
*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

Joacim Rocklöv



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.

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

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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

Computational Statistics in Data Science Walter W. Piegorsch, Richard A. Levine, Hao Helen Zhang, Thomas C. M. Lee, 2022-03-23 Ein unverzichtbarer Leitfaden bei der Anwendung computergestützter Statistik in der modernen Datenwissenschaft In Computational Statistics in Data Science präsentiert ein Team aus bekannten Mathematikern und Statistikern eine fundierte Zusammenstellung von Konzepten Theorien Techniken und Praktiken der computergestützten Statistik für ein Publikum das auf der Suche nach einem einzigen umfassenden Referenzwerk für Statistik in der modernen Datenwissenschaft ist Das Buch enthält etliche Kapitel zu den wesentlichen konkreten Bereichen der computergestützten Statistik in denen modernste Techniken zeitgemäß und verständlich dargestellt werden Darüber hinaus bietet Computational Statistics in Data Science einen kostenlosen Zugang zu den fertigen Eingängen im Online Nachschlagewerk Wiley StatsRef Statistics Reference Online Außerdem erhalten die Leserinnen und Leser eine gründliche Einführung in die computergestützte Statistik mit relevanten und verständlichen Informationen für Anwender und Forscher in verschiedenen datenintensiven Bereichen Umfassende Erläuterungen zu aktuellen Themen in der Statistik darunter Big Data Datenstromverarbeitung quantitative Visualisierung und

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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

Scalable Algorithms for Contact Problems Zdeněk Dostál, Tomáš Kozubek, Marie Sadowská, Vít Vondrák, 2023-10-28 This book presents a comprehensive treatment of recently developed scalable algorithms for solving multibody contact problems of linear elasticity The brand new feature of these algorithms is their theoretically supported numerical scalability i.e. asymptotically linear complexity and parallel scalability demonstrated in solving problems discretized by billions of degrees of freedom The theory covers solving multibody frictionless contact problems contact problems with possibly orthotropic Tresca's friction and transient contact problems In addition it also covers BEM discretization treating jumping coefficients floating bodies mortar non penetration conditions etc This second edition includes updated content including a new chapter on hybrid domain decomposition methods for huge contact problems Furthermore new sections describe the latest algorithm improvements e.g. the fast reconstruction of displacements the adaptive reorthogonalization of dual constraints and an updated chapter on parallel implementation Several chapters are extended to give an independent exposition of classical bounds on the spectrum of mass and dual stiffness matrices a benchmark for Coulomb orthotropic friction details of discretization etc The exposition is divided into four parts the first of which reviews auxiliary linear algebra optimization and analysis The most important algorithms and optimality results are presented in the third chapter The presentation includes continuous formulation discretization domain decomposition optimality results and numerical experiments The final part contains extensions to contact shape optimization plasticity and HPC implementation Graduate students and researchers in mechanical engineering computational engineering and applied mathematics will find this book of great value and interest

Numerical Methods for Scientists and Engineers Zakeriya Altaç, 2024-10-15 Numerical Methods for Scientists and Engineers With Pseudocodes is designed as a primary textbook for a one semester course on Numerical Methods for sophomore or junior level students It covers the fundamental numerical methods required for scientists and engineers as well as some advanced topics which are left to the discretion of instructors The objective of the text is to provide readers with a strong theoretical

background on numerical methods encountered in science and engineering and to explain how to apply these methods to practical real world problems Readers will also learn how to convert numerical algorithms into running computer codes Features Numerous pedagogic features including exercises pros and cons boxes for each method discussed and rigorous highlighting of key topics and ideas Suitable as a primary text for undergraduate courses in numerical methods but also as a reference to working engineers A Pseudocode approach that makes the book accessible to those with different or no coding backgrounds which does not tie instructors to one particular language over another A dedicated website featuring additional code examples quizzes exercises discussions and more <https://github.com/zaltac/NumMethodsWPseudoCodes> A complete Solution Manual and PowerPoint Presentations are available free of charge to instructors at www.routledge.com/9781032754741

High Performance Computing for Computational Science -- VECPAR 2010 José M. Laginha M. Palma, Michel Daydé, Osni Marques, Joao Correia Lopes, 2011-02-23 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

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

Progress in Industrial Mathematics at ECMI 2004 Alessandro Di Bucchianico, Robert M.M. Mattheij, Marc Adriaan Peletier, 2006-01-09 ECMI has a brand name in Industrial Mathematics and organises successful biannual conferences This time the conference on Industrial Mathematics held in Eindhoven in June 2004 Mathematics focused on Aerospace Electronic Industry Chemical Technology Life Sciences Materials Geophysics Financial Mathematics and Water flow The majority of the invited talks on these topics can be found in these proceedings Apart from these lectures a large number of contributed papers and minisymposium papers are included here They give an interesting and impressive overview of the important place mathematics has achieved in solving all kinds of problems met in industry and commerce in particular Acta Numerica

2008: Volume 17 A. Iserles, 2008-06-12 A high impact prestigious annual publication containing invited surveys by subject leaders essential reading for all practitioners and researchers **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

Algorithms and Theory of Computation Handbook, Volume 1 Mikhail J. Atallah, Marina Blanton, 2009-11-20 Algorithms and Theory of Computation Handbook Second Edition General Concepts and Techniques provides an up to date compendium of fundamental computer science topics and techniques It also illustrates how the topics and techniques come together to deliver efficient solutions to important practical problems Along with updating and revising many **High Performance Computing in Science and Engineering** Tomáš Kozubek, Martin Čermák, Petr Tichý, Radim Blaheta, Jakub Šístek, Dalibor Lukáš, Jiří Jaroš, 2018-07-16 This book constitutes the thoroughly refereed post conference proceedings of the Third International Conference on High Performance Computing in Science and Engineering HPCSE 2017 held in Karolinka Czech Republic in May 2017 The 15 papers presented in this volume were carefully reviewed and selected from 20 submissions The conference provides an international forum for exchanging ideas among researchers involved in scientific and parallel computing including theory and applications as well as applied and computational mathematics The focus of HPCSE 2017 was on models algorithms and software tools which facilitate efficient and convenient utilization of modern parallel and distributed computing architectures as well as on large scale applications **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 *Robust Optimization-Directed Design* Andrew J. Kurdila, Panos M. Pardalos, Michael Zabarankin, 2006-06-04 Robust design that is managing design uncertainties such as model uncertainty or parametric uncertainty is the often unpleasant issue crucial in much multidisciplinary optimal design work Recently there has been enormous practical interest in strategies for applying optimization tools to the development of robust solutions and

designs in several areas including aerodynamics the integration of sensing e.g. laser radars vision based systems and millimeter wave radars and control cooperative control with poorly modeled uncertainty cascading failures in military and civilian applications multi mode seekers sensor fusion and data association problems and tracking systems The contributions to this book explore these different strategies The expression optimization directed in this book's title is meant to suggest that the focus is not agonizing over whether optimization strategies identify a true global optimum but rather whether these strategies make significant design improvements

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 Methods for Mixed Finite Element Problems Jean Deteix, Thierno Diop, Michel Fortin, 2022-09-24 This book

focuses on iterative solvers and preconditioners for mixed finite element methods It provides an overview of some of the state of the art solvers for discrete systems with constraints such as those which arise from mixed formulations Starting by recalling the basic theory of mixed finite element methods the book goes on to discuss the augmented Lagrangian method and gives a summary of the standard iterative methods describing their usage for mixed methods Here preconditioners are built from an approximate factorisation of the mixed system A first set of applications is considered for incompressible elasticity problems and flow problems including non linear models An account of the mixed formulation for Dirichlet's boundary conditions is then given before turning to contact problems where contact between incompressible bodies leads to problems with two constraints This book is aimed at graduate students and researchers in the field of numerical methods and scientific computing

Functions of Matrices

Nicholas J. Higham, 2008-09-11 This superb book is timely and is written with great attention paid to detail particularly in its referencing of the literature The book has a wonderful blend of theory and code MATLAB so will be useful both to nonexperts and to experts in the field Alan Laub Professor University of California Los Angeles The only book devoted exclusively to matrix functions this research monograph gives a thorough treatment of the theory of matrix functions and numerical methods for computing them The author's elegant presentation focuses on the equivalent definitions of $f(A)$ via the Jordan canonical form polynomial interpolation and the Cauchy integral formula and features an emphasis on results of practical interest and an extensive collection of problems and solutions Functions of Matrices Theory and Computation is more than just a monograph on matrix functions its wide ranging content including an overview of applications historical references and miscellaneous results tricks and techniques with an $f(A)$ connection makes

it useful as a general reference in numerical linear algebra Other key features of the book include development of the theory of conditioning and properties of the Frchet derivative an emphasis on the Schur decomposition the block Parlett recurrence and judicious use of Pad approximants the inclusion of new unpublished research results and improved algorithms a chapter devoted to the $f(A)b$ problem and a MATLAB toolbox providing implementations of the key algorithms Audience This book is for specialists in numerical analysis and applied linear algebra as well as anyone wishing to learn about the theory of matrix functions and state of the art methods for computing them It can be used for a graduate level course on functions of matrices and is a suitable reference for an advanced course on applied or numerical linear algebra It is also particularly well suited for self study Contents List of Figures List of Tables Preface Chapter 1 Theory of Matrix Functions Chapter 2 Applications Chapter 3 Conditioning Chapter 4 Techniques for General Functions Chapter 5 Matrix Sign Function Chapter 6 Matrix Square Root Chapter 7 Matrix p th Root Chapter 8 The Polar Decomposition Chapter 9 Schur Parlett Algorithm Chapter 10 Matrix Exponential Chapter 11 Matrix Logarithm Chapter 12 Matrix Cosine and Sine Chapter 13 Function of Matrix Times Vector $f(A)b$ Chapter 14 Miscellany Appendix A Notation Appendix B Background Definitions and Useful Facts Appendix C Operation Counts Appendix D Matrix Function Toolbox Appendix E Solutions to Problems Bibliography Index

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