
*Solution of $f(A)x = b$ with Krylov
subspace information*

11.1 Introduction

In this chapter, I expand on an idea for exploiting Krylov subspace information obtained for the matrix A and the vector b . This subspace information can be used for the approximate solution of a linear system $f(A)x = b$, where f is some analytic function, $A \in \mathbb{R}^{n \times n}$, and $b \in \mathbb{R}^n$. I will make suggestions on how to use this for the case where f is the matrix *sign* function. The matrix *sign* function plays an important role in QCD computations, see for instance [147].

In [197] an approach was suggested for the use of a Krylov subspace for the computation of approximate solutions of linear systems

$$f(A)x = b.$$

The approach was motivated by the function $f(A) = A^2$, which plays a role in the solution of some biharmonic systems. The approach is easily generalized for nonsymmetric complex matrices, but we may have to pay more attention to the evaluation of f for the reduced system, associated with the Krylov subspace.

In particular, I will discuss some possible approaches in which the Krylov subspace is used for the computation of $\text{sign}(A)p$ for given vectors p . With the evaluation of the matrix *sign* function we have to be extremely careful. A popular approach, based on a Newton iteration, converges fast, but is sensitive for rounding errors, especially when A is ill-conditioned. We will briefly discuss a computational method that was suggested (and analysed) by Bai and Demmel [15]. This approach can also be combined, in principle, with the subspace reduction technique.

Iterative Krylov Methods For Large Linear Systems

**Gérard Meurant, Jurjen Duintjer
Tebbens**



Iterative Krylov Methods For Large Linear Systems:

Iterative Krylov Methods for Large Linear Systems H. A. van der Vorst, 2003-04-17 Computational simulation of scientific phenomena and engineering problems often depends on solving linear systems with a large number of unknowns. This book gives insight into the construction of iterative methods for the solution of such systems and helps the reader to select the best solver for a given class of problems. The emphasis is on the main ideas and how they have led to efficient solvers such as CG, GMRES and BI-CGSTAB. The author also explains the main concepts behind the construction of preconditioners. The reader is encouraged to gain experience by analysing numerous examples that illustrate how best to exploit the methods. The book also hints at many open problems and as such it will appeal to established researchers. There are many exercises that motivate the material and help students to understand the essential steps in the analysis and construction of algorithms.

Krylov Methods for Nonsymmetric Linear Systems Gérard Meurant, Jurjen Duintjer Tebbens, 2020-10-02 This book aims to give an encyclopedic overview of the state of the art of Krylov subspace iterative methods for solving nonsymmetric systems of algebraic linear equations and to study their mathematical properties. Solving systems of algebraic linear equations is among the most frequent problems in scientific computing; it is used in many disciplines such as physics, engineering, chemistry, biology and several others. Krylov methods have progressively emerged as the iterative methods with the highest efficiency while being very robust for solving large linear systems; they may be expected to remain so independent of progress in modern computer-related fields such as parallel and high performance computing. The mathematical properties of the methods are described and analyzed along with their behavior in finite precision arithmetic. A number of numerical examples demonstrate the properties and the behavior of the described methods. Also considered are the methods' implementations and coding as Matlab-like functions. Methods which became popular recently are considered in the general framework of Q-OR, quasi-orthogonal, Q-MR, quasi-minimum residual methods. This book can be useful for both practitioners and for readers who are more interested in theory. Together with a review of the state of the art, it presents a number of recent theoretical results of the authors, some of them unpublished, as well as a few original algorithms. Some of the derived formulas might be useful for the design of possible new methods or for future analysis. For the more applied user, the book gives an up-to-date overview of the majority of the available Krylov methods for nonsymmetric linear systems, including well-known convergence properties and, as we said above, template codes that can serve as the base for more individualized and elaborate implementations.

Algorithms for Sparse Linear Systems Jennifer Scott, Miroslav Tuma, 2023-04-29 Large sparse linear systems of equations are ubiquitous in science, engineering and beyond. This open access monograph focuses on factorization algorithms for solving such systems. It presents classical techniques for complete factorizations that are used in sparse direct methods and discusses the computation of approximate direct and inverse factorizations that are key to constructing general purpose algebraic preconditioners for iterative solvers. A unified

framework is used that emphasizes the underlying sparsity structures and highlights the importance of understanding sparse direct methods when developing algebraic preconditioners. Theoretical results are complemented by sparse matrix algorithm outlines. This monograph is aimed at students of applied mathematics and scientific computing as well as computational scientists and software developers who are interested in understanding the theory and algorithms needed to tackle sparse systems. It is assumed that the reader has completed a basic course in linear algebra and numerical mathematics.

Handbook of Linear Algebra, Second Edition Leslie Hogben, 2013-11-26. With a substantial amount of new material, the Handbook of Linear Algebra, Second Edition provides comprehensive coverage of linear algebra concepts, applications, and computational software packages in an easy-to-use format. It guides you from the very elementary aspects of the subject to the frontiers of current research. Along with revisions and updates throughout the second edition, this bestseller includes 20 new chapters. New to the Second Edition: Separate chapters on Schur complements, additional types of canonical forms, tensors, matrix polynomials, matrix equations, special types of matrices, generalized inverses, matrices over finite fields, invariant subspaces, representations of quivers, and spectral sets. New chapters on combinatorial matrix theory topics such as tournaments, the minimum rank problem, and spectral graph theory, as well as numerical linear algebra topics including algorithms for structured matrix computations, stability of structured matrix computations, and nonlinear eigenvalue problems. More chapters on applications of linear algebra, including epidemiology and quantum error correction. New chapter on using the free and open source software system Sage for linear algebra. Additional sections in the chapters on sign pattern matrices and applications to geometry. Conjectures and open problems in most chapters on advanced topics. Highly praised as a valuable resource for anyone who uses linear algebra, the first edition covered virtually all aspects of linear algebra and its applications. This edition continues to encompass the fundamentals of linear algebra, combinatorial and numerical linear algebra, and applications of linear algebra to various disciplines, while also covering up-to-date software packages for linear algebra computations.

Spectral Methods for Uncertainty Quantification Olivier Le Maître, Omar M. Knio, 2010-03-11. This book deals with the application of spectral methods to problems of uncertainty propagation and quantification in model-based computations. It specifically focuses on computational and algorithmic features of these methods, which are most useful in dealing with models based on partial differential equations, with special attention to models arising in simulations of fluid flows. Implementations are illustrated through applications to elementary problems as well as more elaborate examples selected from the authors' interests in incompressible vortex-dominated flows and compressible flows at low Mach numbers. Spectral stochastic methods are probabilistic in nature and are consequently rooted in the rich mathematical foundation associated with probability and measure spaces. Despite the authors' fascination with this foundation, the discussion only leads to those theoretical aspects needed to set the stage for subsequent applications. The book is authored by practitioners and is primarily intended for researchers or graduate students in computational mathematics, physics, or fluid dynamics. The book assumes

familiarity with elementary methods for the numerical solution of time dependent partial differential equations prior experience with spectral methods is naturally helpful though not essential Full appreciation of elaborate examples in computational fluid dynamics CFD would require familiarity with key and in some cases delicate features of the associated numerical methods Besides these shortcomings our aim is to treat algorithmic and computational aspects of spectral stochastic methods with details sufficient to address and reconstruct all but those highly elaborate examples

High Performance Computing for Computational Science -- VECPAR 2010 José M. Laginha M. Palma, Michel Daydé, Osni Marques, Joao Correia Lopes, 2011-02-18 This book constitutes the thoroughly refereed post conference proceedings of the 9th International Conference on High Performance Computing for Computational Science VECPAR 2010 held in Berkeley CA USA in June 2010 The 34 revised full papers presented together with five invited contributions were carefully selected during two rounds of reviewing and revision The papers are organized in topical sections on linear algebra and solvers on emerging architectures large scale simulations parallel and distributed computing numerical algorithms

Matrix Analysis and Computations Zhong-Zhi Bai, Jian-Yu Pan, 2021-09-09 This comprehensive book is presented in two parts the first part introduces the basics of matrix analysis necessary for matrix computations and the second part presents representative methods and the corresponding theories in matrix computations Among the key features of the book are the extensive exercises at the end of each chapter Matrix Analysis and Computations provides readers with the matrix theory necessary for matrix computations especially for direct and iterative methods for solving systems of linear equations It includes systematic methods and rigorous theory on matrix splitting iteration methods and Krylov subspace iteration methods as well as current results on preconditioning and iterative methods for solving standard and generalized saddle point linear systems This book can be used as a textbook for graduate students as well as a self study tool and reference for researchers and engineers interested in matrix analysis and matrix computations It is appropriate for courses in numerical analysis numerical optimization data science and approximation theory among other topics

Domain Decomposition Methods in Science and Engineering XX Randolph Bank, Michael Holst, Olof Widlund, Jinchao Xu, 2013-07-03 These are the proceedings of the 20th international conference on domain decomposition methods in science and engineering Domain decomposition methods are iterative methods for solving the often very large linear or nonlinear systems of algebraic equations that arise when various problems in continuum mechanics are discretized using finite elements They are designed for massively parallel computers and take the memory hierarchy of such systems in mind This is essential for approaching peak floating point performance There is an increasingly well developed theory which is having a direct impact on the development and improvements of these algorithms

Numerical Solution of Partial Differential Equations on Parallel Computers Are Magnus Bruaset, Aslak Tveito, 2006-03-05 Since the dawn of computing the quest for a better understanding of Nature has been a driving force for technological development Groundbreaking achievements by great scientists have paved the way from the abacus to the

supercomputing power of today When trying to replicate Nature in the computer's silicon test tube there is need for precise and computable process descriptions The scientific fields of Mathematics and Physics provide a powerful vehicle for such descriptions in terms of Partial Differential Equations PDEs Formulated as such equations physical laws can become subject to computational and analytical studies In the computational setting the equations can be discretized for efficient solution on a computer leading to valuable tools for simulation of natural and man-made processes Numerical solution of PDE based mathematical models has been an important research topic over centuries and will remain so for centuries to come In the context of computer based simulations the quality of the computed results is directly connected to the model's complexity and the number of data points used for the computations Therefore computational scientists tend to fill even the largest and most powerful computers they can get access to either by increasing the size of the data sets or by introducing new model terms that make the simulations more realistic or a combination of both Today many important simulation problems can not be solved by one single computer but calls for parallel computing

Distributed and Parallel Systems Peter Kacsuk, Thomas Fahringer, Zolt Nemeth, 2007-05-03 Distributed and Parallel Systems From Cluster to Grid Computing is an edited volume based on DAPSYS 2006 the 6th Austrian Hungarian Workshop on Distributed and Parallel Systems which is dedicated to all aspects of distributed and parallel computing The workshop was held in conjunction with the 2nd Austrian Grid Symposium in Innsbruck Austria in September 2006 This book is designed for a professional audience composed of practitioners and researchers in industry It is also suitable for advanced level students in computer science

Intelligent Computing Systems Carlos Brito-Loeza, Anabel Martin-Gonzalez, Victor Castañeda-Zeman, Asad Safi, 2022-03-16 This book constitutes the proceedings of the 4th International Symposium on Intelligent Computing Systems ISICS 2022 held in Santiago Chile in March 2022 Due to the COVID 19 pandemic the conference was held online The 9 full papers along with 2 short papers presented in this volume were carefully reviewed and selected from 30 submissions They deal with the field of intelligent computing systems focusing on artificial intelligence computer vision and image processing

Advanced Computational Methods in Science and Engineering Barry Koren, Kees Vuik, 2010-04-29 The aim of the present book is to show in a broad and yet deep way the state of the art in computational science and engineering Examples of topics addressed are fast and accurate numerical algorithms model order reduction grid computing immersed boundary methods and specific computational methods for simulating a wide variety of challenging problems problems such as fluid structure interaction turbulent flames bone fracture healing micro electro mechanical systems failure of composite materials storm surges particulate flows and so on The main benefit offered to readers of the book is a well balanced up to date overview over the field of computational science and engineering through in depth articles by specialists from the separate disciplines

Some Topics in Industrial and Applied Mathematics Rolf Jeltsch, I. H. Sloan, 2007 The Shanghai Forum on Industrial and Applied Mathematics was organized in May 2006 on the occasion that many famous industrial and applied

mathematicians gathered in Shanghai from different countries to participate in the Officers Meeting and the Board Meeting of the ICIAM International Council for Industrial and Applied Mathematics This volume collects the material covered by the majority of the lectures of which reflects panoramically recent results and trends in industrial and applied mathematics This book will be very useful for graduate students and researchers in industrial and applied mathematics *Introduction to Mathematics for Computational Biology* Paola Lecca, Bruno Carpentieri, 2023-09-12 This introductory guide provides a thorough explanation of the mathematics and algorithms used in standard data analysis techniques within systems biology biochemistry and biophysics Each part of the book covers the mathematical background and practical applications of a given technique Readers will gain an understanding of the mathematical and algorithmic steps needed to use these software tools appropriately and effectively as well how to assess their specific circumstance and choose the optimal method and technology Ideal for students planning for a career in research early career researchers and established scientists undertaking interdisciplinary research *Wireless Communications Over Rapidly Time-Varying Channels* Franz Hlawatsch, Gerald Matz, 2011-05-04 As a result of higher frequencies and increased user mobility researchers and systems designers are shifting their focus from time invariant models to channels that vary within a block *Wireless Communications Over Rapidly Time Varying Channels* explains the latest theoretical advances and practical methods to give an understanding of rapidly time varying channels together with performance trade offs and potential performance gains providing the expertise to develop future wireless systems technology As well as an overview of the issues of developing wireless systems using time varying channels the book gives extensive coverage to methods for estimating and equalizing rapidly time varying channels including a discussion of training data optimization as well as providing models and transceiver methods for time varying ultra wideband channels An introduction to time varying channel models gives in a nutshell the important issues of developing wireless systems technology using time varying channels Extensive coverage of methods for estimating and equalizing rapidly time varying channels including a discussion of training data optimization enables development of high performance wireless systems Chapters on transceiver design for OFDM and receiver algorithms for MIMO communication channels over time varying channels with an emphasis on modern iterative turbo style architectures demonstrates how these important technologies can optimize future wireless systems *Fundamentals of Numerical Mathematics for Physicists and Engineers* Alvaro Meseguer, 2020-06-16 Introduces the fundamentals of numerical mathematics and illustrates its applications to a wide variety of disciplines in physics and engineering Applying numerical mathematics to solve scientific problems this book helps readers understand the mathematical and algorithmic elements that lie beneath numerical and computational methodologies in order to determine the suitability of certain techniques for solving a given problem It also contains examples related to problems arising in classical mechanics thermodynamics electricity and quantum physics *Fundamentals of Numerical Mathematics for Physicists and Engineers* is presented in two parts Part I addresses the root

finding of univariate transcendental equations polynomial interpolation numerical differentiation and numerical integration Part II examines slightly more advanced topics such as introductory numerical linear algebra parameter dependent systems of nonlinear equations numerical Fourier analysis and ordinary differential equations initial value problems and univariate boundary value problems Chapters cover Newton's method Lebesgue constants conditioning barycentric interpolatory formula Clenshaw Curtis quadrature GMRES matrix free Krylov linear solvers homotopy numerical continuation differentiation matrices for boundary value problems Runge Kutta and linear multistep formulas for initial value problems Each section concludes with Matlab hands on computer practicals and problem and exercise sets This book Provides a modern perspective of numerical mathematics by introducing top notch techniques currently used by numerical analysts Contains two parts each of which has been designed as a one semester course Includes computational practicals in Matlab with solutions at the end of each section for the instructor to monitor the student's progress through potential exams or short projects Contains problem and exercise sets also with solutions at the end of each section Fundamentals of Numerical Mathematics for Physicists and Engineers is an excellent book for advanced undergraduate or graduate students in physics mathematics or engineering It will also benefit students in other scientific fields in which numerical methods may be required such as chemistry or biology

Numerical Solution of Algebraic Riccati Equations Dario A. Bini, Bruno Iannazzo, Beatrice Meini, 2012-03-31 This treatment of the basic theory of algebraic Riccati equations describes the classical as well as the more advanced algorithms for their solution in a manner that is accessible to both practitioners and scholars It is the first book in which nonsymmetric algebraic Riccati equations are treated in a clear and systematic way Some proofs of theoretical results have been simplified and a unified notation has been adopted Readers will find a unified discussion of doubling algorithms which are effective in solving algebraic Riccati equations as well as a detailed description of all classical and advanced algorithms for solving algebraic Riccati equations and their MATLAB codes This will help the reader gain an understanding of the computational issues and provide ready to use implementation of the different solution techniques

Scientific Computing in Electrical Engineering SCEE 2008 Luis R.J. Costa, Janne Roos, 2010-06-14 This book is a collection of 65 selected papers presented at the 7th International Conference on Scientific Computing in Electrical Engineering SCEE held in Espoo Finland in 2008 The aim of the SCEE 2008 conference was to bring together scientists from academia and industry e.g. mathematicians electrical engineers computer scientists and physicists with the goal of intensive discussions on industrially relevant mathematical problems with an emphasis on modeling and numerical simulation of electronic circuits and devices electromagnetic fields and coupled problems This extensive reference work is divided into five parts 1 Computational electromagnetics 2 Circuit simulation 3 Coupled problems 4 Mathematical and computational methods and 5 Model order reduction Each part starts with an general introduction followed by the actual papers

A Journey through the History of Numerical Linear Algebra Claude Brezinski, Gérard Meurant, Michela Redivo-Zaglia, 2022-12-06 This

expansive volume describes the history of numerical methods proposed for solving linear algebra problems from antiquity to the present day. The authors focus on methods for linear systems of equations and eigenvalue problems and describe the interplay between numerical methods and the computing tools available at the time. The second part of the book consists of 78 biographies of important contributors to the field. *A Journey through the History of Numerical Linear Algebra* will be of special interest to applied mathematicians especially researchers in numerical linear algebra people involved in scientific computing and historians of mathematics.

Spectra and Pseudospectra Lloyd N. Trefethen, Mark Embree, 2005-08-07 Pure and applied mathematicians, physicists, scientists and engineers use matrices and operators and their eigenvalues in quantum mechanics, fluid mechanics, structural analysis, acoustics, ecology, numerical analysis and many other areas. However, in some applications the usual analysis based on eigenvalues fails. For example, eigenvalues are often ineffective for analyzing dynamical systems such as fluid flow, Markov chains, ecological models and matrix iterations. That's where this book comes in. This is the authoritative work on nonnormal matrices and operators written by the authorities who made them famous. Each of the sixty sections is written as a self-contained essay. Each document is a lavishly illustrated introductory survey of its topic, complete with beautiful numerical experiments and all the right references. The breadth of included topics and the numerous applications that provide links between fields will make this an essential reference in mathematics and related sciences.

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