Preface

An important problem that arises in different areas of science and engineering is of computing limits of sequences of vectors $\{x_m\}$, where $x_m \in \mathbb{C}^N$, the dimension N being very large. Such sequences arise, for example, in the solution by fixed-point iterative methods of systems of linear or nonlinear algebraic equations. Given such a system of equations with solution $\mathbf{s}$ and a sequence $\{x_m\}$ obtained from this system by a fixed-point iterative method, we have $\lim_{m\to\infty} x_m = \mathbf{s}$ if $\lim_{m\to\infty} x_m$ exists. Now, in most cases of interest, $\{x_m\}$ converges to $\mathbf{s}$ extremely slowly, making direct use of the x_m to approximate $\mathbf{s}$ with reasonable accuracy quite expensive. This will especially be the case when computing each x_m is very time-consuming. One practical way to remedy this problem is to apply a suitable *extrapolation* (or *convergence acceleration*) method to the available x_m. An extrapolation method takes a finite (and preferably small) number of the vectors x_m and processes them to obtain an approximation to $\mathbf{s}$ that is better than the individual x_m used in the process. A good method is in general nonlinear in the x_m and takes into account, either implicitly or explicitly, the asymptotic behavior of the x_m as $m \to \infty$. If the sequence $\{x_m\}$ does not converge, we may think that no use can be made of it to approximate $\mathbf{s}$. However, at least in some cases, a suitable vector extrapolation method can still be applied to the divergent sequence $\{x_m\}$ to produce good approximations to $\mathbf{s}$, the solution of the system of equations being solved. In this case, we call $\mathbf{s}$ the *antilimit* of $\{x_m\}$; figuratively speaking, we may view the sequence $\{x_m\}$ as *diverging from* its antilimit $\mathbf{s}$.

One nice feature of the methods we study is that they take the vector sequence $\{x_m\}$ as their only input, nothing else being needed. As such, they can be applied to arbitrary vector sequences, whether these are obtained from linear systems or from nonlinear systems or in any other way.

The subject of vector extrapolation methods was initiated by Peter Wynn in the 1960s with an interesting and successful generalization of his famous *epsilon algorithm*, which implements the transformation of Daniel Shanks for accelerating the convergence of sequences of scalars. The works of Shanks and Wynn had a great impact and paved the way for more research into convergence acceleration. With the addition of more methods and their detailed study, the subject of vector extrapolation methods has come a long way since then. Today, it is an independent research area of numerical analysis. It has many practical applications. It also has connections to approximation theory. The relevance of vector extrapolation methods as effective computational tools for solving problems of very high dimension has long been recognized, as can be ascertained by doing a literature search in different computational disciplines.

There are a few books that discuss different aspects of vector extrapolation methods: The 1977 monograph of Brezinski [29] contains one chapter that deals with the epsilon algorithm, its vectorized versions, and a matrix version. The 1991 book by Brezinski and Redivo Zaglia [36] contains one chapter that discusses some of the developments that took place in vector extrapolation methods up to the 1980s. Both books treat vector extrapolation methods as part of the general topic of convergence acceleration. The more recent book by Gander, Gander, and Kwok [93] briefly discusses a few of these methods as tools of scientific computing. So far, however, there has not been a book that is fully dedicated to the subject of vector extrapolation methods and their applications. The present book will hopefully help to fill this void.

The main purpose of this book is to present a unified and systematic account of the existing literature, old and new, on the theory and applications of vector extrapolation methods that is as comprehensive and up-to-date as possible. In this account, I include much of the original and relevant literature that deals with methods of practical importance whose effectiveness has been amply verified in various surveys and comparative studies. I discuss the algebraic, computational/algorithmic, and analytical aspects of the methods covered. The discussions are rigorous, and complete proofs are provided in most places to make the reading flow better. I believe this treatment will help the reader understand the thought process leading to the development of the individual methods, why these methods work, how they work, and how they should be applied for best results. Inevitably, the contents and the perspective of this book reflect my personal interests and taste. Therefore, I apologize to those colleagues whose work has not been covered.

Following the introduction and a review of substantial general and numerical linear algebra background in Chapter 0, which is needed throughout, this book is divided into four parts:

(i) Part I reviews several vector extrapolation methods that are in use and that have proved to be efficient convergence accelerators. These methods are divided into two groups: (i) polynomial-type methods and (ii) epsilon algorithms.

   Chapter 1 presents the development and algebraic properties of four polynomial-type methods: *minimal polynomial extrapolation (MPE)*, *reduced rank extrapolation (RRE)*, *modified minimal polynomial extrapolation (MMPE)*, and the most recent *singular value decomposition–based minimal polynomial extrapolation (SVD-MPE)*. Chapters 2 and 4 present computationally efficient and numerically stable algorithms for these methods. The algorithms presented are also very economical as far as computer storage requirements are concerned; this issue is crucial since most major applications of vector extrapolation methods are to very high dimensional problems. Chapter 3 discusses some interesting relations between MPE and RRE that were discovered recently. (Note that MPE and RRE are essentially different from each other.)

   Chapter 5 covers the three known epsilon algorithms: the *scalar epsilon algorithm (SEA)*, the *vector epsilon algorithm (VEA)*, and the *topological epsilon algorithm (TEA)*.

   Chapters 6 and 7 present unified convergence and convergence acceleration theories for MPE, RRE, MMPE, and TEA. Technically speaking, the contents of the two chapters are quite involved. In these chapters, I have given detailed proofs of some of the convergence theorems. I have decided to present the complete proofs as part of this book since their techniques are quite general and are immediately applicable in other problems as well. For example, the techniques of proof developed in Chapter 6 have been used to prove some of the results presented in Chapters 12, 13, 14, and 16. (Of course, readers who do not want to spend their time on the proofs can simply skip them and study only the statements of the relevant convergence theorems and the remarks and explanations that follow the latter.)

Chapter 8 discusses some interesting recursion relations that exist among the vectors obtained from each of the methods MPE, RRE, MMPE, and TEA.

(ii) Part II reviews some of the developments related to *Krylov subspace methods* for matrix problems, a most interesting topic of numerical linear algebra, to which vector extrapolation methods are closely related.

Chapter 9 deals with Krylov subspace methods for solving linear systems since these are related to MPE, RRE, and TEA when the latter are applied to vector sequences that are generated by fixed-point iterative procedures for linear systems. In particular, it reviews the *method of Arnoldi* that is also known as the *full orthogonalization method (FOM)*, the *method of generalized minimal residuals (GMR)*, and the *method of Lanczos*. It discusses the *method of conjugate gradients (CG)* and the *method of conjugate residuals (CR)* in a unified manner. It also discusses the *biconjugate gradient algorithm (Bi-CG)*.

Chapter 10 deals with Krylov subspace methods for solving matrix eigenvalue problems. It reviews the *method of Arnoldi* and the *method of Lanczos* for these problems. These methods are also closely related to MPE and TEA.

(iii) Part III reviews some of the applications of vector extrapolation methods.

Chapter 11 presents some nonstandard uses for computing eigenvectors corresponding to known eigenvalues (such as the PageRank of the Google Web matrix) and for computing derivatives of eigenpairs. Another interesting application concerns *multidimensional scaling*.

Chapter 12 deals with applying vector extrapolation methods to vector-valued power series. When MPE, MMPE, and TEA are applied to sequences of vector-valued polynomials that form the partial sums of vector-valued Maclaurin series, they produce vector-valued rational approximations to the sums of these series. Chapter 12 discusses the properties of these rational approximations. Chapter 13 presents additional methods based on ideas from *Padé approximants* for obtaining rational approximations from vector-valued power series. Chapter 14 gives some interesting applications of vector-valued rational approximations.

Chapter 15 briefly presents some of the current knowledge about vector generalizations of some scalar extrapolation methods, a subject that has not yet been explored fully.

Chapter 16 discusses vector-valued rational interpolation procedures in the complex plane that are closely related to the methods developed in Chapter 12.

(iv) Part IV is a compendium of eight appendices covering topics that we refer to in Parts I–III. The topics covered are QR factorization in Appendix A; singular value decomposition (SVD) in Appendix B; the Moore–Penrose inverse in Appendix C; fundamental properties of orthogonal polynomials and special properties of Chebyshev and Jacobi polynomials in Appendices D, E, and F; and the Rayleigh quotient and the power method in Appendix G. Appendix G also gives an independent rigorous treatment of the local convergence properties of the Rayleigh quotient *inverse power method with variable shifts* for the eigenvalue problem, a subject not treated in most books on numerical linear algebra. A well-documented and well-tested FORTRAN 77 code for implementing MPE and RRE in a unified manner is included in Appendix H.

The informed reader may pay attention to the fact that I have not included matrix extrapolation methods in this book, even though they are definitely related to vector extrapolation methods; I have pointed out some of the relevant literature on this topic, however. In my discussion of Krylov subspace methods for linear systems, I have also excluded the topic of semi-iterative methods, with Chebyshev iteration being the most interesting representative. This subject is covered very extensively in the various books and papers referred to in the relevant chapters. The main reason for both omissions, which I regret very much, was the necessity to keep the size of the book in check. Finally, I have not included any numerical examples since there are many of these in the existing literature; the limitation I imposed on the size of the book was again the reason for this omission. Nevertheless, I have pointed out some papers containing numerical examples that illustrate the theoretical results presented in the different chapters.

I hope this book will serve as a reference for the more mathematically inclined researchers in the area of vector extrapolation methods and for scientists and engineers in different computational disciplines and as a textbook for students interested in undertaking to study the subject seriously. Most of the mathematical background needed to cope with the material is summarized in Chapter 0 and the appendices, and some is provided as needed in the relevant chapters.

Before closing, I would like to express my deepest gratitude and appreciation to my dear friends and colleagues Dr. William F. Ford of NASA Lewis Research Center (today, NASA John H. Glenn Research Center at Lewis Field) and Professor David A. Smith of Duke University, who introduced me to the general topic of vector extrapolation methods. Our fruitful collaboration began after I was invited by Dr. Ford to Lewis Research Center to spend a sabbatical there during 1981–1983. Our first joint work was summarized very briefly in the NASA technical memorandum [297] and presented at the Thirtieth Anniversary Meeting of the Society for Industrial and Applied Mathematics, Stanford, California, July 19–23, 1982. This work was eventually published as the NASA technical paper [298] and, later, as the journal paper [299]. I consider it a privilege to acknowledge their friendship and their influence on my career in this most interesting topic.

Lastly, I owe a debt of gratitude to my dear wife Carmella for her constant patience, understanding, support, and encouragement while this book was being written. I dedicate this book to her with love.

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