Preface

Systems of linear algebraic equations are ubiquitous in mathematical modeling and scientific computing, and iterative methods are indispensable for the numerical treatment of such systems. What makes iterative solvers so efficient, and what has maintained their state-of-the-art status for almost half of a century? Foremost, these are the optimality property of the Krylov subspaces, which define iterations, and the concept of preconditioning, which gives the approach flexibility and imbues it with mathematical ideas from various fields of applications.

Iterative methods for linear algebraic systems comprise a rapidly developing field of research. The growing variety of applications makes even a nearly complete review of existing preconditioning techniques an overwhelming task. This book gives a mathematically rigorous, consistent introduction to the fundamental and most popular Krylov subspace iterative methods. We review the theory of the Krylov subspaces, including the optimality property, and introduce iterative algorithms following the classic minimization approach. Our analysis of the Krylov subspace methods is concise and rigorous, covering convergence bounds in terms of optimal polynomials, matrix resolvents, numerical range, logarithmic potentials, and alternative estimates. The preconditioning is naturally tied to specific classes of matrices and particular applications which lead to linear systems of equations. We restrict ourselves to the structured (Toeplitz) matrices and to large sparse matrices arising from discretizations of partial differential equations.

The book consists of five chapters. Chapter 1 starts with necessary preliminaries and reviews basic iterative methods. Further, we introduce the Krylov subspaces and prove an important optimality result. Fundamental Krylov subspace methods are defined and considered from algebraic, geometrical, and nonlinear optimization viewpoints. This is followed by the comprehensive convergence analysis of the Krylov subspace methods in a general case and the case of Hermitian matrices. Besides classical estimates, several special topics important in practice are considered, including superlinear convergence and inexact iterations. When we apprehend what properties of the coefficient matrix account for the rate of convergence, we may multiply the original system by some nonsingular matrix, called a *preconditioner*, so that the new coefficient matrix possesses better properties. Chapter 1 closes with a simple observation, which motivates much of the subsequent discussion: any linear consistent iteration defines a preconditioner.

In Chapter 2, we introduce a class of Toeplitz matrices, review their basic properties, and study preconditioners for this class of structured matrices. Chapter 3 deals with multigrid (MG) preconditioners for systems of linear algebraic equations arising from discretizations of partial differential equations. For reference purposes, we review basic principles of a finite element method, taking a two-point boundary value problem and the Poisson equations as model examples. Classic geometric MG preconditioners, in particular, V- and W-cycles are introduced, and a complete analysis is given in the framework of smoothing and approximation properties. Two-dimensional Poisson equations discretized by a conforming finite element method serve to illustrate the convergence analysis. However, less standard situations of nonconforming discretizations and problems without full regularity are also addressed.

Chapter 4 describes preconditioners based on space decompositions. These are multilevel, hierarchical basis, and domain decomposition (including alternating Schwarz, additive Schwarz, and nonoverlapping domains) preconditioners. These preconditioners are analyzed in a uniform framework of space decomposition methods. As in Chapter 3, we use the example of the discrete Poisson equations to apply a general analysis. More examples are collected in Chapter 5, where, we show how the ideas and techniques from the previous chapters apply to the numerical solution of many practical problems. Most of these problems primarily arise in computational physics. Such selection exclusively reflects the authors' own experience and does not indicate any limitation on applicability or efficiency of preconditioned Krylov subspace solvers in other areas of scientific computing.

We believe this book is a useful addition to many excellent texts on iterative methods of linear algebra and their applications, including those by Axelsson [9], Bramble [35], Greenbaum [89], Hackbusch [96, 97], Liesen and Strakoš [131], Marchuk and Kuznetsov [141], Saad [173], Shaidurov [181], Trottenberg, Oosterlee, and Schuller [196], and Varga [210]. It complements other textbooks with its comprehensive and consistent analysis, yet it is still accessible to students with only basic knowledge of linear algebra and calculus. The book includes several topics on Krylov subspace solvers rarely available in texts on numerical linear algebra. Besides this, it also contains all essentials of the multigrid and space decomposition preconditioners via elementary mathematical tools. The final chapter collects many examples of important applications, where the techniques and analysis of previous chapters result in remarkably efficient practical solvers. Most of the material from this chapter had been previously found only in the form of journal publications.

Although the text includes several advanced topics, we strived to achieve a textbook-level of exposition, rather than to write a research monograph. The material included in the book was used by the authors to teach courses on numerical linear algebra and special topics at Moscow State University, the Moscow Institute of Physics and Technology, and the University of Houston, and to give shorter series of lectures at the graduate level. Our teaching experiences and personal tastes largely determined the style of presentation and the topics selection. We complement each section of the book with a list of exercises. Solving these problems is recommended, though not mandatory, for a better understanding the text.

Tribute to Chebyshev and Krylov

Numerical linear algebra owes a lot to the great Russian mathematicians Pafnuty Lvovich Chebyshev (1821–1894) and Alexei Nickolaevich Krylov (1863–1945). In this text on iterative solvers, these two important names can be found in many instances, and we take this opportunity to remember a part of their scientific legacy.

Pafnuty Chebyshev is often considered the founding father of the Russian mathematic school. The marvelous Chebyshev polynomials are defined as monic polynomials on a closed interval with minimal deviation from zero. They appeared in his original memoir of 1857 in French under the title "Sur les questions de minima qui se rattachent á la représentation approximative des fonctions" and were published in the journal *Memoirs of the Imperial Academy of Sciences*, St. Petersburg. Chebyshev's polynomials are recognized as a major milestone that ushered in the beginning of approximation theory. They are essential for the convergence analysis of iterative methods for systems of algebraic equations.

Alexei Krylov was a naval engineer and applied mathematician. He claimed that shipbuilding was his primary profession, or, better to say, the application of mathematics to various questions of maritime science. In linear algebra, the name of Alexei Krylov is given to a special sequence of subspaces in $\mathbb{C}^n$, which is fundamental in most practical numerical methods pervasive in applications, such as conjugate gradient (CG), generalized minimal residual (GMRES), Lanczos bidiagonalization algorithm, etc.

The Krylov subspaces were first introduced in 1931 in the paper "On numerical solution of the equation of technical sciences for frequencies of small oscillations in material systems." In this paper, Alexei Krylov introduced a method for computing the coefficients of characteristic polynomials of matrices. Krylov's idea was to reduce the equation

$$\det(A^T - \lambda I) = \det \begin{bmatrix} a_{11}-\lambda & a_{21} & \dots & a_{n1} \\ a_{12} & a_{22}-\lambda & \dots & a_{n2} \\ \dots & \dots & \dots & \dots \\ a_{1n} & a_{2n} & \dots & a_{nn}-\lambda \end{bmatrix} = 0 \tag{1}$$

to a more computationally affordable form

$$\det \begin{bmatrix} b_{11}-\lambda & b_{21} & \dots & b_{n1} \\ b_{12}-\lambda^2 & b_{22} & \dots & b_{n2} \\ \dots & \dots & \dots & \dots \\ b_{1n}-\lambda^n & b_{2n} & \dots & b_{nn} \end{bmatrix} = 0. \tag{2}$$

He obtained (2) from (1) by a few simple transformations of the equations

$$\begin{aligned} \lambda x_1 &= a_{11}x_1 + a_{21}x_2 + \dots + a_{n1}x_n, \\ \lambda x_2 &= a_{12}x_1 + a_{22}x_2 + \dots + a_{n2}x_n, \\ &\dots \\ \lambda x_n &= a_{1n}x_1 + a_{2n}x_2 + \dots + a_{nn}x_n. \end{aligned}$$

The first step is the multiplication of the first equation by λ and replacing $\lambda x_1, \dots, \lambda x_n$ with the right-hand sides of the original equations. The second step is the multiplication of the new equation by λ and the substitution as previously, and so on. In this way, one obviously finishes with the equation of the required form (2). Denote by $b_1, \dots, b_n$ the column vectors built of the coefficients of the rows of the final equations

$$\begin{aligned} \lambda\, x_1 &= b_{11}x_1 + b_{21}x_2 + \dots + b_{n1}x_n, \\ \lambda^2 x_1 &= b_{12}x_1 + b_{22}x_2 + \dots + b_{n2}x_n, \\ &\dots \\ \lambda^n x_1 &= b_{1n}x_1 + b_{2n}x_2 + \dots + b_{nn}x_n. \end{aligned}$$

Let A be a matrix with the entries a_{ij}. Then it is not difficult to see that

$$b_1 = Ar_0, \quad b_2 = A^2 r_0, \quad \dots, \quad b_n = A^n r_0, \quad \text{where} \quad r_0 = [1, 0, \dots, 0]^T.$$

For any r_0, the vectors $r_0, Ar_0, \dots, A^k r_0$ are now called the *Krylov vectors*, and their linear spans for different k are known as the *Krylov subspaces* generated by r_0 and A.

Equation (1) is equivalent to (2) if the Krylov vectors $r_0, Ar_0, \dots, A^{n-1} r_0$ are linearly independent. If they are not, then the method appears useless at first glance. This is not true, however: Let

$$L_k := \operatorname{span}\{r_0, Ar_0, \dots, A^{k-1} r_0\},$$

and suppose that

$$\dim L_k = \dim L_{k+1} = k.$$

Then L_k is an invariant subspace with respect to A, and the method allows one to obtain the coefficients of a polynomial which is a divisor of the characteristic polynomial. More precisely, one can find the minimal polynomial for a restriction of the matrix A on L_k, and with an appropriate choice of r_0, it is always possible to get the minimal polynomial for A in the whole space; see [74].

In the modern analysis of iterative methods, the names Chebyshev and Krylov both are important and naturally stand close, because the Krylov vectors are *intrinsically linked with polynomials*. To realize this, consider a linear algebraic system $Ax = b$ with a symmetric positive definite matrix A. Then the CG method, with an initial guess x_0, constructs the Krylov subspaces L_k for $r_0 := b - Ax_0$ and defines the kth iterate x_k such that it solves the minimization problem

$$||b - Ax_k||_{A^{-1}} = \min_{x \in x_0 + L_k} ||b - Ax||_{A^{-1}},$$

where

$$||x||_{A^{-1}} := \sqrt{(A^{-1}x, x)}.$$

Obviously, for any $x_k \in x_0 + L_k$ we have $r_k = f_k(A) r_0$, with $f_k \in F_k$, where F_k is the set of all polynomials of degree bounded by k and with the zero order term equal to 1, i.e., $f_k(0) = 1$. From the above minimization property,

$$||b - Ax_k||_{A^{-1}} \le \min_{f_k \in F_k} ||f_k(A) r_0||_{A^{-1}} \le \min_{f_k \in F_k} \max_{m \le \lambda \le M} |f_k(\lambda)| \, ||r_0||_{A^{-1}},$$

where m and M are the minimal and maximal eigenvalues of A. Looking for the minimum of the right-hand side, one inevitably resorts to the Chebyshev polynomials. This is the standard way to obtain the classical convergence estimates for the CG and other Krylov subspace methods.

Acknowledgments

We are grateful to many colleagues for valuable discussions and comments on the manuscript. We would like to thank Nikolai Zamarashkin and Sergei Goreinov, who read the manuscript and suggested many improvements. We give our special thanks to Yuri Vassilevski for informal and insightful discussions of the domain decomposition methods. Valeria Simoncini read a draft of this book and initiated our cooperation with SIAM's book program. We thank Valeria for her encouragement. The research related to the book was supported in part by RFFI and DFG funding agencies. We also acknowledge the support of the University of Houston through the Small Grants Program, which helped us to finalize the manuscript.