the resulting samples. We review different sampling strategies and show how these methods can be used to approximate functions with low-rank tensor methods, in an active learning setting. We do this by coupling iterative algorithms and optimal sampling methods for the projection onto successive linear spaces.

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MS75

An Algebraic Algorithm for the ParaTuck-2 Decomposition

ParaTuck-2 decomposition (PT2D) of 3-rd order tensors is a 2-level extension of the well-known CP (canonical polyadic) decomposition (CPD). It is relevant in several applications, such as chemometrics, telecommunications, and machine learning. As shown in (Harshman, Lundy, 1996), the PT2D enjoys strong uniqueness properties (up to scaling/permutation ambiguities, similarly to the CPD). However, there are very few results on theory and algorithms for the PT2D. In particular, common strategies, such as the alternating least squares, suffer from convergence and initialization issues. We propose an algebraic algorithm for the PT2D decomposition in the case when the ParaTuck-2 ranks are smaller than the frontal dimensions of the tensor. Our approach relies only on linear algebra operations and is based on finding the kernel of a structured matrix constructed from the tensor.

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MS76

Efficient Methods for Hyperparameter Estimation in Large-Scale Bayesian Inverse Problems

Inverse problems arise in a wide variety of applications including biomedicine, environmental sciences, astronomy, and more, but computing reliable solutions to these problems requires the inclusion of prior knowledge, in a process that is often referred to as regularization. Most regularization techniques require suitable choices of regularization parameters or hyperparameters, and estimating these hyperparameters can be one of the main challenges and bottlenecks for large-scale inverse problems. In this work, we describe computationally efficient approaches for hyperparameter estimation using empirical Bayesian approaches.

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MS76

TRIPs-Py: Techniques for Regularization of In-

verse Problems in Python

In this talk we present TRIPs-Py, a new Python package of linear discrete inverse problems solvers and test problems. The solvers available in TRIPs-Py include direct regularization methods (such as truncated singular value decomposition and Tikhonov) and iterative regularization techniques (such as Krylov subspace methods and solvers for $\ell_p - \ell_q$ formulations, some of which have not been publicly available before, which enforce sparse or edge-preserving solutions and handle different noise types). Some of the test problems in TRIPs-Py arise from simulated image deblurring and computerized tomography, while other test problems model realistic problems in dynamic and hyperspectral computerized tomography. During this talk we will give an overview of some of the state-of-the-art TRIPs-Py regularization methods, highlighting similarities and differences, and we will illustrate their use on some of the TRIPs-Py test problems.

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MS76

Preconditioning Studies for Solving Large-Scale Data Assimilation with Ensemble-Variational Methods

The initialization of forecasts for weather and climate prediction employs ensemble-variational methods (EnVAR) which integrate forecasts from earlier times with a large number of heterogeneous observations to calculate the so-called analysis of the current system state of the atmosphere or more general the earth system including atmosphere, land, ocean and surface waves. These methods solve large-scale minimization problems on current supercomputer systems by iterative minimization techniques. Methods used are often mixtures of gradient or conjugate gradient methods with Newton type minimization approaches. Preconditioning plays a key role to control the convergence and convergence speed of the minimizers. Preconditioning in large-scale distributed and parallelized systems involves solving particular purpose-built preconditioners, which employ the particular form and structure of the underlying minimization problems. These depend on the form of the observation operators, for example nonlocal satellite observations through the whole electromagnetic spectrum, as well as on the form and design of background covariance matrices and observation error covariances. We will discuss the design of the EnVAR minimizer and the setup of its preconditioning modules. Further, the construction of different preconditioners will be discussed and their performance within the minimization and subsequent forecasting both with respect to speed as well as quality will be studied.

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MS76

Using the Hessenberg Method for Inverse Problems

Inverse problems involve the reconstruction of hidden objects from possibly noisy indirect measurements and are ubiquitous in a variety of scientific and engineering applications. This kind of problems tend to be ill-posed: the reconstruction is very sensitive to perturbations in the measurements, and therefore need regularization. Moreover, real-world applications are often large-scale: resulting in computationally demanding tasks. In this talk I will recall an inner-product free Krylov solver, CMRH, which is based on the Hessenberg method. More specifically, I will focus on its regularizing properties; as well as presenting a new hybrid variant that incorporates Tikhonov regularization on the projected problems.

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MS77

Monolithic Multigrid Preconditioners for High-Order Discretizations of the Navier-Stokes Equations

Recent years have seen substantial interest in the development of high-order spatial discretizations for the Navier-Stokes equations, using either Scott-Vogelius elements (on suitable meshes) or H(div)-conforming elements to achieve high-order discretizations that strongly enforce the incompressibility constraint. For time-dependent problems, a further complication comes from achieving similar higher-order accuracy for the time-stepping scheme while maintaining optimal cost per time-step, roughly proportional to the number of spatial degrees of freedom. In this talk, we present simulation results using Firedrake for an H(div)-conforming spatial discretization and Irksome for fully implicit Runge-Kutta temporal discretizations, using PETScs PCPatch to define an effective block relaxation scheme for monolithic multigrid applied to the Jacobians of the resulting time-stepping scheme. We show that the scheme is robust in order, and discuss how the cost-per-timestep changes with spatial and temporal resolutions and discretization orders.

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MS77

Constrained Local Approximate Ideal Restriction for Advection-Diffusion Problems

This talk introduces a reduction-based algebraic multigrid method (AMG) that incoporated mode contraints to make it suitable for solving (non)symmetric linear systems ranging from the purely advective to purely diffusive regime. Its initial motivation comes from a new reduction-based algebraic multigrid (AMG) approach, ℓAIR (local approximate ideal restriction), that was developed for solving advection-dominated problems. Motivated by the success of ℓAIR in the advective regime, our aim in this paper is to generalize the AIR framework with the goal of improving the performance of the solver in diffusion dominated regimes. To do so, we propose a novel way to combine mode constraints as used commonly in energy minimization AMG methods with the local approximation of ideal operators used in ℓAIR. The resulting constrained ℓAIR (CℓAIR) algorithm is able to achieve fast scalable convergence on advective and diffusive problems. In addition, it is able to achieve standard low complexity hierarchies in the diffusive regime through aggressive coarsening, something that has been previously difficult for reduction-based methods.

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MS77

Preconditioning and Deflation for Non-Hermitian Positive Definite Matrices

This work considers weighted, preconditioned and deflated GMRES. The objective is to provide a way of choosing:

- a preconditioner,
- deflation operators,
- and an inner product (also called weight)

that ensure fast convergence. The main focus of the article is on Hermitian preconditioning (even for non-Hermitian problems). It is indeed proposed to choose a Hermitian preconditioner H, and to apply GMRES in the inner product induced by H. If moreover, the problem matrix A is positive definite, then a new convergence bound is proved that depends only on how well H preconditions the Hermitian part of A, and on a measure of how non-Hermitian A is. In particular, if a scalable preconditioner is known for the Hermitian part of A, then the proposed method is also scalable. Of course, Hermitian preconditioning finds its limits for significantly non-Hermitian matrix. In collaboration with Daniel B. Szyld, we have proposed new spectral deflation spaces that accelerate convergence in this setup. Both theoretical analysis and numerical results will be presented.

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MS77

Superior Discretizations and AMG Solvers for Extremely Anisotropic Diffusion via Hyperbolic Operators

Heat conduction in magnetic confinement fusion can reach anisotropy ratios of $10^9 - 10^{10}$, and in complex problems the direction of anisotropy may not be aligned with (or is impossible to align with) the spatial mesh. Such problems pose major challenges for both discretization accuracy and efficient implicit linear solvers. Although the underlying problem is elliptic or parabolic in nature, we argue that the problem is better approached from the perspective of hyperbolic operators. The problem is posed in a directional gradient first order formulation, introducing a directional heat flux along magnetic field lines as an auxiliary variable. We then develop novel continuous and discontinuous discretizations of the mixed system, using stabilization techniques developed for hyperbolic problems. The resulting block matrix system is then reordered so that the advective operators are on the diagonal, and the system is solved using AMG based on approximate ideal restriction (AIR), which is particularly efficient for upwind discretizations of advection. Compared with traditional discretizations and AMG solvers, we achieve orders of magnitude reduction in error and AMG iterations in the extremely anisotropic regime.

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MS78

Long Time Electromagnetic Energy Decay in Dissipative Generalized Lorentz Media: a Modal Approach

Electromagnetic dispersive structures such as metamaterials can be modelled by generalized Drude-Lorentz models. In this talk, we are interested in dissipative Drude-Lorentz open structures and we wish to quantify the loss in such media in terms of the long time decay rate of the electromagnetic energy of the corresponding Cauchy problem. In [1], we propose a method based on frequency dependent Lyapunov estimates. Here, we develop a second approach based on the spectral analysis of the underlying non-selfadjoint operator associated to the Maxwell's evolution system. It relies first on a decomposition of this unbounded operator (via a spatial Fourier transform) into

a family of dissipative finite dimensional operators indexed by the wave vector and then on a precise spectral analysis of this family of operators. As in [1], it allows to show the polynomial stability of the Cauchy problem. Technically more involved than the method developed in [1], this approach has two great advantages. The first one is to be closer to physics since it consists in a rigorous modal analysis of the model. The second one is to provide more precise and more optimal results, leading to distinguish the notion of weak and strong dissipation. [1] M. Cassier, P. Joly and L. A. Rossas Martnez, Long time behaviour of the solution of Maxwell's equations in dissipative generalized Lorentz materials (I) A frequency dependent Lyapunov function approach, Z. Angew. Math. Phys., 74 (2023), 115.

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MS78

On the Properties of the Transfer Matrix for Spatio-Temporal Layered Media

We are interested in the band diagrams of a special category of time-modulated composites called space-time laminates. These are standard one-dimensional spatial laminates, in which the pattern of material properties moves at a constant speed, via an external mechanism. The associated dispersion diagram presents directional band gaps, ranges of frequencies at which waves cannot propagate only from the right or only from the left. For material design, it is of paramount importance to be able to identify for which frequencies one has total band gaps (the wave cannot propagate regardless of the direction of propagation) and for which one has directional band gaps. In this talk, we will show that the frequency spectrum of two-component space-time laminates admits a universal structure which is independent of the geometry of the laminate as well as the specific material properties. This is achieved by mapping the band diagram on a torus and using compactness arguments. Furthermore, the maximal width, the expected width, and the density of the band gaps (total and directional) in the spectrum are derived. We will show that these are related to the properties of the transfer matrix (the dispersion relation is given by the trace of such a matrix), which presents a discrete spectrum made up of distinct harmonics, exactly characterized in terms of both the period of their oscillations and their amplitudes.

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MS78

Fractional Time Derivative and Herglotz-Nevanlinna Functions

In the context of anomalous diffusion in disordered materials, the fractional time (FTD) derivative operators are linked to fractional Brownian motions, where the fractional derivative order α is related to the Mean Square Displacement (MSD) of the particles. FTD also shows up in other context such as the Maxwell's equations with the Cole-Cole polarizations, which is a dispersive system. In this talk, we will apply the Herglotz Nevanlinna theory not only to help handle the memory term in the time-domain Maxwell-Cole-Cole equations but also to reveal the analytical structure of the Caputo FTD in this model.

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MS78

Factorization of Divergence-Form and Curl-Curl Operators and Applications to Photonic Crystals

Divergence-form and curl-curl operators arise naturally in the study of composite materials in acoustic and electromagnetic wave propagation. In particular, in composite materials these operators tend to have piecewise-constant periodic coefficients, which enables one to consider the spectrum of the operator in terms of Bloch waves. We will demonstrate how, under relatively loose geometric constraints, one can factorize these operators on certain quasi-periodic Sobolev spaces using layer potentials, separating the geometry of the composite from the material parameter contrast ratio in such a way that leads to useful spectral analysis of the composite.

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MS79

Optimization Without Retraction on the Random Generalized Stiefel Manifold for the Canonical Correlation Analysis

Optimization over the set of matrices that satisfy $X^\top BX = I_p$, referred to as the generalized Stiefel manifold, appears in many applications such as canonical correlation analysis (CCA) and the generalized eigenvalue problem. Solving these problems for large-scale datasets is computationally expensive and is typically done by either computing the closed-form solution with subsampled data or by iterative methods such as Riemannian approaches. Building on the work of Ablin & Peyré (2022), we propose an

inexpensive iterative method that does not enforce the constraint in every iteration exactly, but instead it produces iterations that converge to the generalized Stiefel manifold. We also tackle the random case, where the matrix B is an expectation. Our method requires only efficient matrix multiplications, and has the same sublinear convergence rate as its Riemannian counterpart. Experiments demonstrate its effectiveness in various machine learning applications involving generalized orthogonality constraints, including CCA for measuring model representation similarity.

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MS79

Exploiting Geodesic Convexity in Matrix-Valued Optimization

Matrix-valued optimization tasks arise in many machine learning applications, including maximum likelihood estimation, robust subspace discovery, clustering, and barycenter problems. In such settings, it is often beneficial to exploit non-Euclidean structure in the data for the design of geometric algorithms that can outperform standard nonlinear programming approaches. The tractability of such geometric optimization problems depends crucially on the convexity of the objective. Importantly, a function may be Euclidean nonconvex, but geodesically convex under a suitable Riemannian metric. In this talk, we discuss classes of such functions in matrix-valued optimization, as well as optimization algorithms where such structure enables the derivation of global optimality certificates.

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MS79

Nonnegative Low-rank Factorization for Statistically Optimal K-means Clustering

K-means clustering is a widely used machine learning method for identifying patterns in large datasets. Semidefinite programming (SDP) relaxations have recently been proposed for solving the K-means optimization problem that enjoy strong statistical optimality guarantees, but the prohibitive cost of solving the SDP solver renders these guarantees inaccessible to practical datasets. By contrast, nonnegative matrix factorization (NMF) is a simple clustering algorithm that is widely used by machine learning practitioners, but without a solid statistical underpinning nor rigorous guarantees. In this talk, we introduce an NMF-like algorithm that works by solving a nonnegative low-rank restriction of the SDP relaxed K-means formulation using a nonconvex Burer–Monteiro factorization approach. The resulting algorithm is just as simple and scalable as state-of-the-art NMF algorithms, while also enjoying the same strong statistical optimality guarantees as the SDP. In our experiments, we observe that our algorithm achieves substantially smaller mis-clustering errors compared to the existing state-of-the-art.

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MS79

Riemannian Optimization and Riemannian Langevin Monte Carlo for PSD Fixed Rank Matrices

For optimization under matrix constraints of Hermitian positive semi-definite (PSD) fixed rank, we compare three methodologies. The first approach is the simplest factor-based Burer-Monteiro method. The second approach is to regard the constraint set as an embedded manifold. The third approach is to consider a quotient manifold. We show that nonlinear conjugate gradient (CG) in the first two methodologies is equivalent to CG on the quotient manifold with suitably chosen metrics. The simple Burer-Monteiro approach corresponds to the Bures-Wasserstein metric. We also analyze the condition number of the Riemannian Hessian under these different metrics. The difference in the condition number under different metrics is consistent with the difference in numerical performance. This is joint work with Shixin Zheng at Purdue, Wen Huang at Xiamen University and Bart Vandereycken at University of Geneva. Fo real PSD matrices of fixed rank, we construct efficient sampling schemes to generate samples from the Gibbs distribution, which can be regarded as Monte Carlo sampling on the manifold. Schemes are constructed by adding white noise and a geometric correction to the Riemannian gradient descent method. Numerical verification will be shown. This is joint work with Tianmin Yu and Govind Menon at Brown, Jianfeng Lu at Duke, and Shixin Zheng at Purdue.

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MS80

Linearization of Nonlinear Eigenvector Problems: Numerical Methods, Response and Dynamics

I will review recent work on the structure of nonlinear

eigenvector problems, and some of their applications.

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MS80

Optimizing Convex Compositions of Matrix Traces

The NEPv approach has been increasingly used lately for optimization on the Stiefel manifold arising from machine learning. General speaking, the approach first turns the first order optimality condition, also known as the KKT condition, into a nonlinear eigenvalue problem with eigenvector dependency (NEPv) or a nonlinear polar decomposition problem with orthogonal factor dependency (NPDo) and then solve the nonlinear problem via some variations of the self-consistent-field (SCF) iteration. The difficulty, however, lies in designing a proper SCF iteration so that a maximizer is found at the end. In this talk, we will explain a unifying NPDo framework for optimizing convex compositions of matrix traces.

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MS81

Quasiseparable Representations of Matrices in Numerical Solution of Differential Equations

The appearance of rank-structured matrices in the numerical solution of differential equations is well known. We study concrete numerical methods for various classes of boundary value problems. The first set of results and algorithms is developed for the Dirichlet and related problems for the elliptic biharmonic equations. In the second part of the talk, we consider the Cauchy, the nonlocal, and the inverse problems for the corresponding parabolic equations. Based on quasiseparable representations we develop fast algorithms for the numerical treatment of the problems. This is a joint work with Matania Benartzi, Dalia Fishelov, Luca Gemigniani, Paola Boito, Vladimir Sherstyukov, Ivan Tichonov.

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MS81

Randomized Optimal Experiment Design for Bayesian Inverse Problems via Column Subset Selection

This presentation tackles optimal sensor placement for Bayesian linear inverse problems, a popular version of the more general Optimal Experiment Design (OED) problem, using the D-optimality criterion. This is done by establishing connections between sensor placement and Column Subset Selection Problem (CSSP), which is a well-studied problem in Numerical Linear Algebra (NLA). In particular, we use the Golub-Klema-Stewart (GKS) approach which involves computing the truncated Singular Value Decomposition (SVD) followed by a pivoted QR factorization on the right singular vectors. The algorithms are further accelerated by using randomization to compute the low-rank approximation as well as for sampling the indices. The resulting algorithms are robust, computationally efficient, require virtually no parameter tuning, and come with strong theoretical guarantees. We also propose a new approach for OED, called reweighted sensors, that selects k sensors but judiciously recombines sensor information to dramatically improve the D-optimality criterion. Numerical experiments on model inverse problems involving the heat equation and seismic tomography in two spatial dimensions demonstrate the performance of our approaches.

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MS81

One-element Commutation Classes: Counting and Generating

A word s in the alphabet $1, 2, \cdots, n$ is said to be formed by consecutive integers if every factor of length 2 is of the form $i,\ i+1$ or $i+1,\ i$, for some $1 \leq i < n$. When s is also a reduced word for some permutation, we say that s is a one-element commutation class. We give a necessary and sufficient condition for a word formed by consecutive integers to be a one-element commutation class and construct an efficient algorithm to generate all one-element commutation classes of a given permutation.

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MS82

Progress with Minimal Height Structured Companions

The **height** of a matrix $\mathbf{A}$ is $\|\text{vec}(\mathbf{A})\|_\infty$. The **characteristic height** of $\mathbf{A}$ for a particular polynomial basis $\phi_j(\lambda)$ is $\|\mathbf{c}\|_\infty$ where the characteristic polynomial of $\mathbf{A}$, written in the basis $\phi_j(\lambda)$, is $\sum_{j=0}^{n} c_j \phi_j(\lambda)$. If we start with a polynomial $p(\lambda)$ and find a structured companion matrix $\mathbf{C}$ for it, then we can compare the height of the polynomial with the height of the companion matrix. These notions are not useful without some other restriction on either the entries of the matrix or on the polynomial coefficients, but if, say, these entries or coefficients must be integers, then one may ask for such things as minimal height companions, or minimal height structured companions. This talk will report on progress in understanding minimal height structured companions (or, in some cases, linearizations of matrix polynomials). As of the date I write this abstract, we have some examples where one can find exponentially better companions than the standard ones. We have two algorithms for finding such things, but both are expensive; more progress is needed. What is also needed is more clarity on just why a minimal height structured companion is, or might be, useful; and I hope to have at least a partial answer by the time of the conference.

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MS82

Companion Forms for Scalar and Matrix Polyno-

mials: a Personal Review

I will review some features of companion forms for scalar and matrix polynomials, together with an overview of some families of companion matrices introduced during the last 20 years, namely: Fiedler and Fiedler-like pencils and block companion pencils, as well as companion l-ifications. The preservation of the symmetries in the coefficients of the matrix polynomial to construct structured companion forms will be also considered. The basic properties of these families will be reviewed, and we will also pay attention to some structural features, like the sparsity.

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MS82

A Skew Symmetric Matrix Polynomial Canonical Form

Spectral symmetries show up time and again in applications where matrix polynomials naturally arise. Over the decades, this has lead researchers to study structured matrix polynomials whose (matrix polynomials whose spectrum admits some symmetry property) most notably are the alternating, palindromic, and skew-symmetric structures. In the early 2010s, Mackey, Mackey, Mehl, and Mehrmann (MMMM) published a trio of papers fully exploring the spectra of matrix polynomials that admit the alternating, palindromic, or skew-symmetric structures. In this talk, we will be using the results from the MMMM paper on skew-symmetric matrix polynomials along with techniques from my 2020 dissertation to construct a canonical form for regular, skew-symmetric matrix polynomials whose spectrum does not include the infinite eigenvalue. This canonical form will be skew-symmetric, have the same degree as the original matrix polynomial, and allow for the recovery of the spectral data without numerical computations.

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MS82

Low Rank Perturbation of Symplectic Matrices

In this talk, the effect of generic structure-preserving low-rank perturbations on symplectic matrices is considered. In a first step, the question is answered which symplectic matrices can be written as a product of k symplectic reflectors when the given symplectic matrix is a rank-k perturbation of the identity. In a second step, the previous result is used to extend the theory of generic structure-preserving rank-one perturbations of symplectic matrices to perturbations of arbitrary rank. This is joint work with Julio Moro and Fredy Sosa.

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MS83

Block Sparse Structures in the Tensor Train Representation of the Quantum Chemical Hamiltonian in the Presence of Symmetries

QC-DMRG is regarded as a powerful method for the resolution of the ground state energy of the many-body electronic Schrödinger equation. The construction of the quantum chemical Hamiltonian operator in matrix product or tensor train (TT) form is at the core of the QC-DMRG algorithm. Although the ranks of the exact TT representation grow quadratically with the system size d, $O(d^2)$, it can be reduced using the TT-SVD algorithm. However, this might destroy the sparsity as well as the symmetries of the original operator if it is not carefully done. In this talk, we show that the TT format of the Hamiltonians in QC-DMRG has an inherent structure that can be exploited to get a sparse and symmetry-preserving scheme. [1] Bachmayr, Markus and Götte, Michael and Pfeffer, Max. Particle Number Conservation and Block Structures in Matrix Product States. Calcolo,2021 [2] Sebastian Wouters and Dimitri Van Neck. The density matrix renormalization group for ab initio quantum chemistry. Springer Science and Business Media LLC,2014 [3] Sebastian Keller and Michele Dolfi and Matthias Troyer and Markus Reiher. An efficient matrix product operator representation of the quantum chemical Hamiltonian. The Journal of Chemical Physics,2015 [4] Claudius Hubig. Symmetry-protected tensor networks. Ludwig-Maximilians-Universität München,2017

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MS83

Regularization Through Quantization

Kernel machines have emerged as a well-established model in the field of machine learning. However, their application has been limited due to the challenges associated with solving large inverse problems. This limitation has confined their usage to scenarios involving either low-dimensional data or small datasets. In recent years, the utilization of tensor decompositions has proven to be a successful approach in overcoming these restrictions and enhancing the capabilities of kernel machines. In this talk, I will outline a novel technique that enables an additional tensorization of the problem. This approach leads to more expressive models without increasing the number of model parameters, all while incurring no additional computational costs. Moreover, the introduced tensorization technique serves as a regularization mechanism, promoting the utilization of the most significant features within the dataset during model training.

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MS83

Adaptive Low-Rank Methods for High-Dimensional Parabolic PDEs

We present a space-time adaptive method for parabolic PDEs that combines sparse wavelet expansions in time with adaptive low-rank approximations in the spatial vari-

ables. We use a perturbed Richardson iteration, where we apply two reduction operators to the iterates to keep the support as well as the arising ranks of the low-rank approximations near-optimal for a given error tolerance. This iteration is applied to a bi-infinite matrix-vector problem based on a space-time variational formulation. One of the main challenges is the fact that the parabolic operator is an isomorphism with respect to spaces not endowed with a cross norm. Therefore we use a method for preconditioning operators in low-rank format by exponential sum approximations. The method is shown to converge and satisfy similar complexity bounds as the existing adaptive low-rank method for elliptic problems and does not suffer from the curse of dimensionality. The construction also yields computable rigorous a posteriori error bounds for the total error depending on the activated basis functions and ranks in the approximation. The results are illustrated by numerical experiments for the heat equation in high dimensions. We also consider a second model problem motivated by Magnetic Particle Imaging, where we obtain a Fokker-Planck equation based on the particle direction and magnetization. Here we can also use tensor methods to separate between particle direction, magnetization, and parameter space.

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MS83

Algebraic Programming for Tensor Computations

Algebraic Programming, or ALP for short, allows for programming with explicit algebraic structures. Originating from the GraphBLAS, ALP's initial and most mature interface concerns generalised sparse linear algebra. In recent work, we extended this interface to cover dense linear algebra and its canonical numerical algorithms, including computing matrix decompositions. A next logical step is to cover both sparse and dense tensor computations as well. This talk first overviews the ALP API for sparse and dense linear algebra, while noting both differences and similarities with the GraphBLAS, and while discussing relevant implementation concepts such as nonblocking execution and NUMA-aware allocation and parallelisation. We then move to cover multi-linear algebra: for dense tensor computations we focus on deep learning operators, while for sparse tensor computations we focus on novel data structures. A performance comparison in terms of peak throughput as well as versus state of the art concludes the talk. Preliminary results for our novel sparse tensor format indicate compression ratios of up to 38 percent versus the canonical coordinate storage, while the tensor API does indeed allow for the multi-linear formulation of some important and canonical deep learning operators.

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MS84

Solving Quadratic Lyapunov Equations

Lyapunov equations are, in general, linear, symmetric matrix equations. They occur in multiple application, foremost in stability analysis and model order reduction of dynamical systems. Recently, a Lyapunov-type equation with a quadratic nonlinearity in Kronecker product form was suggested for model order reduction of dynamical systems with quadratic nonlinearities. We will study theoretical properties of this matrix equation, including the existence of symmetric positive (semi-)definite (spsd) solutions. Furthermore, we discuss different approaches to solving these "quadratic Lyapunov equations" and in particular pursue those approaches that allow to compute a low-rank approximation of the spsd solution. This includes a solver based on the matrix sign function implemented in the MATLAB and Octave model order reduction toolbox MORLAB.

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MS84

Inexact Low-Rank Methods for Matrix Equations

One established strategy to solve large-scale algebraic matrix equations is to compute a low-rank approximations of the solution by iterative methods. Often, these methods work internally with rational Krylov subspaces which necessitates to solve a large and sparse linear system of equations inside each iteration step. In this contribution, we will look at inexact variants of rational Krylov subspace and low-rank ADI methods for Lyapunov and Sylvester equations, where "inexact" refers to the scenario when the occurring *inner* linear systems are solved inexactly by iterative methods such as, e.g., preconditioned Krylov subspace methods. We present estimates for the required accuracies regarding the inner linear systems which dictate when the employed inner Krylov subspace methods can be safely terminated. The goal is to save some computational effort without endangering the functionality of the outer low-rank method. Ideally, the inexact method mimics the convergence behavior of the more expensive exact method. If time permits, we will also look at inexact matrix-valued low-rank Krylov methods for general linear matrix equations, where inexactness also occurs in the form of low-rank truncations.

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MS84

Truncated LSQR for Least Squares Matrix Prob-

lems

Sylvester-like linear matrix least squares problems arise in different applications. In particular, we consider the generalized Sylvester $AXB + EXD = C_1C_2^T$ and T-Sylvester $AX^T + XB^T = C_1C_2^T$ problems, in the unknown matrix X, with rectangular coefficient matrices. Matrix-oriented least squares methods such as LSQR [Paige and Saunders, 1982] and Conjugate Gradients on the normal equation are viable strategies. However, problems of large dimensions make their classical implementation unappealing. In this presention it is shown how truncation can be used to enhance the effectiveness of the matrix-oriented LSQR algorithm, also compared with the truncated version of the matrix CG method [Simoncini and Hao, 2023].

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MS84

Using Indefinite Low-Rank Factorizations for Solving Large-Scale Riccati Equations

The continuous-time symmetric algebraic Riccati equation (CARE) is a special type of nonlinear matrix-valued equation and an essential component of many applications, including controller design, model order reduction and game theory. While there have been many developments in recent years regarding new solution methods of CAREs in the setting of large-scale sparse coefficient matrices, these methods are typically based on semi-definite low-rank factorizations of their solutions and assume certain structure of the equation, such as positive semi-definite factorizations of data matrices in the quadratic and constant equation terms. In this work, we present a new Newton-type approach for solving the most general formulation of CAREs that does not require assumptions on the definiteness of these terms. To this end, we are utilizing low-rank LDL^T factorizations of the CARE solution, which enables efficient computations especially in the case of large-scale sparse coefficient matrices.

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MS85

Stand-Alone Multigrid for Indefinite Systems Revisited: An Application to the Helmholtz Equation

Many applications ranging from imaging to the design of nuclear fusion devices rely on simulations of certain partial differential equations using numerical solvers. While state-of-the-art solvers exist for symmetric and positive-definite problems, nonsymmetric indefinite problems, such as the Helmholtz problem, remain notoriously difficult to solve numerically. By example of the Helmholtz equation, we will consider the convergence properties and bottlenecks for multigrid algorithms, which are known to diverge for Helmholtz. We will introduce theory and algorithms developed for this highly indefinite problem, and pose how these can serve as a baseline for other PDEs leading to indefinite systems.

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MS85

Preconditioning Non-Symmetric Systems with Positive Definite Hermitian Part

For several classes of mathematical models that yield linear systems, the splitting of the matrix into its Hermitian and skew Hermitian parts is naturally related to the underlying model. This is particularly so for discretizations of dissipative Hamiltonian ODEs, DAEs and port-Hamiltonian systems where, in addition, the Hermitian part is positive definite or semi-definite. It is then possible to develop short recurrence optimal Krylov subspace methods in which the Hermitian part is used as a preconditioner. In this talk, we present new, right preconditioned variants of this approach which, as their crucial new feature, allow the systems with the Hermitian part to be solved only approximately in each iteration while keeping the short recurrences. We present some theoretical results about te speed of convergence of this flexile method as well as new approximate a posteriori error bounds which can be computed at very low additional cost and can be used within a stopping criterion. Several numerical examples will be presented. This is joint work with Malak Diab and Karsten Kahl.

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MS85

Multiscale Spectral Generalised Finite Elements: Preconditioning and Model Reduction Beyond SPD

Multiscale PDEs with heterogeneous, highly oscillatory coefficients pose severe challenges for standard numerical methods. Two prominent approaches to tackle such problems are numerical multiscale methods with problem-adapted coarse spaces and structured (approximate) inversion techniques that exploit a low-rank property of the associated Greens function. They can also be used to precondition the resulting large-scale and typically very ill-conditioned linear equation systems. This work presents an abstract framework for the design and analysis of the Multiscale-Spectral Generalized FEM (MS-GFEM), a partition of unity method based on optimal local approximation spaces constructed from local eigenproblems, which is closely related to the GenEO coarse space more familiar in the DD community. We establish a general local approximation theory demonstrating, under certain assumptions, an exponential convergence w.r.t the local degrees of freedom and an explicit dependence on key parameters. Our framework applies to a broad class of multiscale PDEs with L^∞-coefficients, including convection-dominated diffusion or high-frequency Helmholtz/Maxwell. Notably, we prove a nearly exponential, local convergence rate on all those problems. As a corollary, the MS-GFEM space can be used within a robust two-level DD preconditioner to achieve condition numbers arbitrarily close to one. Numerical experiments support the theoretical results and demonstrate huge

efficiency gains.

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MS85

Neural Network Preconditioned Subspace Methods for the Solution of the Helmholtz Equation

In recent years, scientific machine learning, utilizing deep learning methodologies, has found widespread application in the fields of scientific computing and computational engineering. In this talk, we present the details of training various learning techniques, incorporating different neural network architectures, for generating a preconditioner and/or for solving the heterogeneous Helmholtz equation. For the neural network preconditioner, the purpose is once the neural networks are adequately trained, their inferences can be applied as a nonlinear preconditioner in the classical subspace methods, like the fexible GMRES or flexible FOM method for solving Helmholtz equations with different domain and sound velocity distribution. This presentation demonstrates the efficiency of employing neural networks as preconditioner and showcases the advantages of these neural network preconditioned approaches.

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MS86

Tight Scattering and Antenna Bounds

Fundamental limits play a crucial role in defining the boundaries of performance for various systems and devices, establishing theoretical maximum or minimum performance that can be achieved. They offer valuable insights into the trade-offs and constraints inherent in different designs, aiding in making informed decisions to enhance device functionality. The significance of tight limits is even more pronounced, as they provide a more precise measure of the performance boundaries within a given design. When a limit is tight, it signifies that the disparity between the limit and the actual performance that can be obtained, allowing for the creation of optimal devices. In such instances, identifying areas for improvement is more straightforward, enabling strategic modifications that yield substantial advancements. Physical bounds have recently been investigated for many radiation and scattering scenarios based on duality and convex optimization. This method involves optimizing over source distributions while adhering to power constraints. Radiation (antenna) problems are naturally posed as optimization over the current distribution, with a feed only constrained by its supplied power. The resulting bounds are hence valid for all antenna structure and feed locations restricted to the design region. In this presentation, we discuss tightness of these type of limits and show that some of them are tight, providing valuable insights for future design considerations.

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MS86

Fast Multi-Channel Full-Wave Solver and Inverse Design with Augmented Partial Factorization

Multi-channel optical systems such as disordered media and aperiodic metasurfaces are challenging to model: full-wave solutions of Maxwell's equations are necessary, the system size is large, and many simulations are needed to characterize the multi-channel response. In this talk, I will present a new strategy for such computations: augment the frequency-domain Maxwell operator with all the input source profiles and all the output projection profiles, followed by a single partial LU factorization that directly yields the complete multi-channel response. This "augmented partial factorization" (APF) approach directly computes the projected outputs of interest, bypassing the forward and backward substitutions traditionally used to compute the full-basis solution. It is exact with no approximation beyond discretization, and it applies to any linear partial differential equation. Benchmarks on large disordered media and aperiodic metasurfaces in 2D yield three to seven orders of magnitude in the speed-up compared to conventional methods. We are developing an open-source software called MESTI (Maxwells Equations Solver with Thousands of Inputs) that implements APF in both 2D and 3D. I will also present multi-channel gradient computation and inverse design using APF that leads to record-breaking efficiency reaching fundamental bounds.

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MS86

Accelerated First-Order Optimization Methods with Applications to Inverse Problems

In this talk, I will first give an overview of first-order methods in convex optimization. Then, I will talk about two types of effort for improving theoretical and practical performance of first-order methods. Specifically, the first one is on improving iteration complexity or accelerating convergence rate of first-order methods by incorporating Nesterovs acceleration schemes. The second one is about developing backtracking strategies to search for larger stepsize. For the third part, I will discuss the applications of accelerated first-order methods in linear inverse problems arising from imaging science, particularly the conductivity map reconstruction from Scanning Tunneling Potentiometry.

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MS86

Convex Nanophotonics: Hidden Structure in Maxwells Equations

In optimization theory, one clear dividing line between "easy" and "hard" problems is convexity. In convex optimization problems, all local optima are global optima, which can be found by highly efficient computational algorithms. By contrast, nonconvex problems can have highly oscillatory landscapes, and one must typically use local optimization techniques or black-box approaches. Nanophotonic design problems, and many design problems across physics, reside squarely in the latter category of nonconvex optimization problems. Or do they? I will show that there is a surprising amount of mathematical structure hidden in the typical differential equations of physics, and that this structure enables new connections to modern techniques in convex optimization. The key differential-equation constraints can be transformed to infinite sets of local conservation laws, which have a structure amenable to quadratic and semidefinite programming. This approach can lead to global bounds ("fundamental limits") for many design problems of interest, and potentially to dramatically new approaches to identifying designs themselves. I will discuss applications of this approach to the photonics problem of extracting maximal radiation from dipolar radiators, with connections to the minimum mode size for eigenfunctions of wave physics.

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MS87

GMRES and FGMRES in variable accuracy storage

In the context where the representation of the data is decoupled from the arithmetic used to process it, we investigate the backward stability of GMRES and FGMRES. Considering that data may be compressed to reduce memory requirements, we are interested in the situation where the leading part of the rounding error is related to the data representation. We illustrate the backward stability with numerical experiments in two different practical contexts. The first one corresponds to the use of an agnostic compressor, where the vector compression is controlled in norm-wise. The second arises in the solution of tensor linear systems, where low-rank tensor approximations based on Tensor-Train are considered to overcome the curse of dimensionality. We discuss the existing and missing theory to fully explain the observed numerical behavior.

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MS87

Mixed Precision Strategies for Solving Sparse Linear Systems with Bicgstab

Most numerical simulations are carried out in double precision, however the emergence of efficient hardware using lower precision has motivated its introduction in hope to decrease the energy consumption and to have an optimal use of the memory. Iterative linear solvers based on Krylov subspace like BiCGStab or GMRES are often used in combination with a preconditioner to speed up their convergence. In this presentation, we propose different solutions for using lower precision in BiCGStab while maintaining a convergence to high accuracy. First, we show that the use of the flexible variant of BiCGStab allows for the preconditioner to be applied in lower precision. Second, we show that we can even switch the rest of the operations to lower precision and refine the solution to high accuracy with an iterative refinement algorithm. We assess the potential of our algorithms for solving large linear systems coming from various industrial applications.

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MS87

Approximate Batched Solvers for Patch-Based Relaxation

For many large-scale applications with complex multi-

physics interactions, domain decomposition approaches focused on spatial regions related to mesh geometry are often used to reduce iteration counts. These patches are domains typically based around mesh cells or vertices to perform an overlapping domain decomposition method. One of the major challenges for domain decomposition methods currently is the large cost associated with inverting every patch matrix. To this end, we propose an approach that exploits redundancy by detecting and constructing a database of patches, which is a reduced set of patches that may be inverted for multiple patch solves. This may be done in a truly approximate fashion or an exact fashion, and errors may then be accounted for accordingly. In doing so, the reduction in data required for the algorithm allows for larger and faster batched solves. We present scaling results utilizing batched solves on GPUs in the Trilinos library and formal error analysis to validate the method.

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MS87

Randomized Implicitly Restarted Arnoldi algorithm for the unsymmetric eigenvalue problem

In this talk we introduce an algorithm for the non symmetric eigenvalue problem called randomized Implicitly Restarted Arnoldi (rIRA). Building upon the already existing IRA algorithm, we show how randomization can reduce the computational cost in the orthogonalization process. We justify this method through an analysis in exact arithmetic that gives hindsight on its behavior and show that we maintain the useful properties of IRA, such as restarting without adding errors and being able to focus on user-defined part of the spectrum. Numerical examples are presented to validate the performances on large scale sparse systems.

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MS88

Computing the Graph P-Laplacian Eigenpairs As Constrained Linear Eigenpairs

The study of the graph p-Laplacian spectrum, especially in the limit cases $p = 1$ and $p = \infty$, yields different topological information about the graph itself. In particular, the 1-Laplacian and the ∞-Laplacian spectrum provide approximations of the Cheeger cuts and the packing radii of the graph. These and other applications open the problem of computing the p-Laplacian eigenpairs. In this work, we study this last problem in the case $p \in (2, \infty]$. To this aim, we first reformulate the graph p-Laplacian eigenproblem in terms of a constrained weighted 2-Laplacian eigenvalue problem. Then, based on this reformulation, we introduce a class of energy functions whose differentiable saddle points correspond to p-Laplacian eigenpairs. In particular, any such eigenpair is such that the Morse index of the p-Rayleigh quotient in the eigenfunction matches the index of the energy function. Finally, based on gradient flows for the energy functions, we propose numerical methods for the computation of nonlinear p-Laplacian eigenpairs as limit points of sequences of linear generalized eigenpairs.

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MS88

Multi-View Clustering with Block Spectral Clustering

In this presentation, we study several novel numerical algorithms for data clustering mainly applied on multi-view data. For multi-view clustering, more accurate results can be achieved by integrating information from multiple sources. However, Most of existing multi-view clustering method assume the degree of association among all the views are the same. However, one significant truth is some views may be strongly or weakly associated with other views in reality. We propose several methods based on spectral clustering to cluster multi-view data and determine the degree of association among views simultaneously. The spectral clustering is formulated as the generalized eigenvalue problem, and different cluster structures can be obtained in each view by making use of different sets of eigenvectors. Then, we update the degree of association based on cluster structure of each view. We employ our proposed method on several real sets from different real-world applications, including face recognition, bioinformatics to illustrate the effectiveness of proposed algorithm.

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MS88

Revisit NEPv Approaches for Optimization of Sum of Rayleigh Quotients

NEPv approach is increasingly used to solve optimization problems with orthogonality constraints. It provides a distinctive way to characterize the optimal solution, often surpassing the conventional first- and second-order optimality conditions. However, why NEPv characterization is superior in this regard remains unclear. The aim of this talk is to shed light on this through a case study on optimizing the sum of Rayleigh quotients. We show that by a change

of variables, the original optimization problem can be expressed as an optimization over the joint numerical range. This reformulation preserves the global optimizer while potentially reducing the number of local minimizers, making it a better problem to solve. The standard first-order optimization condition for this reformulation simply aligns with a NEPv, revealing the nature of NEPv characterization and why it works so well. Finally, we will discuss how to extend this interpretation to establish NEPv characterization for more general optimization problems with orthogonality constraints and demonstrate the effectiveness of the NEPv approaches.

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MS88

On a matrix-Newton-type framework for solving NEPv

This talk focuses on introducing a novel framework for the use of Newton's method for solving NEPv. We show how to fit NEPv into the framework of matrix-valued root finding problems and derive Newton-type algorithms for solving these types of problems. The approach is particularly well-suited for problems of multiple eigenvectors, since the application of Newton's method on a matrix level allows for fast local convergence without vectorizing the problem. Numerical experiments indicate the benefits of this framework compared to SCF-based solution techniques.

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MS89

Random Restrictions of High-Rank Tensors and Polynomial Maps

Motivated by a problem in computational complexity, we consider the behavior of rank functions for tensors and polynomial maps under random coordinate restrictions. We show that, for a broad class of rank functions called *natural rank functions*, random coordinate restriction to a dense set will typically reduce the rank by at most a constant factor.

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MS89

Questions and Progress on the Ranks of Tensors

I will introduce several of the notions of rank that have been defined on tensors, and which each extend the matrix rank in a different direction. The basic properties, techniques and viewpoints which hold for the matrix rank often do not immediately extend to the ranks of tensors. I will highlight some of the difficulties in understanding these ranks, but also some of the progress that has recently been made.

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MS89

The Symmetric Geometric Rank

Inspired by recent work of Kopparty-Moshkovitz-Zuiddam and motivated by problems in combinatorics and hypergraphs, we introduce the notion of symmetric geometric rank for a symmetric tensor. We first derive fundamental properties of the symmetric geometric rank. Then, we study spaces of symmetric tensors with prescribed symmetric geometric rank. These turn out to be spaces of homogeneous polynomials whose corresponding hypersurfaces have a singular locus of bounded codimension.

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MS89

Discreteness of Asymptotic Tensor Ranks

Tensor parameters that are amortized or regularized over large tensor powers, often called "asymptotic" tensor parameters, play a central role in several areas including algebraic complexity theory, quantum information, and additive combinatorics. Recent works have investigated notions of discreteness (no accumulation points) or "gaps" in the values of such tensor parameters. We prove a general discreteness theorem for asymptotic tensor parameters of order-three tensors and use this to prove that (1) over any finite field (and in fact any finite set of coefficients in any field), the asymptotic subrank and the asymptotic slice rank have no accumulation points, and (2) over the complex numbers, the asymptotic slice rank has no accumulation points. Central to our approach are two new general lower bounds on the asymptotic subrank of tensors, which measures how much a tensor can be diagonalized. The first lower bound says that the asymptotic subrank of any concise three-tensor is at least the cube-root of the smallest dimension. The second lower bound says that any concise three-tensor that is "narrow enough" has maximal asymptotic subrank. Our proofs rely on new lower bounds on the maximum rank in matrix subspaces that are obtained by slicing a three-tensor in the three different directions. We prove that for any concise tensor, the product of any two such maximum ranks must be large, and as a consequence there are always two distinct directions with large max-rank.

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MS90

Some Structured Matrix Pencils and Polynomials and Associated Distance Problems

We consider the distance from a given Hermitian matrix pencil to a nearest one of the same structure that has no real eigenvalues and find upper and lower bounds on the distance. The principal tool used for the upper bound is a canonical form under unitary congruence for Hermitian matrix pencils. Numerical experiments show that the upper and lower bounds can be tight in many cases. The lower bounds extend to the corresponding distance problems for Hermitian quadratic matrix polynomials. Upper bounds on the distance for the Hermitian quadratic matrix polynomials are obtained from eigenvalue localization techniques. Analogous results are obtained for the distance from a given $*$-even or $*$-odd matrix polynomial of degree at most 2 to a nearest one of the same structure that has no purely imaginary eigenvalues.

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MS90

The Hamiltonian Extended Krylov Subspace Method

Extended Krylov subspaces $\text{span}\{b, A^{-1}b, Ab, A^{-2}b, A^2b, \ldots, A^{k-1}b, A^{-k}b\} = \mathcal{K}_k(A, b) + \mathcal{K}_k(A^{-1}, A^{-1}b)$ for general nonsingular matrices $A \in \mathbb{C}^{n\times n}$ and a vector $b \in \mathbb{C}^n$ have been used for the numerical approximation of $f(A)b$ for a function f and a large matrix A at least since the late 1990s. In case an orthogonal matrix V has been constructed such that $\text{range}(V) = \mathcal{K}_k(A, b) + \mathcal{K}_k(A^{-1}, A^{-1}b)$, an approximation to $f(A)b$ can be obtained as $f(A)b \approx Vf(V^TAV)V^Tb$. We will present an algorithm for constructing a J-orthogonal basis of the extended Krylov subspace $\mathcal{K}_{r,s} = \mathcal{K}_{2r}(H, u) + \mathcal{K}_{2s}(H^{-1}, H^{-1}u)$, where $H \in \mathbb{R}^{2n\times 2n}$ is a large (and sparse) Hamiltonian matrix (for $r = s + 1$ or $r = s$). Surprisingly, this allows for short recurrences involving at most five previously generated basis vectors. Projecting H onto the subspace $\mathcal{K}_{r,s}$ yields a small Hamiltonian matrix. The resulting HEKS algorithm may be used in order to approximate $f(H)u$ where f is a function which maps the Hamiltonian matrix H to, e.g., a (skew-)Hamiltonian or symplectic matrix. Numerical experiments illustrate that approximating $f(H)u$ with the HEKS algorithm is competitive for some functions compared to the use of other (structure-preserving) Krylov subspace methods.

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MS90

On Condition Numbers

We discuss a variety of problems revolving around matrix condition numbers for linear systems and eigenvalue problems, including whether various standard bounds hold and are sharp for unitarily invariant norms.

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MS90

Eigenstructure Perturbations of a Class of Hamiltonian Matrices and Solutions of Related Riccati Equations/inequalities

We study the positive definite solutions of a class of algebraic Riccati equations/inequalities from robust control and passive control systems. We use the relation between the solutions and the Lagrangian invariant subspaces of Hamiltonian matrices. We characterize the Riccati equation/inequality solution set by applying global structured perturbation techniques to Hamiltonian matrices. This is a joint work with Volker Mehrmann.

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MS91

Batch Normalization Preconditioning for Neural Network Training

Batch normalization (BN) is a popular and ubiquitous method in deep neural network training that has been shown to decrease training time and improve generalization performance. Despite its success, BN is not theoretically well understood. It is not suitable for use with very small mini-batch sizes or online learning. In this talk, we will review BN and present a preconditioning method called Batch Normalization Preconditioning (BNP) to accelerate neural network training. We will analyze the effects of mini-batch statistics of a hidden variable on the Hessian matrix of a loss function and propose a parameter transformation that is equivalent to normalizing the hidden variables to improve the conditioning of the Hessian. Compared with BN, one benefit of BNP is that it is not constrained on the mini-batch size and works in the online learning setting. We will present several experiments demonstrating competitiveness of BNP. Furthermore, we will discuss a connection to BN which provides theoretical insights on how BN improves training and how BN is ap-

plied to special architectures such as convolutional neural networks. The talk is based on a joint work with Susanna Lange and Kyle Helfrich.

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MS92

On the Relation Between Port-Hamiltonian Systems, Passivity and the Solution of KYP's

Passive systems are usually characterized by a special type of linear matrix inequality called the Kalman-Yakubovich-Popov (KYP) inequality. More recently, port Hamiltonian systems defined a framework that allows the representation of passive systems in a more structured way. In this talk, we will see how the solution of the KYP inequality is related to pH systems and how the solution of the KYP can help in modeling and simulating passive systems. We start with a discussion on linear time-invariant descriptor systems. Then, we consider time-varying systems and use the solution of the KYP to define port Hamiltonian systems for time-varying systems.

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MS92

Time-Limited Balanced Truncation Within Variational Data Assimilation

Balanced truncation is a well-established model order reduction method in system theory that has been applied to a variety of problems. Recently, a connection between linear Gaussian Bayesian inference problems and the system theoretic concept of balanced truncation was drawn for the first time. Although this connection is new, the application of balanced truncation to data assimilation is not a novel concept: It has already been used in four-dimensional variational data assimilation (4D-Var) in its discrete formulation. In this talk, the link between system theory and data assimilation is further strengthened by discussing the application of balanced truncation to standard linear Gaussian Bayesian inference, and, in particular, the 4D-Var method. similarities between both data assimilation problems allow a discussion of established methods as well as a generalisation of the state-of-the-art approach to arbitrary prior covariances as reachability Gramians. Furthermore, we propose an enhanced approach using time-limited balanced truncation that allows to balance Bayesian inference for unstable systems and in addition improves the numerical results for short observation periods.

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MS92

Generalizations of Data-Driven Balancing: What to Sample for Different Riccati Equation-Based Variants

In this work we present generalizations of the Quadrature-based Balanced Truncation (QuadBT) framework of Gosea, Beattie, and Gugercin to other types of balancing. QuadBT is an entirely "non-intrusive" reformulation of balanced truncation; a classical projection-based model-order reduction technique for linear systems. QuadBT is non-intrusive in the sense that it builds approximate balanced reduced-order models entirely from system response data (e.g., transfer function measurements) without the need to reference an explicit state-space realization of the underlying full-order model. We extend this data-driven framework to other types of balancing, those involving solutions to algebraic Riccati equations (AREs); namely, balanced stochastic truncation, positive-real balanced truncation, and bounded-real balanced truncation. We show that the data-driven construction of these balanced reduced-order models requires sampling certain spectral factorizations derived from the relevant AREs. Numerical examples are included in each case to validate our approach.

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MS92

Solving Sequences of Parametrized Lyapunov Equations with Recycling

Sequences of parametrized Lyapunov equations can be encountered in many application settings. Moreover, solutions of such equations are often intermediate steps of an overall procedure whose main goal is the computation of quantities of the form f(X), where X denotes the solution of a Lyapunov equation. We are interested in addressing problems where the parameter dependency of the coefficient matrix is encoded as a low-rank modification to a seed, fixed matrix. We present two numerical procedures that fully exploit such a common structure. The first one builds upon recycling Krylov techniques, aims to solve moderate size problems as it makes use of dense numerical linear algebra tools. The second algorithm can instead address large-scale equations by relying on state-of-the-art projection techniques based on the extended Krylov subspace. We demonstrate how our algorithms can beat the previous state-of-the-art algorithms on test cases arising in the study of damped vibrational systems and the analysis of output synchronization problems for multiagent systems.

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MS93

Measurements of Entanglement

A d-partite state is d-tensor T in d-tensor products of finite dimensional Hilbert spaces. It is unentangled if it is a rank one tensor . It is "easy' (poly-time computable) to determine if T is entangled or not. In this talk we will survey some known results on the standard notions of entanglements of T: the rank, the geometric measure of entanglement, the nuclear norm and nuclear rank. The problem with the above notions is that they are NP-hard to compute if d¿2, hence hard to measure experimentally. In the end of the talk we will discuss some simple measurement of entanglement based on bipartite states.

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MS93

On the Minimal Algebraic Complexity of the Rank-one Approximation Problem for General Inner Products

In this talk, we discuss the algebraic complexity of Euclidean distance minimization from a generic tensor to a variety of rank-one tensors. The Euclidean Distance (ED) degree of the Segre-Veronese variety counts the number of complex critical points of this optimization problem. In a recent joint work with Kozhasov, Muniz, and Qi, we regard this invariant as a function of inner products and conjecture that it achieves its minimal value at Frobenius inner product. We prove our conjecture in the case of matrices. We discuss the above optimization problem for other algebraic varieties, classifying all possible values of the ED degree. Our approach combines tools from Singularity Theory, Morse Theory, and Algebraic Geometry.

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MS94

Randomized Preconditioning for Least Squares Solvers on Gpus

In this talk we will present experimental results about the convergence behaviour and performance improvements that are attainable by performing critical components of randomized solvers in reduced precision formats. In order to establish this, we have developed mixed precision implementations of gaussian sketching and sparse sketching, via the countsketch algorithm, to generate randomized preconditioners for the LSQR-IR and FGMRES-IR procedures. All of the software components we designed allow for composition of operators of different types (dense or sparse) and precisions. This allows us to easily experiment with the various precision formats supported by the NVIDIA A100 GPU to solve a) least squares and b) noisy least squares problems. We showcase that both refinement schemes can recover from the loss of accuracy in (a), leading to significant performance improvements. Additionally, we demonstrate that the reduced precision solvers implicitly regularize the regression problem and thus provide a competitive advantage over their high-precision versions for tackling (b).

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MS94

Randomized Orthogonalization Techniques for Krylov Subspace Solvers

In this talk we will review recent research on using randomization for orthogonalizing a set of vectors. We will then present the usage of those orthogonalization processes in the context of Krylov subspace methods and discuss their accuracy.

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MS94

Sketched and Truncated Krylov Methods for Core Linear Algebra Problems

Randomized methods based on the sketch-and-solve paradigm have originally been developed for applications with rather crude accuracy demands. Yet, by comining them with (polynomial) Krylov subspace methods, they have recently been succesfully been applied for linear algebra problems with high accuracy requirements, like solving linear systems and matrix equations or approximating matrix functions. The key idea in many of these algorithms is combining a truncated orthogonalization with an oblivious subspace embedding that mitigates the negative effects of lack of orthogonality and this way (almost) restores convergence properties of the full method, while significantly reducing cost, storage demands and communication. This comes at a cost, though: Implementation becomes more cumbersome (particularly for more involved problems like

matrix equations) and hyperparameters like the embedding dimension are introduced. At the same time, an analysis of the methods also becomes highly nontrivial, as sketching might alter the spectral properties of the problem significantly, to a point where one would often not expect the methods to work at all. Yet, almost magically, they still perform very well for many problems of interest. In this talk, we give an overview of recent advances both on the algorithmic front and concerning convergence analysis and theoretical guarantees, in order to explain why the great practical performance might be less magical than it seems at first sight.

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MS94

A Sketch-and-Select Arnoldi Process

In recent literature, sketching has been used to improve Krylov subspace methods for several linear algebra tasks, such as the solution of linear systems or eigenvalue problems. By solving a sketched version of the problem projected on the Krylov subspace, the solution of the original problem can be efficiently approximated even when the Krylov subspace basis is not orthonormal. This makes it possible to reduce orthogonalization costs, and in sketched Krylov subspace methods the basis is usually constructed using the k-truncated Arnoldi process with a (small) fixed integer k, in which each vector is orthogonalized only against the last k basis vectors, instead of the usual full orthogonalization. As an alternative to k-truncated Arnoldi, in this talk we propose a sketch-and-select Arnoldi process that, at each iteration, utilizes sketching to select k of the previously computed basis vectors to project out of the current basis vector. This procedure very often produces a basis with a smaller condition number compared to the basis constructed with truncated Arnoldi, for a comparable computational cost. The subset selection problem is approximately solved using a number of different heuristic algorithms, and the most effective ones are identified using performance profiles. This is a joint work with Stefan Gttel.

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MS95

Algebraic Spectral Multilevel Preconditioners for Sparse Least-Squares Problems

Solving the normal equations corresponding to large sparse linear least-squares problems is an important and challenging problem. For very large problems, an iterative solver is needed and, in general, a preconditioner is required to achieve good convergence. In recent years, a number of preconditioners have been proposed. These are largely serial and reported results demonstrate that none of the commonly used preconditioners for the normal equations matrix is capable of solving all sparse least-squares problems. In this work, we present new preconditioners for the normal equations that are efficient, robust, and scalable. Our proposed preconditioners can be constructed efficiently and algebraically. We exploit the sparsity structure of the symmetric positive definite normal equations matrix to define algebraic local symmetric positive semi-definite splitting matrices that allow us to introduce two-level Schwarz preconditioners for least-squares problems. The condition number of the preconditioned normal equations is shown to be theoretically bounded independently of the number of subdomains. This upper bound can be adjusted using a single parameter τ that the user can specify. Problems arising from practical applications are used to compare the performance of the proposed preconditioner with that of other preconditioners. We also show how the proposed preconditioner can be used to precondition saddle-point systems arising from PDE-constraint optimization.

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MS95

Recent Advances on Sparse Direct Solver Using Block Low-Rank and Mixed Precision for Large Scale Applications.

The solution of sparse systems of linear equations is a key computational kernel in scientific computing. It often represents the most time, memory and energy consuming part of the whole numerical simulation process. In this talk, we focus on sparse direct solvers, and more particularly on MUMPS sparse multifrontal solver (https://mumps-solver.org/). We present recent features that enable to efficiently solve large real and complex systems, and that have led to a strong gain of interest of these methods in many applications. We also illustrate how today challenges related to heterogeneity of computers, mixed-precision arithmetics, new models and applications, motivate activity in the field of sparse direct solvers.

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MS95

Multifrontal LU Factorization with Block Low Rank Compression on Multi-GPU Systems

We present a scalable, robust, and purely algebraic fast sparse solver or preconditioner based on multifrontal LU factorization with block low rank compression. The low rank decomposition is done using an adaptive randomized approximation scheme, which offers good performance as well as high accuracy. The talk focuses on the implementation on modern HPC systems, including those from multiple different vendors. The code runs on NVIDIA, AMD and Intel GPUs using the CUDA, HIP/ROCm, and SYCL programming runtimes respectively. Several numerical issues are also discussed in detail and illustrated by several large scale applications relevant to DOE. The solver is implemented in the STRUMPACK library, and relies on MAGMA, SLATE and KBLAS for high performance dense linear algebra kernels on GPU.

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MS95

Hierarchical matrix preconditioning for dominated convection problems

Hierarchical matrices (H-matrices) refer to compression schemes leading to a drastic acceleration of linear algebra operations. They rely on two main ingredients: recursive partitioning of the matrix, and compression of certain so-called admissible blocks of the partition. H-matrices typically target a certain class of fully populated matrices stemming from the discretization of PDEs. They perform very well in the case where the underlying PDE is strongly elliptic, which has been well documented and received a solid theoretical justification, but the performance a priori deteriorates when ellipticity is lost. In this work, we shall focus on the case of matrices stemming from the discretization of convection-dominated problems. We shall first discuss where the standard proof of approximability fails in the case of dominating convection. Then we shall explain how to modify the partitioning and the admissibility criterion so as to overcome this issue and restore the performance of H-matrix compression. We will conclude by presenting numerical results.

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MS96

Tight Spectral Clustering Approximations in Graph Neural Networks for Vertex Partitioning in Attributed Graphs

Graph Neural Networks (GNNs) can be used to partition the vertices of attributed graphs, i.e., graphs with features associated with their vertices and edges. This talk will first introduce the recent GNN models that are adopted for this task. These models are trained with an unsupervised minimum cut objective, approximated by a Spectral Clustering (SC) relaxation. While it offers a closed-form solution, the SC relaxation is loose and yields overly smooth cluster assignments that poorly separate the vertices. The second part of the talk will present a new GNN architecture that computes cluster assignments by optimizing a tighter relaxation of the minimum cut based on graph total variation (GTV). The model consists of two core components: i) a message-passing layer that minimizes the L1 distance in the features of adjacent vertices, which is key to achieving sharp transitions between clusters; ii) an unsupervised loss function that minimizes the GTV of the cluster assignments while ensuring balanced partitions. Two different applications are presented. The first is the vertex clustering. The second is graph classification: here, the clustering result is used to hierarchically coarsen the graph and gradually distill the class information.

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MS96

Changing the Ranking in Eigenvector Centrality of a Weighted Graph

In this talk we consider eigenvector centrality of a weighted graph G and focus our attention on the robustness of this

popular centrality measure. An indicator of robustness of eigenvector centrality consists in looking for a nearby perturbed graph G_1, with the same structure as G (i.e. with the same vertices and edges), but with a weighted adiacency matrix W_1 such that the highest m entries ($m \geq 2$) of the Perron eigenvector of W_1 coalesce, making the ranking at the highest level ambiguous. To compute a solution to this matrix nearness problem, a nested iterative algorithm is proposed that makes use of a constrained gradient system of matrix differential equations in the inner iteration and a one-dimensional optimization of the perturbation size in the outer iteration. The objective here is to provide a sharp theoretical concept and a computational tool, to be compared to more empirical results obtained with inexpensive heuristic criteria. As an interesting by-product, the algorithm also provides the *optimal* perturbation of the graph which determines the coalescence and thus the ambiguity, and is thus potentially able to compute a nearby perturbation which determines an arbitrary change of the highest m positions. Due to this it can be used to influence the ranking.

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MS96

Graph Adjacency Matrix Estimation Via Maximum Likelihood

Learning graphs represented by M-matrices via an ℓ_1-regularized Gaussian maximum-likelihood method is a popular approach, but also one that poses computational challenges for large scale datasets. Recently proposed methods cast this problem as a constrained optimization variant of precision matrix estimation. In this talk, we build on a state-of-the-art sparse precision matrix estimation method and introduce an algorithm that learns M-matrices, which capture the adjacency structure and edge weights of the graph. We demonstrate the effectiveness, accuracy, and performance of the method with numerical examples and comparative results with modern open-source packages, that reveal that the proposed algorithm can accelerate the learning of graphs by up to 3 orders of magnitude.

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MS96

The Fiedler Connection to Graph Clustering with Resolution Variation

There are connections and distinctions between graph partition and graph clustering, a.k.a. community detection in a network. In this talk, we first describe a formal connection of the Fiedler vector of the graph Laplacian to the modularity method by Newman and Girvan for community detection, following the quadratic form associated with the modularity matrix introduced by Newman. This algebraic connection and analysis offer insight into the so-called resolution limit in graph clustering/community detection. We extend the analysis to the generalized modularity equipped with the resolution parameter $\gamma\,(\gamma > 0)$ introduced by Reichardt and Bornholdt, which recovers the original modularity model at $\gamma = 1$. Next, we establish the concept of the Pseudo Fiedler Set (PFS) and the use of its properties to distinguish split criteria between regulated graph partition and autonomous detection of innate community structures. Thirdly, we introduce the use of PFS to the graph minors in the BlueRed method for graph clustering across resolution variation. BlueRed can be applied to many existing and novel graph clustering models. We present numerical results with real-world networks and model-generated synthetic graphs. Finally, we discuss the broader implications of our theoretical and empirical findings and identify several new issues that arise in graph clustering with resolution variation and warrant further investigation.

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MS97

Tensor decomposition for spatiotemporal data analysis in spread of Covid-19 and wildfires

In this talk, I will give an overview of tensor decompositions in biological applications as well as describe new techniques, including sampling methods, for the canonical polyadic decomposition. Numerical results for forecasting Covid-19 infection densities, identification of hotspots, and wildfire analysis will be discussed.

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MS97

Deblurring, Denoising and Coloring of Biomedial Images

Blind deconvolution is a challenging low-level vision problem with many applications. Given a blurred image the goal is to not only deblur the image but also find the blur kernel. In this talk we will present an approach using convolutional neural network to find the blur kernel which is in turn used to deblur our input image through an extension

of the classical ROF functional for variational deblurring to the tensor case by employing multi-dimensional total variation regularization. The resulting minimization problem is calculated by generalizing iterative soft thresholding to the tensor case, where the circulant structure of the tensor is exploited to allow for an efficient implementation. This method is tested using biomedical images like covid-19 lung x-rays and mri data.

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MS97

Tensor Methods for Multi-Modal Genomics Data

Genomics datasets often involve multiple dimensions, incorporating factors such as genes, samples, and experimental conditions. Moreover, multi-omics integrates diverse omics data and explores molecular events occurring at distinct levels, encompassing DNA variations, epigenetic modifications, transcriptional activities, metabolite profiles, and clinical phenotypes. Such intricate data find effective representation with tensors, and tensor methods emerge as powerful tools in genomics analysis, uniquely equipped to unravel the complex and multi-dimensional nature of genomics data. In this presentation, I will delve into tensor-based methods across various genomics applications, including tumor-microenvironment modeling, deconvolution of cell-cell communication, and imputation of single-cell RNA-sequencing data. The talk will also touch on the limitations of tensor methods and highlight potential areas for future development, fostering a comprehensive understanding of their potential in advancing genomics research.

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MS97

Dissection and reconstruction of live-cell fluorescence microscopy data using dynamic mode decomposition

Fluorescence microscopy of living cells is a major tool for the analysis of the fundamental processes of life. The analysis of the complex and often non-linear spatiotemporal datasets, however, represents a major challenge, and a variety of methods have been developed for that purpose. Dynamic mode decomposition (DMD) is a method for dissecting complex dynamics into distinct modes based on a linear approximation of the Koopman operator. In this contribution, several applications of DMD to analysis of live-cell fluorescence imaging data are presented. This includes segmentation of fluorescence images based on fluorophore-specific photobleaching dynamics [1], dissection of protein dynamics and aggregation based on fluorescence loss in photobleaching (FLIP) experiments [2], calcium imaging as well as denoising and high-fidelity reconstruction of multiphoton and super-resolution microscopy data. It is shown, how DMD and its variants, higher order and multi-resolution DMD, can provide insight into the dynamics in each application. Limitations of the method are also discussed. [1] D. Wstner, Image segmentation and separation of spectrally similar dyes in fluorescence microscopy by dynamic mode decomposition of photobleaching kinetics., BMC Bioinformatics, 23(2022)1-23. [2] D. Wstner, Dynamic Mode Decomposition of Fluorescence Loss in Photobleaching Microscopy Data for Model-Free Analysis of Protein Transport and Aggregation in Living Cells., Sensors, 22(2022)4731.

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MS98

Beyond Rosenbrocks Theorem

Rosenbrocks theorem on polynomial system matrices is a classical result that relates the Smith-McMillan form of a rational matrix G with the Smith forms of two polynomial matrices: one is an irreducible polynomial system matrix P and the other is a submatrix A of P, whose Schur complement in P is precisely G. This theorem has been essential in the development of algorithms for computing the poles and zeros of a rational matrix via linearizations and generalized eigenvalue algorithms. Though the irreducibility hypothesis is essential in Rosenbrock's theorem, it is not always guaranteed to hold in numerical practice. Thus, in this talk, we investigate in detail the information that can be extracted about the Smith-McMillan form of G when the polynomial system matrix P is reducible. We will consider not only the case of polynomial matrices P, but also the most general case when the entries of P are in an arbitrary elementary divisor domain and the entries of G are in its field of fractions. This is the second of two talks on this subject in the minisymposium. In a previous talk, my coauthor V. Noferini will discuss the extension of Rosenbrock's theorem to system matrices with entries in an arbitrary elementary divisor domain.

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MS98

Hidden Structure in the Sign Characteristic of Hermitian Matrix Polynomials

The sign characteristic is a structural feature of Hermitian matrix polynomials that is important for both theory and applications. It consists of a plus or minus sign associated to each elementary divisor corresponding to a real or infinite eigenvalue; these $\pm$ signs are invariants under unimodular congruence. When all eigenvalues are simple, these signs can be naturally ordered to form a *sign sequence*. For an $n \times n$ Hermitian polynomial of degree d with dn simple real eigenvalues, there are 2^{dn} possible sign sequences,

not every one of which can actually be realized by some degree d Hermitian polynomial. Is it possible to characterize exactly which sign sequences are realizable and which are not? And does the degree play any role in the story? This talk explores these questions, discussing several new constraints on signs beyond the well-known signature constraint (1), as well as an underlying group of symmetries on the collection of all sign sequences that sheds light on the characterization question. (1) V. Mehrmann, V. Noferini, F. Tisseur, and H. Xu, *On the sign characteristics of Hermitian matrix polynomials*, Linear Alg. App., 511 (2016), p.328–364.

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MS98

Hypocoercivity and Stability of Differential-Algebraic Equations and Their Representations

For the classes of finite-dimensional linear semi-dissipative Hamiltonian first and second order systems of ordinary differential equations or differential-algebraic equations with constant coefficients, stability and hypocoercivity are discussed and related to concepts from control theory. For the second order case particular trimmed linearization schemes are used to generate first order formulations.

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MS98

Rosenbrocks Theorem over Elementary Divisor Domains

Rosenbrocks theorem on polynomial system matrices is a classical result in linear systems theory that relates the Smith-McMillan form of a rational matrix G with the two Smith forms of an irreducible polynomial system matrix P, of which G is a Schur complement, and of a certain submatrix of P. This theorem has been essential in the development of algorithms for computing the poles and zeros of a rational matrix via linearizations and generalized eigenvalue algorithms. In this talk, we extend Rosenbrocks theorem to system matrices with entries in an arbitrary elementary divisor domain $\mathcal{R}$ and matrices G with entries in the field of fractions of $\mathcal{R}$. These are the most general rings where the involved Smith-McMillan and Smith forms both exist, and hence, where the problem makes sense. This is the first of two talks on this subject in the minisymposium. In a subsequent talk, my coauthor F. Dopico will discuss what happens when the system matrix P is not irreducible. The talk is based on joint work with F. Dopico and I. Zaballa.

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MS99

Online Machine Learning for Solving a Sequence of Linear Systems

For solving a sequence linear systems using (preconditioned) SOR where the SOR acceleration parameter must be chosen for each system, we experimentally study the use of multi-armed bandit algorithms. We first assume that each matrix from the sequence is independent and drawn from an unknown distribution. We then assume that the distribution varies over time. Finally, we assume that the matrices are diagonal shifts of each other, and that knowledge of each diagonal shift can be used to choose the acceleration parameter. The above cases correspond to using stochastic, adversarial, and contextual bandits, respectively. This is joint work with Mikhail Khodak, Maria-Florina Balcan, and Ameet Talwalkar.

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MS99

Preconditioning the Nfft Based Interior Point Method for Support Vector Machines

In this talk we discuss an approach to solve the support vector machine optimization via an interior point method (IPM). In the IPM method a large linear system in saddle point form needs to be solved. The key ingredient in this KKT system is a large-scale kernel matrix, typically dense, and we propose a Fourier based approach to approximate the matrix vector product of the kernel matrix. Additionally, we perform a feature grouping method for large feature space dimensions that can also be accelerated based on the Fourier scheme. The IPM requires a preconditioner to accelerate the convergence of linear solver and we propose the use of low-rank approaches. Namely, we use Cholesky-based approaches, a Nystrom method and random Fourier features to solve the IPM method efficiently. We compare these methods and then additionally compare the accuracy of the IPM prediction with the know libsvm library.

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MS99

Multigrid-Augmented Deep Learning for the Helmholtz Equation: Better Scalability with Com-

pact Implicit Layers

We present a deep learning-based iterative approach to solve the discrete heterogeneous Helmholtz equation for high wavenumbers. Combining classical iterative multigrid solvers and convolutional neural networks (CNNs) via preconditioning, we obtain a learned neural solver that is faster and scales better than a standard multigrid solver. Our approach offers three main contributions over previous neural methods of this kind. First, we construct a multilevel U-Net-like encoder-solver CNN with an implicit layer on the coarsest grid of the U-Net, where convolution kernels are inverted. This alleviates the field of view problem in CNNs and allows better scalability. Second, we improve upon the previous CNN preconditioner in terms of the number of parameters, computation time, and convergence rates. Third, we propose a multiscale training approach that enables the network to scale to problems of previously unseen dimensions while still maintaining a reasonable training procedure. Our encoder-solver architecture can be used to generalize over different slowness models of various difficulties and is efficient at solving for many right-hand sides per slowness model. We demonstrate the benefits of our novel architecture with numerical experiments on a variety of heterogeneous two-dimensional problems at high wavenumbers.

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MS100

Projected Exponential Methods for Stiff Dynamical Low-Rank Approximation Problems

The numerical integration of stiff equations is a challenging problem that needs to be approached by specialized numerical methods. Exponential integrators form a popular class of such methods since they are provably robust to stiffness and have been successfully applied to a variety of problems. On the other hand, the dynamical low-rank approximation is a recent technique for solving high-dimensional differential equations by means of low-rank approximations. However, the domain is lacking numerical methods for stiff equations since existing methods are either not robust-to-stiffness or have unreasonably large hidden constants. In this talk, we focus on solving large-scale stiff matrix differential equations with a Sylvester-like structure,

$$\dot{X}(t) = AX(t) + X(t)B + G(t, X(t)), \quad X_0 = X(0),$$

that admit good low-rank approximations. We propose two new methods that have good convergence properties, small memory footprint and that are fast to compute. The theoretical analysis shows that the new methods have order one and two, respectively. We also propose a practical implementation based on Krylov techniques. The approximation error is analyzed, leading to a priori error bounds and, therefore, a mean for choosing the size of the Krylov space. Numerical experiments are performed on several examples, confirming the theory and showing good speedup in comparison to existing techniques.

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MS100

Functional Tensor Train Cross Approximation with Gradient Data

Tensor Train (TT) decomposition is an efficient function approximation method, particularly due to TT Cross algorithms that can construct the TT approximation in a quasi-direct way using adaptive samples of the function. If the function admits an accurate TT approximation and can be evaluated exactly, the TT Cross is usually faster than regression of random samples. However, practically available samples can be noisy - for example, due to measurement errors, or inexact computation of the function. This noise can inflate the TT ranks of the approximation and slow down the convergence of TT Cross methods. We develop a gradient-enhanced functional TT Cross algorithm that minimizes the total misfit of the values of the function and its gradient. This extra optimization reduces the noise and allows one to compute a more accurate low-rank TT approximation. We use the proposed gradient cross to synthesize optimal feedback control of nonlinear dynamics, where the value function and its gradient are approximated by the solution of the State-Dependent Riccati Equations (SDRE). The latter is a fast but inexact way to produce feedback control. In particular, samples of the SDRE function alone lead to a large-rank and inaccurate TT decomposition. Adding the gradient information reduces both the rank and error, and allows one to compute the full value function in up to 100-dimensional Cucker-Smale model.

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MS100

Krylov Subspace Methods for Large Multidimensional Eigenvalue Computation

In this paper, we describe Krylov subspace methods for computing eigentubes and eigenvectors (eigenslices) for large and sparse third-order tensor tensors. This work provides some projection method tools for computing a section of eigentubes and eigenslices utilizing the T-product. The intended computed eigentubes and eigenslices are either associated with the greatest or smallest eigentubes. In particular, we describe the tensor Arnoldi's approach for the non-hermitian case and the tensor Lanczos's approach for f-hermitian tensors. We also propose the tensor block Arnoldi's method. Computed examples are given to illustrate the effectiveness of these methods.

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MS100

Low-Rank Methods for IGA with Multiple Patches

Isogeometric analysis (IGA) has become one of the most popular methods for the discretization of PDEs on complex domains, which arise in various applications of science and engineering. Thereby, it is often required to describe the computational domain of a complex geometry as multiple patches, where each patch is given by a tensor product B-spline parametrization and two such patches of a geometry are connected by an interface. In this setup the crucial challenge lies in the solution of the discretized equations of a PDE problem, for which the discretization results in a system of large mass and stiffness tensors, which are typically very costly to assemble and may become infeasible to treat with conventional methods due to its size. Furthermore, the continuity of the approximation must always be guaranteed on the interfaces. In this talk we illustrate that low-rank methods based on the tensor train format in combination with the Block-AMEn (alternating minimal energy) iterative solver, where the discretization of the PDE can be formulated as a low-rank structure with Kronecker products between its individual spatial dimensions, can be generalised for multi-patch geometries by integrating an isogeometric tearing and interconnecting (IETI) approach, by extending the linear system with constraint tensors and Lagrange multipliers which enforce continuity on the respective interfaces. Numerical tests implemented in MATLAB using the GeoPDEs toolbox confirm this theory.

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MS101

On Perfect Tensors and Multipartite Entanglement

We define the notion of a perfect tensor and explain its relevance in quantum information theory, especially in description of multipartite quantum entanglement.The existence of such objects in Hilbert space of arbitrary dimension is currently investigated from theoretical and practical point of view.We present a solution to the particular case of four parties with six degrees of freedom each, which contains additional features simplifying its experimental realization.

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MS101

Positive Maps from the Walled Brauer Algebra

We present positive maps and matrix inequalities for variables from the positive cone. These inequalities contain partial transpose and reshuffling operations, and can be understood as positive multilinear maps that are in one-to-one correspondence with elements from the walled Brauer algebra. Using our formalism, these maps can be obtained in a systematic and clear way by manipulating partially transposed permutation operators under a partial trace. Additionally, these maps are reasonably easy in construction by combining an algorithmic approach with graphical calculus.

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MS101

Perfect and Almost-perfect Tensors: Some New Constructions

A perfect tensor with for indices, each running from one to d, reshaped into a square matrix U of size d^2 is unitary, for any choice of two pairs of indices determining the matrix. For any $d > 3$ besides $d = 6$ such tensors can be constructed from a pair of orthogonal Latin squares of order d. We present novel solutions of such tensors for $d = 7$ and discuss the case of almost perfect tensors, related to dual-unitary matrices, in which some constraints are relaxed.

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MS102

GMRES with Sketching and Deflated Restarting

We introduce a sketched GMRES variant for solving large sparse linear systems of equations, called GMRES-SDR. The method uses approximate harmonic Ritz vectors to reduce convergence delays caused by restarting. As opposed to GMRES-DR, GMRES-SDR can easily be applied for the solution of sequences of nearby linear systems of equations. As opposed to GCRO-DR, GMRES-SDR requires a number of inner products and projection steps that grows only linearly in the restart length. This can result in improved memory locality and faster time-to-solution. We characterize GMRES-SDR as a projection method using a semi-inner product and discuss some practical aspects of this method.

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MS102

Using Tools from Matrix Sketching to Analyze Classical Krylov Methods for Low-Rank Approx-

imation

Krylov subspace methods are a ubiquitous tool for computing near-optimal rank k approximations of large matrices. Until recently, our strongest theoretical guarantees for such methods only held in the "large block' setting, where the Krylov method is run with a randomly chosen starting block of size at least k. This setting can be analyzed using tools from the matrix sketching literature. However, in practice, block size one (a single vector) or a small constant is often preferred. Despite their popularity, we have lacked theoretical bounds on the performance of such "small block' Krylov methods for low-rank approximation. I will discuss a recent result that addresses this gap between theory and practice by proving that small block Krylov methods essentially match all known low-rank approximation guarantees for large block methods. As an example, we show that the standard single vector Krylov method run for t iterations obtains the same error bounds as a Krylov method with block size $l \geq k$ run for $O(t/l)$ iterations, up to a logarithmic dependence on the smallest gap between singular values. That is, for a given number of matrix-vector products, single vector methods are essentially as effective as the best choice of large block size. Our analysis proceeds via a black-box reduction, which interesting allows us to use tools from matrix sketching to analyze single vector and small block methods. Based on joint work with Raphael Meyer and Cameron Musco.

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MS102

A Nested Divide-and-Conquer Method for Tensor Sylvester Equations with Positive Definite Hierarchically Semiseparable Coefficients

Linear systems with a tensor product structure arise naturally when considering the discretization of Laplace type differential equations or, more generally, multidimensional operators with separable coefficients. In this work, we focus on the numerical solution of linear systems of the form

$$(I \otimes \cdots \otimes I \otimes A_1 + \cdots + A_d \otimes I \otimes \cdots \otimes I)\, x = b,$$

where the matrices $A_t \in \mathbb{R}^{n \times n}$ are symmetric positive definite and belong to the class of hierarchically semiseparable matrices. We propose and analyze a nested divide-and-conquer scheme, based on the technology of low-rank updates, that attains the quasi-optimal computational cost $\mathcal{O}(n^d \log(n))$. Our theoretical analysis highlights the role of inexactness in the nested calls of our algorithm and provides worst case estimates for the amplification of the residual norm. The performances are validated on 2D and 3D case studies.

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MS102

Krylov Subspace Solvers with Randomized Orthogonal Projection for Solving Symmetric Positive Definite Systems of Linear Equations

Given a symmetric positive definite system of linear equations $Ax = b$, we show how randomization can relax the energy minimization step of Krylov solvers, allowing significant reduction of the computational cost in the case of full orthogonalization method (FOM). Through theoretical and numerical observations, we show that such modified solvers have quasi-optimal convergence, and discuss their implementation.

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MS103

Large Scale Finite-Element Multigrid Using the HyTeG Framework

HyTeG is a scalable software framework for the implementation of massively parallel multigrid methods and other linear solvers. HyTeG is based on hybrid tetrahedral meshes as a compromise between unstructured and structured meshes. This leads to special matrix structures that support the design of scalable and highly efficient iterative solvers. In this talk we will present an analysis of the convergence and scalability of HyTeG for challenging applications, such as from geodynamics or for fusion energy research.

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MS103

Highly Parallel Smoothers for Psctoolkit on Gpus

Sparse linear algebra is essential for a wide variety of scientific and industrial applications. The availability of massively parallel sparse solvers and preconditioners lies at the core of almost all traditional multi-physics and multi-scale simulations and many more recent AI and machine learning

procedures. Technology is nowadays expanding to target exascale platforms and we try to face the new challenges by developing algorithmic and theoretical strategies to make exascale computing possible. We developed PSCToolkit [DAmbra Durastante Filippone, Parallel Sparse Computation Toolkit, Software Impacts 15 (2023): 100463] aiming for highly efficient parallel operations with sparse matrices capable of running on machines with thousands of parallel cores. These tools have enabled the construction of iterative linear solvers and AMG preconditioners for the solution of problems deriving from fluid dynamics and the simulation of systems related to the production of renewable energy. We will focus on some new advances in the direction of designing polynomial smoothers which optimize error bounds of AMG V-cycle. The new smoothers rely on the first-type Chebyshev polynomial recurrences and improve error lower bound with respect to similar approaches recently proposed in the literature. We will present the optimal recurrences, discuss implementation issues and show results on clusters of heterogeneous nodes exploiting GPU accelerators.

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MS103

Domain Decomposition Preconditioning Methods Using Block Low Rank Compression in CFD

Solving very large sparse linear problems may require the use of iterative methods such as Krylov methods. Responding to the divide-and-conquer paradigm, Restricted Additive Schwarz methods used as preconditioners allow the work to be distributed among different workers. Each subdomain is provided with a local solver such as ILU(0), ILU(K) or even direct LU. For large CFD cases, ILU(0) is no longer an adequate preconditioner as matrices are too ill-conditioned. On the other hand, LU solvers require too much memory and CPU time. Thus, in this work, we investigate the use of approximate factorizations from the MUMPS solver which relies on Block Low-Rank compression to reduce the cpu and memory cost of the preconditioner. We assess its potential as a preconditioner for CFD applications on parallel computer architectures, depending on the problem size and the resource distribution strategy, with a focus on load balancing and memory footprint.

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MS103

Adaptive and Scalable Domain Decomposition Preconditioners

Recent advances in adaptive domain decomposition methods have made it possible to solve large systems of equations that where previously challenging for both algebraic multigrid (because of lack of robustness) and exact factorization (because of large FLOP count and memory cost). In this presentation, I will present some recent improvements and developments in HPDDM, a framework for defining efficient preconditioners. Its interface to PETSc will be explained, and numerical results for solving large linear systems of various types (indefinite, nonsymmetric) will be showcased.

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MS104

Multi-Class Graph Clustering Via Approximated Effective P-Resistance

In this talk we develop an approximation to the (effective) p-resistance and apply it to multi-class clustering. Spectral methods based on the graph Laplacian and its generalization to the graph p-Laplacian have been a backbone of non-euclidean clustering techniques. The advantage of the p-Laplacian is that the parameter p induces a controllable bias on cluster structure. The drawback of p-Laplacian eigenvector based methods is that the third and higher eigenvectors are difficult to compute. Thus, instead, we are motivated to use the p-resistance induced by the p-Laplacian for clustering. For p-resistance, small p biases

towards clusters with high internal connectivity while large p biases towards clusters of small "extent," that is a preference for smaller shortest-path distances between vertices in the cluster. However, the p-resistance is expensive to compute. We overcome this by developing an approximation to the p-resistance. We prove upper and lower bounds on this approximation and observe that it is exact when the graph is a tree. We also provide theoretical justification for the use of p-resistance for clustering. Finally, we discuss experiments comparing our approximated p-resistance clustering to other p-Laplacian based methods.

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MS104

Nonlinear PageRank for Local Graph Partitioning

A modified nonlinear version of the PageRank problem is developed for local graph partitioning purposes, which involves the p-norm. It is shown that the solution is subject to a tighter upper bound with decreasing p-values under certain conditions. The Levenberg-Marquardt method is proposed for tackling the problem. An approach for improving the conditioning of the Jacobian through subset selection and then preconditioning is put forward. A number of experiments on both synthetic and real-world graphs demonstrate the consistently strong, and often superior, performance of the modified PageRank problem.

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MS104

Sublinear-Time Clustering Oracle for Signed Graphs

Social networks are often modeled using signed graphs, where vertices correspond to users and edges have a sign that indicates whether an interaction was positive or negative. The arising signed graphs typically contain a clear community structure in the sense that the graph can be partitioned into a small number of polarized communities, each defining a sparse cut and indivisible into smaller polarized sub-communities. We provide a local clustering oracle for signed graphs with such a clear community structure, that can answer membership queries, i.e., "Given a vertex v, which community does v belong to?", in sublinear time by reading only a small portion of the graph. Formally, when the graph has bounded degrees and at most $O(\log n)$ communities, then with $\tilde{O}(\sqrt{n}(1/\varepsilon)^{O(1)})$ preprocessing time, our oracle can answer each membership query in $\tilde{O}(\sqrt{n}(1/\varepsilon)^{O(1)})$ time, and it correctly classifies a $(1-\varepsilon)$-fraction of vertices w.r.t. a set of hidden ground-truth communities. Previously, such local clustering oracles were only known for unsigned graphs; our generalization to signed graphs requires a number of new ideas and gives a novel spectral analysis of the behavior of random walks with signs. We evaluate our oracle data structure for answering membership queries on both synthetic and real-world datasets, validating its performance in practice.

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MS104

Max-Flow for Circular Mapper Graphs

Graph shaped topological summaries are appear in all kinds of data analysis situations. Merge trees, Reeb graphs, mapper graphs, and many other skeletonization techniques are frequently used to analyze images, functions, shape, atomic structures and environmental data. For this reason, researchers are working on methods that can help understanding the variance of a population of such graphs, with respect to some learning tasks. To this end, we can distinguish between two approaches: the first one aims at defining metrics, possibly with some stability properties, to compute the similarity between different graphs in the population. When the computational complexity of the data makes this approach infeasible, one usually resorts to some sufficient statistics, or incomplete invariant, which must be interpretable depending on the aim of the analysis. In this talk I will present a sufficient statistic based on the idea of a source-target max flow, which I designed and used to compare point clouds with periodic boundary conditions.

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MS105

The Scaling Techniques for the Polynomial Eigenvalue Problem Solved by a Contour Integral Method

The contour integral method is a class of efficient methods for computing partial eigenvalues of polynomial eigenvalue problems (PEPs). Among them, the recently developed SakuraiSugiura method with RayleighRitz projection (SS-RR) method has received much attention for its effectiveness. However, the SS-RR method may suffer from numerical instability when the coefficient matrices of the projected PEP vary widely in the norm. To improve the numerical stability, we incorporate the tropical scaling technique into the SS-RR method and establish upper bounds for the backward error of an approximate eigenpair of the original eigenvalue problem. These bounds shed light on the mechanism that the tropical scaling improves the numerical stability of the original SS-RR method. Numerical experiments show that the actual backward errors can be successfully reduced by scaling and the bounds can predict well the errors occurring before and after scaling.

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MS105

Interior Eigensolver Based on Rational Filter with

Composite Rule

Contour integral based rational filter leads to interior eigensolvers for non-Hermitian generalized eigenvalue problems. Based on the Zolotarev's problems, this talk shows the asymptotic optimality of the trapezoidal quadrature of the contour integral in terms of the rational function separation. A composite rule of the trapezoidal quadrature is also derived, based on which two interior eigensolvers are proposed. Both eigensolvers adopt direct factorization and multi-shift generalized minimal residual method for the inner and outer rational functions, respectively. The first eigensolver fixes the order of the outer rational function and applies the subspace iteration to achieve convergence, whereas the second eigensolver doubles the order of the outer rational function every iteration to achieve convergence without subspace iteration. The efficiency and stability of proposed eigensolvers are demonstrated on synthetic and practical sparse matrix pencils.

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MS105

A Contour Integral-based Method for Nonlinear Eigenvalue Problems for Semi-infinite Photonic Crystals

In this study, we introduce an efficient algorithm for determining the isolated singular point of semi-infinite photonic crystals with perfect electric conductor and quasi-periodic mixed boundary conditions. This specific problem can be modelled by a Helmholtz equation, which becomes an eigenvalue problem of an infinite-dimensional Toeplitz matrix after discretization. Through ingenious matrix transformations, our computational goal is to obtain the closest eigenvalue to a given value and its corresponding eigenvector of a nonlinear eigenvalue problem. The contour integration method can be used elegantly for this purpose. Moreover, this particular eigenpair holds significant importance in the examination of edge states in photonic crystals.

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MS105

Computing Generalized Singular Value Decomposition Through Contour Integration

We propose a contour integral-based algorithm for computing a few generalized singular values of a matrix pencil and the corresponding generalized singular vectors. Mathematically, generalized singular values of a matrix pencil are eigenvalues of the Jordan-Wielandt which is an equivalent Hermitian-definite matrix pencil. However, direct application of the FEAST solver does not fully exploit the structure of this problem. We analyze several project strategies on the Jordan-Wielandt matrix pencil, and propose an effective and robust projection scheme tailored to GSVD. Both theoretical analysis and numerical experiments demonstrate that our algorithm achieves rapid convergence and satisfactory accuracy.

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MS106

Communication in Multiplex Networks

Modeling complex systems that consist of different types of objects leads to multilayer networks, in which vertices are connected by both inter-layer and intra-layer edges. We deal with vertex-aligned multiplex networks, in which the inter-layer edges are the coupling edges. A multiplex with N vertices and L layers may be represented by the third-order adjacency tensor $\mathcal{A} \in \mathbb{R}^{N\times N\times L}$ and a parameter $\gamma \geq 0$, which is associated with the ease of communication between layers. We focus on the multiplex average inverse geodesic length, which we refer to as the *global efficiency* $e_{\mathcal{A}}(\gamma)$, and determine non-decreasing lower bounds $e^K_{\mathcal{A}}(\gamma)$ to $e_{\mathcal{A}}(\gamma)$, by means of path length matrices $P^K \in \mathbb{R}^{N\times N}$ that only take into account multiplex paths made up of at most K intra-layer edges. A different point of view in analyzing the communication in the multiplex takes into account the Perron vectors and the Perron root ρ of the supra-adjacency matrix $B(\gamma)$. Both the sensitivity of $e^K_{\mathcal{A}}(\gamma)$ and the structured sensitivity of ρ to changes of the positive entries of $\mathcal{A}$ are investigated to determine the intra-layer edges that should be strengthened to enhance the global efficiency or the *total communicability* the most and those that could be removed to simplify the multiplex.

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MS107

Extending Elman's Bound for GMRES

When the numerical range of a matrix is contained in the right half-plane, the GMRES algorithm makes progress at every step. In his PhD dissertation, Howard Elman derived a bound that guarantees convergence. When the numerical range contains the origin, GMRES need not progress at each step, and Elman's bound does not apply. By solving a Lyapunov equation, one can obtain an inner product in which the numerical range is contained in the right half-plane, allowing use of Elman's bound (and other GMRES convergence bounds based on the numerical range), at the cost of a multiplicative constant. Lyapunov inverse iteration can produce a family of suitable inner products. This approach complements techniques recently proposed by Greenbaum and colleagues for eliminating the origin from the numerical range for GMRES convergence analysis.

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MS107

Advances in Resource-Constrained Matrix Krylov Methods for Space-Time Discretizations

Time dependent partial differential equations are ubiquitous in mathematical modelling. The need for time discretizations beyond time marching procedures has recently emerged, to guarantee a sufficiently accurate solution approximation in case of, e.g., low data regularity or nonlocal phenomena. Among the most successful techniques are space-time discretizations, which lead to algebraic matrix equations able to naturally maintain the separation between the space and time operators, thus better designing a tensorized approximation. Still, two- and three-dimensional discretizations in space lead to large computational and memory requirements, which need to be addressed to make the overall procedure feasible. We discuss recently developed techniques in the linear matrix equation context, such as truncation, sketching and structure-aware strategies, to significantly reduce memory allocations and CPU time consumptions of space-time discretizations.

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MS107

Convergence of Randomized and Greedy Relaxation Schemes for Solving Nonsingular Linear Systems of Equations

We extend results known for the randomized Gauss-Seidel and the Gauss-Southwell methods for the case of a Hermitian and positive definite matrix to certain classes of non-Hermitian matrices. We obtain convergence results for a whole range of parameters describing the probabilities in the randomized method or the greedy choice strategy in the Gauss-Southwell-type methods. We identify those choices which make our convergence bounds best possible. Our main tool is to use weighted ℓ_1-norms to measure the residuals. A major result is that the best convergence bounds that we obtain for the expected values in the randomized algorithm are as good as the best for the deterministic, but more costly algorithms of Gauss-Southwell type.

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MS107

Preconditioning Least Squares

Preconditioning has been extremely successful in rendering feasible the solution of extremely large-dimensional linear systems via iterative methods. For linear least squares problems the picture is much more limited. I will make some observations on possible approaches for such least squares problems.

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MS108

The AAA Algorithm for Fitting Second-Order Dynamical Systems from Frequency Response Data

The AAA (Adaptive Antoulas Anderson) algorithm is a robust rational approximation tool used for fitting rational functions to measured data. Consequently, it can also be used as a system identification tool for linear, unstructured (first-order) dynamical systems using frequency-response data, i.e., samples of the underlying system's transfer function. In this work, we develop an extension of the AAA algorithm for fitting systems with second-order dynamics (structured case), which we call SO-AAA. Toward this goal, we first develop various structured barycentric forms associated with the transfer function of second-order systems. These allow the iterative construction of reduced-order models from given frequency domain data, by combining interpolation and least-squares fit, together with the preservation of the desired structure (mostly appearing in mechanical systems). The newly developed algorithm is tested on various numerical examples with second-order structure, illustrating its efficiency.

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MS108

Barycentric Forms for Optimal Multivariate Rational Approximations for Dynamical Systems with Quadratic Output

Barycentric form of rational functions is a fundamental tool in modeling linear dynamical systems from frequency-response data. In this talk, we develop the barycentric forms for linear dynamical systems with quadratic-nonlinearity in their output (LQOs) and then employ them in learning these systems from data. LQOs are fully explained by two rational functions, a single-variable and a two-variable one. We first develop the barycentric forms corresponding to these two rational functions. These barycentric forms are constructed jointly in such as a way that together they correctly model a LQO. We then introduce the AAA framework in this setting.

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MS108

The Short-Term Rational Lanczos Method and Applications

Rational Krylov subspaces have become a reference tool

in dimension reduction procedures for several application problems. When data matrices are symmetric, a short-term recurrence can be used to generate an associated orthonormal basis. In the past, this procedure was abandoned because it requires twice the number of linear system solves per iteration than with the classical long-term method. We propose an implementation that allows one to obtain key rational subspace matrices without explicitly storing the whole orthonormal basis, with a moderate computational overhead associated with sparse system solves. Several applications are discussed to illustrate the advantages of the proposed procedure.

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MS108

Rectifying Unstable Rational Representations in Sequence Models

State-space models (SSMs) have recently gained prominence as a framework for addressing long-range sequence tasks by leveraging large linear time-invariant (LTI) systems. What sets SSMs apart from other recurrent sequence models is their ability to be trained in the frequency domain, using samples of the transfer functions of the LTI systems. Given that the transfer function of an LTI system is a rational function, we exploit a simplified rational representation, such as the partial fraction formula, to facilitate sampling. Representing the transfer function in partial fractions is equivalent to diagonalizing a state matrix; however, this process encounters conditioning issues due to the inherent non-normality of the state matrices in SSMs. We use the concept of approximate diagonalization to craft a backward stable algorithm for converting the transfer function into partial fractions. While the resulting partial fractions may appear distinct from the true ones, we demonstrate that a modest backward error ensures good performance of SSMs. To assess the effectiveness of our approach, we compare it with existing methods found in the literature, such as enforcing normality in state matrices and incorporating a barycentric rational formula in lieu of partial fractions.

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MS109

Jacobi-Type Methods for Tensor Decompositions

In this talk we are going to discuss two closely related problems, an SVD-like tensor decomposition and an (approximate) tensor diagonalization. For a general third-order tensor $\mathcal{A} \in \mathbb{R}^{n\times n\times n}$, we develop a Jacobi-type algorithm that works on $2\times 2\times 2$ subtensors. We use two approaches, one where the Frobenius norm of the diagonal is maximized, and the other one where the tensor trace is maximized. For both cases we show how the rotation angles are calculated and prove the convergence of the algorithms. Different initializations of the algorithms will be discussed, as well as the special cases of symmetric and antisymmetric tensors.

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MS109

Compression of Convolution Layers via CPD: Matrix Representation and Bounds on Convolution Error

A convolutional layer is a fundamental component of convolutional neural networks (CNNs) that performs feature extraction by applying filters to input data in a localized manner, enabling the network to capture spatial dependencies. It is known that the convolution operation can be represented as matrix multiplication, where the matrix is constructed using Toeplitz matrices, and the vector is a vectorization of the input in the convolutional layer. The weights of the convolutional operator are stored in a tensor called the kernel tensor. To compress the convolutional layer, a low-rank tensor approximation of the kernel tensor is employed. In this talk, we demonstrate how 1D and 2D convolutions, for both the original convolution and the compressed convolution via CPD, can be represented as matrix multiplications, providing explicit structured matrix forms. We then utilize this matrix construction to establish upper bounds on the convolution errori.e., the residual error between the output obtained from the original convolutional layer and the output obtained by applying the compressed convolutional layer via CPDin relation to the kernel tensor rank approximation error. This analysis helps explain the reduction in accuracy typically observed when replacing the original model with the compressed one, which is usually remedied through the use of the fine-tuning step.

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MS109

Dynamical Tucker Low-Rank Factorization of Convolutional Neural Networks

We present a rank-adaptive algorithm to train convolutional neural networks in low-rank tensor Tucker format via a form of Riemannian optimization scheme. We discuss theoretical guarantees of convergence and approximation and we provide extensive numerical evidence of performance, showing that the method drastically reduces model dimension while retaining the full-model performance on standard computer vision benchmarks.

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MS109

Decomposition of a Tensor into Multilinear Rank-$(M_r, N_r, \cdot)$ Terms

Rank-1 terms play a crucial role in countless applications as they can be interpreted thanks to the mild uniqueness conditions of the canonical polyadic decomposition. However, rank-1 terms may be too simple, and instead of looking at these 'atoms', we might be interested in more expressive 'molecules' or block terms. In this talk, we focus on the decomposition into multilinear rank $(M_r, N_r, \cdot)$ terms. We present new deterministic and generic uniqueness results that are constructive and lead to an algebraic algorithm that can be used to estimate all required parameters. To avoid the high cost of computing the null space needed in the algebraic algorithm, a fast direct method is derived. Finally, we illustrate the tremendous improvements in success rate and computation time as an initialization for standard optimization algorithms compared to random initializations.

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MS110

Negative Curvature and Newton Steps for Fast Nonconvex Optimization

A class of second-order algorithms is proposed for minimizing smooth nonconvex functions that alternate between regularized Newton and negative curvature steps. In most cases, the Hessian matrix is regularized with the square root of the current gradient and an additional term to account for moderate negative curvature; a negative curvature step is theoretically required but not so efficient in practice. Practical variants that allow Krylov subspaces to compute a step, or the use of gradient information only, are also proposed. The complexity is up to a logarithm of the optimal second order, and first numerical experiments suggest some merits of our approach.

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MS110

Optimization Landscape of Matrix Square Root Approximation

The efficacy of deep neural networks has spurred extensive research into their training processes. Landscape analysis, emphasizing loss function critical points, has been particularly successful in studying linear networks. Loss landscape exploration has also been conducted for continuous-in-depth architectures inspired by NeuralODE, a recently introduced architecture based on ordinary differential equations. However, this analysis does not apply to practical NeuralODE implementations. In this talk, we focus on a discretized NeuralODE implementation obtained using the forward Euler method, and analyze the landscape of its training process. Assuming whitened training data and a symmetric positive definite target matrix, we classify global minima and identify two strict saddle point classes, including a novel class absent in linear networks. A full landscape description is provided for a scalar target matrix and we show that in that case the loss landscape satisfies the strict saddle property.

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MS110

Minimum Eigenvalue Routines and Nonconvex Optimization

In this talk, we will survey the use of negative curvature estimation routines in nonconvex optimization. We will first present the notion of minimum eigenvalue oracle, that encompasses a variety of routines for computing the smallest eigenvalue of a matrix. Our focus will be on using randomized variants of Krylov subspace methods, such as Lanczos' method and conjugate gradient, as oracles with probabilistic guaranteed. We will then describe how these routines can be incorporated in nonconvex optimization algorithms to obtain non-asymptotic convergence rates.

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MS110

Trust-Regions for Ill-Conditioned Low-Rank Problems

When reconstructing a low-rank matrix from linear measurements, it is classical to write the matrix as the product of two "thin" matrices and optimize directly over the factors. This approach, called the Burer-Monteiro factorization, saves computational time and storage space, compared to optimizing over the full matrix. When the size of the factors is stricly larger than the rank of the underlying unknown matrix (the "overparametrized setting"), the factorization introduces ill-conditioning in the problem, making straightforward first-order methods slow. To overcome this issue, preconditioned gradient methods have been proposed. In this talk, we will discuss the performance of a

second-order method, namely trust-regions.

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MS111

An Inertial Multiplicative Update for Nonnegative Matrix Factorization with the Kullback-Leibler Divergence

We propose a Block Majorization Minimization method with Extrapolation (BMMe) for solving a class of multiconvex optimization problems. The extrapolation parameters of BMMe are updated using a novel adaptive update rule. By showing that block majorization minimization can be reformulated as a block mirror descent method, with the Bregman divergence adaptively updated at each iteration, we establish subsequential convergence for BMMe. We use this method to design efficient algorithms to tackle nonnegative matrix factorization problems with the β-divergences (β-NMF) for $\beta \in [1, 2]$, $\beta = 1$ corresponding to the Kullback-Leibler divergence widely used in topic modeling and imaging. These algorithms, which are multiplicative updates with extrapolation, benefit from our novel results that offer convergence guarantees. We also empirically illustrate the significant acceleration of BMMe for β-NMF through extensive experiments.

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MS111

Adventures in PCA for Heterogeneous Quality Data

PCA is a workhorse method in statistics, machine learning, and data science for discovering underlying low-rank signals in noisy data. This talk discusses what happens when the data are of heterogeneous quality, i.e., when some samples are noisier than others. Data with heterogeneous quality are common in modern data analysis (e.g., in genomics, astronomy, and RADAR to name just a few). We will present some surprising discoveries (inverse noise variance weighted PCA is suboptimal!) as well as some new PCA methods that rigorously account for the noise heterogeneity.

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MS112

Spectral Elements of Positive Definite Matrices Over Symmetrized Tropical Algebra

The images by the valuation of symmetric positive semidefinite matrices over the field of real Puiseux series have been characterized by Josephine Yu (2015) as the matrices over the tropical semiring such that all the principal 2×2 minors are "nonnegative". The symmetrized tropical algebra is a semiring extension of the tropical semifield, which is isomorphic to the "signed tropical" hyperfield, and can be used to define the signed valuation, which associate to the valuation an information of sign. The sign valuation is then almost a morphism from the field of real Puiseux series to the symmetrized tropical semiring. In a recent work, the 2 first co-authors together with Allamigeon and Sergeev (2023) characterized the signed valuation of symmetric positive semidefinite matrices over the field of real Puiseux series, as the symmetric positive semidefinite matrices over the symmetrized tropical semiring. In this talk, we present characterizations of the eigenvalues and eigenvectors of symmetric positive definite matrices over the symmetrized tropical semiring, and show in some cases that they coincide with the signed valuations of the eigenvalues and eigenvectors of symmetric positive definite matrices over the field of Puiseux series. We shall also discuss how such results can be used in the numerical computation of eigenvalues and eigenvectors of real symmetric positive definite matrices.

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MS112

Diagonal Scalings in Matrix Perturbation Theory

Matrix perturbation theory becomes rather complicated when the original matrix has repeated eigenvalues: although perturbation series are nominally available, computing the relevant terms is a headache. It is known from the tropical algebra literature that some computations simplify when the matrix has entries that differ in magnitude. In this talk we will give precise and easy-to-use results on matrix perturbations that exploit diagonal scalings. Our method has applications to the study of kernel matrices which we will sketch.

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MS112

Solving Linear Equations over Maxmin-Omega Systems

Maxmin-ω dynamical systems were previously introduced as an "all-in-one package' that can yield a solely min-plus, a solely max-plus, or a max-min-plus dynamical system by varying a parameter $\omega \in (0, 1]$. With such systems in mind, it is natural to introduce and consider maxmin-ω linear systems of equations of the type $A \otimes_\omega x = b$. However, to our knowledge, such maxmin-ω linear systems have not been studied before and in this paper we present an approach to solve them. We show that the problem can be simplified by performing normalization and then generating a "canonical' matrix which we call the principal order matrix. Instead of directly trying to find the solutions, we search the possible solution indices which can be identified using the principal order matrix and the parameter ω. The fully active solutions are then immediately obtained from these solution indices. With the fully active solutions at hand, we then present the method to find other solutions by applying a relaxation, i.e., increasing or decreasing some components of fully active solutions. This approach can be seen as a generalization of an approach that could be applied to solve max-plus or min-plus linear systems. Our results also shed more light on an unusual feature of maxmin-ω linear systems, which, unlike in the usual linear algebra, can have a finite number of solutions in the case where their solution is non-unique.

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MS112

Exploiting Tropical Algebra in Numerical Linear Algebra

The tropical semiring consists of the real numbers and infinity along with two binary operations: addition defined by the max or min operation and multiplication. Tropical algebra is the tropical analogue of linear algebra, working with matrices with entries on the extended real line. There are analogues of eigenvalues and singular values of matrices, and matrix factorizations in the tropical setting, and when combined with a valuation map these analogues offer 'order of magnitude' approximations to eigenvalues and singular values, and factorizations of matrices in the usual algebra. What makes tropical algebra a useful tool for numerical linear algebra is that these tropical analogues are usually cheaper to compute than those in the conventional algebra. They can then be used in the design of preprocessing steps to improve the numerical behaviour of algorithms. In this talk I will review the contributions of tropical algebra to numerical linear algebra and discuss recent results on the selection of Hungarian scalings prior to solving linear systems and eigenvalue problems.

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MS113

Truncated Qr Factorization with Pivoting in Mixed Precision

Low-rank approximations are widely used to reduce the memory footprint and operational complexity of numerous linear algebra algorithms in scientific computing and data analysis. In some of our recent work we have demonstrated that low-rank approximations can be stored using multiple arithmetic precisions to further reduce the storage and execution time. In this talk we present a method that can produce this mixed-precision representation directly using a mixed-precision truncated rank-revealing QR (RRQR) factorization with pivoting. We present a floating-point error analysis and provide bounds on the error of the approximation demonstrating that the use of multiple precisions does not alter the overall accuracy. Finally, we present experimental results showing the execution time reduction for the cases where either classical or randomized pivoting are used.

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MS113

Approximate Coarsest-Level Solves in Multigrid V-Cycle Methods

Multigrid methods are frequently used when solving systems of linear equations, applied either as standalone solvers or as preconditioners. Within each cycle, the approximation is computed using smoothing on fine levels and solving on the coarsest level. With growth of the size of the problems that are being solved, the size of the problems on the coarsest level is also growing and their solution can become a computational bottleneck. In practice the problems on the coarsest level are often solved approximately, for example by Krylov subspace methods or direct methods based on low-rank approximation; see, e.g., [Buttari et al., Numerical Linear Algebra with Applications (2022)]. The accuracy of the coarsest-level solver is typically determined experimentally in order to balance the cost of the solves and the total number of multigrid cycles required for convergence. In this talk, we present an approach to analyzing the effect of approximate coarsest-level solves in the multigrid V-cycle method for symmetric positive definite problems. We discuss how the choice of the tolerance in a relative residual stopping criterion for an iterative coarsest-level solver may affect the convergence of the V-cycle method. We present new coarsest-level stopping criteria, which yields that the computed V-cycle approximation is "close' to the approximation which would be obtained by solving the coarsest-level problem exactly. The

results are illustrated through numerical experiments.

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MS113

A Backward Error Analysis Framework for Gmres Using Approximate Computing Techniques

The Generalized Minimal Residual methods (GMRES) for the solution of general square linear systems is a class of Krylov-based iterative solvers for which there exist backward error analyses that guarantee the computed solution in inexact arithmetic to reach certain attainable accuracies. Unfortunately, these existing backward error analyses cover a relatively small subset of the possible GMRES variants and cannot be used straightforwardly in general to derive new backward error analyses for variants that do not yet have one. In this talk, we will present a backward error analysis framework for GMRES that substantially simplifies the process of determining error bounds of most existing and future variants of GMRES; in particular, those using approximate computing techniques. This framework describes modular bounds for the attainable normwise backward and forward errors of the computed solution that can be specialized for a given GMRES variant under minimal assumptions. We further explained how our framework can be used to derive error bounds on GMRES algorithms using approximate computing techniques.

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MS114

Application of Numerical Linear Algebra in Signal Processing: Convergence Analysis of Iterative Filtering Applied on the Sphere

Since real-life data are non-stationary, it would be better to study them through non-stationary techniques, and 'Fast Iterative Filtering has proven to be an interesting and useful method to achieve this goal, especially in classic 1D or 2D cases [A. Cicone, H. Zhou, Multidimensional Iterative Filtering method for the decomposition of high-dimensional non-stationary signals, Cambridge Core in Numerical Mathematics: Theory, Methods and Applications, Volume 10, Issue 2, Pages 278-298]. But some problems arise in non-Euclidean settings since the filtering relies on convolution. After developing a continuous operator we analysed its discretisation through the Generalised Locally Toeplitz (GLT) sequences of matrices [C. Garoni, S. Serra-Capizzano, Generalized Locally Toeplitz Sequences: Theory and Applications, 2017]. Using some property from the GLT theory we studied the convergence of this procedure [G. Barbarino, A. Cicone, Conjectures on spectral properties of ALIF algorithm, Linear Algebra and its Applications, Volume 647, Pages 127-152, 2022]. In this talk, after a brief review on the topic, we will describe some problems related to this setting and what we have obtained so far to overcome them. We conclude our talk with a few examples of applictions of this method to real life signals.

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MS114

An Alternating Direction Multiplier Method for the Inversion of FDEM Data

This paper aims to solve an inverse problem arising in geophysics. We wish to determine the electrical conductivity and magnetic permeability dsitributions of the ground by inverting Frequency Domain Electromagnetic (FDEM) data. Inverting FDEM data is a very challenging inverse problem, as the problem is extremely ill-posed, i.e. sensible to the presence of noise in the measured data, and nonlinear. Therefore, we need to regularize the problem. In this work, we propose an Alternating Direction Multiplier Method (ADMM) algorithm for the inversion of the problem, we show the convergence of the obtained method, and propose an automated strategy to determine the parameters involved in the method. In particular, we propose to compute a regularized solution by solving a minimization of an $\ell^2 - \ell^q$ functional for which we construct an ADMM algorithm that decouples the ℓ^2 part from the ℓ^q part of the functional. At each iteration of ADMM, the solution of two minimization problems are performed. The first one is a least-squares non-linear problem. The second one is an $\ell^2 - \ell^q$ minimization problem, where all the operators involved are linear. To solve this minimization problem we use an adaptation of the Majorization-Minimization algorithm. Some selected numerical examples on synthetic data show the good performances of our proposal.

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MS114

A Generalized Krylov Subspace Method for Nonlinear Inverse Problems

The solution of nonlinear inverse problems is a challenging task in numerical analysis. In most cases, this kind of problems is solved by iterative procedures that, at each iteration, linearize the problem in a neighborhood of the currently available approximation of the solution. The linearized problem is then solved by a direct or iterative method. Among this class of solution methods, the Gauss-Newton method is one of the most popular ones. We propose an efficient implementation of this method for large-scale problems. Our implementation is based on projecting the nonlinear problem into a sequence of nested subspaces, referred to as Generalized Krylov Subspaces, whose dimension increases with the number of iterations, except for when restarts are carried out. Numerical experiments demonstrate the performance of the method.

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MS114

A Projection Method for Large Scale Linear Inverse Problems with a General Form Regularizing Term

One of the possible approaches for the solution of ill-conditioned linear least-squares problems in general form, for a chosen regularization operator L, projects the problem in the null space of L and in its orthogonal complement. We will present various computational schemes for an efficient implementation of such an approach, including an algorithm based on the Golub-Kahan partial factorization, particularly suited for large scale problems. This work is in collaboration with Federica Pes (University of Cagliari, Italy).

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MS115

An Augmented Lagrangian Preconditioner for the Control of the Navier-Stokes Equations

We consider the distributed control problem for the flow of an incompressible viscous Newtonian fluid in a bounded domain. The problem consists in the minimization of a cost functional subject to the stationary incompressible Navier-Stokes equations with the introduction of a control variable that is assumed to be defined on the whole domain. The first-order optimality conditions and discretization using finite elements lead to a large-scale nonlinear system of equations that is solved by a Gauss-Newton approach. At each step, the resulting linear system of equations is solved by a preconditioned Krylov subspace method. We present an effective block preconditioner of augmented Lagrangian type and illustrate its performance for a wide range of problem parameters by means of numerical experiments. This is joint work with Patrick Farrell (Oxford University) and Santolo Leveque (Scuola Normale Superiore).

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MS115

To Schur Or Not to Schur

Schur complements arise in several flavors in the design of block preconditioners for the iterative solution of block-structured indefinite linear system. They often exist but are hard to form and solve for, and at times they do not exist due to singularity of the blocks of the matrix. Altogether, they are an indispensable way of dealing with this type of linear systems, and their efficient use or approximation is a central aspect in the design and performance of the underlying solvers. In this talk we will discuss some spectral properties of Schur complements and will focus on the role they play in the numerical solution of double saddle-point systems.

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MS115

Operator Preconditioning for Stochastic Galerkin Saddle Point Matrices

Stochastic Galerkin (SG) approximation is a popular approach for performing forward uncertainty quantification (UQ) in PDE models with uncertain inputs. Unlike sampling methods, SG schemes yield approximations that are functions of the random inputs so that all realisations of the PDE solution are effectively approximated simultaneously. Standard SG schemes give rise to huge linear systems with coefficient matrices with a characteristic Kronecker product structure. The number of equations may run into the hundreds of millions, even for relatively simple physical models. Tailored linear algebra tools are required. If sufficient memory is available to store vectors of the appropriate length, standard preconditioned Krylov methods can be applied. The key challenge is to construct suitable preconditioners that are cheap and robust not only with respect to the SG discretisation parameters and any physical model parameters, but also with respect to the number of random inputs and their statistical properties. In this talk, we consider mixed formulations of linear elasticity and poroelasticity problems with uncertain inputs and discuss how the now well-known operator approach to preconditioning can be applied in the SG setting. In this approach, the preconditioner is chosen to provide a discrete representation of a weighted norm with respect to which the weak

formulation of the mixed problem is provably stable.

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MS115

A New Algebraic Multigrid Algorithm for Curl-Curl Systems That Explicitly Enforces Commutator Relationships Associated with the De Rham Complex

A new AMG algorithm is proposed for curl-curl electromagnetics problems that are discretized with 1st order edge elements. The algorithm enforces a commuting relationship between interpolation and gradient operators, which was originally highlighted by Reitzinger and Schoberl. Specifically, interpolation of coarse nodal quantities followed by application of an appropriate discrete gradient operator should be equivalent to first applying the discrete gradient on the coarse level and then interpolating the resulting edge quantities. When this commuting holds, important near null space properties are preserved on coarse levels and good AMG convergence rates can be obtained. The new algorithm is based on energy minimization AMG. It takes an already-computed nodal interpolation operator to then define an edge interpolant that satisfies commuting and energy minimization properties. Unlike previous works, this new algorithm is general in that it can essentially start with any standard nodal interpolation operator. Thus, it is possible to leverage traditional AMG schemes to first generate nodal interpolation operators. We show that the new algorithm can produce "ideal geometric" edge interpolants in some limited cases. Numerical results are provided showing the overall efficacy, comparing with traditional Reitzinger and Schoberl schemes and with traditional auxiliary-based AMG methods.

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MS116

Optimal Super-Resolution of Close Point Sources and Decimated Prony's Method

We consider the problem of recovering a linear combination of Dirac masses from noisy Fourier samples, also known as the problem of super-resolution. Following recent derivation of min-max bounds for this problem when some of the sources collide, we develop an optimal algorithm which provably achieves these bounds in such a challenging scenario. Our method is based on the well-known Prony's method for exponential fitting, and a novel analysis of its stability in the near-colliding regime, combined with the decimation technique for improving the conditioning of the problem. Based on joint works with D. Batenkov and R.Katz: [1] R. Katz, N. Diab and D. Batenkov. Decimated Prony's Method for Stable Super-Resolution. IEEE Signal Processing Letters. 2023. doi: 10.1109/LSP.2023.3324553. [2] R. Katz, N. Diab, D. Batenkov. On the accuracy of Prony's method for recovery of exponential sums with closely spaced exponents. 2023. http://arxiv.org/abs/2302.05883

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MS116

Phase Retrieval in Dynamical Sampling

Considering finite-dimensional signals evolving in time under the action of a matrix, our aim is to recover the signal up to a global phase from the absolute value of certain space-time measurements. The loss of the phase turns the well-posed dynamical sampling into a severe ill-posed inverse problem. Here, we combine phase retrieval in dynamical sampling with the identification of the system in case that the evolving matrix is unknown. Using Prony's method, we establish several recovery guarantees for signal and system. The proofs are constructive, yield analytic recovery methods and the required assumptions are satisfied by almost all signals, operators, and sampling vectors.

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MS116

Stability of the Sparse Super-Resolution Problem

Since the work by Abbe and Rayleigh the difficulty of super resolution where one wants to recover a collection of point sources from low-resolved measurements (a.k.a. low degree trigonometric moments) is thought to be dependent on whether the distance between the sources is below or above a certain threshold. Numerically, this gives rise to huge or moderate condition numbers, respectively. While this threshold is one and perfectly understood in the univariate situation, we present our recent findings for the multivariate case.

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MS116

Stability and Super-Resolution of Esprit and Related Problems

The Rayleigh length in optics refers to the minimum distance between two particles that can be resolved by an imaging system. Although this is a widely used principle, there is experimental evidence suggesting that in certain situations, it is possible to image objects at distances smaller than the traditional resolution limit. Motivated by such discoveries, we examine this phenomenon from a mathematical viewpoint. Super-resolution asks whether it is possible to stably recover point sources, possibly closer than the Rayleigh length, from noisy Fourier measurements. We study the fundamental limits of super-resolution from an information theoretic viewpoint and the stability of subspace methods such as ESPRIT. We derive novel multiscale lower bounds for the minimum singular value of Fourier/Vandermonde matrices and a perturbation bound for subspace algorithms that depends on the local geometry of the point sources. These results indicate that it is possible to bypass the resolution limit in an almost optimal way.

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MS117

A Multilinear Nystrm Algorithm for Low-Rank Approximation of Tensors in Tucker Format

Several applications lead to problems involving data or solutions that can be represented by tensors. Dealing with these multidimensional arrays is often prohibitively expensive and some type of compression in data-sparse formats has to be performed. For this aim several low rank tensor factorizations have been proposed. In this work, we focus on the Tucker decomposition. We extend to tensors the Generalized Nystrm method by Nakatsukasa providing a randomized algorithm for the computation of the Tucker Decomposition: Multilinear Nystrm method. The accuracy of the approximation is close to the optimal truncated Higher Order SVD; moreover from a complexity point of view is cheaper than existing alternatives.

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MS117

Efficient Algorithms for Regularized Nonnegative Scale-Invariant Factorization Models

Regularized nonnegative low-rank approximations such as sparse Nonnegative Matrix Factorization or Sparse Nonnegative Tucker Decomposition are important variants of dimensionality reduction models with enhanced interpretability. However, from a practical perspective, the choice of regularizers and regularization coefficients is often challenging because of the multifactor nature of these models and the lack of theory to back these choices. Moreover, existing optimisation algorithms to infer these models do not handle many combinations of loss functions and regularization terms. This paper aims at improving upon these issues. By studying a more general model called the Homogeneous Regularized Scale-Invariant, we prove that the scale-invariance inherent to low-rank approximation models causes an implicit regularization with unexpected beneficial or detrimental effects. This observation enables to better understand the effect of regularization functions in low-rank approximation models, to guide the choice of the regularization hyperparameters, and to design balancing strategies to enhance the speed of dedicated optimization algorithms. We also derive a generic Majorization Minimization algorithm that handle many regularized nonnegative low-rank approximations, with convergence guarantees. We showcase our contributions on sparse Nonnegative Matrix Factorization, ridge-regularized Canonical Polyadic decomposition and sparse Nonnegative Tucker Decomposition.

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MS117

Decoupling of Multivariate Functions Using Tensor Decompositions

Defining and reducing the complexity, as well as increasing the interpretability of nonlinear multivariate vector functions are important but challenging problems. We propose a decomposition of nonlinear functions [1], which we view as a generalization of the singular value decomposition. In this decomposition, univariate nonlinear mappings replace the scaling performed by the singular values. The computation of the decomposition is based on tensor techniques. Finally, we also mention applications in nonlinear system identification and recent extensions in neural network compression. [1] P. Dreesen, M. Ishteva, and J. Schoukens. Decoupling multivariate polynomials using first-order information and tensor decompositions. SIMAX, 36:864–879, 2015.

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MS117

Iteratively Reweighted Least Squares Recovery on Tensor Networks

One fundamental approach to matrix recovery, being a predecessor to tensor recovery, traces back to the affine rank minimization problem. While there are various surrogate approaches within that setting, we emphasize here that the asymptotic minimization of the well-known, so called *log-det* objective functions always yields the desired, minimal rank matrices within the given, affine set; whereas such may or may not recover an a-priorly sought for ground truth. Concerning the commonly applied method of iteratively reweighted least squares (IRLS-0), one thus remains with two concerns. How problematic are local minima inherent to the log-det approach truly; and opposingly, how influential instead is the numerical realization. With higher dimensions in mind, based on the concept of matricization, affine sum-of-ranks minimization then generalizes the setting from matrices to tensors. While convergence properties are directly transferable, we demonstrate that in numerical experiments, the corresponding IRLS-0 method can be exhausted in order to observe the theoretical phase transition for generic tensor recoverability. In large-scale applications in turn, alternating, reweighted optimization on tensor tree networks allows to avoid exponential computational complexity, without substantial loss of approximation quality.

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MS118

Randomized Kaczmarz Linear Discriminant Analysis

We present randomized Kaczmarz linear discriminant anal-

ysis (rkLDA), an iterative randomized approach to binary-class Gaussian model linear discriminant analysis (LDA) for very large data. We harness a least squares formulation and mobilize the stochastic gradient descent framework to obtain a randomized classifier with performance that can achieve comparable accuracy to that of full data LDA. We present analysis for the expected change in the LDA predictions if one employs the rkLDA solution in lieu of the full-data least squares solution that accounts for both the Gaussian modeling assumptions on the data and algorithmic randomness. Our analysis shows how the expected difference depends quantities inherent in the data such as the scaled condition number and Frobenius norm of the input data, how well the linear model fits the data, and choices from the randomized algorithm. Our experiments demonstrate that rkLDA can offer a viable alternative to full data LDA on a range of step-sizes and numbers of iterations.

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MS118

Stochastic Iterative Methods for Linear Problems with Adversarial Corruption

Stochastic iterative methods, like stochastic gradient descent or the randomized Kaczmarz method, have gained popularity in recent times due to their amenability to large-scale data and distributed computing environments. This talk will focus on variants of the randomized Kaczmarz methods developed for problems with significant or adversarial corruption present in the data. This type of corruption arises frequently in applications like medical imaging, sensor networks, and error correction. We will focus on recent results for systems of inequalities and tensor regression problems.

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MS118

Linear Convergence of Kaczmarz Methods With Sparse Constraints

"In this talk, I will discuss recent developments in hybrid methods that combine the Kaczmarz method (KZ) and the iterative thresholding (IHT) method to solve linear systems with sparse constraints. The Kaczmarz method (KZ) and its variants, which are types of stochastic gradient descent (SGD) methods, have been extensively studied due to their simplicity and efficiency in solving linear equation systems. The iterative thresholding (IHT) method has gained popularity in various research fields, including compressed sensing or sparse linear regression. Recently, a hybrid method called Kaczmarz-based IHT (KZIHT) has been proposed, combining the benefits of both approaches, but its theoretical guarantees are missing. In this paper, we provide the first theoretical convergence guarantees for KZIHT by showing that it converges linearly to the solution of a system with sparsity constraints up to optimal statistical bias when the reshuffling data sampling scheme is used. We also propose the Kaczmarz with periodic thresholding (KZPT) method, which generalizes KZIHT by applying the thresholding operation for every certain number of KZ iterations and by employing two different types of step sizes. I will discuss several numerical experiments to support our theory. This is joint work with Deanna Needell. "

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MS118

An Optimal Scheduled Learning Rate for a Randomized Kaczmarz Algorithm

We consider using the randomized Kaczmarz algorithm to solve a consistent linear system perturbed by noise with i.i.d. components. We show how it is possible to break through the convergence horizon and converge to the ground truth by choosing an appropriate learning rate and derive a closed form expression for the optimal learning rate, in terms of two hyperparameters that can be inferred from the system. Based on joint work with Nicholas F. Marshall.

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MS119

A Data-Dependent Regularization Method Based on the Graph Laplacian for Image Reconstruction

We investigate a Tikhonov method that embeds a graph Laplacian operator in the penalty term (graphLa+). The novelty lies in building the graph Laplacian based on a first approximation of the solution derived by any other reconstruction method. Consequently, the penalty term depends on and adapts to the observed data and noise. We demonstrate that graphLa+ is a regularization method and we rigorously establish both its convergence and stability properties. We present some selected numerical experiments in 2D computerized tomography, where we combine the graphLa+ method with several reconstructors: Filter Back Projection (graphLa+FBP), standard Tikhonov (graphLa+Tik), Total Variation (graphLa+TV), and a trained deep neural network (graphLa+Net). The quality increase of the approximated solutions granted by the graphLa+ approach is outstanding for each given method. In particular, graphLa+Net outperforms any other method, presenting a robust and stable implementation of deep neural networks for applications involving inverse problems.

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MS119

Variable Projection Methods for Separable Nonlinear Inverse Problems

Variable projection methods are among the classical and efficient methods to solve separable nonlinear least squares problems. In this talk, I will introduce the variable projection method, its use to solve large-scale blind deconvolution problems, and some new variants that preserve the edges in the solution. Some theoretical results on the convergence of VarPro when using approximate Jacobians obtained using Krylov methods as an inner solver will also be presented.

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MS119

A Scalable Interior-Point Gauss-Newton Method for PDE-Constrained Optimization with Bound Constraints

We present a scalable method for large-scale elliptic PDE- and bound-constrained optimization. Such problems are a means to learn unknown aspects of PDE-based models. It is assumed that such model uncertainty is mathematically manifest in an unknown spatially distributed parameter field, $\rho(x)$. Bound-constraints $\rho(x) \geq \rho_\ell(x)$ are a natural means to introduce additional knowledge of an unknown parameter field, e.g., nonnegativity of a diffusivity parameter field. Bound-constraints are, however, the source of additional computational challenges as they introduce complementarity conditions in the nonlinear optimality system. We utilize a robust, full-space, interior-point method to solve the optimization problem. In order to avoid the computational costs required to regularize the inertia of the linearized optimality system matrix, we use a Gauss-Newton search direction. We discuss two related preconditioned Krylov-subspace solution strategies for said linear system. We show that the number of preconditioned Krylov-subspace iterations is independent of not only discretization but also the ill-conditioning that notoriously plagues interior-point linear systems. We conclude with parallel scaling results on a nonlinear elliptic PDE- and bound-constrained optimization example problem. The results were generated with a native implementation of the computational framework that makes extensive use of MFEM, a scalable C++ finite element library.

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MS119

Multilevel Proximal Methods for Image Restoration : Application to Radio-Interferometry

Solving large scale optimization problems is a challenging task and exploiting their structure can alleviate its computational cost. In this work, we focus on the multiresolution structure at the core of multilevel optimization methods. These approaches leverage the definition of coarse approximations of the objective function to minimize it. In this talk, we present a multilevel proximal algorithm IML FISTA, Inexact Multilevel FISTA applicable to solve composite optimization problem which are not proximable exactly for their non-smooth part.The proposedmethod is then extended to solve problems with reweighted penalizations and its the effectiveness is illustrated on color images reconstruction problems for radio-interferometry.

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MS120

Low tensor rank dynamics of neural learning

Recent work has shown that the weight matrices of task-trained RNNs are typically low rank, but how this low rank structure unfolds over learning is unknown. To address this, we investigate the rank of the 3-tensor formed by the weight matrices throughout learning. We present a set of mathematical results bounding the matrix and tensor ranks of gradient descent learning dynamics which show that low-tensor-rank weights emerge naturally in RNNs trained to solve low-dimensional tasks. We next validate the observation of low-tensor-rank learning on an RNN trained to solve tasks. Finally, by fitting RNNs of varying rank to large-scale neural recordings during a motor learning task, we find that the inferred weights are low-tensor-rank and therefore evolve over a fixed low-dimensional subspace throughout the entire course of learning. Taken together, our findings provide insight on the evolution of population connectivity over learning in both biological and artificial neural networks, and enable reverse engineering of learning-induced changes in recurrent dynamics from large-scale neural recordings.

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MS120

More Is Less: Understanding Compressibility of Neural Networks Via Implicit Bias and Neural Collapse

Despite their recent successes in various tasks, most modern machine learning algorithms lack theoretical guarantees, which are crucial to further development towards delicate tasks such as designing self-driving cars. One mysterious phenomenon is that, among infinitely many possible ways to fit data, the algorithms always find the "good" ones, even when the definition of "good" is not specified by the designers. In this talk I will cover the empirical and theoretical study of the connection between the good solutions in neural networks and the sparse solutions in compressed sensing with four questions in mind: What happens? When does it happen? Why does it happen?

How can we improve it? The key concepts are implicit bias/regularization, Bregman divergence, neural collapse, and neural tangent kernel.

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MS120

Gradient Descent for Low-Rank Functions

Several recent empirical studies demonstrate that important machine learning tasks, e.g., training deep neural networks, exhibit low-rank structure, where the loss function varies significantly in only a few directions of the input space. In this talk, we leverage such low-rank structure to reduce the high computational cost of canonical gradient descent method (GD). Our proposed Low-Rank Gradient Descent (LRGD) algorithm finds an epsilon-approximate stationary point of a p-dimensional smooth, lower-bounded function by first identifying $r < p$ significant directions, and then estimating the true p-dimensional gradient at every iteration by computing directional derivatives only along those r directions. We establish that the "directional oracle complexities" of LRGD is $O(r/\epsilon^2 + rp)$. When $r << p$, this is smaller than the known complexity of $O(p/\epsilon^2)$ of GD. Thus, LRGD reduces the computational cost of gradient-based methods for sufficiently low-rank functions. In the course of our analysis, we define and characterize a classes of exact and approximately low-rank functions.

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MS120

Dynamical Low-Rank Training of Neural Networks

Neural networks have achieved tremendous success in a wide variety of applications. However, their memory footprint and computational demand can render them impractical in application settings with limited hardware or energy resources. An optimal trade-off is then to be found in order to reduce networks dimensions while maintaining high performance. Popular approaches in the current literature are based on pruning techniques that look for subnets capable of maintaining approximately the initial performance. Nevertheless, these techniques are often not able to reduce the memory footprint of the training phase, and approximation guarantees are not clear. In this talk, we will present DLRT, a training algorithm that looks for low-rank lottery tickets by interpreting the training phase as a continuous ODE and integrating it within the manifold of low-rank matrices while maintaining desirable approximation properties.

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MS121

Krylov Subspace Recycling With Randomized Sketching For Matrix Functions

I will discuss a new augmented Krylov subspace method which allows for the efficient evaluation of a sequence of matrix function applications on a set of vectors using Krylov subspace recycling. If selected appropriately, the recycling subspace can be used to accelerate the convergence of each problem in the sequence, leading to an overall reduction in the computational overhead required to evaluate the full sequence of function applications, in comparison to standard Krylov subspace methods. Our new algorithm exploits the technique of randomized sketching in order to avoid excessive orthogonalization costs.

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MS121

FGMRES in Four Precisions

The flexible generalized minimum residual method (FGMRES) can be used to iteratively solve systems of linear equations. It is well known that preconditioning is needed to achieve high performance. We consider a case where a general split-preconditioner, and four potentially different precisions are used for computations with the coefficient matrix, application of the left preconditioner, application of the right preconditioner, and the working precision. In this talk, we discuss how the backward and forward error can be bounded, and how the various precisions should be chosen.

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MS121

Effective Approximate Preconditioners for Linear Inverse Problems

Many problems in science and engineering give rise to linear systems of equations that are commonly referred to as large-scale linear discrete ill-posed problems. These problems arise for instance, from the discretization of Fredholm integral equations of the first kind. The matrices that define these problems are typically severely ill-conditioned and may be rank deficient. Because of this, the solution of linear discrete ill-posed problems may not exist or be extremely sensitive to perturbations caused by error in the available data. These difficulties can be reduced by applying regularization to iterative refinement type methods which may be viewed as a preconditioned Landweber method. Using a filter factor analysis, we demonstrate that low precision matrix approximants can be useful in the construction of these preconditioners.

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MS121

Randomized Nystrom Method for Symmetric In-

definite Matrices

In this talk, we present a variant of the Nystrm method for symmetric indefinite matrices. The Nystrm method is a popular choice for symmetric positive semi-definite matrices. However, the method can fail when the matrix is indefinite, for which the error can be large. We first identify the main challenges in finding a robust Nystrm approximation to symmetric indefinite matrices and describe an algorithm, whose robustness for symmetric indefinite matrices is illustrated with experiments.

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MS122

Solving a Fractional Differential Equation Using the Matrix Mittag-Leffler Function

Anomalous diffusion problems can be described by a time-dependent diffusion equation featuring a fractional time derivative. Initially derived within the framework of continuous-time random walk with heavy-tailed waiting times, this equation has evolved into a standard framework for describing subdiffusive dynamics. To find approximate solutions to this type of equation we can start to discretize the spatial operator and arrive at a time-fractional matrix equation whose solution has a closed form representation in terms of the Mittag-Leffler function with a matrix argument times a vector. The main purpose of our presentation is to find approximate solutions for this equation using matrix techniques such as matrix functions and Krylov subspaces. A set of experiments will be presented to compare our method with the already existing ones and highlight its advantages and disadvantages.

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MS122

Functions and Means of Quasi-Toeplitz Operators

We consider functions and means in the Toeplitz algebra of semi-infinite matrices that can be written as the sum of a Toeplitz operator $T(a)$ associated with a continuous function a plus a compact operator F. These objects are also known as quasi-Toeplitz matrices. For any continuous function f defined in the spectrum of $T(a)$ we show that $f(T(a) + E) = T(f \circ a) + F$, where F is a compact operator. Moreover, we prove that it is possible to extend the usual notions of geometric mean of operators to the quasi-Toeplitz matrices associated with the continuous and positive functions $a_1, \ldots, a_\ell$, and the resulting quasi-Toeplitz means are associated with the geometric mean $(a_1 \cdots a_\ell)^{1/\ell}$, with different compact part. We show by numerical tests that fractional powers and means of quasi-Toeplitz operators can be practically approximated.

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MS122

Mixed-Precision Paterson-Stockmeyer Method for Evaluating Matrix Polynomials

The Paterson–Stockmeyer method is an evaluation scheme for matrix polynomials with scalar coefficients that arise in many state-of-the-art algorithms based on polynomial or rational approximants, for example, those for computing transcendental matrix functions. We derive a mixed-precision version of the Paterson–Stockmeyer method that can be faster than its fixed-precision counterpart while delivering the same level of accuracy.

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MS122

Numerical and Quantum Algorithms for Matrix Functions Based on Some Quadrature Formulas

Matrix fractional power, matrix logarithm, and matrix exponential are fundamental matrix functions, which arise from a rich variety of applications such as fractional partial differential equations, control theory, lattice quantum chromodynamics, and quantum information. Among many approaches to computing matrix functions, we are interested in integral representations of the matrix functions for computing the large matrix functions, especially focusing on element-wise computation of the matrix functions so that only mat-vec is available. In this talk, the recent progress of our error-controlled numerical algorithms based on some double exponential formulas is presented: matrix fractional power [Tatsuoka et al., ETNA, 2020], matrix logarithm [Tatsuoka et al., JCAM, 2021], matrix exponential [Tatsuoka et al., arXiv:2306.14197, 2023]. Further, quantum algorithms based on some quadrature formulas for matrix functions are also presented: a basic quantum algorithm [Takahira et al., Quantum Inf. Comput., 2020] and a block encoding [Takahira et al., Quantum Inf. Comput., 2022].

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MS123

Iterative Methods for Linear Systems and Sampling

Iterative methods, both stationary, polynomial and rational, have been used not only for solving linear systems of

equations, but also for eigenvalue computations, model reduction and the evaluation of matrix functions. In this talk we present an overview of their applications to sampling from probability distributions on high-dimensional state spaces. Such sampling techniques are, among others, a key component of Markov chain Monte Carlo algorithms for sampling from the posterior a Bayesian inverse problem.

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MS123

Multifidelity Methods for a Pollutant Dispersion Model

Air pollution is a pressing issue challenging modern society from both public health and environmental perspectives. Recent advances in computational mathematics have made it feasible to model some of the key processes contributing to air quality problems over a range of parameter values in order to gain some insight into the factors that influence pollutant concentration. Here we use a parametric differential equation as a pollutant dispersal model and assign probability distribution functions to model uncertainties associated with various parameters. For realistic problems, the cost of such modelling can still be high. To improve computational efficiency, we introduce a control variate method using a combination of high and low fidelity models for variance reduction. The choice of numerical model and the efficient solution of the resulting linear systems of equations can play an important role in the feasibility and robustness of this process. In this talk, we will highlight some of these important aspects with reference to a simple advection-diffusion model of pollution dispersal, and focus on appropriate model selection strategies. The ultimate aim is to be able to carry out a global sensitivity analysis which shows how the variability in the pollutant concentration can be attributed to the variability in the model parameters across the problem domain.

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MS123

Scalable Preconditioning of a Fully-Implicit VMS Visco-Resistive MHD Formulation with Application to MCF

A scalable multiphysics block preconditioner for an implicit low Mach number compressible resistive magnetohydrodynamics (MHD) formulation based on a variational multiscale (VMS) finite element (FE) method is presented. The VMS formulation stabilizes the strongly convective flow effects, and saddle point structure of the magnetic field elliptic divergence cleaning term and the low Mach number nearly incompressible flow limit. The MHD model is intended to simulate macroscopic plasma instabilities and disruptions in complex 3D Tokamak devices used for exploring magnetic confinement fusion (MCF). In this talk the block structure of the Newton linearized discrete system is presented along with a brief description of the approximate block factorization and Schur complement operators that encode the critical cross-coupling physics of the system. The discussion includes a few simulation results on MCF relevant problems in ITER geometry. The numerical results will then present representative strong and weak scaling of the block preconditioner along with the Lundquist number robustness of the method. This work is in collaboration with J. Bonilla, P. Ohm, E. Phillips, M. Crockatt, R. Tuminaro, J. Hu, and X. Tang. This work was partially supported by the U.S. DOE, Office of Science, Office of Advanced Scientific Computing Research (ASCR), Applied Mathematics Program. It has also been partially supported by the DOE, ASCR and Fusion Energy Sciences SciDAC Partnership program.

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MS123

Fast Solution of Incompressible Flow Problems with Two-Level Pressure Approximation

This talk discusses efficient preconditioned iterative solvers for incompressible flow problems discretised by an enriched Taylor–Hood mixed approximation, in which the usual pressure space is augmented by a piecewise constant pressure to ensure local mass conservation. This enrichment process causes over-specification of the pressure, which complicates the design and implementation of efficient solvers for the resulting linear systems. This is joint work with Jennifer Pestana.

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MS124

Nonlinear Approximations for Efficient Kernel Methods

Kernel methods are an important class of tools within machine learning, spatial statistics, and more. However, scaling up these methods to large data sets of practical interest (both in terms of data set size and latent dimension) can be challenging. This talk will discuss two ways that nonlinear approximations can be used to accelerate common kernel computations including sampling and matrix vector products.

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MS124

Differential Prony-Type Method for Approximation of the Gaussians

We propose a differential Prony-type method to approximate the Gaussian function on $\mathbb{R}$ by a short exponential

sum. We prove that the optimal frequency parameters $\lambda_1, \ldots, \lambda_N$ for our method in the approximation problem $\min_{\lambda_1,\ldots,\lambda_N,\gamma_1\ldots\gamma_N} \|\mathrm{e}^{-\cdot^2/2\sigma} - \sum_{j=1}^{N} \gamma_j \, \mathrm{e}^{\lambda_j \cdot}\|_{L_2(\mathbb{R},\mathrm{e}^{-t^2/2\rho})}$, are zeros of a scaled Hermite polynomial. This observation leads us to a numerically stable approximation method with low computational cost of $O(N^3)$ operations. Furthermore, we derive a direct algorithm to solve this approximation problem based on a matrix pencil method for a special structured matrix. The entries of this matrix are determined by hypergeometric functions. For the weighted L_2-norm, we prove that the approximation error decays exponentially with respect to the length N of the sum.

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MS124

Optimal Pole Placement for the Approximation of Branch Point Singularities

An important setting where rational functions outperform polynomials significantly is the approximation of functions with singularities; the best rational approximation to x^α on $[0, 1]$ converges root-exponentially, while polynomials only converge algebraically for non-integer α. On the other hand, rational approximation is generally much more computationally demanding due to its nonlinear nature. Recently developed "lightning methods" are able to linearize the problem while still achieving root-exponential convergence when the locations of the singularities are known in advance. Their key characteristic is the pre-assignment of poles exponentially clustered towards the singularities. A series of optimizations has surprisingly led to the identification of poles resulting in rational approximations converging at the optimal rate as shown by Stahl for the approximation of x^α on $[0, 1]$.

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MS125

Low-Rank Tensor Decompositions for Quaternion Multiway Arrays

Quaternion multiway arrays appear naturally as compact representations of 3D or 4D multidimensional signals. However, the non-commutativity of quaternion multiplication prevents a straightforward extension of standard tensor algebra to analyze and process quaternion multiway arrays. In this talk, we will start by reviewing the theoretical difficulties related to quaternion tensor algebra and propose the construction of quaternion tensors as representation of dedicated quaternion multilinear forms. We will demonstrate that this theoretical construction ensures that usual tensor algebraic properties such as mode products properties are preserved. In a second step, we will exploit this novel framework to extend standard low-rank tensor decompositions (e.g. CP) to the quaternion case, including quaternion-domain algorithms and identifiability guarantees.

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MS125

Algorithms and Uniqueness of Tensor Decompositions

In contrast to matrices, tensor rank decompositions are often unique (up to trivialities). Uniqueness is useful in applications, as it corresponds to a unique interpretation of the information stored in a tensor. I will talk about recent work on (i) developing algorithms for tensor rank decompositions, and (ii) certifying that a given tensor rank decomposition is unique.

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MS125

Fuzzy Clustering Using Matrix Factorization

It has been shown that k-means clustering is equivalent to a matrix factorization of the data matrix with orthogonality and nonnegativity constraints. However, these constraints are hard to impose in practice. We develop a relaxed version of k-means that is akin to fuzzy clustering, where cluster membership is probabilistic. This leads to a continuous matrix factorization problem that can be solved using Riemannian optimization. The proposed format can also be applied in data fusion, i.e., when several data sets are available for the same samples. We test our method both on synthetic and real world data sets.

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MS125

Data Fusion and Unmixing with the Regularized Non-Negative Block-Term Decomposition: Blind Approach and Automatic Model Order Selection

This talk introduces a family of coupled tensor optimization problems for joint super-resolution and unmixing in remote sensing. Using β-divergences allows the proposed methods to account for various noise statistics. A family of simple, efficient and flexible algorithms is proposed, that are capable of solving the two problems at hand. Moreover, the proposed algorithms are able to estimate the degradation operators mapping the HSI and MSI to the unknown SRI. We introduce penalized versions of our optimization problems, with an emphasis on the minimum-volume reg-

ularization approach. This approach is designed to efficiently identify the number of factors in the tensor decomposition, and to effectively manage scenarios involving potential rank deficiencies in the estimated mixing factors. It facilitates the computation of interpretable and meaningful tensor decompositions, and enhances the identifiability of the decomposition model. The proposed algorithms demonstrate competitive performance against state-of-the-art methods for joint fusion and unmixing, even in scenarios with various noise statistics and challenging cases, including partially unknown degradation operators, almost collinear materials, and estimation of the number of endmembers.

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MS126

Implicit Preconditioning in Stochastic Linear System Solvers

In this talk, I will present new algorithms and convergence guarantees for solving linear systems via sketch-and-project, a framework which unifies many known iterative methods including randomized Kaczmarz, coordinate descent, and others. Our new results uncover a connection between stochastic iterative solvers and randomized preconditioning algorithms: Whenever the spectral structure of a linear system is amenable to constructing a strong preconditioner via low-rank approximation, then one can construct a stochastic solver based on sketch-and-project that will implicitly take advantage of this spectral structure. In particular, I will show how this leads to faster solvers for linear systems with not too many large singular values.

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MS126

SlimTrain: Iterative Sampling for Training of Separable Deep Neural Networks

Deep neural networks (DNN) have become the workhorse of data science because of their ability to approximate a wide range of functions and thereby act as surrogate models. Despite their success and prevalence, DNNs are notoriously difficult to train. The training problem is often posed as a high-dimensional, nonconvex stochastic optimization problem with numerous hyperparameters that are chosen through trial-and-error. In this talk, we will make DNN training easier by employing an iterative sampling scheme that automatically adapts hyperparameters during training. We will demonstrate the efficacy of our approach on various tasks, including surrogate modeling and dimensionality reduction.

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MS126

Low Rank Approximation for Faster Optimization

Low rank structure is pervasive in real-world datasets. This talk shows how to accelerate the solution of fundamental computational problems, including eigenvalue decomposition, linear system solves, and stochastic optimization (including deep learning), by exploiting this low rank structure. We review a simple method based on randomized numerical linear algebra for efficiently computing approximate top eigendecompositions, which can be used to replace large matrices (such as Hessians and constraint matrices) with low rank surrogates that are faster to apply and invert. The resulting solvers for linear systems (NystromPCG) and stochastic optimization (SketchySGD and PROMISE) demonstrate strong theoretical and numerical support, outperforming state-of-the-art methods in terms of speed and robustness to hyperparameters.

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MS126

Minimal Error Momentum Bregman-Kaczmarz

"The Bregman-Kaczmarz method solves strongly convex problems with linear constraints using a single or selected number of rows of the system matrix each iteration, thereby making it amenable for large-scale systems. Here, the strongly convex regularization can incorporate prior knowledge such as sparsity, which opens for applications like data compression or reconstruction. We present two adaptive Heavy Ball accelerations in the dual update to enhance convergence. We demonstrate that, both numerically and theoretically, our algorithms converge at least as quickly as the basic method, a feature not previously proven for other Heavy Ball accelerations."

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MS127

Ocean Seabed Tomography Using Acoustic Waves

The accurate understanding of the structure of the seabed is essential in designing effective solutions to combat and mitigate the negative global impacts of climate change. The seabed serves as a critical source of information for various applications, including the safety assessment of offshore wind farms, establishing global transport routes, and identifying potential locations for catastrophic oceanic events. However, current technologies are limited in their ability to provide accurate seabed location data, especially for large-scale and deep ocean areas. This work introduces a novel approach that leverages elastic waves to explore the seabed. By considering the seabed as a thin interface, we are able to significantly reduce the complexity of the problem. Additionally, we employ regularization techniques that exploit the regularity of the seabed, resulting in accelerated computations. Another key contribution of our method is the estimation of uncertainty levels in the regularity of the seabed, which can play a crucial role in risk assessments for global solutions aimed at combating climate change. This talk will showcase the significant ad-

vancements in accuracy, efficiency, and reliability for large-scale and deep ocean imaging.

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MS127

Edge-Preserving Kaczmarz-Type Methods for Solving Inverse Problems

Inverse problems have many applications, such as image deblurring, super-resolution imaging, and X-ray tomography. Inverse problems involving large datasets present challenges for both storage and computation time. For large-scale inverse problems in which our data is too large to use all at once, we consider Kaczmarz-type methods, which allow us to work with just a subset of the data at a time. This talk presents an edge-preserving Kaczmarz-type method for solving inverse problems.

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MS128

Oblique Projection for Efficient Solution of High-Dimensional Dynamical Systems on Low-Rank Matrix Manifolds

Dynamical low-rank approximation (DLRA) and dynamically orthogonal (DO) decomposition are two equivalent low-rank approximation schemes that have successfully been used for approximating the solution to nonlinear random partial differential equations (PDEs). While both DLRA and DO can lead to an order of magnitude reduction in computational cost for linear quadratic PDEs, they both become inefficient for general nonlinearities and moreover they require intrusive implementation. To this end, we present a scalable method for solving high-dimensional dynamical systems on low-rank manifolds that is computationally efficient, minimally intrusive, robust in the presence of small singular values, rank-adaptive and highly parallelizable. These favorable properties are achieved via oblique projections that require evaluating the matrix differential equations at a small (order of rank) number of rows and columns. The columns and rows are selected using the discrete empirical interpolation method (DEIM), which yields near-optimal matrix low-rank approximations. We show that the proposed algorithm is equivalent to a CUR matrix decomposition. Numerical results demonstrate the accuracy, efficiency and robustness of the new method for a diverse of problems.

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MS128

Numerical Solution of Poisson Partial Differential Equation in High Dimension Using Two-Layer Neural Networks

The aim of this work is to analyze numerical schemes using two-layer neural networks with infinite width for the resolution of the high-dimensional Poisson partial differential equation (PDE) with Neumann boundary condition. Using Barrons representation of the solution with a probability measure defined on the set of parameter values, the energy is minimized thanks to a gradient curve dynamic on the 2-Wasserstein space of the set of parameter values defining the neural network. Inspired by the work from Bach and Chizat, we prove that if the gradient curve converges, then the represented function is the solution of the elliptic equation considered. In contrast to previous works, the activation function we use here is not assumed to be homogeneous to obtain global convergence of the flow. Numerical experiments are given to show the potential of the method.

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MS128

The Rank-Reduced Kalman Filter: Approximate Dynamical-Low-Rank Filtering in High Dimensions

Inference and simulation in the context of high-dimensional dynamical systems remain computationally challenging problems. In this talk, we discuss a novel approximate Gaussian filtering and smoothing method, which propagates low-rank approximations of the covariance matrices. This is accomplished by projecting the Lyapunov equations associated with the prediction step to a manifold of low-rank matrices, which are then solved by dynamical low-rank integrator. Meanwhile, the update steps are made tractable by noting that the covariance update only transforms the column space of the covariance matrix, which is low-rank by construction. The algorithm differentiates itself from existing ensemble-based approaches in that the low-rank approximations of the covariance matrices are deterministic, rather than stochastic. Crucially, this enables the method to reproduce the exact Kalman filter as the low-rank dimension approaches the true dimensionality of the problem. Our method reduces computational complexity from cubic (for the Kalman filter) to quadratic in the state-space size in the worst-case, and can achieve linear complexity if the state-space model satisfies certain criteria. Through a set of experiments in classical data-assimilation and spatio-temporal regression, we show that the proposed method consistently outperforms the ensemble-based methods in terms of error in the mean and covariance with respect to the exact Kalman filter.

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MS128

Solving Schroedinger's Equation with Principle-driven Neural Network Methods

Part of the success of Machine Learning owes to the development of neural-networks, variational approximators that can efficiently represent unknown functions living in high-dimensional spaces. Recently, those techniques have been ported to the field of numerical physics and used to approximate inherently high dimensional objects such as the Many-Body Wave-Function [G. Carleo and M. Troyer, Science 355, 602 (2017)] or Density-Matrix [F Vicentini, A Biella, N Regnault, C Ciuti, Phys. Rev. Lett 122, 250503 (2019)] in an approach known as Neural-Network Quantum States. This Ab-Initio computational method is not data-driven, and is therefore more well behaved than standard machine learning algorithms. In this seminar I will discuss some advances in the field of Variational Monte Carlo that could have impact outside of that field: - First, i will discuss how we can compress exponentially-large positive-definite density operators in small neural networks by leveraging low-rank structures [F. Vicentini, R. Rossi and G. Carleo, ArXiV:2206.13488], and how we can use those structures to obtain the steady-state of open-quantum systems. - Second, I will discuss recent improvements to the Naturale Gradient Descent method that can enourmously lower the computational cost and make it viable for multi-million parameter neural networks [F. Vitteritti, R. Rende, et Al., arXiv:2310.05715].

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MS129

Hardware-Accelerated Stochastic Rounding for Floating-Point Arithmetic: Applications to DNN Training

Rounding errors pose a prominent challenge when performing floating-point computations. While there are some applications like DNN training that exhibit a certain tolerance to these errors, their ultimate impact can lead to substantial information loss. Within this setting, stochastic rounding has emerged as a particularly effective strategy for damping the effects of rounding errors (such as stagnation, in particular). Still, its efficient implementation in hardware is not obvious. In this talk we will present some recent results in designing efficient implementations of hardware floating-point stochastic rounding and look at their effect within dot product and matrix multiply operations during neural network training workflows.

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MS129

Subspace Embedding with Random KhatriRao Products and Its Application to Eigensolvers

Sketching provides a powerful dimensionality reduction tool for speeding up numerical linear algebra algorithms. Its effectiveness relies on the oblivious subspace embedding property (OSE) of the random test matrix, i.e., it is an approximate isometry for a low-dimensional space with high probability. In this study, we establish the OSE property of Khatri-Rao products formed from two standard Gaussian matrices. We show that for an arbitrary k-dimensional space, it is sufficient to take a number of columns proportional to $k^{3/2}$ to guarantee that it has the OSE property. Compared to an unstructured random matrix, the random Khatri-Rao product matrix yields advantages when multiplying with matrices that admit the Kronecker product structure. This advantage becomes evident through a contour-based eigensolver and a gradient-type eigensolver. Using the OSE property, we demonstrate how well the approximation overlaps with the target eigenspace after one iteration when using Khatri-Rao products of standard Gaussian matrices as an initial guess in the context of the contour-based eigensolver.

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MS129

Matrix-Free Multigrid with Surrogate Polynomials

Numerical simulations of extreme scale systems may lead to linear systems with trillions of unknowns. As an example, consider Earth mantle convection, modeled by Stokes equations with a resolution of 1km on the surface. Our finite element framework HyTeG (Hybrid Tetrahedral Grids) provides efficient, flexible data structures and highly scalable algorithms to handle such systems from a wide range of problems such as curl-curl, convection-diffusion and Stokes equations. To reduce the memory requirements, we employ matrix-free methods. Of course, repeated evaluation of bilinear forms leads to a substantial increase in operation count. To mitigate that, we make use of surrogate techniques: It can be shown that the system matrix can be approximated with sufficient accuracy by a set of polynomials. The efficient implementation of this approach requires special mesh structures. In HyTeG this is realized by using block structured, tetrahedral grids, resulting from subsequently refining an initially unstructured coarse grid. This not only provides an inherent hierarchy of nested grids for geometric multigrid solvers but also allows for various optimizations and automatically generated kernels. In particular, the local mesh structure allows defining surrogate operators where the evaluation of the coefficients can be performed with linear complexity with respect to the polynomial degree. We provide analysis as well as numerical examples to demonstrate the benefits of this approach.

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MS129

Ham: Hierarchical Approximate Maps

Obtaining a suitable, effective preconditioner is often a tall task – both theoretically and computationally. In many applications we face a *sequence* of linear systems

$$A_k \mathbf{x}_k = \mathbf{b}_k, \quad k = 1, 2, \ldots,$$

and obtaining a solid preconditioner for each of them *separately* is a harder task still, especially from the point of view of the computational costs. Moreover, the naive approach of calculating a powerful preconditioner P_1 for the first system ($k = 1$) and using it "as is' also for the subsequent ones ($k > 1$) usually leaves a lot to be desired. Here, we address this issue by using the so-called *preconditioner maps* that approximately map the consecutive systems ($k > 1$) back to the original one ($k = 1$) for which we already have an effective preconditioner. This idea has been already proposed before, but the new contribution here lies in the way this map is constructed. We use the hierarchical matrix formats (HODLR and HSS), proposing the so-called *Hierarchical Approximate Maps* for preconditioner updating to obtain efficient preconditioners also for the subsequent systems. We analyze these preconditioners using the pseudospectral bounds for GMRES and numerically investigate further directions to enhance these.

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MS130

Tensor Oriented Splitting of Exponential-Like Matrix Functions with Applications

In this talk, we present how to efficiently approximate actions of φ-functions for matrices K that have d-dimensional Kronecker sum structure, i.e., $K = A_d \oplus A_{d-1} \oplus \cdots \oplus A_1$. The technique is based on a suitable directional splitting of the exponential-like matrix functions, which allows for an efficient tensor oriented evaluation through Tucker operators. The implementation of such an approach is done by exploiting the high performance level 3 BLAS, which are available for many kinds of modern computer architectures. In the context of exponential integrators, the employment of the proposed technique allows for the efficient numerical integration of many stiff problems from the applications. In particular, in this presentation we show the results on two- and three-dimensional semidiscretized (systems of) Advection–Diffusion–Reaction equations, in comparison with state-of-the-art techniques.

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MS130

Computing the Square Root of a Low-Rank Perturbation of the Scaled Identity Matrix

We consider the problem of computing the square root of a perturbation of the scaled identity matrix, $A = \alpha I_n + UV^*$, where U and V are $n \times k$ matrices with $k \leq n$. This problem arises in various applications, including computer vision and optimization methods for machine learning. We derive a new formula for the pth root of A that involves a weighted sum of powers of the pth root of the $k \times k$ matrix $\alpha I_k + V^*U$. This formula is particularly attractive for the square root, since the sum has just one term when $p = 2$. We also derive a new class of Newton iterations for computing the square root that exploit the low-rank structure. We test these new methods on random matrices and on positive definite matrices arising in applications. Numerical experiments show that the new approaches can yield a much smaller residual than existing alternatives and can be significantly faster when the perturbation UV^* has low rank.

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MS130

Fast Monte Carlo Methods for Evaluating Matrix Functions

Many scientific problems can be expressed in matrix form and their direct solution often requires the calculation of some function over these matrices. Yet, most numerical methods developed so far struggle to evaluate these functions over large matrices due to very high computational requirements and the poor utilization of parallel resources. In this talk, we propose an alternative method based on Monte Carlo that randomly samples the rows and columns of the matrix as a way to approximate each term of the corresponding power series. We show that our approach converges much faster than other Monte Carlo methods and is particularly effective for determining the total communicability and the subgraph centrality of large complex networks.

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MS130

A New Legendre Polynomial Approach for Computing the Matrix Exponential

The solution of a linear autonomous ODE system can be expressed by a matrix exponential. An alternative method for solving such ODEs is based on a product that gener-

alizes the convolution, and it is known as the $\star$-product. A new approach, based on the Legendre discretization of the $\star$-product has been recently proposed. In this presentation, we propose a new method for computing the matrix exponential based on this approach. It enables us to find the matrix exponential efficiently. Our approach allows the ODEs solution to be expressed through a linear system that can be alternatively formulated as a matrix equation. We use a Krylov subspace model reduction approach to solve the matrix equation and compute the matrix exponential. We provide numerical results to demonstrate the effectiveness and efficiency of the new method.

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MT1

An Introduction to Randomized Algorithms in Linear Algebra and Scientific Computing

The goal of this tutorial is to give a high-level overview of the ways randomization can be used to speed up fundamental algorithms in linear algebra (with probabilistic guarantees of accuracy). Attendees should leave with a taste of the practical benefit of randomized algorithms, some idea of proof techniques, and starting points for further exploration. The tutorial will assume background in linear algebra but will cover the necessary results in probability theory. (1) Randomized Rangefinder and Randomized SVD: In many applications, we want to find a subspace that captures most of the information in a set of vectors (e.g. principal component analysis, manifold learning). If we stack the vectors into a matrix, this goal corresponds to capturing most of its range, i.e. the subspace spanned by its columns. We present the randomized range finder (RRF) and show how this technique can be leveraged to quickly approximate the SVD. (2) Randomized Least Squares: Approximating the solution of an overdetermined least squares problem is fundamental in both data science and statistics. Here we consider how sketching such a least squares problem can produce a smaller system that is easier to solve but still provides a solution close to that of the original problem. We focus on producing this sketch via row sampling according to a weighted probability distribution and give the associated guarantees on the sketched solutions accuracy.

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MT1

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MT2

Linear Algebra Challenges in Electronic Structure Simulations

In the physical sciences electronic structure simulations are an indispensable tool to provide an accurate description of electrons in matter from first principles. From a computational linear algebra perspective these simulations have a wealth of interesting structure: high-dimensional eigenvalue problems, non-linear eigenvalue problems, fixed-point problems, Riemannian optimization, nested problems, etc. Classical and new tools in linear algebra such as low-rank compression, randomized linear algebra methods or tensor methods have also been used to accelerate computations. The goal of this minitutorial is to provide a hands-on introduction to density-functional theory (DFT), the most widely employed electronic structure method. It is targeted at a general audience wanting to understand how interesting linear algebra problems arise from electronic structure simulations, and assumes no prior knowledge in quantum mechanics. The planned structure of the tutorial is as follows: - Introduction to electronic structure theory - DFT and its underlying non-linear eigenvector-dependent eigenvalue problem - Numerical setting and challenges of DFT: discretization, fixed-point problem and acceleration, eigensolvers - Hands-on session on getting and solving linear algebra problems from DFTK, a Julia-based toolkit for DFT - Open problems and future research directions

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MT2

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MT2

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MT3

A Hands-on Tutorial on lt;Tgt;LAPACK

The sustainability of legacy software libraries, in particular legacy numerical libraries, has been seriously deteriorated by several recent radical changes in microprocessor and system designs. These have rendered most legacy software infrastructure obsolete. The Linear Algebra PACKage (LAPACK) is a community standard for dense linear algebra and has been adopted and supported by a large community of users, computing centers, and high-performance computing (HPC) vendors. The lt;Tgt;LAPACK library is one proposal to close the gap between LAPACK and the new and emerging computing platforms. It uses C++ templates to provide (1) datatype-neutral algorithms, i.e., which work with single, double, half, and multiprecision types, but also, in some cases, more general sets like integer, rationals and complex; (2) different data layouts under a single interface, like column-major, row-major, banded layout, tiled layout, etc. In the long term, we hope that some of the framework of lt;Tgt;LAPACK could be used to develop new implementations of state-of-the-art numerical linear algebra libraries. In this tutorial, we prepare the audience to use and collaborate with lt;Tgt;LAPACK. We also present the modern C++ features that is rich in semantics without compromising performance.

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MT3

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MT3

A Hands-on Tutorial on lt;Tgt;LAPACK

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MT4

Petsc, the Portable Extensible Toolkit for Scientific Computations

PETSc, the portable extensible toolkit for scientific computations, is used as an algebraic backend in many scientific libraries around the world. It has been deployed on various architectures, from laptops to large exascale systems. In the tutorial, we will cover the basics of PETSc, first by describing its elementary classes, and then by providing examples, showcasing how it can be used to solve linear systems, using simple or more advanced preconditioners, with an emphasis on their connection with applied linear

algebra. We will also present some other advanced capabilities, for example, using its sister library SLEPc, the scalable library for eigenvalue problem computations, to solve eigenvalue problems or compute singular value decomposition. Most of these exemples will be implemented live, in either C, Fortran or Python, depending on the attendees preference.

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MT4

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MT5

Kirchoff Forests for Graph Linear Algebra

Much of graph theory revolves around a matrix called the "graph Laplacian". Tasks including community detection, signal denoising, centrality estimation, the computation of graph embeddings, etc. can all be framed in terms of computing certain quantities related to the Laplacian (its spectrum, its eigenvectors, its pseudo-inverse, etc.). In large graphs all these operations are cubic in the number of nodes, and in practice approximate algorithms are often necessary. Kirchoff forests are random processes on graphs that are strongly tied to the Laplacian (Avena & Gaudillire, 2018, Pilavci et al., 2021). They are easy and fast to simulate, and can be used to create stochastic estimators of various graph quantities. In this tutorial we aim to introduce Kirchoff forests as a tool for approximate computation in problems involving the graph Laplacian. For more information, an extended abstract is available at: https://hal.science/hal-04104124/document

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MT5

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PP1

Solving An Inverse Eigenvalue Problem via Discrete Integrable Systems

An inverse eigenvalue problem (IEP) is an important subject in numerical linear algebra. To construct a matrix with prescribed eigenvalues and a given structure is called the structured IEP (SIEP) [M. T. Chu and C. T. Golub, Inverse Eigenvalue Problem: Theory, Algorithms, and Applications, Oxford Univ., 2005]. A discrete integrable system is a discrete dynamical system which has explicit solutions. The author proposed algorithms for constructing band matrices with prescribed eigenvalues by using Toda-type discrete integrable systems (for example, [K. Akaiwa, A. Yoshida and K. Kondo, An improved algorithm for solving an inverse eigenvalue problem for band matrices, Electronic Journal of Linear Algebra, 38 (2022), 745–759] etc.). In this talk, we show how to solve an SIEP for matrices with a certain band structure via discrete integrable systems.

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PP1

Analyzing the Relationship Between Atmospheric Co2 and Ocean Heat Content

Our planet is currently facing a climate crisis largely associated with the increased use of fossil fuels over time causing an abundance of greenhouse gases, notably CO2, in the atmosphere. Examining the Keeling Curve shows an alarming result: there has been a steady increase in CO2 concentrations over time, greatly contributing to the Greenhouse House Gas Effect. This research investigates the role that CO2 plays in Ocean Heat Content (OHC) since the ocean is one of Earths biggest climate drivers and it also absorbs CO2. Through regression analysis, we uncovered a linear relationship between the yearly increase in OHC and the concentration of atmospheric CO2. This relationship can succinctly be described by a simple ODE model: $\frac{dy}{dt} \quad cx(t)$ where y represents OHC and x denotes CO2 concentrations measured in parts per million (ppm). Our findings underscore the intrinsic link between escalating CO2 levels and the rising OHC, emphasizing the need for comprehensive investigation. While this is ongoing research on the interaction between atmospheric CO2 levels and ocean heat content, this holds promise for advancing our understanding of climate change and may contribute

to the development of effective solutions.

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PP1

Modularity-Based Community Detection in Multiplex Networks by Balanced Total Variation Minimization

The unsupervised detection of communities, i.e., densely connected subsets of nodes is one of the most studied problems in network science and machine learning. We consider the popular approach of modularity maximization by its intrinsic linear algebraic formulation in terms of the modularity matrix. Recent works proved the equivalence of modularity maximization and the minimization of certain balanced graph cut and balanced graph total variation problems, which can be solved via gradient flows of suitable Ginzburg–Landau energy functionals. We generalize this approach to multiplex networks in which the same set of nodes is connected by different types of interactions represented by different network layers. We provide multiplex balanced total variation formulations for multiplex networks with and without edges across layers and discuss the efficient numerical solution of the corresponding graph Allen–Cahn equations by exponential integration and pseudo-spectral IMEX schemes.

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PP1

Preconditioned Low-Rank Riemannian Optimization for Multiterm Linear Matrix Equations

We focus on the development and analysis of Riemannian optimization methods for solving multiterm linear matrix equations, when the associated linear operator is symmetric positive definite. Assuming low-rank approximability of the solution, we employ first- and second-order Riemannian optimization algorithms on low-rank matrix manifolds. To enhance competitiveness with existing solvers on realistic problems, significant efforts are dedicated to developing efficient Riemannian preconditioners, which are interpreted as changing the Riemannian metric. By alternating between fixed-rank Riemannian optimization and rank updates, we devise a rank-adaptive algorithm that does not require fixing the rank a priori. In numerical experiments, we illustrate the effectiveness of the developed Riemannian preconditioners, comparing our approach with established solvers such as Conjugate Gradient with truncation. Results indicate that the Riemannian optimization approach, in both its fixed-rank and rank-adaptive variants, is competitive with other solvers and can avoid excessive growth of ranks in intermediate iterations.

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PP1

Numerical Methods for Fem-Bem Coupling

In simulations of the time-harmonic acoustic wave propagation, which is modeled by the Helmholtz equation, the domain in which the wave propagates is often unbounded, so that its direct discretization is not possible. In a homogeneous medium, this issue can be circumvented by reformulating the problem as an integral equation posed on the boundary, using Boundary Integral Operators. In practice, a domain is not homogeneous, but can often be split into a homogeneous subdomain and a heterogeneous one. In order to exploit this knowledge we want to solve the heterogeneous problem with the Finite Element Method (FEM) and the homogeneous one with the Boundary Element Method (BEM): it is known as FEM-BEM coupling. The linear system of the discretized problem involves a block matrix with sparse and dense blocks: such a problem is hard to precondition efficiently. In this poster, we establish a comparative study of several FEM-BEM coupling techniques using GMRES (classical or restarted), and explore some preconditioning strategies on either FEM blocks or BEM blocks, or on both simultaneously. In particular, we examine the number of iterations with increasing wavenumber for different obstacles and incident angles; we observe that, when using restarted GMRES, combined FEM-BEM couplings are more robust than classical coupling techniques, and that all couplings can become equivalent when preconditioning both FEM and BEM blocks.

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PP1

Double Randomized Generalized SVD Regularization Algorithm

Randomized algorithms are gaining more interest since they offer faster alternative to some of the standard numerical algorithms. Our focus is on creating randomized algorithms that are a replacement for the standard regularization algorithms which employ generalized singular value decomposition (GSVD). These standard algorithms can be effective in solving the ill posed inverse problem $\mathbf{Ax} = \mathbf{b}$, but they are also known for their slow execution time. In this work we present a new algorithm based on Tikhonov regularization that uses double randomized generalized SVD of the matrix pair $(\mathbf{A}, \mathbf{L})$. The matrix $\mathbf{L}$ denotes the discrete version of the first derivative operator. Double randomization produces smaller scale inverse problem than single randomization, leading to a faster algorithm. We will show different strategies for selecting the parameters ℓ_1 and ℓ_2, inherent in the randomized algorithm, and their influence on the accuracy of the regularized solution. Our new algorithm is compared to standard one and tested in numerical simulation on the inverse problem where the singular values of matrix $\mathbf{A}$ decay slowly.

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PP1

The Semi-Positive Tensors and Associated Special Structured Tensors

In multi-linear algebra, several topics have attracted considerable attention in recent years. Tensors generalize the concept of matrices in linear algebra. In this context, the term tensor refers to a hyper-matrix or a multi-dimensional array. Here, special structured tensors play a significant role. The class of (strictly) semi-positive tensors is a generalization of the class of (strictly) copositive tensors, which contains (positive) nonnegative tensors. The construction and detection challenge is one of the main concerns with strictly semi-positive and semi-positive tensors. To move closer to our aim of constructing a new characterization of (strictly) semi-positive tensors, we found it useful to extend the idea of almost (strictly) semimonotone matrices (which has been extensively investigated in the field of linear complementarity) to tensors. We provide insights into the characteristics of the entries within these tensors, and we explore some interesting tensor theoretic properties of these special structured tensors. Besides the significance of (strictly) semi-positive tensors in matrix analysis, the class of (strictly) semi-positive tensors plays an important role in the theory of the tensor complementarity problem. We provide examples to support our results.

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PP1

Contractive Systems Improve Graph Neural Networks Against Adversarial Attacks

Graph Neural Networks (GNNs) have established themselves as a key component in addressing diverse graph-based tasks. Despite their notable successes, GNNs remain susceptible to input perturbations in the form of adversarial attacks. This paper introduces an innovative approach to fortify GNNs against adversarial perturbations through the lens of contractive dynamical systems. Our method introduces graph neural layers based on differential equations with contractive properties, which, as we show, improve the robustness of GNNs. A distinctive feature of the proposed approach is the simultaneous learned evolution of both the node features and the adjacency matrix, yielding an intrinsic enhancement of model robustness to perturbations in the input features and the connectivity of the graph. We mathematically derive the underpinnings of our novel architecture and provide theoretical insights to reason about its expected behavior. We demonstrate the efficacy of our method through numerous real-world benchmarks, reading on par or improved performance compared to existing methods.

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PP1

CPFloat: A C Library for Simulating Low-Precision Arithmetic

CPFloat is a header-only C library that offers efficient routines for rounding arrays of binary32 or binary64 numbers to lower precision. The library is distributed as free software, is fully documented, is accompanied by a comprehensive test suite, and is hosted on GitHub. The repository also contains a MEX interface for MATLAB and Octave, and an object-oriented interface for C++. The library implements a variety of rounding modes: round-to-nearest with several tie-breaking rules, directed rounding, two variants of stochastic rounding, and round-to-odd. Any format that can fit into binary64 is supported, but if round-to-nearest is used then only formats with up to 26 digits of precision are recommended, as these are immune from double rounding. The underlying techniques exploit the bit level representation of these formats, and perform only low-level bit manipulations and integer arithmetic without relying on costly library calls. In numerical experiments the new techniques bring a considerable speedup (typically one order of magnitude or more) over existing C/C++ alternatives, such as GNU MPFR and the FloatX library. To the best of our knowledge, CPFloat is currently the most efficient and complete library for rounding floating-point numbers to a custom low-precision format.

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PP1

Adaptive Mesh Refinement with Quantum Computing

High precision electromagnetic simulations are time and resource consuming. Adaptive mesh refinement allows to allocate these resources in a smart way by concentrating the degrees of freedom where they will have the most impact on the accuracy of the solution. We consider solving the time Harmonic Maxwell equations in a cavity with an obstacle. To this end, a mesh adaptation loop is implemented where the problem is solved on more and more refined meshes. A well-chosen *a posteriori* estimate allows to choose which areas must be refined. The question addressed by this work is how quantum computing can be included in a mesh adaptation loop. It is assumed that each linear system is solved by the HHL (Harrow, Hassidim, and Lloyd) algorithm so that the solution is encoded in the amplitudes of a quantum state. This state is then sampled with amplitude amplification as proposed by Montanaro to obtain an approximated estimate of the field in a classical register. It is then possible to compute a posteriori estimates from these values. We study the impact of the fields uncertainties on the convergence rate of the

mesh adaptation loop.

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PP1

An Optimal Error Bound for Shiftedcholeskyqr3 in Oblique Inner Product

The shiftedCholeskyQR3 algorithm has been proposed as an optional choice of the orthogonalization algorithms recently. We extend the error analysis result for oblique inner product and show that the new error bound is optimal. We also discuss the loss of orthogonality and verify our conclusions through numerical experiments.

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PP1

Subspace Acceleration for a Sequence of Linear Systems and Application to Plasma Simulation

We present an acceleration method for sequences of large-scale linear systems, such as the ones arising from the numerical solution of time-dependent partial differential equations coupled with algebraic constraints. We leverage the subspace containing the history of solutions computed at previous time steps in order to generate a good initial guess for the iterative solver. In particular, we propose a novel combination of reduced-order projection with randomized linear algebra techniques, which drastically reduces the number of iterations needed for convergence. The accuracy of the initial guess produced by the reduced-order projection is analyzed when the coefficients of the linear system depend analytically on time, showing that it improves rapidly as the size of the history increases. The developed method is applied to the simulation of plasma turbulence in the boundary of a fusion device, showing that the time needed for solving the linear systems is significantly reduced.

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PP1

Randomized Simultaneous Diagonalization Via Congruence of Symmetric Matrices

A family of symmetric matrices A is Simultaneously Diagonalizable via Congruence (SDC) if A = Ak = V DkV T d k=1 where Dk is diagonal and V is invertible, we consider the task of Simultaneous Diagonalization via Congruence that computes an invertible matrix that diagonalizes every matrix in the family by congruence. In this work, we propose and analyze randomized Simultaneous Diagonalization via Congruence (RSDC) for performing this task. RSDC only diagonalizes two random linear combinations of the matrices via congruence. Unlike existing optimization-based methods, RSDC is simple to implement and leverages existing highquality linear algebra software packages. Our main novel contribution is to prove the exact and robust recovery: Given an SDC family, RSDC diagonalizes every matrix in the family with probability 1. Given a family that is ?-close to an SDC family, RSDC diagonalizes this family via congruence, with high probability, up to an error of norm O(?) in the first order. We also discuss how the algorithm can be further improved by optimization and demonstrate its state-of-the-art performance by numerical experiments with synthetic and real-world data.

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PP1

Optimization of Approximate Maps for Linear Systems Arising in Discretized PDEs

Generally, discretization of partial differential equations (PDEs) creates a sequence of linear systems $A_k x_k = b_k, k = 1, 2, ..., N$ with structured sparsity patterns. When solving these linear systems using iterative solvers, we can use preconditioner updates instead of computing preconditioners for each system from scratch. One such preconditioner update is the Sparse Approximate Map (SAM) (Carr et al., 2021), which is based on the sparse approximate inverse preconditioner using a least squares approximation and maps one matrix in the sequence to another nearby one for which we have an effective preconditioner. To efficiently compute these preconditioner updates, we seek to compute an optimal sparsity pattern. In this poster, we examine several sparsity patterns for computing the SAM update in an effort to characterize optimal or near-optimal sparsity patterns for linear systems arising from discretized PDEs. These sparsity patterns should allow for enough nonzeros to compute an accurate enough map efficiently. We focus our attention on level 1 and level 2 neighbors in the graph representation of the matrices A_k based on analysis in (Chow, 2000), as well as an element-wise analysis on the difference matrix between two nearby matrices e.g., k^{th} and $(k-1)^{st}$ matrix. We extend the existing analysis to show that if our sequence of linear systems satisfies simple subset assumptions, we can characterize properties of the sparsity pattern of the exact map.

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PP1

Fast Eigenvalue Decomposition of Arrowhead and Diagonal-Plus-Rank-k Matrices of Quaternions

Quaternions are a non-commutative associative number system that extends complex numbers, first described by Hamilton in 1843. We present algorithms for solving the eigenvalue problem for Arrowhead and DPRk (diagonal-plus-rank-k) matrices of quaternions. The algorithms use the power method, Rayleigh quotient iteration (RQI), and modified Rayleigh quotient iteration (MRQI) combined with the Wielandt deflation technique, and the fact that the eigenvector matrices have Cauchy-like structure. The algorithms require $O(n^2)$ floating-point operations, n being the order of the matrix. The algorithms are elegantly implemented in Julia, using its polymorphism feature. The code, along with examples, is available on GitHub.

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PP1

Heuristics for Robust Factorization of Sparse Symmetric Indefinite Matrices

Efficiently factorizing sparse symmetric and indefinite matrices into triangular factors requires exploiting symmetry and preserving sparsity as much as possible. However, numerical pivoting, which can adversely affect symmetry, is required to ensure stability. In Cholesky factorization, which works for symmetric positive definite matrices, the use of supernodes enables attaining high performance. A supernode consists of columns that have essentially the same sparsity pattern. In this work, we exploit the techniques developed for the factorization of sparse symmetric positive definite matrices and make use of the supernodal structure. We attempt to limit numerical pivoting within the diagonal block of a supernode, since interchanging columns and rows within the diagonal block does not affect sparsity. Our pivoting strategy is based on the Bunch-Kaufman algorithm, which is designed for dense matrices. If a good pivot cannot be found in the current supernode, we delay the column to the parent supernode. Before delaying a column, we relax the conditions and re-test the column to keep the fill-in low at the expense of decreasing stability. Experiments show that the proposed algorithm has an error rate comparable to that of the Bunch-Kaufman algorithm. We also show that the proposed algorithm achieves more accurate results while generating less fill-in compared to state-of-the-art sparse factorization algorithms.

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PP1

Algorithms for Boolean Matrix Factorization Using Integer Programming

Boolean matrix factorization (BMF) approximates a given binary input matrix as the product of two smaller binary factors. As opposed to binary matrix factorization which uses standard arithmetic, BMF uses the Boolean OR and Boolean AND operations to perform matrix products. This leads to factors being more flexible, as the support sets of each rank-1 factor do not need to be disjoint anymore, as well as lower reconstruction errors. In this work, we first show an alternating optimization (AO) strategy that solves the subproblem in one factor matrix in BMF using an integer program (IP). To solve integer programs, we utilize the mixed integer programming (MIP) software, Gurobi. When solving for each factor, we show in detail how we transform the initial non-linear matrix least squares problem into a convex quadratic optimization problem with linear constraints over binary variables, so we can use the solver. We also provide two ways to initialize the factors within AO. Then, we show how several solutions of BMF can be combined optimally using another IP. This allows us to come up with a new algorithm: it generates several solutions using AO and then combines them in an optimal way. We then explore the performance of our algorithms on real world binary data sets. Our experiments also consider data sets that contain missing entries. We show that our algorithms outperform the state of the art on medium-scale problems.

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PP1

The I/O Requirements of Various Numerical Linear Algebra Kernels

When designing an algorithm, one cares about arithmetic/computational complexity, but data movement (I/O) complexity is playing an increasingly important role that highly impacts performance and energy consumption. The objective of I/O complexity analysis is to compute, for a given program, its minimal I/O requirement among all valid schedules. We consider a sequential execution model with two memories, an infinite one, and a small one of size S on which the computations retrieve and produce data. The I/O is the number of reads and writes between the two memories. From this model, we review various Numerical Linear Algebra kernels that are increasingly complicated from matrix-matrix multiplication, to LU factorization, then to symmetric rank-k update, to Cholesky factorization, then to Modified Gram-Schmidt to Householer QR factorization. We will show pratical examples of these results too.

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PP1

An Aggressive Shrinkage Technique for Block

Eigensolvers

In block eigenvalue algorithms, such as the subspace iteration algorithm and the locally optimal block preconditioned conjugate gradient (LOBPCG) algorithm, larger block sizes are often employed to achieve more robust and faster convergence. However, larger block sizes also lead to an increase in computational cost. Traditionally, the block size is only reduced after convergence of some eigenpairs, known as deflation. In this work, we propose a non-deflation-based, more aggressive technique where the block size is adjusted dynamically during the algorithm. This technique can be widely applied to most block eigenvalue algorithms, reducing computational cost without compromising convergence speed. We present three adaptive strategies for adjusting the block size and apply them in four well-known eigenvalue solvers as examples. Theoretical analysis and numerical experiments are provided to illustrate the efficiency of the proposed technique. In practice, an overall acceleration by 20% to 30% is observed.

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PP1

Mixed Precision Algorithms for Symmetric Eigenvalue Problems

In this work, we consider to use mixed precision idea to accelerate algorithms for the symmetric eigenvalue problem. For dense problem, we propose a mixed precision Jacobi algorithm for computing the SVD. After appropriate preconditioning, the proposed algorithm computes the SVD in lower precision as an initial guess, and then performs one-sided Jacobi rotations in working precision as iterative refinement. By carefully transforming a lower precision solution to a working precision one, our algorithm achieves about 2× speedup on the x86-64 architecture compared to the usual one-sided Jacobi SVD algorithm in LAPACK, without sacrificing the accuracy. We propose a mixed precision variant of LOBPCG, for computing a few smallest eigenpairs of a large Hermitian positive definite matrix A, that uses a (sparse) Cholesky factorization of A computed in lower precision as the preconditioner. To further enhance performance, a mixed precision orthogonalization strategy is proposed. To analyze the impact of reducing precision in the preconditioner on performance, we carry out a rounding error and convergence analysis of PINVIT, a simplified variant of LOBPCG. Our theoretical results predict and our numerical experiments confirm that the impact on convergence remains marginal. In practice, our mixed precision LOBPCG algorithm typically reduces the computation time by a factor of 1.4–2.0 on both CPUs and GPUs.

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PP1

Optimization of a Lattice Spring Model with Elastoplastic Conducting Springs: A Case Study

We consider a simple lattice spring model in which every spring is elastoplastic and is capable to conduct current. The elasticity bounds of spring i are taken as $[-c_i, c_i]$ and the resistance of spring i is taken as $1/c_i$, which allows us to compute the resistance of the system. The model is further subjected to a gradual stretching and, due to plasticity, the response force increases until a certain terminal value. We demonstrate that the recently developed sweeping process theory can be used to optimize the interplay between the terminal response force and the resistance on a physical domain of parameters c_i. The proposed methodology can be used by practitioners for the design of multi-functional materials as an alternative to topological optimization. In this way we introduce a simple conceptual model for the design of optimal multi-functional materials. We stick to a particular feasible domain of parameters c_i for which a formula for the terminal response force has been recently obtained in the literature over a sweeping process approach.

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PP1

Spectral Analysis of Random Geometric Graphs

Random geometric graphs have been recently used as a model of spatial networks for various real-world applications. In this work, we combine theoretical analyses and computational techniques to study the spectral properties of random geometric graphs. In particular, we study how the connectivity and Hamiltonicity of random geometric graphs affect their spectral properties. Numerical simulations on a large variety of random geometric graphs in different spaces are presented.

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PP1

LibHSL: the Ultimate Collection for Large-Scale Scientific Computation

The Harwell Subroutine Library (HSL) is a renowned suite of efficient and robust numerical algorithms designed to tackle complex mathematical problems such as solving sparse linear systems or computing eigenvalues and eigenvectors of sparse matrices. LibHSL is a comprehensive collection of HSL packages that facilitates their integration into C, Fortran or Julia projects. One of the notable features of libHSL is its innovative compilation system based on Meson. The new build system not only significantly

accelerates compilation, but also ensures portability across multiple operating systems. To further streamline the user experience, libHSL provides a precompiled version called HSL_jll.jl, specifically designed for the Julia ecosystem. This eliminates the need for users to compile anything on their local machines, offering ready-to-use functionality right away.

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PP1

Tensor Train Decomposition for Primal Methods in Global Polynomial Optimization

In global optimization of polynomials one can either solve the associated relaxed semi-definite programming on the moments or consider the primal problem based on finding a sum-of-squares relaxation. The latter approach allows to use augmented Lagrangian methods to solve the constrained optimization task. Both methods, the moments approach and the sum-of-squares approach, scale combinatorial in the space dimension of the polynomial. However, in many application the objective functions have some additional structure, for example the number of variables involved in the monomials. We propose to use a Tensor Train operator parametrization of a subset of the sum-of-squares polynomials in combination with an Alternating Direction Method of Multipliers on low-rank tensors to provide lower bounds for the minimum of polynomial optimization while avoiding the combinatorial scaling. We illustrate the resulting algorithm by numerical examples in medium to high-dimensions.

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PP1

Searching for Cyclic-Invariant Fast Matrix Multiplication Algorithms

Fast matrix multiplication algorithms correspond to exact CP decompositions of tensors that encode matrix multiplication of fixed dimensions. This 3-way matrix multiplication tensor M has cyclic symmetry: the entry values are invariant under cyclic permutation of the indices. The CP decomposition of Strassens original fast matrix multiplication algorithm for 2x2 matrices is cyclic invariant, and cyclic invariant decompositions are known to exist for 3x3 and 4x4 matrix multiplication as well. Cyclic invariance means a cyclic permutation of the CP factors results in the same CP components, just in a different order. We describe how to search for these solutions, which involve one third of the variables of generic solutions, using the damped Gauss-Newton optimization method along with heuristic rounding techniques, and we summarize the algorithms discovered so far.

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PP1

Convergence Study of Gmres for Helmholtz Problems Close to Resonance

The iterative solution of linear systems resulting from the finite element discretization of time-harmonic wave propagation problems (e.g. Helmholtz problems) can be numerically expensive. This is especially the case for problems with phenomena close to resonance, where the convergence behavior can be difficult to interpret. Our goal is to interpret of the properties of the system matrix in relation to convergence of Krylov-type iterative methods. Results from the literature use the notions of conditioning, spectrum, pseudo-spectrum, numerical range, Ritz values and Harmonic Ritz values. In this study, we use numerical experiments to identify the factors that delay convergence, in relation to the initial time-harmonic problems, in order to propose appropriate acceleration strategies.

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PP1

A Conceptual Model for Permafrost Thawing: a Numerical Solution Scheme

Permafrost thaw, driven by climate change, releases stored carbon, intensifying the global climate crisis. Our poster introduces a conceptual model, combining principles from planetary energy balance and heat equation to estimate carbon emissions from degrading permafrost. Our research develops a robust framework, presenting a conceptual model with complex feedback mechanisms and specific boundary conditions to describe the degradation process. We devise a numerical solution scheme, a method of lines, for a linear system of ordinary differential equations. We address stiffness with a modified scheme. We perform a detailed parameter using least squares approximation.

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PP1

A Pinn Approach to Linear Eigenvalue Problems with Non-Trivial Boundary Conditions

Recently, machine learning based techniques for solving differential equations in a mesh-free manner have experienced an increase in attention. These so called physics informed neural networks (PINN) have been applied to various problems in engineering and physics, such as forward and inverse problems in electromagnetism, and optical waveguide design. Traditional methods of simulating waveguides, like the finite element method, use a perfectly matched layer (PML) to efficiently obtain free-space solutions from a finite simulation domain. PINNs, on the other hand, can be equipped with any mathematical function representing boundary conditions (BC) as a soft constraint in the loss term. This keeps the opportunity to implement a PML, but a proper choice of BCs can be used to make this obsolete by solving an eigenvalue-dependent boundary value problem in a self-consistent way. To showcase this approach, we employ Sommerfeld BCs to a one-dimensional slab waveguide and use PINNs to solve the resulting hermitian eigenvalue problem. This optimization problem solely relies on satisfying the differential equation and boundary conditions on a set of collocation points. Hence, the approach is unsupervised and no expensive data preparation has to be performed. As the eigenpair varies insignificantly with respect to a small variation of the wavelength, an already converged PINN can be used as the starting point for a new simulation to efficiently obtain the waveguide dispersion.

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PP1

Householder Orthogonalization with a Non-Standard Inner Product

Householder orthogonalization plays an important role in numerical linear algebra. It attains perfect orthogonality regardless of the conditioning of the input. However, in the context of a non-standard inner product, it becomes difficult to apply Householder orthogonalization, partly due to the lack of an initial orthonormal basis. We propose strategies to overcome this obstacle and discuss algorithms and variants of Householder orthogonalization with a non-standard inner product. Theoretical analysis and numerical experiments demonstrate that our approach is numerically stable under mild assumptions.

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PP1

The Twisted Factorization Method with Preprocessing Based on Cyclic and Stride Reductions in Eigenvector Computations

The Twist factorization method is a known technique for computing eigenvectors of symmetric tridiagonal matrices. The cyclic and stride reductions are techniques for solving equations of linear systems with tridiagonal matrices. In this poster, we propose a twist factorization method employing cyclic and stride reductions as a preprocessing to compute the eigenvectors of symmetric tridiagonal matrices.

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PP1

Coded Computing for Fault-Tolerant Parallel Qr Decomposition

QR decomposition is an essential operation for solving linear equations and obtaining least-squares solutions. In high-performance computing systems, large-scale parallel QR decomposition often faces node faults. We address this issue by proposing a fault-tolerant algorithm that incorporates 'coded computing' into the parallel Gram-Schmidt method, commonly used for QR decomposition. Coded computing introduces error-correcting codes into computational processes to enhance resilience against intermediate failures. While traditional coding strategies cannot preserve the orthogonality of Q, recent work has proven a post-orthogonalization condition that allows low-cost restoration of the degraded orthogonality. In this paper, we construct a checksum-generator matrix for multiple-node failures that satisfies the post-orthogonalization condition and prove that our code satisfies the maximum-distance separable (MDS) property with high probability. Furthermore, we consider in-node checksum storage setting where checksums are stored in original nodes. We obtain the minimal number of checksums required to be resilient to any f failures under the in-node checksum storage, and also propose an in-node systematic MDS coding strategy that achieves the lower bound. Extensive experiments validate our theories and showcase the negligible overhead of our coded computing framework for fault-tolerant QR decomposition.

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PP1

Efficiently Computing Solutions to Matrix Equations in MATLAB and Octave

Matrix equations such as Lyapunov, Sylvester and Riccati equations are essential tools throughout the disciplines. They occur in many different variants and sizes, and it is of particular importance to obtain numerical solutions to these equations in an efficient and reliable way. On this poster, we present two free and open source toolboxes that provide the computational backend for the solution of small, medium and large-scale matrix equations in MathWorks MATLAB and GNU Octave. The MORLAB, Model Order Reduction LABoraty, toolbox utilizes spectral projection as well as Newton methods for the solution of small and medium-scale matrix equations, while the M-M.E.S.S., Matrix Equations Sparse Solvers, library is well suited for

equations with large-scale sparse coefficient matrices.

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PP1

A Fortran Idr(s) Package for Solving Nonsymmetric Linear Systems

IDR(s) is a fast and robust Krylov method for solving large nonsymmetric systems of linear equations $Ax = b$. It uses short recurrences of depth $s + 2$. For $s = 1$, the method is equivalent with BiCGSTAB, while for larger s the convergence becomes increasingly closer to that of GMRES. After its first introduction in 2008, several new variants have been proposed. These include a variant based on quasi-minimisation, a flexible method that allows varying preconditioners, specialised methods for simultaneously solving shifted systems for multiple shifts, and recycling techniques to speed-up the solution of sequences of linear systems. We have brought all these variants together in one software package written in modern Fortran. The package strictly conforms to the Fortran 2018 standard and does not require external libraries. Parallelisation is done using co-array Fortran, which is part of the standard. The package comes with a set of polynomial preconditioners. Other preconditioners are easy to incorporate. A user-supplied matrix-vector multiplication routine is all that is needed for the package to work. Moreover, interfaces are provided for matrices in matrix-market and in CRS format. The package comes with many examples to illustrate its use. These examples also illustrate the excellent performance of IDR(s).

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