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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

Wolfgang Guggemos

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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 **Iterative Methods for Large Linear Systems** David R. Kincaid,Linda J. Hayes,2014-05-10 Iterative Methods for Large Linear Systems contains a wide spectrum of research topics related to iterative methods such as searching for optimum parameters using hierarchical basis preconditioners utilizing software as a research tool and developing algorithms for vector and parallel computers This book provides an overview of the use of iterative methods for solving sparse linear systems identifying future research directions in the mainstream of modern scientific computing with an

eye to contributions of the past present and future Different iterative algorithms that include the successive overrelaxation SOR method symmetric and unsymmetric SOR methods local ad hoc SOR scheme and alternating direction implicit ADI method are also discussed This text likewise covers the block iterative methods asynchronous iterative procedures multilevel methods adaptive algorithms and domain decomposition algorithms This publication is a good source for mathematicians and computer scientists interested in iterative methods for large linear systems **Recherches physiques sur la lumière, la pesanteur, les marées, le cours des astres et sur la comète de 1860** ,1760 **Matrix Computations** Gene Howard Golub,Charles F. Van Loan,2013-02-15 This revised edition provides the mathematical background and algorithmic skills required for the production of numerical software It includes rewritten and clarified proofs and derivations as well as new topics such as Arnoldi iteration and domain decomposition methods **Fundamentals of Numerical Mathematics for Physicists and Engineers** Alvaro Meseguer,2020-05-26 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 Mathematics and Advanced Applications 2011 Andrea Cangiani,Ruslan L Davidchack,Emmanuil Georgoulis,Alexander N. Gorban,Jeremy Levesley,Michael V. Tretyakov,2013-01-20

The European Conferences on Numerical Mathematics and Advanced Applications ENUMATH are a series of conferences held every two years to provide a forum for discussion of new trends in numerical mathematics and challenging scientific and industrial applications at the highest level of international expertise ENUMATH 2011 was hosted by the University of Leicester UK from the 5th to 9th September 2011 This proceedings volume contains more than 90 papers by speakers of the conference and gives an overview of recent developments in scientific computing numerical analysis and practical use of modern numerical techniques and algorithms in various applications New results on finite element methods multiscale methods numerical linear algebra and finite difference schemes are presented A range of applications include computational problems from fluid dynamics materials image processing and molecular dynamics **Parallelism in Matrix Computations** Efstratios Gallopoulos,Bernard Philippe,Ahmed H. Sameh,2015-07-25 This book is primarily intended as a research monograph that could also be used in graduate courses for the design of parallel algorithms in matrix computations It assumes general but not extensive knowledge of numerical linear algebra parallel architectures and parallel programming paradigms The book consists of four parts I Basics II Dense and Special Matrix Computations III Sparse Matrix Computations and IV Matrix functions and characteristics Part I deals with parallel programming paradigms and fundamental kernels including reordering schemes for sparse matrices Part II is devoted to dense matrix computations such as parallel algorithms for solving linear systems linear least squares the symmetric algebraic eigenvalue problem and the singular value decomposition It also deals with the development of parallel algorithms for special linear systems such as banded Vandermonde Toeplitz and block Toeplitz systems Part III addresses sparse matrix computations a the development of parallel iterative linear system solvers with emphasis on scalable preconditioners b parallel schemes for obtaining a few of the extreme eigenpairs or those contained in a given interval in the spectrum of a standard or generalized symmetric eigenvalue problem and c parallel methods for computing a few of the extreme singular triplets Part IV focuses on the development of parallel algorithms for matrix functions and special characteristics such as the matrix pseudospectrum and the determinant The book also reviews the theoretical and practical background necessary when designing these algorithms and includes an extensive bibliography that will be useful to researchers and students alike The book brings together many existing algorithms for the fundamental matrix computations that have a proven track record of efficient implementation in terms of data locality and data transfer on state of the art systems as well as several algorithms that are presented for the first time focusing on the opportunities for parallelism and algorithm robustness **Computational Methods for Nanoscale Applications** Igor Tsukerman,2020-08-21 Positioning itself at the common boundaries of several disciplines this work provides new perspectives on modern nanoscale problems where fundamental science meets technology and computer modeling In addition to well known computational techniques such as finite difference schemes and Ewald summation the book presents a new finite difference calculus of Flexible Local Approximation Methods FLAME that qualitatively improves

the numerical accuracy in a variety of problems **Parallel Computing is Everywhere** Sanzio Bassini,Gerhard R. Joubert,Frans Peters,2018-03-15 The most powerful computers work by harnessing the combined computational power of millions of processors and exploiting the full potential of such large scale systems is something which becomes more difficult with each succeeding generation of parallel computers Alternative architectures and computer paradigms are increasingly being investigated in an attempt to address these difficulties Added to this the pervasive presence of heterogeneous and parallel devices in consumer products such as mobile phones tablets personal computers and servers also demands efficient programming environments and applications aimed at small scale parallel systems as opposed to large scale supercomputers This book presents a selection of papers presented at the conference Parallel Computing ParCo2017 held in Bologna Italy on 12 to 15 September 2017 The conference included contributions about alternative approaches to achieving High Performance Computing HPC to potentially surpass exa and zetascale performances as well as papers on the application of quantum computers and FPGA processors These developments are aimed at making available systems better capable of solving intensive computational scientific engineering problems such as climate models security applications and classic NP problems some of which cannot currently be managed by even the most powerful supercomputers available New areas of application such as robotics AI and learning systems data science the Internet of Things IoT and in car systems and autonomous vehicles were also covered As always ParCo2017 attracted a large number of notable contributions covering present and future developments in parallel computing and the book will be of interest to all those working in the field A Survey of Preconditioned Iterative Methods Are Magnus Bruaset,2018-12-13 The problem of solving large sparse linear systems of algebraic equations is vital in scientific computing even for applications originating from quite different fields A Survey of Preconditioned Iterative Methods presents an up to date overview of iterative methods for numerical solution of such systems Typically the methods considered are w **SIAM Journal on Scientific Computing** ,2009 Iterative Methods and Preconditioning for Large and Sparse Linear Systems with Applications Daniele Bertaccini,Fabio Durastante,2018-02-19 This book describes in a basic way the most useful and effective iterative solvers and appropriate preconditioning techniques for some of the most important classes of large and sparse linear systems The solution of large and sparse linear systems is the most time consuming part for most of the scientific computing simulations Indeed mathematical models become more and more accurate by including a greater volume of data but this requires the solution of larger and harder algebraic systems In recent years research has focused on the efficient solution of large sparse and or structured systems generated by the discretization of numerical models by using iterative solvers *Krylov Subspace Methods with Fixed Memory Requirements* Kirk McLane Soodhalter,2012 Krylov subspace iterative methods provide an effective tool for reducing the solution of large linear systems to a size for which a direct solver may be applied However the problems of limited storage and speed are still a concern Therefore in this dissertation work we present iterative Krylov

subspace algorithms for non Hermitian systems which do have fixed memory requirements and have favorable convergence characteristics This dissertation describes three projects The first project concerns short term recurrence Krylov subspace methods for nearly Hermitian linear systems In 2008 Beckermann and Reichel introduced a short term recurrence progressive GMRES algorithm for nearly Hermitian linear systems However we have found this method to be unstable We document the instabilities and introduce a different fixed memory algorithm to treat nearly Hermitian problems We present numerical experiments demonstrating that the performance of this algorithm is competitive The other two projects involve extending a strategy called Krylov subspace recycling introduced by Parks and colleagues in 2005 This method requires more overhead than other subspace augmentation methods but offers the ability to recycle subspace information between cycles for a single linear system and recycle information between related linear systems In the first project we extend subspace recycling to the block Krylov subspace setting A block Krylov subspace is a generalization of Krylov subspace where a single starting vector is replaced with a block of linearly independent starting vectors We then apply our method to a sequence of matrices arising in a Newton iteration applied to fluid density functional theory and present some numerical experiments In the second project we extend the methods of subspace recycling to a family of linear systems differing only by multiples of the identity These problems arise in the theory of quantum chromodynamics a theory of the behavior of subatomic particles We wish to build on the class of Krylov methods which allow the simultaneous solution of all shifted linear systems while generating only one subspace However the mechanics of subspace recycling complicates this situation and interferes with our ability to simultaneously solve all systems using these techniques Therefore we introduce an algorithm which avoids this complication and present some numerical experiments demonstrating its effectiveness *Iterative Methods for Solving Linear Systems* Anne Greenbaum,1997-01-01 Mathematics of Computing Numerical Analysis *High-quality Preconditioning Techniques for Multi-length-scale Symmetric Positive Definite Matrices and Their Applications to the Hybrid Quantum Monte Carlo Simulation of the Hubbard Model* Ichitaro Yamazaki,2008 *Computational Methods for Acoustics Problems* Frédéric Magoulès,2008 This volume presents in eleven chapters key computational methods for acoustics and vibro acoustics problems Each chapter written by different authors presents a state of the art of well established or innovative methods techniques or algorithms A bibliography is included at the end of each chapter BOOK JACKET The Journal of the Acoustical Society of America Acoustical Society of America,2006 **Reduced Order Modeling of Incompressible Flow Using Proper Orthogonal Decomposition and Galerkin Projection** Mohamed S. Ebeida,2009 Simulation of Unsteady Incompressible Turbulent Flows Using Galerkin Finite Element and Adaptive Grids Mohamed S. Ebeida,2008

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