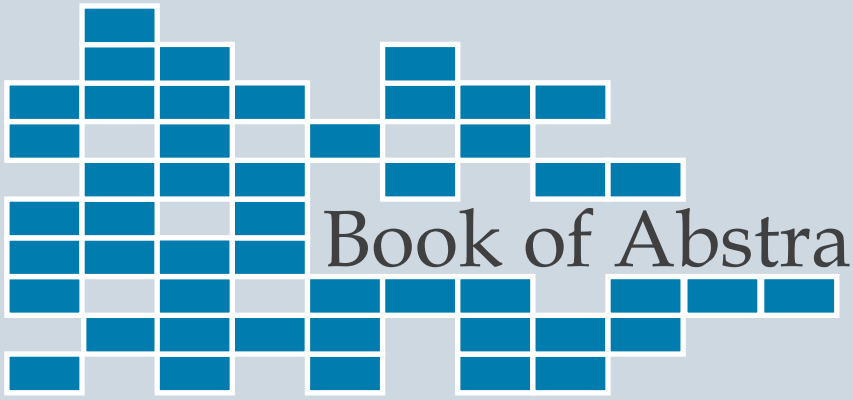

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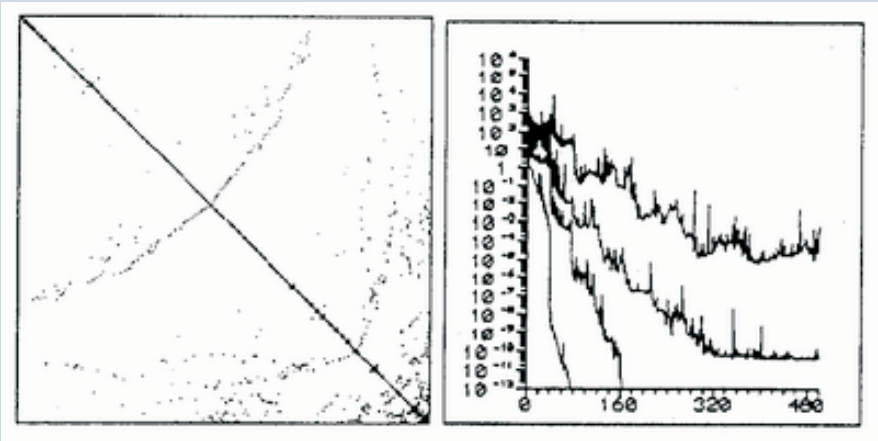

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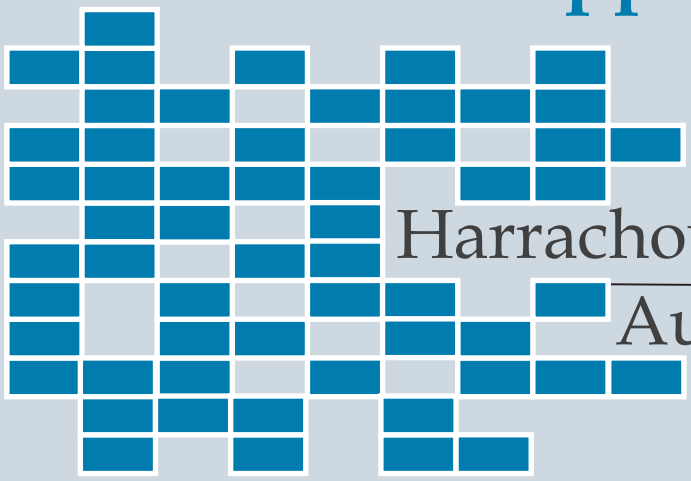

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Contents

A PRECONDITIONED DOMAIN DECOMPOSITION ALGORITHM FOR CONTACT PROBLEM

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Keywords: domain decomposition, Schur complement, preconditioner, seminorm

Abstract

The purpose of this work is to study for small strains, the quasistatic two-body contact problem without friction. The mechanical interation between the bodies is modeled, under the assumption of small displacement, by the bilateral or unilateral contact condition [1]. An algorithm is introduced to solve the resulting finite element system by a non-overlapping domain decomposition method. The global problem is transformed to a independent local problems posed in each bodie and a problem posed on the contact surface (the interface problem). The central aspect of this work is the adaptation of a preconditioner construction developed by B. Kiss at al., in [2] for non-overlapping decomposition domain method to the contact problem. The circulant matrix representations of the $H^{\frac{1}{2}}$ seminorm has been proved to be spectrally equivalent to the Schur Complement in [3]. The advantage of this preconditioner construction is, that its preconditioning property is optimal and this technique allows us to reduce the storage and the matrix-vector multiplication costs. Using this equivalence, the interface problem is transformed to an equivalent problem which is solved with adequate mathematical programming methods [4]. The developed algorithm is validated for two-dimensional and three-dimensional problems.

Reference

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KRYLOV SUBSPACE METHODS FOR AN INITIAL VALUE PROBLEM ARISING IN TEM

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Keywords: TEM, matrix exponential, restarted Arnoldi approximation

Abstract

A popular geophysical exploration technique, known as Transient Electromagnetics (TEM) cf. [1], is based on observing the decay of a low-frequency electromagnetic field in the subsurface in order to infer geological properties of interest. The governing equations for this phenomenon are the time-dependent Maxwell's equations in the diffusive limit of vanishing displacement currents. The typical configuration of a current shutoff leads to a linear constant-coefficient initial value problem for the electric field

$$E_t = -\sigma\Big(\nabla \times (\mu^{-1}\nabla \times E)\Big), \qquad E(t_0) = E_0,$$

which, after discretization by e.g. the Yee finite difference scheme or Nédélec finite elements, becomes the ODE system

$$u'(t) = -Au, \quad u(t_0) = u_0, \tag{1}$$

in which the matrix A denotes the discrete approximation of the differential operator $\sigma\big(\nabla \times (\mu^{-1}\nabla \times \cdot)\big)$. The ODE system (1) is typically solved using explicit time-stepping algorithms such as the Du Fort-Frankel scheme (see, e.g., [1]). Other possible methods include ODE solvers designed especially for parabolic initial value problems such as Runge-Kutta-Chebyshev methods.

In this talk we present some comparisons of such time-stepping techniques with Krylov subspace approximations of the matrix exponential $u(t) = \exp(-A(t-t_0))u_0$, including in particular restarted variants such as proposed in [2].

Acknowledgement: This research was supported by the German Research Foundation (DFG) Projekt *Numerische Simulation der Ausbreitung transienter elektromagnetischer Felder zur Erkundung des Untergrundes.*

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A SCALABLE MULTI-LEVEL PRECONDITIONER FOR MATRIX-FREE μ-FINITE ELEMENT ANALYSIS OF HUMAN BONE STRUCTURES

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Keywords: micro-finite element analysis, algebraic multigrid, aggregation methods, matrix-free preconditioning

Abstract

The recent advances in microarchitectural bone imaging are disclosing the possibility to assess both the apparent density and the trabecular microstructure of intact bones in a single measurement. Coupling these imaging possibilities with microstructural finite element (μFE) analysis offers a powerful tool to improve bone stiffness and strength assessment for individual fracture risk prediction.

Many elements are needed to accurately represent the intricate microarchitectural structure of bone; hence, the resulting μFE models possess a very large number of degrees of freedom. In order to be solved quickly and reliably on state-of-the-art parallel computers, the μFE analyses require advanced solution techniques. In this paper, we investigate the solution of the resulting systems of linear equations by the conjugate gradient algorithm, preconditioned by aggregation-based multigrid methods. We introduce a variant of the preconditioner that does not need assembling the system matrix but uses element-by-element techniques to build the multilevel hierarchy. The preconditioner exploits the voxel approach that is common in bone structure analysis, it has modest memory requirements, while being at the same time robust and scalable. Using the proposed methods, we have solved in less than 10 minutes a model of trabecular bone composed of 247'734'272 elements, leading to a matrix with 1'178'736'360 rows, using only 1024 CRAY XT3 processors.

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GMRES PRECONDITIONED BY A PERTURBED LDL^T DECOMPOSITION WITH STATIC PIVOTING

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Keywords: LDL^T factorization, right preconditioned GMRES, flexible GMRES, roundoff error

Abstract

A strict adherence to threshold pivoting in the direct solution of symmetric indefinite problems can result in substantially more work and storage than forecast by an sparse analysis of the symmetric problem. One way of avoiding this is to use static pivoting where the data structures and pivoting sequence generated by the analysis are respected and pivots that would otherwise be very small are replaced by a user defined quantity. This can give a stable factorization but of a perturbed matrix.

The conventional way of solving the sparse linear system is then to use iterative refinement (IR) but there are cases where this fails to converge. We will discuss the use of more robust iterative methods, namely GMRES and its variant FGMRES and their backward stability when the preconditioning is performed by HSL_M57 with a static pivot option.

Reference

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RATE OF CONVERGENCE OF A NEW BLOCK MATRIX FACTORIZATION VARIABLE PRECONDITIONING METHOD

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Abstract

Classical block-matrix approximate factorization methods for matrices in a two-by-two block form, corresponding to a partitioning of a finite element mesh or of a matrix graph in some fine-coarse set of points, involve at each iteration step two solutions of systems with the approximation of the pivot block, in addition to the solution of the system approximating the Schur complement with respect to the pivot block.

A new method is presented where, in addition to the Schur complement preconditioner, only one solution of the approximate pivot block (or a matrix-vector multiplication with its approximate inverse) is required. This method assumes, however, an initial transformation with a fixed approximation of the off-diagonal block matrix.

Additionally, the method has the advantage that both the outer and inner iterations can be performed using a conjugate gradient method. The use of such inner iterations leads to a variable preconditioner and therefore generalized conjugate gradient methods must be used.

The method is not only applicable for symmetric positive definite systems but also for nonsymmetric and indefinite problems of saddle point form. It is shown that the preconditioned matrix can be written in a form which readily enables estimates of the rate of convergence of the method.

Some numerical tests illustrate the method and show its robustness.

ON MULTIGRID METHODS FOR THE CAHN–HILLIARD EQUATION WITH OBSTACLE POTENTIAL

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Keywords: Cahn–Hilliard equation, finite elements, multigrid methods

Abstract

Numerical simulations of the Cahn–Hilliard equation with obstacle potential require the solution of a saddle-point system with inequality constraint. Based on a preconditioned Uzawa-Multigrid algorithm that has been proposed in [1], the authors recently developed an efficient solution method for a finite element approximation of a degenerate Cahn–Hilliard equation in 3D, see [2]. The Uzawa-Multigrid algorithm can be viewed as an active set strategy, that requires the solution of an unconstrained saddle-point problem. The unconstrained problem can be effectively solved by standard multigrid methods for linear saddle-point problems, however an outer iteration is needed to obtain an approximation of the active set. Here we present a new full multigrid method that is applied directly to the original problem with the inequality constraint, i.e. no outer iterations are needed. Finally, we present some 3D experiments where we illustrate the performance of both multigrid methods.

Acknowledgement: The work of the first author was supported by the EPSRC grant EP/C548973/1.

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MODEL REDUCTION BY A CROSS-GRAMIAN APPROACH FOR DATA-SPARSE SYSTEMS

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Keywords: model reduction, hierarchical matrices, Sylvester equations, Cross-Gramian

Abstract

We consider linear time-invariant (LTI) systems of the following form

$$\Sigma : \begin{cases} \dot{x}(t) &= Ax(t) + Bu(t), \qquad t > 0, \qquad x(0) = x^0, \\ y(t) &= Cx(t) + Du(t), \qquad t \geq 0, \end{cases}$$

with stable state matrix $A \in \mathbb{R}^{n\times n}$ and $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$, $D \in \mathbb{R}^{p\times m}$, arising, e.g., from the discretization and linearization of parabolic PDEs. Typically, in practical applications, we have a large state-space dimension $n = \mathcal{O}(10^5)$ and a small input and output space, $n \gg m, p$. We further assume that the system is square, i.e., $p = m$. We show how to compute an approximate reduced-order system $\hat{\Sigma}$ of order $r \ll n$ with a balancing-related model reduction method. The method is based on the computation of the cross-Gramian X, which is the solution of the Sylvester equation

$$AX + XA + BC = 0.$$

As standard algorithms for the solution of Sylvester equations are of limited use for large-scale systems, we investigate approaches based on the matrix sign function method [2]. To make this iterative method applicable in the large-scale setting, we propose a modified iteration scheme for computing low-rank factors of the solution X and we incorporate structural information from the underlying PDE model into the approach. By using data-sparse matrix approximations, hierarchical matrix formats, and the corresponding formatted arithmetic we obtain an efficient solver having linear-polylogarithmic complexity [1]. We show that the reduced-order model can then be computed from the low-rank factors directly.

Note this continues the talk submitted by P. Benner.

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NUMERICAL RANGE ERROR ESTIMATES FOR EVALUATING FUNCTIONS OF MATRICES VIA THE ARNOLDI METHOD

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Keywords: Arnoldi method, numerical range, Faber polynomials

Abstract

In this talk we propose explicit a priori error bounds for approaching $f(A)b$ by help of the Arnoldi method. Here A is a large real not necessarily symmetric matrix, and f some function analytic on the field of values or numerical range $W(A) = \{y^*Ay : \|y\| = 1\}$. An essential tool in our work is the inequality $\|F_n(A)\| \leq 2$ derived in [1] where F_n is the nth Faber polynomial corresponding to $W(A)$, and $\|\cdot\|$ denotes euclidean vector norms and the induced spectral matrix norm. We show in a first step how to improve bounds given by Knizhnerman [3] and by Hochbruck and Lubich [2]. Subsequently we give some simple bounds in terms of the numerical range for the exponential function as well as for Stieltjes functions like the pth power of A.

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MATHEMATICAL MODEL OF MULTI-PHASE FLOW IN CONCRETE EXPOSED TO HIGH TEMPERATURE

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Keywords: multi-phase flow, coupled problem, finite element method, finite difference method

Abstract

We present a nonlinear mathematical model for numerical analysis of hygro-thermal behavior of concrete segment exposed to transient heating according to the standard ISO fire curve. One- and two dimensional problems for numerical analysis are considered.

The governing equations of the present model are the dry air conservation equation, liquid water conservation equation, water vapor conservation equation coupled with the energy conservation equation (general nonlinear heat equation). Dry air, water vapour and their mixture are assumed to behave as perfect gases, therefore Dalton's law and the Clapeyron equation are assumed as state equations. Water vapour pressure, p_{gw}, is obtained from the Kelvin equation. As the constitutive equations for fluid phases (capillary water, gas phase) the multi-phase Darcy's law is applied.

The numerical algorithm connecting finite element method for the numerical solution of the energy equation and Euler method for the mass balance equations is presented.

Acknowledgement: This research has been supported by Ministry of Education, Youth and Sports of the Czech Republic, No. 1M6840770001 within the frame of research centre CIDEAS.

BALANCING-RELATED MODEL REDUCTION FOR DATA-SPARSE SYSTEMS

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Keywords: model reduction, hierarchical matrices, Lyapunov equations, balanced truncation

Abstract

Model reduction is an ubiquitous tool to facilitate or even enable the simulation, optimization and control of large-scale dynamical systems. Application areas range from microelectronics (device and circuit simulation) over computational biology, control of mechanical and electrical systems to flow control and PDE-constrained optimization. In this talk, we will focus on problems from the latter application areas. In particular, we will discuss model reduction techniques based on system balancing for (optimal) control of parabolic partial differential equations. After discretization of the elliptic (spatial) differential operator by FEM or BEM methods, large-scale, sparse (in case of FEM) or data-sparse (in case of BEM) linear control systems are obtained. Due to the cubic complexity of standard implementations of balanced truncation and relatives, it is not possible to apply these methods directly to such systems.

Here, we will discuss how the use of hierarchical matrices and the corresponding formatted arithmetic enables us to implement balanced truncation and related algorithms for model reduction in almost linear complexity. Our approach is based on the sign function method for solving Lyapunov equations, where matrix inversions, additions, and multiplications are replaced by the corresponding operations for hierarchical matrices [1]. Numerical experiments will demonstrate the applicability of this approach to control problems for several types of parabolic PDEs.

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DOI: 10.1007/s00607-006-0178-y.

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UPDATING PRECONDITIONERS FOR SEQUENCES FROM COMPRESSIBLE FLOW

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Keywords: nonsymmetric preconditioning, preconditioner updates, sequences of linear systems, compressible flow, finite volume methods

Abstract

This contribution illustrates the application of preconditioner updates as in [2] to model problems from compressible flow, that represent a broad range of typical sequences of nonsymmetric linear systems. There, a typical technique is freezing with periodic recomputation of ILU decompositions [3]. This can be improved by updating between refactorizations. In particular, the extension to block matrices is discussed, as well as different strategies for the adaptive choice of the update and the effect of renumbering on the performance of the new method, as in [1]. This is illustrated by theoretical results.

Acknowledgement: The work of the first two authors is supported by the German Science Foundation as part of the Sonderforschungsbereich SFB/TR TRR 30. The work of the second two authors is supported by the Program Information Society under project 1ET400300415 and by project number KJB100300703 of the Grant Agency of the Academy of Sciences of the Czech Republic.

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ALGEBRAIC MULTILEVEL PRECONDITIONERS WITH AGGREGATIONS

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Keywords: multilevel preconditioners, aggregations, finite elements

Abstract

Multilevel preconditioners can be used for solving systems arising from discretization of boundary value problems by the finite element method. Standard multilevel preconditioners use a hierarchy of nested finite element grids and corresponding finite element spaces. In some situations, it can be difficult or impossible to create such hierarchies. In these cases, it is still possible to construct similar hierarchies of spaces in algebraic way by aggregation. This approach can be used e.g. for both conforming and nonconforming linear finite elements and has several favourable properties discussed in the contribution. Beside preconditioning, both geometric and algebraic hierarchies can be also used for aposteriori error estimation.

Acknowledgement: This research is supported by the project 1ET400300415 under the program Information Society granted by the Academy of Sciences of the Czech Republic.

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MODEL REDUCTION USING MULTI-LEVEL SUBSTRUCTURING

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Keywords: model reduction, multi-level substructuring

Abstract

The numerical treatment of linear time-invariant dynamical systems requires in many cases the use of model reduction techniques to reduce the complexity of the system. But the applicability of those methods, particularly SVD-based methods, to large systems is often limited. We present a framework based on multi-level substructuring to treat very large systems. The idea is to decompose the original system hierarchically into several sufficiently small systems. Thus, the reduction methods are applied only to the smaller subsystems. We will use this framework to apply different kinds of reduction methods and show that it can be extended to second order systems.

DECOMPOSITIONAL ANALYSIS OF KRONECKER STRUCTURED MARKOV CHAINS

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Keywords: Markov chains, Kronecker representation, decomposition

Abstract

This contribution proposes a decompositional iterative method for the steady-state analysis of Kronecker structured Markov chains [1]. The Markovian system, which is formed by a composition of subsystems using the Kronecker sum operator for local transitions and the Kronecker product operator for synchronized transitions, is assumed to have irreducible subsystem matrices associated with local transitions. However, in contrast with [2], the interactions among subsystems, which are captured by synchronized transitions, are not assumed to be weak. On a variety of problems the merit of the proposed solver is investigated.

Acknowledgement: This research is partially supported by grants from TÜBA-GEBİP and TÜBİTAK.

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APPROXIMATE INVERSES AND INCOMPLETE DECOMPOSITIONS

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Keywords: preconditioning, approximate inverses, incomplete decompositions, Shermam-Morrison formula

Abstract

In this work we consider the approximate inverse preconditioners AISM based on the Sherman-Morrison formula [1]. We will show some of theoretical properties of the factors of AISM in function of the value of parameter s considered in the decomposition. In particular, we will show that one of the factors hides a scaled factor of the standard incomplete LDU decomposition of the system matrix A. Thus the AISM decomposition can be considered as a way to get an incomplete decomposition via a factorizad approximate inverse. We will show that the LDU decomposition obtained in this way can be useful in preconditioned iterative methods. Numerical experiments illustrate the efficiency of this incomplete decomposition where some dropping strategies are used where the entries and the norms of the inverse factors are considered.

Acknowledgement: This research was fully supported by Spanish grant DGI grant MTM2004-02998 and by the project 1ET400300415 within the National Program of Research "Information Society".

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A REFINED UNSYMMETRIC LANCZOS EIGENSOLVER FOR COMPUTING ACCURATE EIGENTRIPLETS OF A REAL UNSYMMETRIC MATRIX

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Keywords: eigensolver, unsymmetric matrices, Lanczos algorithm

Abstract

For most unsymmetric matrices it is difficult to compute many accurate eigenvalues using the primitive form of the unsymmetric Lanczos algorithm (ULA). In this talk I present a modification of the ULA. Using the refined ULA, the calculation of accurate extremal and interior eigenvalues is feasible. The refinement we is very simple: approximate right and left eigenvectors computed using the ULA are used to form a small projected matrix whose eigenvalues and eigenvectors are easily computed. There is no re-biorthogonalization of the Lanczos vectors and no need to store large numbers of vectors in memory. The method can therefore be used to compute eigenvalues of very large matrices.

SECOND-ORDER TIME-ACCURATE ALE METHODS

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Keywords: second-order time-accuracy, ALE method, flux time-averaging

Abstract

In this paper, we propose second-order time-accurate Lagrangian-Eulerian methods for a compressible fluid in a moving domain. Instead of using rezoning and remapping technique, we discretize unsteady and compressible Euler equations for moving grid points directly to consider the effect of movement of grids on flux. Our approach is based on time-averaging flux. Numerical analysis shows our approach is formally second-order time-accuracy. Numerical results prove that our approach is convergent and stable.

Acknowledgement: This research was fully supported by the Technology Fund of Chinese Academy of Engineering under Project 20060108.

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H-MATRIX THEORY AND ITS APPLICATIONS

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Keywords: H-matrices, strictly diagonally dominant matrices, diagonal scaling

Abstract

The most important property of the class of H-matrices, in the sense of applications presented here, is the following: every H-matrix can be diagonally scaled into a strictly diagonally dominant form. When the scaling matrix is chosen to be a diagonal matrix of the special form, we are able to characterize the corresponding subclass of H-matrices by relatively simple conditions. Precisely this fact allows us to improve known results in several different linear algebra fields: eigenvalue localization, bounds of determinants, Perron root estimates, or convergence of some relaxation methods. The aim of the talk is to present general idea of this approach.

Acknowledgement: This research is partly supported by Provincial Secretariat of Science and Technological Development of Vojvodina, grant 01123.

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ORTHOGONALIZATION VIA DEFLATION: A MINIMUM NORM APPROACH FOR LOW - RANK APPROXIMATIONS OF A MATRIX

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Abstract

In this talk we introduce a new orthogonalization method. Given a real $m \times n$ matrix A, the new method constructs an SVD-type decomposition of the form $A = U\Sigma V^T$. The columns of U and V are orthogonal, or nearly orthogonal, while Σ is a diagonal matrix whose diagonal entries approximate the singular values of A. The method has three versions. A "left-side" orthogonalization scheme in which the columns of U constitute an orthonormal basis of Range(A). A "right-side" orthogonalization scheme in which the columns of V constitute an orthonormal basis of Range(A^T). In the third version both U and V have orthonormal columns, but the the decomposition is not exact.

Starting from $A_1 = A$ the deflation process generates a sequence of matrices $A_1, A_2, A_3, \ldots$, by the rule

$$A_{k+1} = A_k - \sigma_k \mathbf{u}_k (\mathbf{v}_k)^T, \quad k = 1, 2, 3, \ldots,$$

where $\{\sigma_k, \mathbf{u}_k, \mathbf{v}_k\}$ denotes a computed estimate of a singular triplet of A_k. The estimated singular vectors are obtained by a few "rectangular iterations" for solving the minimum norm problem

$$\text{minimize } F(\mathbf{u}, \mathbf{v}) = \|A_k - \mathbf{u}\mathbf{v}^T\|_F^2.$$

The resulting orthogonal decomposition may substitute the SVD in many applications. The advantage of the new method lies in problems with missing data. That is, when some entries of A are unknown. Standard SVD algorithms are unable to handle such matrices. Yet the minimum norm approach overcomes this difficulty in an elegant way: The objective function is redefined as

$$F(\mathbf{u}, \mathbf{v}) = \Sigma(a_{ij} - u_i * v_j)^2,$$

where the sum is restricted to known entries of A. This modification enables us to construct a low-rank approximation of A, or a "pseudo SVD" of A, in spite of the missing data. Once a pseudo SVD of A is constructed, it can be used for estimating the missing data. Numerical experiments illustrate the usefulness of the proposed methods.

REDUCED ORDER MODELING IN A DATA ASSIMILATION PROCEDURE USING PROPER ORTHOGONAL DECOMPOSITION

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Keywords: reduced order model, proper orthogonal decomposition, data assimilation, convection-diffusion equation, optimal control

Abstract

The proper orthogonal decomposition (POD) represents an efficient way to carry out reduced order modeling by identifying the few most energetic modes in a sequence of snapshots from a time-dependent system, and providing a means of obtaining a low-dimensional description of the system's dynamics. Many researchers have applied the POD technique to optimal control problems. The variational data assimilation for oceanographic and atmospheric models is an example of optimal control problem, where initial condition is the control variable. A difficult task in the operational use of data assimilation for such kind of models is the large dimension of the control space which is the size of the discrete model initial conditions ($10^6 - 10^8$). Order reduction procedures aim to alleviate the computational effort of the variational data assimilation by performing the optimization in a low-order control space.

In this paper the POD approach to model reduction is used to construct a reduced-order control space for one-dimensional convection-diffusion equations. We perform several data assimilation experiments associated with such transport models using the reduced control space. A comparative study with these experiments in the full model space shows that with appropriate basis functions the optimization in the POD space is able to provide good results at a reduced computational cost.

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STUDY OF THE BDF-DGFE METHOD FOR THE SOLUTION OF THE COMPRESSIBLE NAVIER-STOKES EQUATIONS

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Keywords: Navier-Stokes equations, discontinuous Galerkin finite element method, backward difference formulae, linearization

Abstract

Our aim is to developed a sufficiently robust, accurate and efficient numerical scheme for the simulation of a viscous compressible flow, which is described by the system of the *Navier-Stokes equations*. Among several types of numerical schemes the *discontinuous Galerkin finite element* (DGFE) method seems to be a promising technique for the discretization of this system. DGFE method is based on a discontinuous piecewise-polynomial approximation. The main advantages of this approach are the discontinuous approximation (important for transonic flow regimes), high order of approximation, local character of the method and easy parallelization.

Within this contribution we present a semi-implicit numerical scheme which is based on DGFE method for the space semi-discretization and the *backward difference formula* (BDF) for the time discretization presented in [1]. A suitable *linearization* of inviscid as well as viscous fluxes leads to a linear algebraic problem at each time step which should be solved by a suitable solver.

We study the implementation and algoritmization aspects of this approach, namely the choice of basis functions, matrix solver and preconditioning of the linear algebraic problem. We present several numerical examples.

Acknowledgement: This work is a part of the research project MSM 0021620839 financed by the Ministry of Education of the Czech Republic.

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PRECONDITIONING FOR BOUND CONSTRAINED QUADRATIC PROGRAMMING PROBLEMS ARISING FROM DISCRETIZATION OF VARIATIONAL INEQUALITIES

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Keywords: quadratic programming, rate of convergence, bound constraints

Abstract

The active set based MPRGP (modified proportioning with reduced gradient projection) [1] for the solution of partially bound constrained quadratic programming problems turned out to be an important ingredient in development of scalable algorithms for the solution of variational inequalities by FETI [3] and BETI [4] domain decomposition methods. The algorithm was proved to have R-linear rate of convergence in terms of the spectral condition number of the Hessian matrix. Our poster considers the preconditioning of MPRGP active set based algorithm [1] with goal to get improved rate of convergence of the algorithm. We are interested in results which concern the overall rate of convergence, which requires not only the preconditioning of the solution of auxiliary linear solvers, but also the preconditioning of nonlinear steps. We first report improved bounds on the rate of convergence of MPRGP with preconditioning by conjugate projector applied to a model boundary variational inequality [2] and give results of numerical experiments that are in agreement with the theory. The method uses, similarly as related multigrid algorithms, the auxiliary subspace which is not effected by the constraints. Then we give numerical examples which indicate the ways how to overcome this limitation in the framework of FETI based domain decomposition methods.

Acknowledgement: This research has been supported by the grants GA CR 201/07/0294 and 1ET400300415 and the institutional project MSM6198910027.

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OPTIMAL ALGORITHMS FOR LARGE SCALE QUADRATIC PROGRAMMING PROBLEMS

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Abstract

First we describe an active set based algorithm [1] for the solution of bound constrained quadratic programming problems. The working set based algorithm combines the the conjugate gradient method to explore the face of the feasible region defined by the current iterate with the reduced gradient projection with the fixed steplength. The precision of approximate solutions of the auxiliary unconstrained problems is controlled by the structure of violation of the Karush-Kuhn-Tucker conditions at the active constraints. The algorithm has R-linear rate of convergence in terms of the spectral condition number of the Hessian matrix and the finite termination property preserved even for the dual degenerate problems. The algorithm is then combined with a variant of the augmented Lagrangian type algorithm for strictly convex quadratic programming problems with equality constraints to obtain and algorithm for the solution of the bound and equality constrained problems. The update rule for the penalty parameter is introduced that is related to the increase of the augmented Lagrangian. A qualitatively new feature of the algorithm is a bound on the feasibility error that is independent of conditioning of the constraints and is valid even for dependent constraints and the quadratic functions with semidefinite Hessian. The algorithm turned out to be a key ingredient in the development of scalable algorithms for the solution of variational inequalities by FETI [3] and BETI [4] domain decomposition methods.

Acknowledgement: This research has been supported by grant 1ET400300415 and the institutional project MSM6198910027.

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COMPUTING A LOW-RANK APPROXIMATION OF A TENSOR

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Keywords: tensor, low-rank, approximation, multilinear, Newton's method, Grassmann, manifold

Abstract

We investigate various properties of the best rank-(r_1, r_2, r_3) approximation of a tensor, and their implications in the development of algorithms for computing the approximation. The problem is formulated as an optimization problem on a product of Grassmann manifolds, which we solve by Newton's method. We develop a notation that makes it possible to derive the Newton equation without extensive index manipulation (which is rather common in tensor contexts). Numerical examples are given, where we compare the Newton method with the alternating least squares method.

This is joint work with Berkant Savas.

Acknowledgement: This research was partially supported by the Swedish Research Council.

POTENTIAL THEORY AND PRACTICAL ASPECTS OF THE SOLUTION OF LYAPUNOV EQUATIONS

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Keywords: ADI iteration, condenser capacity, Sylvester equation

Abstract

The Lyapunov equation $AX+XA^* = -BB^*$ poses considerable computational challenges when the dimension of A is large, for the solution X is typically dense regardless of the sparsity of A. However, in many applications the right-hand side has low rank, and under broad hypotheses the solution X inherits this trait. Effective algorithms, such as the modified Smith method, efficiently approximate X in a low-rank factored form.

Numerous issues must be addressed to translate this observation into an algorithm viable for the kind of large-scale problems that arise, for example, in balanced truncation model reduction. In this talk, we shall describe estimates on the decay of the singular values of X derived from potential theory (work in collaboration with Christopher Beattie). Such analysis suggests both the rank of X and asymptotically optimal shifts for use in the modified Smith method. Practical considerations naturally restrict the number of shifts, and we shall demonstrate how one can often achieve more effective convergence by repeatedly applying a small set of shifts determined via an optimization scheme. Several other important considerations, ranging from the order in which shifts are applied and the use of inexact inner iterations, to techniques for efficiently computing the residual norm [1], shall also be discussed.

Acknowledgement: This research was supported in part by US National Science Foundation Grant DMS-CAREER-0449973.

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MULTILEVEL KRYLOV METHOD FOR THE HELMHOLTZ EQUATION

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Keywords: multilevel Krylov method, GMRES, Helmholtz equation, shifted Laplace preconditioner

Abstract

In the first part of the talks on multilevel Krylov methods, Reinhard Nabben discussed the underlying concept of the method and showed by some numerical examples the effectiveness of the method. In this talk, we extend the application of the multilevel Krylov method to the indefinite, high wavenumber Helmholtz equation.

In this case, we consider the preconditioned Helmholtz system, where the preconditioner is the discrete formulation of the shifted Laplace preconditioner [1] and is solved by one multigrid iteration. With this preconditioning, the eigenvalues of the system are clustered around zero and one. To speed up the convergence, multilevel Krylov method is applied to the preconditioned system, based on shifting of small eigenvalues to one. To construct the coarse grid problem associated with the projected small eigenvalues, an approximation based on a product of low dimension matrices is introduced. This approximation will require a multigrid iteration of reduced level in the preconditioning step at every level in the projection step.

Numerical examples show that the convergence of Krylov iteration applied to 2D high wavenumber Helmholtz problems can be made independent of both grid size and wavenumber.

Acknowledgement: The research was supported by the *Deutsche Forschungsgemeinschaft* (DFG), Project Number NA248/2-2.

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KARHUNEN-LOÈVE APPROXIMATION OF RANDOM FIELDS USING HIERARCHICAL MATRIX TECHNIQUES

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Keywords: random field, Karhunen-Loève expansion, covariance operator, hierarchical matrix approximation, restarted Lanczos method

Abstract

In stochastic finite element computations for modelling uncertainty a popular approach for separating the deterministic and stochastic dependencies of a random field is to compute the first few terms of its Karhunen-Loève (KL) expansion. This entails approximating the dominant eigenpairs of its covariance operator, leading to a large dense eigenvalue problem, in particular since the operator typically acts on functions defined on a domain, not only its boundary.

In this talk we emphasize the relation of the KL expansion to the singular value decomposition and present our experiences in computing approximate covariance eigenpairs based on Galerkin discretization and Krylov subspace projection. The latter requires efficient matrix-vector multiplication routines. Recent work has explored fast multipole techniques [2]. Here we employ the hierarchical matrix approximation technique [1].

Acknowledgement: This research was partially supported by the German Academic Exchange Service (DAAD) under the project *Uncertainty Quantification in Computer Simulations of Groundwater Flow Problems with Emphasis on Contaminant Transport.*

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ON A QUADRATIC EIGENVALUE PROBLEM ARISING IN THE ANALYSIS OF DELAY EQUATIONS

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Keywords: polynomial eigenvalue problem, structured linearization, eigenvalue pairing

Abstract

The analysis of retarded linear m-delay time delay systems

$$\begin{array}{ll} \dot{x}(t) = \sum_{k=0}^{m} A_k x(t-h_k), & t > 0 \\ x(t) = \phi(t), & t \in [-h_m, 0] \end{array}$$

with $h_0 = 0 < h_1 < \ldots < h_m, x : [-h_m, \infty) \to \mathbb{R}^n, A_k \in \mathbb{R}^{n\times n}$, leads to a quadratic eigenvalue problem $Q(\lambda)u = 0$ where

$$Q(\lambda) = \lambda^2 E + \lambda F + G$$

with $E = A_m \otimes I, G = I \otimes A_m$, and $F = \sum_{k=0}^{m-1} I \otimes A_k e^{-i\phi_k} + A_k \otimes I e^{i\phi_k}, \phi_k = \omega h_k$ where $\otimes$ denotes the Kronecker product.

As there exists a permutation matrix P such that $P^T(A \otimes B)P = B \otimes A$ for all real $n \times n$ matrices A, B, the quadratic matrix polynomial Q satisfies

$$P^T \mathrm{rev}(\overline{Q}(\lambda))P = Q(\lambda), \tag{1}$$

where $\overline{Q}(\lambda) = \lambda^2\overline{E} + \lambda\overline{F} + \overline{G}$ and $\mathrm{rev}(Q(\lambda)) = \lambda^2 Q(\frac{1}{\lambda})$. Matrix polynomials which satisfy (1) remind of the different palindromic polynomial definition given in [1], e.g., a palindromic polynomial is given by $\mathrm{rev}(Q(\lambda)) = Q(\lambda)$, while a $\star$-palindromic polynomial satisfies $\mathrm{rev}(Q^\star(\lambda)) = Q(\lambda)$, where $\star$ is used as an abbreviation for transpose T in the real case and either T or conjugate transpose $*$ in the complex case.

Following the derivations in [1], we will discuss the spectral symmetry of matrix polynomials (1) as well the structured linearizations where we continue the practise stemming from Lancaster of developing theory for polynomials of degree k where possible in order to gain the most insight and understanding.

Acknowledgement: Work done in collaboration with Elias Jarlebring, TU Braunschweig, Germany and Nil and Steve Mackey, Western Michigan.

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INEXACT SHIFT-AND-INVERT ARNOLDI'S METHOD AND IMPLICIT RESTARTS WITH PRECONDITIONING FOR EIGENCOMPUTATIONS

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Keywords: eigenvalue approximation, shift-and-invert Arnoldi's method, iterative methods, preconditioning

Abstract

We consider the computation of a few eigenvectors and corresponding eigenvalues of a large sparse nonsymmetric matrix. In order to compute eigenvalues in an isolated cluster around a given shift we apply shift-and-invert Arnoldi's method with and without implicit restarts. For the inner iterations we use GMRES as the iterative solver. The costs of the inexact solves are measured by the number of inner iterations needed by the iterative solver at each outer step of the algorithm.

We first extend the relaxation strategy developed by Simoncini [2] to implicitely restarted Arnoldi's method which yields an improvement in the overall costs of the method.

Secondly we apply a new preconditioning strategy to the inner solver. We show that small rank changes of the preconditioner can produce significant savings in the total number of iterations. This property has been observed in [1]. Numerical experiments illustrate the theory.

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ORDER REDUCTION OF TRULY LARGE-SCALE LINEAR DYNAMICAL SYSTEMS

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Keywords: dimension reduction, order reduction, Krylov subspace method, Padé approximation, Padé-type approximation, projection

Abstract

In recent years, Krylov subspace methods have become widely-used tools for order reduction of large-scale linear dynamical systems; see [1] for a recent survey of such reduction techniques. Despite all the progress in this area, the development of algorithms that are applicable to truly large-scale systems and at the same time preserve the key structures of the large-scale system remains a challenging task. For example, state-of-the-art algorithms, such as SPRIM [2], for structure-preserving order reduction of the large-scale systems arising in VLSI circuit simulation are based on explicit projection. They first generate a basis matrix of the underlying Krylov subspace and then employ projection using some suitable partitioning of the basis matrix to obtain a structure-preserving reduced-order model. There are two major problems with the use of such explicit projections. First, it requires the storage of the basis matrix, which becomes prohibitive in the case of truly large-scale linear dynamical systems. Second, the approximation properties of the resulting structure-preserving reduced-order models are far from optimal, and they show that the available degrees of freedom are not fully used.

In this talk, we first present an overview of Krylov subspace-based reduction techniques for large-scale linear dynamical systems. We then discuss some recent variants of these techniques that avoid explicit projection and are thus applicable to truly large-scale systems.

Acknowledgement: This research was supported in part by the National Science Foundation grant DMS-0613032.

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PARALLEL ACCESS TO NETCDF FILES IN HIGH PERFORMANCE APLICATIONS FROM HIGH-LEVEL FRAMEWORKS

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Keywords: parallel architectures, MPI, netCDF, climate variability, scalable applications

Abstract

The analysis of climate variability requires to perform operations with netCDF files [1], Empirical Orthogonal Functions analysis (EOF), and Singular Value Decompositions (SVD) of coupled data sets. As example, PyClimate [2] is a Python package designed to accomplish these tasks sequentially. However, the huge data volume in this kind of applications requires high performance routines that can be executed in distributed memory architecture platforms. High performance linear algebra operations can be performed with the high-level framework PyACTS [3]. Also, huge volume of the netcdf files requires a parallel tool for Python. In this way, we present PyPnetCDF like a Python package that implements parallel access to netCDF files using PnetCDF library [4]. The results show a scalable tool with very lower execution times than the sequential application when the data volume is high.

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DISCRETE SCHWARZ METHODS: DISCRETIZATIONS OF CONTINUOUS SCHWARZ METHODS?

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Keywords: dimension reduction, order reduction, Krylov subspace method, Padé approximation, Padé-type approximation, projection

Abstract

Schwarz domain decomposition methods have been developed at two different levels: at the continuous level for partial differential equations (the historical Schwarz alternating method by Schwarz himself in 1869, and a parallel Schwarz method by Lions in 1988), and at the discrete level for linear systems (multiplicative and additive Schwarz by Dryja and Widlund in 1987, and more recently restricted additive Schwarz and additive Schwarz with harmonic extension by Cai and Sarkis en 1999, discovered by a programming error).

I will first show in my talk similarities and differences between the classical continuous and discrete Schwarz methods. I will then introduce at the algebraic level a new class of Schwarz methods, called optimized Schwarz methods, which converge significantly faster than classical Schwarz methods, at the same cost per iteration. I will conclude with three important open problems in this area of research.

STABILIZATION OF RESTARTED KRYLOV METHODS FOR MATRIX FUNCTIONS

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Keywords: matrix function, restarted Krylov subspace method, Lyapunov equation

Abstract

In [1] Eiermann and Ernst proposed a restarting scheme for Krylov subspace approximations to $f(A)b$ where f is a suitable function, A a square matrix and b a vector. The approximates are of the form

$$f(A)b \approx \beta V_m f(H_m) e_1,$$

where

$$AV_m = V_m H_m + \eta_{m_1,m} v_{m+1} e_1^\top$$

is an Arnoldi-like decomposition and $\beta v_1 = b$. The most straightforward implementation is based on the evaluation of an expression for the error which involves repeated divided differences of f where the nodes are the Ritz values associated with the successive Krylov subspaces generated in the course of the restart algorithm. Since the direct evaluation of this error formula is in general unstable, a somewhat more expensive variant was proposed in [1] which required applying the function f to an aggregate Hessenberg matrix and which was found to be stable.

In this talk we present an alternative stable variant based on the Schur-Parlett approach for evaluating matrix functions by solving Lyapunov equations. This variant is stabilized by repeated swapping of diagonal blocks inside the Schur form (cf. [2]).

Acknowledgement: This research was supported by the German Research Foundation (DFG) Projekt *Numerische Simulation der Ausbreitung transienter elektromagnetischer Felder zur Erkundung des Untergrundes.*

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THE TECHNIQUE OF HIERARCHICAL MATRICES

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Abstract

The discretisation of partial differential equations (PDEs) leads to large systems of equations. In particular, the boundary element method (BEM) produces fully populated matrices. Several methods try to reduce the costs for storage and matrix-vector multiplication from $\mathcal{O}(n^2)$ to $\mathcal{O}(n \log^* n)$. The technique of hierarchical matrices presented here supports *all* matrix operations, i.e., addition, multiplication, inversion of matrices and LU decompositions up to certain approximation errors. This is of interest also for the sparse matrices from FEM, since the dense inverse or certain Schur complements can be approximated.

Concerning the applications, we mention several topics.

FEM preconditioning: Linear equations with sparse FEM matrices A are usually solved iteratively, provided a good preconditioner is available. The technique of hierarchical matrices allows to approximate the LU-factors (if they exist) which lead to a perfect black-box preconditioner. The most efficient version uses domain decomposition ideas for the construction of the cluster tree.

Matrix equations: The Lyapunov and Riccati equations arise in control theory and define a system of n^2 equations for the n^2 unknown entries of X. Therefore the best possible solve seems to need a work of $O(n^2)$. If the coefficient matrix A arises from an elliptic operator (as in control problems with a state governed by an elliptic boundary value problem), it turns out that the solution X can be well approximated by a hierarchical matrix. The costs add up to $O(nk^2 \log^3 n)$ even in the case of the nonlinear Riccati equation.

Matrix functions: The matrix exponential function $\exp(-tA)$ is of general interest. We are able to compute $\exp(-tA)$ with accuracy ε with a cost of order $O(n \log^p \frac{1}{\varepsilon} \log^q n)$. Similarly, other matrix functions can be computed, in particular, the sign-function $sign(A)$ is a very interesting function.

Beyond the hierarchical matrix technique, one can consider similar constructions involving Kronecker tensor products instead of low-rank matrices. Here we present some problems in high spatial dimensions.

USING EXTRAPOLATION FOR THE SOLUTION OF THE LINEAR COMPLEMENTARITY PROBLEM

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Keywords: Linear Complementarity Problem (LCP), positive stable matrices, $P-$matrices, positive definite matrices, iterative schemes, extrapolation, Möbius transformations

Abstract

The *Linear Complementarity Problem* (LCP) has many applications as, e.g., in the solution of Linear and Convex Quadratic Programming, in Free Boundary Value problems of Fluid Mechanics, etc. In the present work we consider the case where the matrix coefficient $A \in \mathbf{R}^{n,n}$ of LCP is a *positive stable matrix*. Considering a known iterative method for the solution of LCP we introduce the principle of *Extrapolation* and find the best *extrapolation* parameter ω for which the corresponding extrapolated iterative scheme converges asymptotically faster. Various simple and more complicated numerical examples show that it is worth using extrapolation to solve an LCP.

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IMAGE DEBLURRING IN THE LIGHT OF DCT

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Keywords: regularization, regularizing iterations, discrete cosine transform

Abstract

In the setting of matrix computations, the model for the blurring of the image is $A\,x = b$, where the vectors x and b represent the exact and blurred images, and the matrix A represents the blurring process. Since image deblurring is a discrete ill-posed problem, it is necessary to use regularization in order to compute stable solutions [1]. Moreover, it is often advantageous to impose boundary conditions on the reconstruction, which is achieved by a simple modification of the coefficient matrix [2], [3].

This paper focuses on *regularizing iterations* where we apply a Krylov subspace method directly to the problem $Ax = b$. The regularization comes from the projection of the solution on the Krylov subspace associated with the method, and the number of iterations plays the role of the regularization parameter.

We use the two-dimensional discrete cosine transform (DCT) to perform a spectral analysis of the solutions to the image deblurring problem, computed by means of regularizing iterations, and we focus on CGLS/LSQR and GMRES and their variants MINRES, RRGMRES and MR-II. To the best of our knowledge, a thorough study of the spectral and visual quality of the reconstructions computed by these methods has not been carried out.

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GMRES METHODS FOR LEAST SQUARES PROBLEMS

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Keywords: linear least squares problem, iterative method, Krylov subspace method, GMRES, CGLS, LSQR, robust incomplete factorization (RIF), reorthogonalization

Abstract

The standard iterative method for solving large sparse least squares problems $\min_{\boldsymbol{x}\in\mathbf{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|_2$, $A \in \mathbf{R}^{m\times n}$ is the CGLS method, or its stabilized version LSQR, which applies the (preconditioned) conjugate gradient method to the normal equation $A^{\mathrm{T}}A\boldsymbol{x} = A^{\mathrm{T}}\boldsymbol{b}$.

In this talk, we will consider alternative methods [1] using a matrix $B \in \mathbf{R}^{n\times m}$ and applying the Generalized Minimal Residual (GMRES) method to $\min_{\boldsymbol{z}\in\mathbf{R}^m} \|\boldsymbol{b} - AB\boldsymbol{z}\|_2$ or $\min_{\boldsymbol{x}\in\mathbf{R}^n} \|B\boldsymbol{b} - BA\boldsymbol{x}\|_2$.

First, we give a sufficient condition concerning B for the GMRES methods to give a least squares solution without breakdown for arbitrary $\boldsymbol{b}$, for over-determined, under-determined and possibly rank-deficient problems. Next, we give a convergence analysis of the GMRES methods as well as the CGLS method. Then, we propose using the robust incomplete factorization (RIF) [2] for B.

Finally, we show by numerical experiments on over-determined and under-determined problems that, for large problems, the GMRES methods with RIF, give least squares solutions faster than the CGLS and LSQR methods with RIF. We will also discuss the effect of reorthogonalization on the CGLS method.

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WOVEN CONVOLUTIONAL CODES FOR NO BINARY FINITE FIELDS

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Keywords: woven convolutional codes, concatenated convolutional codes, parallel iterative encoder

Abstract

Binary woven convolutional codes was introduced by S. Host, R. Johannesson, and V. Zyablov [1], [2]. This construction, considered as a powerful method to obtain convolutional codes with very large free distance, can be regarded as generalization of cascade convolutional codes. In this contribution we consider some practical iterative encoder implementations of no binary woven convolutional codes. For the purpose to introduce the parallel iterative encoder algorithm, we use the linear system modelization of woven convolutional codes for any finite fields introduced by Climent, Herranz, and Perea [3]. We have developed a parallel environment, integrating Matlab and MPI, that implements the encoder proposed. We show the results obtained in a distributed memory architecture. Finally, to select some good examples, we take into account the lower bound for the free distance of the concatenated convolutional codes from system viewpoint that appears in [4].

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NUMERICAL ANALYSIS OF THE MATRIX LOGARITHM

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Keywords: matrix, function, logarithm, exponential, Fréchet derivative

Abstract

We present the theory of the matrix logarithm and algorithms for computing it and its condition number. The matrix logarithm arises in a number of applications and we begin by outlining some of them. We classify all logarithms of a matrix, analyze when $\log(AB) = \log(A) + \log(B)$ for matrices A and B, and characterize the Fréchet derivative and the condition number. The inverse scaling and squaring method based on Padé approximation and repeated square roots is then developed for both triangular and full matrices and compared with a Schur–Parlett algorithm. Finally, numerical evaluation of the Fréchet derivative and exact computation and estimation of the condition number are treated.

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ON TOTAL LEAST SQUARES FORMULATION IN LINEAR APPROXIMATION PROBLEMS WITH MULTIPLE RIGHT-HAND SIDES

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Based on the joint work with **Diana Sima**, *K. U. Leuven, Belgium.*

Keywords: total least squares, multiple right-hand sides, core problem

Abstract

Consider an orthogonally invariant linear approximation problem $Ax \approx b$. In [3] it is proved that the partial Golub-Kahan bidiagonalization [1] of the matrix $[b, A]$ determines a *core approximation problem* $A_{11}x_1 \approx b_1$ containing the necessary and sufficient information for solving the original problem. It is shown how the core problem can be used in a simple and efficient way for solving different formulations of the original approximation problem.

In this contribution we concentrate on the total least squares formulation [2] of a linear approximation problem $AX \approx B$ with *multiple right-hand sides*. Here a concept of the solution, and, consequently, of a minimally dimensioned approximation problem containing the necessary and sufficient information for solving the original problem, is still under development, cf. [4].

We will discuss several difficulties which have to be resolved in formulation of the total least squares problem with multiple right-hand sides, and investigate techniques that could possibly lead to an extension of the core problem theory.

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NUMERICAL SOLUTION OF POROUS MEDIA TRANSPORT PROBLEM WITH DOUBLE POROSITY AND NON-LINEAR ADSORPTION

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Keywords: advection-diffusion problem, non-equilibrium, mobile-immobile

Abstract

We describe a numerical scheme for a coupled problem of the advection-diffusion equation and the first-order non-equilibrium interaction process, with non-linear terms. In the field of groundwater contamination modelling, it represents the solute transport with non-equilibrium diffusive exchange between mobile and immobile pores or fractures and equilibrium non-linear adsorption on solid surface. The presented problem and its solution is a generalisation of two standard approaches, each with one of the features excluded (non-linearity or non-equilibrium).

We formulate the scheme on the basis of the finite volume method, applied for both the advection-diffusion equation in the mobile zone and the first-order interaction in the immobile zone. The time discretisation allows arbitrary weighting between explicit and fully implicit scheme. The resulting system of non-linear equation is solved with standard Newton-Raphson iterations, assuming all the necessary properties of non-linear coefficients. Next we use a block substitution method, transforming the double-sized algebraic system (mobile and immobile unknowns) to the size and sparse form of the simple advection-diffusion problem.

We also present results of numerical experiments on physically illustrative problems.

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A FEM/MULTIGRID SOLVER FOR MONOLITHIC ALE FORMULATION OF FLUID-STRUCTURE INTERACTION PROBLEM

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Keywords: fluid-structure interaction, monolithic ALE, mixed FEM, multigrid

Abstract

In this contribution we investigate a monolithic algorithm to solve the problem of time dependent interaction between an incompressible, possibly non-newtonian, viscous fluid and an elastic solid. The continuous formulation of the problem and its discretization is done in a monolithic way, treating the problem as one continuum and discretized by the Q2/P1 finite elements. The resulting set of nonlinear algebraic system of equations is solved by an approximate Newton method with coupled geometric multigrid linear solver for solving the linear subproblems. We discuss possible efficient strategies of setting up the resulting system and its solution. A 2-dimensional configuration is presented to test the developed method. It is based on the DFG benchmark *flow around cylinder* for incompressible laminar fluid flow and extendet to fluid-structure interaction in [1].

Acknowledgement: This research was supported by NCMM, project LC06052, financed by MSMT CR.

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ON SINGULAR VALUES OF PARAMETER DEPENDENT MATRICES

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Keywords: SVD, ASVD, continuation, singularity theory

Abstract

We consider the *Analytic Singular Value Decomposition*, ASVD, of matrix valued functions. ASVD is smooth up to isolated parameter values at which either a multiple singular value or a zero singular value turns up on the path. These exceptional points are called *non-generic*, see [1]. They were classified in [2]. Note that ASVD-computations, see e.g. [1], [2], require information on *all* singular values on the path and hence the algorithms were not able to cope with large sparse input data. In [3], we investigated a pathfollowing of just *one* simple singular value and the corresponding left/right singular vector. A breakdown of the continuation is related to non-generic points on the path. We apply Singularity Theory to analyze and classify these non-generic points. Our analysis will include the questions concerning *structural stability*. The classification will result in precise localization technique of these points. We compare our classification list with [2].

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A NOTE ON COMPUTATION OF PSEUDOSPECTRA

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Keywords: pseudospectra, pathfollowing

Abstract

The aim is to contribute to pseudospectra computation via a pathfollowing, see e.g. [1], [2].

Let $A = A(t) \in \mathbb{R}^{m\times n}$, $m \geq n$. In [3], we proposed a continuation technique to follow the path of simple singular values and the corresponding left/right singular vectors of $A(t)$. For example we may wish to follow the path of the smallest singular values.

In ALA 06, Stratis Gallopoulos suggested to apply the above technique in order to compute pseudospectrum curves: Given $B \in \mathbb{C}^{n\times n}$, follow the contours $\partial\Lambda_\epsilon = \{z|\sigma_{\min}(zI - B) = \epsilon\}$.

After a "realification" and some transformations, we consider a curve $f : \mathbb{R}^{2+4n} \longrightarrow \mathbb{R}^{1+4n}$. The coordinates of the state space $\mathbb{R}^{2+4n}$ are interpreted as the parameter z, and u, $v \in \mathbb{C}^n$, respectively, are the right/left singular vectors of $(zI - B)$ related to $\sigma_{\min}(zI - B) = \epsilon$. The pathfollowing f yields the contours $\partial\Lambda_\epsilon$.

Acknowledgement: The research of both authors was partially supported by the Grant Agency of the Czech Republic (grant No. 201/06/0356).

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AN APPLICATION OF THE BAUER-FIKE THEOREM TO NONLINEAR EIGENPROBLEMS

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Keywords: the Bauer-Fike theorem, nonlinear eigenvalue problems, eigenvalue perturbation analysis, time-delay systems

Abstract

We consider the problem of characterizing the approximation accuracy of a set of eigenvalues of the *nonlinear eigenvalue problem*

$$(-sI + A_0 + A_1 h(s))\, v = 0,\ v \neq 0,$$

for an analytic function h. The analysis is done by successively applying *the Bauer-Fike theorem*, generating a sequence of conditions which relates the approximation with the solution. The sequence can be treated as a *fixpoint iteration* which is necessary to converge for the theory to yield accuracy information. We apply the analysis to an approximation of a *time-delay system*, where we find necessary and sufficient conditions for the fixpoint iteration to converge and show that it converges to a value explicitly expressible with the *Lambert W function*.

STABILIZING ITERATIVE METHODS: LIMITS OF PERFORMANCE VIA REACHABLE SETS

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Keywords: GMRES(m), Rayleigh Iteration, stability of numerical methods

Abstract

Numerical algorithms can be interpreted as discrete-time control systems, incorporating shift parameters as control variables. We analyze the geometric structure of the reachable sets for two well-known algorithms: GMRES(m) and Rayleigh Iteration. Our results provide fundamental limitations on the possibility of feedback stabilization. Necessary as well as sufficient conditions for the existence of convergent shift strategies are derived.

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PARALLEL SOLUTION OF THERMOELASTICITY PROBLEMS USING AGGREGATIONS

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Keywords: thermoelasticity, FEM, conjugate gradients, aggregations

Abstract

The contribution concerns the FE solution of the thermoelasticity problem. The numerical solution of this problem leads to the repeated solution of large systems of linear equations. For the solution of the system we use preconditioned CG method with overlapping Schwarz type preconditioners. If the Schwarz method is used for elliptic problems, the efficiency of the preconditioner decreases with increasing number of subproblems and for avoiding this problem it is necessary to involve coarse mesh correction. We use the algebraic coarse space created by aggrregation. For the parabolic problem the corresponding system matrix depends on the time stepsize. In this case even one level Schwarz methods is efficiet for suitable small stepsizes. The numerical tests are realised on a large geotechnical problem arising from the assessment of nuclear waste repositories.

Acknowledgement: The work was supported of the program Information Society and by the Ministry of Education, Youth and Sports under the project 1M0554.

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S-SDD CLASS OF MATRICES AND ITS APPLICATIONS

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Keywords: H-matrices, strictly diagonally dominant matrices, diagonal scaling, S-SDD matrices

Abstract

S-SDD class of matrices has been introduced in [1] as a generalization of Ostrowski class, known in the literature also as doubly diagonally dominant matrices. As it was shown in [2], this class can be characterized by the special form of its "scaling" into an SDD matrix. Due to this fact, we can use S-SDD matrices as a tool for measuring and exploiting the magnitude of diagonal dominance. How this leads to improvement, for example, in convergence theory of relaxation methods will be the main goal of this talk.

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DASHNIC-ZUSMANOVICH CLASS OF MATRICES AND ITS APPLICATIONS

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Keywords: H-matrices, strictly diagonally dominant matrices, diagonal scaling, Dashnic-Zusmanovich class of matrices

Abstract

Dashnic-Zusmanovich class of matrices has been introduced in [1] as a generalization of the well-known strictly diagonally dominant class. In the same paper it has been shown that this class can be characterized by the special form of its "scaling" into an SDD matrix. Due to this fact, we can improve some known results about, for example, determinant estimation or Perron root estimation in the case of SDD matrices. Moreover, we can develop corresponding estimations for a larger class of matrices. Some simple numerical examples will show how significant this improvement could be.

Acknowledgement: This research is partly supported by Ministry of Science and Environmental Protection, Serbia, grant 144025.

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A TECHNIQUE FOR COMPUTING MINORS OF ORTHOGONAL MATRICES

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Keywords: orthogonal matrices, determinant calculus, symbolic computations, Gaussian elimination, growth problem

Abstract

We introduce a technique for computing all possible principal determinants (minors) of order $(n-j)\times(n-j)$ of various orthogonal $n\times n$ matrices, which works also for orthogonal matrices in a generalized sense, e.g. for binary Hadamard matrices S ($S^TS=\frac{1}{4}(n+1)(I_n+J_n)$). The method takes advantage of the orthogonality property $A^TA=kI_n$ of an orthogonal matrix A and of the symmetry of B^TB, where B is a principal submatrix of A. The idea is facilitated by algebraic computations based on determinant formulas for matrices of the form $(k-\lambda)I_n+\lambda J_n$ and for block matrices of the form $\left[\begin{smallmatrix}B_1 & B_2\\ B_3 & B_4\end{smallmatrix}\right]$. The whole process can be standardized and implemented as a computer algorithm, which overcomes the difficulties occurring due to strenuous calculations done by hand. Theoretically, the algorithm works for every values n and j, and specifically for small values of j it provides general (i.e. they are valid of general n), analytical formulas. The symbolic implementation of the algorithm guarantees its precision. Finally, we justify the usefulness of such a method with an application to a problem of Numerical Linear Algebra, the growth problem. The results presented here are a generalization of an idea discussed in [2] for larger values j and also for other classes of orthogonal matrices. Extensive information on orthogonal matrices can be found in [1].

Acknowledgement: This research was financially supported by PENED 03ED 740 of the Greek General Secretariat for Research and Technology.

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THE EFFECT OF AGGRESSIVE EARL DEFLATION ON THE CONVERGENCE OF THE QR ALGORITHM

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Keywords: QR algorithm, convergence

Abstract

Aggressive early deflation [1] has proven to significantly enhance the convergence of the QR algorithm for computing the eigenvalues of a nonsymmetric matrix. It is shown that this deflation strategy is equivalent to extracting converged Ritz vectors from certain Krylov subspaces. As a special case, the single-shift QR algorithm enhanced with aggressive early deflation corresponds to a Krylov subspace method whose starting vector undergoes a Rayleigh-quotient iteration. These observations are used to derive improved convergence bounds for the QR algorithm.

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ANALYSIS OF REACTOR VESSEL BY DOMAIN DECOMPOSITION METHODS

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Keywords: domain decomposition, Schur complement method, FETI-DP method, parallel computing

Abstract

Detailed and complex analyses of reactor vessels of nuclear power plants are very complicated and computationally demanding. This contribution deals with mechanical and thermal analyses of an existing reactor vessel made from prestressed concrete. The analyses has to described 33 years of construction and life of the vessel. The vessel has to be modelled as a threedimensional problem. With respect to symmetry, only one eighth of the vessel is used in the analysis.

The specified analyses are very computationally demanding and they take several weeks on a modern single-processor computer. Therefore, the analyses are conducted in parallel and domain decomposition methods are applied. The Schur complement method is used in all analyses while the FETI-DP method is applied for some of them. Both methods are described in reference [1].

Very demanding analyses have been conducted on a cluster of PC's. Application of the cluster speeds up the analyses significantly and solves some problems with sizes of output files.

Acknowledgement: Financial support for this work was provided by project 103/07/1455 of Czech Science Foundation. The financial support is gratefully acknowledged.

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AN ALGORITHM FOR SOLUTION OF NON-SYMMETRIC SADDLE-POINT SYSTEMS

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Keywords: saddle-point system, Schur complement, orthogonal projectors, BiCGSTAB algorithm, multigrid

Abstract

The contribution deals with fast solving of non-symmetric saddle-point systems

$$\begin{pmatrix} A & B_1^\top \\ B_2 & 0 \end{pmatrix} \begin{pmatrix} u \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}, \tag{1}$$

where an $(n \times n)$ diagonal block A is possibly singular and $(m \times n)$ off-diagonal blocks B_1, B_2 have full row-rank and they are highly sparse. We will be interested especially in systems (1) with n large, m much smaller than n and with the defect l of A, $l = n - rankA$, much smaller than m.

Our algorithm is based on the Schur complement reduction. If A is singular, the reduced system has again the saddle-point structure (1), however its size is considerably smaller. After applying orthogonal projectors, we obtain an equation in terms of λ only that can be solved by a *projected* Krylov subspace method for non-symmetric operators. For this purpose, we derive a projected variant of the BiCGSTAB algorithm from the non-projected one, whose iterations can be accelerated by a multigrid strategy.

The presented method can be viewed as a generalization of algebraic ideas used in FETI domain decomposition methods [1], where A is symmetric positive semidefinite and $B_1 = B_2$.

Acknowledgement: This research was supported by grants 1ET400300415, IAA1075402 and MSM6198910027.

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THE DISCONTINUOUS GALERKIN METHOD FOR THE COMPRESSIBLE NAVIER-STOKES EQUATIONS

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Keywords: compressible Navier-Stokes equations, discontinuous Galerkin method, wide range of Mach numbers, shock capturing

Abstract

This work deals with the numerical solution of viscous compressible flows. Our goal is to develop a sufficiently accurate and robust method allowing the solution of problems with a wide range of Mach numbers. The compressible Navier-Stokes equations which describe such problems are discretized in space using the discontinuous Galerkin finite element method (DGFEM). In order to overcome severe restrictions imposed on the time step in order to obtain a stable scheme, semi-implicit time stepping is used. The arising linear systems are solved either by a direct solver or preconditioned GMRES. Special treatment of transparent boundary conditions and a suitable limiting procedure near discontinuities play an important role in the resulting scheme. Numerical experiments demonstrate the robustness of the method in cases when the exact solution of the governing equations is available, or test cases where the character of the solution is well known.

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COMPUTING SPARSE SOLUTIONS OF UNDERDETERMINED STRUCTURED SYSTEMS BY GREEDY METHODS

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Keywords: underdetermined systems, compressive sampling, greedy methods, sparse Fourier analysis, FFT

Abstract

Recently, the surprising fact that it is possible to recover functions having only few non-zero coefficients with respect to some basis from vastly incomplete information has gained much attention. Such functions are commonly called sparse or compressible and they naturally appear in a wide range of applications. We study *sparse trigonometric polynomials*

$$f(x) = \sum_{k \in I_N} \hat{f}_k \mathrm{e}^{-2\pi \mathrm{i} k x}, \qquad I_N := \{-\frac{N}{2}, \dots, \frac{N}{2} - 1\},$$

with non-zero Fourier coefficients $\hat{f}_k \in \mathbb{C}$ only on a set $\Omega \subset I_N$ with size $|\Omega| \ll N$. However, a priori nothing is known about Ω apart from a maximum size. Our aim is to sample f at M randomly chosen nodes $x_j \in [-\frac{1}{2}, \frac{1}{2}]$ and try to reconstruct f from these samples.

Thus, we wish to solve the strongly underdetermined consistent linear system

$$A\hat{f} = y \qquad \left(a_{j,k} = \mathrm{e}^{-2\pi \mathrm{i} k x_j},\ y_j = f(x_j),\ j = 1, \dots, M,\ k \in I_N\right),$$

for the vector $\hat{f} = (\hat{f}_k)_{k \in I_N}$ with the smallest number of non-zero entries.

For an appropriate number M of samples, greedy methods like *(Orthogonal) Matching Pursuit* or *Thresholding* succeed in this task with high probability. We focus on the computational complexity of the proposed methods when using the nonequispaced FFT and particular updating techniques. Illustration of our observations is given by numerical experiments.

STABILITY OF KRYLOV SUBSPACE SPECTRAL METHODS

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Keywords: spectral methods, Gaussian quadrature, variable-coefficient, Lanczos method

Abstract

This talk summarizes recent analysis of an alternative approach to the solution of diffusion problems and wave propagation problems in the variable-coefficient case that leads to a new class of numerical methods, called Krylov subspace spectral methods [3].

The basic idea behind these methods, applied to a PDE of the form $du/dt + L(x, D)u = 0$, is to use Gaussian quadrature in the spectral domain to compute Fourier components from elements of $\exp[-L\Delta t]$ for a matrix L discretizing $L(x, D)$ and time step Δt, using algorithms developed by Golub and Meurant [1], as opposed to applying Gaussian quadrature in the spatial domain as in traditional spectral methods. This strategy allows accurate resolution of all desired components, for both high and low frequencies, without having to resort to smoothing techniques to ensure stability.

This talk focuses on the stability properties of these methods. By describing the Fourier components of the computed solution in terms of directional derivatives of moments, we can demonstrate unconditional stability for parabolic problems, given sufficient smoothness of the coefficients of $L(x, D)$. We also discuss generalizations to systems of equations, including a simple high-order scheme for the second-order wave equation [2]. In this case, we demonstrate that Krylov subspace spectral methods, although they are explicit, are not restricted by the CFL condition.

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ON THE INCOMPRESSIBLE FLUID FLOW IN A JOURNAL BEARING, THE VISCOSITY DEPENDING ON PRESSURE

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Keywords: continuum mechanics, incompressible fluid, viscous fluid, pressure-thickening, journal bearing

Abstract

The steady flow of the incompressible viscous fluid is addressed, the viscosity of which depends on the pressure and on the share rate. An engineering application to flows of a lubricant in the journal bearing is emphasized.

The geometry of the journal bearing can be approximated by the plane geometry of the eccentric annulus; the small gap between the inner and the outer circle being filled by the fluid. The flow is induced by the rotation of the journal around its axis, the bearing being kept steady. In the words of corresponding partial differential equations, the flow is induced by these boundary conditions: a zero velocity is prescribed on the outer circle while some constant tangential velocity is prescribed on the inner circle. In the resulting flow the region of huge pressure develops eventually. In the engineering applications, the viscosity of the lubricant is considered to grow with increasing pressure.

The existence of a solution for the mathematical model is obtained by generalizing the existence result given in [1]. This assumes, however, that the viscosity model is both pressure-thickening and shear-thinning in a specific way. For the model, where the viscosity depends only on the pressure in a way observed from experiments and often used by engineers, the well-posedness of the mathematical model is not known, however.

In this contribution, the numerical simulations performed via the finite element method are presented, both for the model which the existence result applies to and for the model for which the well-posedness is not clear so far.

Acknowledgement: Research supported by the project GAČR 201/06/0321.

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ON OPTIMAL SHORT RECURRENCES FOR GENERATING ORTHOGONAL KRYLOV SUBSPACE BASES

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Keywords: Krylov subspace methods, orthogonal bases, short recurrences, conjugate gradient like methods

Abstract

In this talk I will discuss necessary and sufficient conditions on a nonsingular matrix A, such that for *any* initial vector r_0, an orthogonal basis of the Krylov subspaces $\mathcal{K}_n(A, r_0)$ is generated by a short recurrence. Orthogonality here is meant with respect to some unspecified positive definite inner product. This question is closely related to the question of existence of *optimal* Krylov subspace solvers for linear algebraic systems, where optimal means the smallest possible error in the norm induced by the given inner product. The conditions on A were first derived and characterized more than 20 years ago by Vance Faber and Tom Manteuffel (SIAM J. Numer. Anal., 21 (1984), pp. 352–362). Their main theorem is often quoted and appears to be widely known. Its details and underlying concepts, however, are quite intricate, with some subtleties not covered in the literature.

The talk will be based on joined work with Zdeněk Strakoš [1], and with Vance Faber and Petr Tichý [2].

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NUMERICAL SIMULATION OF 3D FLUID-STRUCTURE INTERACTION

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Keywords: arbitrary Lagrangian-Eulerian (ALE) formulation, fluid-structure interaction, large deformation, three-dimensional deformation

Abstract

The problem of interaction of an incompressible fluid and an incompressible elastic material in the so-called Arbitrary Lagrangian-Eulerian formulation, including suitable numerical schemes in three space dimensions is studied. We deal with suitable numerical implementation and we compute either an incompressible Newtonian or an incompressible power-law fluid for the liquid part, and Neo-Hookean or Mooney-Rivlin rubber-like materials for the solid part.

The easiest approach, where the problem is decoupled into the fluid part and solid part and the interaction is treated as external boundary condition, is alternated by single continuum formulation. There is the interaction treated as an internal boundary, which does not require any special treatment. This approach is described among others in [1].

Acknowledgement: This research was supported by the project The Nečas Center for Mathematical Modeling, project LC06052 (MŠMT ČR).

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A NUMERICAL ALGORITHM FOR FLUID FLOW IN POROUS MEDIA

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Keywords: fluid flow, nonlinear parabolic equation, iterative scheme

Abstract

Fluid flow model in porous media is considered. The governing equation is strong nonlinear parabolic differential equation. We develop an efficient algorithm for the numerical solution of the problem. It depends on an iterative scheme that developed recently. We prove the convergence of this scheme. Numerical results demonstrate the efficiency of the algorithm.

Acknowledgement: I would like to thank Professor Heike Faßbender for her encourage.

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MATHEMATICAL ANALYSIS AND COMPUTATIONAL SIMULATIONS FOR FLOWS OF INCOMPRESSIBLE FLUIDS

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Abstract

Dealing with models describing steady flows of incompressible fluids with the viscosity that may depend on the shear rate and the presure, we survey the recent developments concerning theoretical analysis of relevant boundary value problems and comment on a few computational tests.

MULTILEVEL BDDC IN THEORY AND PRACTICE

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Abstract

The BDDC algorighm has quickly become one of the most popular substructuring methods for symmetric, positive definite variational problems. Like other substructuring method, the method is conjugate gradients preconditioned by independent problems on substructures, solved in parallel, and a coarse problem. For large number of processors, the coarse problem becomes a bottleneck. Therefore, three-level BDDC was proposed, which add another, yet coarser level. Here we extend the three-level BDDC and its theory to an arbitrary number of levels.

We present the formulation and new condition number bounds for a multilevel version of the BDDC algorithm. The condition number bound grows polylogarithmically with the ratio of the substructure sizes between levels, but it is not bounded independently of the number of levels. Numerical results show that this may indeed occur. Since in practice the substructures are large and the number of levels is small, this is acceptable and provides a superb domain decomposition method.

The condition number bounds are based on a new multilevel algebraic theory for nested substructuring methods. The BDDC preconditioner on a finite element space is given by an extension of the variational form of the problem to a direct sum of energy orthogonal spaces and by projections from each of the spaces into the original finite element space. The abstract BDDC preconditioner then consists of solving the variational problem on each space from the direct sum, and adding the solutions projected into the original space. It turns out that both the original BDDC and the multilevel BDDC can be written in this form with a judicious selection of the spaces in the direct sum. Taking maximal advantage of orthogonality is what assures fast convergence of the method, and also leads to an elegant mathematical theory.

CONVERGENCE ISSUES OF ITERATIVE AGGREGATION/DISAGGREGATION METHODS IN PRESENCE OF CYCLIC PARTS IN THE SPECTRUM OF THE ITERATION MATRIX

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Keywords: stochastic matrices, iterative aggregation/disaggregation methods, block cyclic iteration matrices

Abstract

Many methods designed for computing eigenvalues and eigenvectors share one characteristic and namely that their convergence similarly as the power method requires the computed eigenvalue to be the dominant point of the spectrum of the iteration matrix. To computing eigenvectors of stochastic matrices this requirement is easy to achieve by using matrix $\frac{1}{1+\gamma}[T+\gamma I], \gamma > 0$, in place of the original iteration matrix T. This procedure stops being efficient if the index of cyclicity of T becomes large. In this report we show that various variants of iterative aggregation/disaggregation (IAD) methods [1] remain convergent independent of the index of cyclicity of the corresponding iteration matrix. This fact allows us to claim that IAD methods possess the following property: The larger index of cyclicity of the iteration matrix the faster convergence. We give a proof of an appropriate convergence result and accompany it by a rather large number of computations showing the efficiency of IAD methods.

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TRUST REGION INTERIOR POINT METHODS FOR LARGE SPARSE OPTIMIZATION

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Keywords: unconstrained optimization, large-scale optimization, trust region methods, interior point methods

Abstract

Trust-region methods are globally convergent techniques widely used, for example, in connection with the Newton's method for unconstrained optimization. They can be advantageously used when the Hessian matrix of the objective function (or its approximation) is indefinite, ill-conditioned or singular so the standard line-search methods cannot be used.

The most commonly-used iterative approaches for solving the trust-region subproblems are the factorization-based Moré-Sorensen method and the matrix-free Steihaug-Toint method. A method which combines both of these approaches is very efficient in practice [1].

Interior point methods are an effective tool for solving general large sparse nonlinear programming problems. They can be realized as the trust region methods where the direction vector is found by solving a corresponding quadratic programming subproblem.

Large sparse l_1 optimization problem [2] can be converted to a nonlinear KKT system by primal interior point method based on a standard logarithmic barrier function. The structure of the problem allows advantageous using of the trust region subproblem for a direction determination.

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NUMERICAL SOLUTION OF OPTIMAL CONTROL PROBLEMS FOR DESCRIPTOR SYSTEMS

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Keywords: descriptor system, optimality condition, strangeness index, even matrix polynomial

Abstract

We discuss optimal control problems for general unstructured linear differential-algebraic equations of arbitrary index. We discuss controllability and observability in the higher order case and show that order reduction may lead to false results. We then derive necessary conditions in the case of linear-quadratic control problems and show how these lead to eigenvalue problems for for even matrix polynomials.

We discuss the numerical solution of these structured eigenvalue problems and present some examples.

Acknowledgement: This research was partially supported by the research-in-pairs program at Mathematisches Forschungsinstitut Oberwolfach and partially by the DFG Research Center MATHEON in Berlin.

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COMPUTATIONAL METHODS IN IMAGE ANALYSIS

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Keywords: numerical methods, advection-diffusion equations, semi-implicit scheme, finite volume method, image processing, biology

Abstract

In many applications computers analyse images or image sequences quality of which can be poor, e.g., they are contaminated by a noise and/or boundaries of image objects are partly missing (e.g. in bio-medical imaging, in scene with occlusions or ilusory contours). We will discuss how nonlinear partial differential equations can be used to denoise and segment such images and extract further useful information from large-scale 3D image sequences arising e.g. in cell developmental biology. We apply finite volume spatial discretizations and semi-implicit time discretizations to geometrical advection-diffusion equations related to level set formulation of the surface evolution problems. The methods are unconditionally stable, robust, fast and naturally parallelizable.

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THEORETICAL AND NUMERICAL COMPARSION OF ABSTRACT PROJECTION METHODS DERIVED FROM DEFLATION, DOMAIN DECOMPOSITION AND MULTIGRID METHODS

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Keywords: deflation, domain decomposition, multigrid, projection methods, Krylov subspace iterations

Abstract

For various applications, it is well-known that a two-level-preconditioned Krylov method is an efficient method for solving large and sparse linear systems. Beside a traditional preconditioner like incomplete Cholesky decomposition, a projector has been included as preconditioner to get rid of a number of small and large eigenvalues of the matrix. In literature, various projection methods are known coming from the fields of deflation, domain decomposition and multigrid.

From an abstract point of view these methods are closely related. The aim of this talk is to compare these projection methods both theoretically and numerically. We investigate their convergence properties and stability by considering implementation issues, rounding-errors, inexact coarse solves and severe termination criteria. Finally, we end up with a suggestion of the optimal second-level preconditioner, which is as stable as the balancing preconditioner and as cheap and fast as the deflation preconditioner.

This talk is based on joint papers with K. Vuik, Y. Erlangga, and J. Tang.

ON STEIN-ROSENBERG TYPE THEOREMS FOR NONNEGATIVE SPLITTINGS

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Keywords: Stein-Rosenberg theorem, nonnegative splittings, Perron-Fronenius theory

Abstract

The Stein-Rosenberg theorem is extended and generalized to the classes of nonnegative splittings $A = M_1 - N_1 = M_2 - N_2$, of the first kind ($M_1^{-1}N_1 \geq 0$, $M_2^{-1}N_2 \geq 0$) and also of the second kind ($N_1M_1^{-1} \geq 0, N_2M_2^{-1} \geq 0$). Two types of the Stein-Rosenberg theorem are stated and proved under the main assumption that the series of inequalities $M_1^{-1}N_1 \geq M_1^{-1}N_2 \geq 0$, $M_1^{-1}N_1 \neq M_1^{-1}N_2$, $M_1^{-1}N_2 \neq 0$ or $M_2^{-1}N_1 \geq M_2^{-1}N_2 \geq 0$, $M_2^{-1}N_1 \neq M_2^{-1}N_2$, $M_2^{-1}N_2 \neq 0$ hold. These theorems allow us to obtain comparison results for the rate of convergence of the associated iterative methods. Specific assumptions are given under which the inequalities of the spectral radii become equalities or strict inequalities. The theoretical results are confirmed by numerical examples. Finally, some ideas as to how the present theory can be extended to cover the Perron-Frobenius splittings are presented.

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EFFICIENT SIMULATION OF CONVECTION DIFFUSION EQUATIONS

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Keywords: a posteriori error estimates, convection diffusion equations, adaptive methods

Abstract

In this talk we address efficient methods for the discretization of convection diffusion equations. Efficiency is obtained by using grid adaptive discretization schemes on parallel computers. We will discuss recent results of a posteriori error estimates for convection diffusion equations on the one hand [3], [4], [5], [6], [7], and present generic implementation concepts within the software environment DUNE on the other hand [1], [2].

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SPEEDING THE TRAINING OF SUPPORT VECTOR MACHINES

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Keywords: SVM, support vector machines, quadratic programming, clustering

Abstract

Data classification is a fundamental task in science and engineering. For example, given data gathered about a patient's tumor, we might need to decide whether the tumor is malignant or benign. Ideally, we would like to determine a mathematical function whose evaluation would indicate the classification of the tumor. Linear discriminant analysis provides one such function, but functions more general than a separating hyperplane are needed in many applications.

Support vector machines (SVMs) provide a means to classify data into two groups (positive and negative) using criteria more descriptive than separating hyperplanes. SVMs are *trained* using a large set of positive and negative examples. Classifiers such as neural networks are trained by an iterative process of presenting examples and adjusting network weights until convergence. In contrast, the training of an SVM is acccomplished by solving a single quadratic programming problem whose size is determined by the number of examples and the number of parameters in the classifier. This simple training regime is a major advantage of the SVM framework.

These quadratic programming problems can, however, be quite large. In this work we use two approaches to improve computational efficiency. First, we apply an adaptive constraint reduction method in an interior point method for

solving the quadratic programming problem. This has the effect of allowing later iterations to focus on only a few of the example datapoints. Second, we cluster the data and initially train on a small number of examples drawn from each cluster. This has the effect of reducing computation time in the early iterations.

We discuss our algorithm and its convergence theory and illustrate its performance on a variety of examples.

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ON A PARALLEL IMPLEMENTATION OF THE ONE-SIDED BLOCK JACOBI SVD ALGORITHM

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Keywords: preconditioned Jacobi method, fast block rotations, parallel implementation

Abstract

Recent progress in the serial one-sided Jacobi method is the consequence of two main ideas. The first one is that of preconditioning of an original matrix by one (two) QR (and LQ) decomposition(s) with column pivoting. Drmač and Veselić [1] have shown (experimentally and, to some degree, also theoretically) that such a preconditioning leads to a significant concentration of an off-diagonal matrix norm near the main diagonal. Then the one-sided Jacobi method is applied to the R-factor (L-factor) together with a clever modification of a cyclic ordering. Consequently, less sweeps are needed for the convergence, and the efficiency of the one-sided Jacobi method with preconditioning is suddenly comparable to that of bidiagonalization or divide-and-conquer approach.

The second idea is that of working with matrix blocks instead of matrix elements, which is usually much more efficient on modern computer architectures (serial or parallel) due to the hierarchical memory organization. Hari [2] has shown how to use matrix blocks and cyclic matrix orderings in the one-sided Jacobi method and how to organize fast computations using the CS decomposition of those matrix blocks.

In this contribution we design the parallel one-sided block Jacobi SVD algorithm using both above mentioned ideas. The data layout, computational and communication complexity are discussed in detail, and the results of first numerical experiments obtained on a cluster of personal computers are presented.

Acknowledgement: This research was partially supported by the VEGA Grant no. 2/7143/27.

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RITZ VALUES OF HERMITIAN MATRICES

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Keywords: Hermitian matrices, invariant subspaces, Ritz approximations

Abstract

If $x, y \in \mathbb{C}^n$ are unit-length vectors ($x^H x = y^H y = 1$) where y is an approximation to an eigenvector x of $A = A^H \in \mathbb{C}^{n\times n}$ with $Ax = x\lambda$, $\lambda = x^H Ax \in \mathbb{R}$, then it is well known that the Rayleigh quotient $y^H Ay$ satisfies

$$|\lambda - y^H Ay| \leq \sin^2\theta(x, y).\text{spread}(A). \tag{1}$$

Here if $\lambda_1(A) \geq \cdots \geq \lambda_n(A)$ are the eigenvalues of A in descending order then $\text{spread}(A) \equiv \lambda_1(A) - \lambda_n(A)$, and $\theta(x, y) \equiv \cos^{-1}|x^H y| \in [0, \pi/2]$ is the acute angle between x and y. This shows that the Rayleigh quotient approximation $y^H Ay$ to the eigenvalue λ of A can be far more accurate than the approximation of range(y) to the invariant subspace range(x) of A. We generalize this result to a higher dimensional subspace $\mathcal{Y}$ approximating an invariant subspace $\mathcal{X}$.

Let $X, Y \in \mathbb{C}^{n\times k}$ be such that $X^H X = Y^H Y = I_k$, the $k \times k$ unit matrix, where $\mathcal{Y} \equiv \text{range(Y)}$ is an approximation to the invariant subspace $\mathcal{X} \equiv \text{range(X)}$ of A, so that $AX = X.X^H AX$. Let $\lambda(X^H AX)$ and $\lambda(Y^H AY) \in \mathbb{R}^k$ be the vectors of eigenvalues in descending order of $X^H AX$ and $Y^H AY$ respectively. The elements of $\lambda(Y^H AY)$ are called Ritz values in the Rayleigh-Ritz method for approximating the eigenvalues $\lambda(X^H AX)$ of A. Such approximations are used in numerical computing, and computed for example via the Lanczos method for the Hermitian eigenproblem. Let $\theta(\mathcal{X}, \mathcal{Y}) \in \mathbb{R}^k$ be the vector of angles (in descending magnitude) between the subspaces $\mathcal{X}$ and $\mathcal{Y}$, so that $\cos\theta(\mathcal{X}, \mathcal{Y}) = (\sigma_k, \ldots, \sigma_1)^T$ where $\sigma_1 \geq \cdots \geq \sigma_k$ are the singular values of $X^H Y$. Then we show, see [1], that for many practical cases (*c.f.* (1)

$$|\lambda(X^H AX) - \lambda(Y^H AY)| \prec_w \sin^2\theta(\mathcal{X}, \mathcal{Y}).\text{spread}(A), \tag{2}$$

where " $\prec_w$ " denotes weak (sub-) majorization: that is, if $u, v \in \mathbb{R}^k$ and $u^\downarrow = (u_1^\downarrow, \ldots, u_k^\downarrow)^T$ is u with its elements rearranged in descending order, then

$$u \prec_w v \quad \Leftrightarrow \quad \sum_{i=1}^{j} u_i^\downarrow \leq \sum_{i=1}^{j} v_i^\downarrow \quad \text{for} \quad j = 1, \ldots, k. \tag{3}$$

Let $e \equiv (1, \ldots, 1)^T$. We say u is *majorized* by v (written $u \prec v$) if $e^T u = e^T v$ as well as (3). We suspect that the Ritz value result (2) holds in general, but have only been able to prove that a slightly weaker version *always* holds.

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HARMONIC RAYLEIGH-RITZ FOR THE MULTIPARAMETER EIGENVALUE PROBLEM

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Keywords: multiparameter eigenvalue problem, harmonic extraction, Jacobi-Davidson method, Rayleigh-Ritz, subspace method

Abstract

Harmonic extraction methods for the multiparameter eigenvalue problem will be presented. These techniques are generalizations of their counterparts for the standard and generalized eigenvalue problem. The methods aim to approximate interior eigenpairs, generally more accurately than the standard extraction does. The process can be combined with any subspace expansion approach, for instance a Jacobi-Davidson type technique, to form a subspace method for multiparameter eigenproblems of high dimension.

We will focus on the two-parameter eigenvalue problem

$$\begin{aligned} A_1 x_1 &= B_1 x_1 + C_1 x_1, \\ A_2 x_2 &= B_2 x_2 + C_2 x_2, \end{aligned}$$

for given $n_i \times n_i$ (real or complex) matrices A_i, B_i, C_i for $i = 1, 2$; we are interested in eigenpairs $((\lambda_1, \lambda_2), x_1 \otimes x_2)$ where x_1 and x_2 have unit norm.

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A HYBRID KACZMARZ – CG ALGORITHM FOR INCONSISTENT SYSTEMS ARISING IN IMAGE RECONSTRUCTION

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Keywords: Kaczmarz projection method, CG algorithm, inconsistent least squares problems, image reconstruction from projections

Abstract

Tomographic image reconstruction is the process of reconstructing an object or its cross section from several images of its projections. In the 2D case the object is illuminated by a fan-beam of X-rays, where the signal is attenuated by the object. This leads to a linear system of equations with a sparse matrix, because each observation is influenced only by the pixels on the corresponding beam path. The drawbacks of all Algebraic Reconstruction Techniques (ART) are the computational costs of the iterative formula applied to huge data sets; as an example, in practice the reconstruction of a 256^3 volume and 150 X-ray images of size 1024^2 is a common situation leading us to dimension $16777216 \times 157286400$ for the problem matrix. In such cases, the matrix A cannot be any more stored in the computer memory (not even in a compressed form !), thus it has to be re-generated (row by row) during each iteration of an iterative solver. Moreover, because of measurements errors for the X-rays intensities which give us the right-hand side of the problem, the corresponding system of equations becomes also inconsistent. In this paper, we propose a hybrid algorithm for overcoming both storage and inconsistency difficulties mentioned before. It combines in an efficient way an Extended Kaczmarz method from [2] with the general CG algorithm from [1]. We prove convergence of our algorithm for inconsistent linear least squares problems. Numerical experiments are presented on some real medical 2D data sets.

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A POSTERIORI ERROR ESTIMATES FOR HIERARCHICAL FINITE ELEMENTS

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Keywords: a posteriori estimates, hierarchical bases, elliptic problems

Abstract

Hierarchical finite element bases are widely used for preconditioning large systems solving elliptic partial differential equations. The a posteriori energy based error estimates have been developed for multilevel function spaces, e.g. [2].

There are two main objectives in our presentation. We have derived new types of the estimates, that exploit the quantities which are easily computed when using iterative multilevel methods [1]. As the second result, we compute the constants in the strengthened Cauchy - Bunyakowski – Schwarz inequality for the hierarchical finite element functions on rectangles. We study both of the h [3] and p hierarchical refinement and we compare the accuracy of the introduced error estimates for these cases. Several numerical examples are included.

Acknowledgement: The research was supported by the Information Society project No. 1ET400300415, by the project CEZ MSM 6840770001 and by the Grant Agency of Czech Republic under the contract No. 201/05/0453.

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NUMERICAL SOLUTIONS OF POPULATION BALANCES IN PARTICULATE SYSTEMS

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Keywords: population balance models, finite volume schemes, method of characteristics, hyperbolic conservation laws, particles

Abstract

The dynamic behavior of a population of small particles is a subject of interest in various engineering fields. These areas include atmospheric physics, precipitation, crystallization, pharmaceutical manufacture, aerosol formation, colloid chemistry, growth of microbial and cell populations, and so on. Most of such systems involve simultaneous nucleation, growth, aggregation and breakage of particles. Population balances, in their integro-differential equation form, are a widely used tool for simulating these processes. Since, population balance equations can only be solved exactly in simplified cases, numerical solutions are usually needed.

This work focuses on the derivation of numerical schemes for solving population balance models with simultaneous nucleation, growth, aggregation and breakage processes. Two numerical methods are proposed for this purpose. The first method combines a method of characteristics (MOC) for growth process with a finite volume scheme (FVS) for aggregation and breakage processes. For handling nucleation terms, a cell of nuclei size is added at a given time level. The second method purely uses a semi-discrete finite volume scheme for nucleation, growth, aggregation and breakage of particles. Note that both schemes use the same finite volume scheme for aggregation and breakage processes. The proposed techniques are tested for various combination of these processes. The numerical results are validated against available analytical solutions.

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THERMODYNAMICS OF MATERIALS UNDERGOING DISSIPATIVE PROCESSES

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Abstract

In this talk, a general thermodynamic approach will be presented for modeling a class of material responses that has as its basis the notion that during a process that the material is subject to, the "natural configuration" from which the response of the body is described can change: the evolution of the "natural configurations" being determined by a certain thermodynamic criterion.

The body can also have different material symmetries with regard to these different natural configurations and this allows one to model processes during which the symmetry of the body changes. We consider bodies that can be described by a family of non-dissipative responses characterized by stored energy functions parameterized from an evolving set of "natural configurations". The evolution of the "natural configurations" is accompanied by dissipation and entropy production. The way in which the natural configurations change is determined by the maximization of "entropy production". By choosing different forms for the stored energy, rate of dissipation, etc., we can capture different types of dissipative responses as that evidenced in: classical plasticity, twinning, solid to solid phase transition, deformation of multi-network polymers, response of viscoelastic bodies, crystallization in polymers, flows of liquid crystals, the response of geological materials, growth and adaptation of biological materials, etc. The body possessing different natural configurations leads naturally to ideas introduced by Eshelby concerning configurational forces. The thermodynamic setting also provides a natural setting for generalizing the reciprocal relations due to Onsager.

AN ADVANCED ILU PRECONDITIONER FOR THE INCOMPRESSIBLE NAVIER STOKES PROBLEM

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Keywords: AILU, reordering, preconditioner, Navier Stokes

Abstract

In this paper, we solve the incompressible Navier Stokes problem with an ILU preconditioned Krylov subspace methods. The finite element discretization and linearization of the Navier Stokes problem gives rise to a linear system having large number of zeros on the main diagonal. ILU factorization of the original system matrix may fail due to zeros on the main diagonal. To avoid breakdown of the ILU decomposition, we present here different ordering techniques of the grid points and the unknowns. The reordering techniques used with ILU preconditioning makes that the iterative methods applied to the system of equations converge rapidly. We call this the AILU preconditioner. With the reordering techniques, a direct solver can also be used to solve the coupled system without pivoting. It is observed that AILU converges rapdily for both Picard's and Newton's linearization for the Navier Stokes problem.

Results are compared with ILUPACK that show that AILU takes a larger number of iterations than ILUPACK. However, AILU is cheaper in construction of the preconditioner and memory, and consumes less CPU time in computations.

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ANALYSIS AND DEVELOPMENT OF ALGORITHMS FOR REGULARIZATION PARAMETERS IN THE SOLUTION OF LINEAR PARAMETER ESTIMATION PROBLEMS

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Keywords: least squares, regularization, confidence interval

Abstract

Solution of the regularized least squares problem for linear parameter estimation requires the use of regularization parameters. Typical approaches for finding an appropriate parameter choice involve methods such as the L-curve and cross-correlation methods. Recently, a new technique was introduced by Mead (2007) in which the weights on the parameter misfits are found by solving an optimization problem, for which it can be shown that the penalty functional follows a χ^2 distribution with n degrees of freedom, where n is the dimension of the data space. Here, our focus is on the impact of the formulation of this optimization problem for determing best possible confidence intervals on the parameter estimates, given the covariance structure on the data. The given optimization problem is reformulated to become more feasible. Experiments to show the validity of the new model, and theoretical results will be presented.

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LSTRS: MATLAB SOFTWARE FOR LARGE-SCALE TRUST-REGION SUBPROBLEMS AND REGULARIZATION

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Keywords: trust regions, large eigenvalue problems, regularization

Abstract

We describe a MATLAB implementation [6] of the method LSTRS [5] for the large-scale trust-region subproblem:

$$\min \ \frac{1}{2}x^T Hx + g^T x \ \text{ subject to (s.t.) } \ \|x\|_2 \leq \Delta, \tag{1}$$

where H is an $n \times n$, real, large, symmetric matrix, g is an n-dimensional real vector, and Δ is a positive scalar. Problem (1) arises in connection with the trust-region globalization strategy in optimization. A special case of problem (1), namely, a least squares problem with a norm constraint, is equivalent to Tikhonov regularization [7] for discrete forms of ill-posed problems.

LSTRS is based on a reformulation of the trust-region subproblem as a parameterized eigenvalue problem, and consists of an iterative procedure that finds the optimal value for the parameter. The adjustment of the parameter requires the solution of a large-scale eigenvalue problem at each step. The method relies on matrix-vector products only and has low and fixed storage requirements, features that make it suitable for large-scale computations. In the MATLAB implementation, the Hessian matrix of the quadratic objective function can be specified either explicitly, or in the form of a matrix-vector multiplication routine. Therefore, the implementation preserves the matrix-free nature of the method. The MATLAB implementation offers several choices for the eigenvalue calculation and it also allows the users to specify their own eigensolver routine.

We present a brief description of the LSTRS method from [5] and describe the main components and features of the MATLAB software. We include comparisons with the following state-of-the-art, large-scale techniques for solving problem (1): the Semidefinite Programming approach of Fortin and Wolkowicz [1], the Sequential Subspace Method of Hager [3], and the Generalized Lanczos Trust Region method of Gould et al. [2] as implemented in the HSL library [4]. We present examples of use of the software as well as results from the regularization of large-scale discrete forms of ill-posed problems.

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A ROBUST AND EFFICIENT PARALLEL SVD SOLVER BASED ON RESTARTED LANCZOS BIDIAGONALIZATION

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Keywords: SVD, Lanczos bidiagonalization, thick restart

Abstract

The computation of singular subspaces associated with the k largest or smallest singular values of a large, sparse (or structured) matrix A is commonplace. Example applications are the solution of discrete ill-posed problems or the construction of low-rank matrix approximations in areas such as signal processing or information retrieval.

Lanczos bidiagonalization can exploit matrix sparsity, thus being competitive with other methods in many situations. However, the straightforward algorithm may encounter convergence problems and some effective restarting technique is required. In this work, we present a Lanczos bidiagonalization procedure implemented in SLEPc (Scalable Library for Eigenvalue Problem Computations), a software library for the solution of large, sparse eigenvalue problems on parallel computers. Our solver is based on a thick restart variant [1] and it also incorporates the following features:

- A one-sided variant [2] that can reduce computational and storage requirements, while allowing for better parallel performance.
- Robust Gram-Schmidt orthogonalization balancing numerical reliability and computational efficiency and scalability.

We use the solver to investigate different restarting strategies, including locking, non-locking and hybrid, in practical applications.

Acknowledgement: Work supported by Valencia Regional Administration, Directorate of Research and Technology Transfer, grant number GV06/091.

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EFFICIENT IMPLEMENTATION OF LARGE SCALE LYAPUNOV AND RICCATI EQUATION SOLVERS

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Abstract

The Newton-ADI-method has shown to be an efficient tool for the solution of large scale sparse Lyapunov and Riccati matrix equations. The Lyapack software package has obtained acceptance as a valuable and efficient MATLAB tool implementing this method. Since its application in PDE control often involves usage of the MATLAB `mex` interface, thus producing a noticeable overhead especially in large scale, one is interested in applying the Newton-ADI-method directly using the matrix multiplication and solver routines from the chosen PDE solver library or toolbox. Here we want to compare a C implementation of the Newton-ADI-method with the Lyapack version. We also implement some improvements for the case where underlying system involves a mass matrix ($M\dot{x} = Ax + Bu$) regarding the transformation of these systems to standard form ($\dot{\tilde{x}} = \tilde{A}\tilde{x} + \tilde{B}u$). Furthermore we discuss variants of the Newton-ADI-method that may lead to improvements in computational time and memory usage for practical applications.

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USING URV–DECOMPOSITIONS TO SOLVE PALINDROMIC AND EVEN EIGENVALUE PROBLEMS

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Keywords: URV decomposition, palindromic/even eigenvalue problem, structure preserving method

Abstract

A generalized eigenvalue problem $Ax = \lambda Bx$ is called palindromic, if $B = A^T$. It is called even, if A is symmetric, while B is skew symmetric. The eigenvalues of a palindromic problem come in pairs $(\lambda, \frac{1}{\lambda})$. The eigenvalues of an even problem come in pairs $\pm\lambda$, [1].

A URV decomposition of a matrix A is a factorization of the form $A = URV^*$ where U and V are unitary and R is triangular.

In this talk algorithms for both, the palindromic and the even problem are presented, yielding eigenvalues that fulfill the spectral symmetry even in finite precision arithmetic. Both algorithms are based upon a URV-type matrix decomposition.

Acknowledgement: Supported by Deutsche Forschungsgemeinschaft through MATHEON, the DFG Research Center *Mathematics for key technologies* in Berlin.

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A COUNTEREXAMPLE FOR CHARACTERIZING INVARIANT SUBSPACES OF MATRICES BY SINGULARITY SYSTEMS

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Keywords: eigenvalue, invariant subspace, singularity system, Newton

Abstract

Let λ_1 be a simple eigenvalue of a matrix A with right and left eigenvectors x_1, y_1, resp., and $x_1^H x_1 = y_1^H x_1 = 1$. Consider the singularity system

$$C(\lambda; u, v) \begin{bmatrix} x \\ \mu \end{bmatrix} = \begin{bmatrix} A - \lambda I & v \\ u^H & 0 \end{bmatrix} \begin{bmatrix} x \\ \mu \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{1}$$

where u, v are sufficiently good approximations to x_1, y_1, resp. Then the bordered matrix $C(\lambda_1; u, v)$ is nonsingular so (1) uniquely defines $x = x(\lambda)$, $\mu = \mu(\lambda)$ for λ close to λ_1, and for $\lambda = \lambda_1$ we have $x(\lambda_1) = x_1/u^H x_1$, $\mu(\lambda_1) = 0$. Hence, $\lambda = \lambda_1$ may be determined by using the scalar singularity condition $\mu(\lambda) = e_{n+1}^T C(\lambda; u, v)^{-1} e_{n+1} = 0$ via, e.g., applying Newton's method as done in the Generalized Rayleigh Quotient Iteration of Schwetlick/Lösche [ZAMM 2000].

Now let $\operatorname{im} X_1$, $X_1^H X_1 = I_p$, be a p-dimensional invariant subspace of A which implies $AX_1 - X_1\Lambda_1 = 0$ with $\Lambda_1 = X_1^H A X_1$. With U, V such that $\operatorname{im} U \approx \operatorname{im} X_1$, $\operatorname{im} V \approx \operatorname{im} Y_1$ sufficiently good where $\operatorname{im} Y_1$ is the corresponding left invariant subspace with $Y_1^H X_1 = I_p$, we try to define $X = X(\Lambda)$, $M = M(\Lambda)$ as functions of Λ by generalizing (1) to the block singularity system

$$C(\Lambda; U, V)[X, M] = \begin{bmatrix} AX - X\Lambda + VM \\ U^H X \end{bmatrix} = \begin{bmatrix} 0 \\ I_p \end{bmatrix} \tag{2}$$

For $\Lambda = \Lambda_* = S^{-1}\Lambda_1 S$ with $S = (U^H X_1)^{-1}$, the linear system (2) is solved by $X = X_* = X_1 S$, $M = M_* = 0$. Hence, when the linear operator $C(\Lambda_*; U, V) : [X, M] \to C(\Lambda_*; U, V)[X, M]$ defined in (2) would be nonsingular, $[X, M]$ would be uniquely defined by (2) for Λ close to Λ_*, and the $(p \times p)$ singularity condition $M(\Lambda) = 0$ could be exploited for computing Λ_* as in case $p = 1$ above.

Since we did not succeed in proving nonsingularity of $C(\Lambda_*; U, V)$ we started looking for a counterexample and, finally, constructed a (5×5)-matrix A with a two-dimensional simple invariant subspace such that even the optimal borderings $U = X_1$ (which leads to $\Lambda_* = \Lambda_1$) and $V = Y_1$ give an operator

$C(\Lambda_1, X_1, Y_1)$ that has rank drop 1. Here we used that the Sylvester equation (2) can equivalently be written as standard linear system

$$\begin{aligned}\mathcal{C}(\Lambda; U, V)\begin{bmatrix}\mathrm{vec}(X)\\ \mathrm{vec}(M)\end{bmatrix} &= \begin{bmatrix} I_p \otimes A - \Lambda^T \otimes I_n & I_p \otimes V \\ I_p \otimes U^H & 0\end{bmatrix}\begin{bmatrix}\mathrm{vec}(X)\\ \mathrm{vec}(M)\end{bmatrix} = \\ &= \begin{bmatrix}\mathrm{vec}(0)\\ \mathrm{vec}(I_p)\end{bmatrix}.\end{aligned}$$

ON THE DIRECT SOLUTION OF VERY LARGE SPARSE LINEAR SYSTEMS USING OUT-OF-CORE TECHNIQUES

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Keywords: sparse linear systems, multifrontal, out-of-core solver

Abstract

An effective way of extending the size of problem that can be successfully solved using a sparse direct solver is to allow the system matrix and its factors to be held out-of-core. In this talk, we discuss the design and development of new sparse out-of-core solvers that will be included in the next release of the HSL mathematical software library [1]. An important feature of the codes is that all input and output to disk is performed through a set of Fortran subroutines that manage a virtual memory system so that actual input/output occurs only when really necessary. We describe this system and highlight other key features of the new packages. Numerical results for a range of large-scale problems arising from practical applications are presented and comparisons made with existing HSL solvers.

Acknowledgement: This work was supported by the EPSRC grant GR/S42170.

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LEVEL CHOICE IN TRUNCATED TOTAL LEAST SQUARES

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Keywords: truncated singular value decomposition, truncated total least squares, filter factors, effective number of parameters, model selection

Abstract

The method of truncated total least squares [2] is an alternative to the classical truncated singular value decomposition used for the regularization of ill-conditioned linear systems $Ax \approx b$ [3]. Truncation methods aim at limiting the contribution of noise or rounding errors by cutting off a certain number of terms in an expansion such as the singular value decomposition. To this end a truncation level k must be carefully chosen.

The truncated total least squares solution becomes more significantly dominated by noise or errors when the truncation level k is overestimated than the truncated singular value decomposition solution does. Model selection methods that are often applied in the context of the truncated singular value decomposition can be modified to be applied in the context of the truncated total least squares. The proposed modified generalized cross validation combined with the truncated total least squares method performs better than the classical generalized cross validation [1] combined with the truncated singular value decomposition, especially when both the coefficient matrix A and the right-hand side vector b are contaminated by noise.

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ON A WEIGHTED QUASI-RESIDUAL MINIMIZATION STRATEGY OF QMR FOR SOLVING COMPLEX SYMMETRIC SHIFTED LINEAR SYSTEMS

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Keywords: shifted linear systems, complex symmetric matrices, QMR

Abstract

We consider the solutions of complex symmetric shifted linear systems of the form

$$(A + \sigma_k I)\boldsymbol{x}^{(k)} = \boldsymbol{b}, \quad k = 1, 2, \ldots, m, \tag{3}$$

where $A + \sigma_k I$ is a nonsingular n-by-n complex symmetric matrix with scalar shifts $\sigma_k \in C$, and $\boldsymbol{x}^{(k)}, \boldsymbol{b}$ are complex vectors of length n. The systems (1) arise in large-scale electronic structure calculation, e.g. [3], and there is a strong need for the fast solutions of the systems.

In this talk, to solve the systems (1) efficiently, we will derive an iterative method (referred to as shifted QMR_SYM) from the combination of the two important results given in [1, 2]. Since we found that the most time consuming part of shifted QMR_SYM was to update approximate solutions when the number of systems m in (1) was large enough, we will present a weighted quasi-residual minimization strategy of shifted QMR_SYM and give a specific weight such that it reduces the computational cost of recurrence formulas for updating approximate solutions. To show the efficiency of the present strategy, we will report the results of some numerical experiments.

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STATISTICAL PERTURBATION THEORY FOR SPECTRAL CLUSTERING WITH APPLICATION TO THE ANALYSIS OF GENE EXPRESSION DATA

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Keywords: statistical perturbation, eigenvectors, singular vectors, clustering, gene expression data

Abstract

In biology, microarrays generate huge gene expression data sets that require reliable algorithms for their analysis. An important problem is to cluster genes (or samples) into groups, and this is often achieved by spectral clustering, for example, using the Fiedler vector of the Laplacian matrix of a network or a singular vector of the adjacency matrix of a network. A major difficulty is that the biological data is subject to many random errors and the clustering results can be very sensitive to perturbation.

In this talk we first discuss some spectral perturbation theory for a symmetric matrix where the perturbation parameter is a random variable. Second, we extend this to the statistical perturbation of singular vectors of a rectangular matrix. We illustrate the theory with numerical results obtained from gene expression data arising from the analysis of certain cancer tissue samples.

RELAXING CONDITIONS FOR THE BRAMBLE PASCIAK CG

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Abstract

In 1988 Bramble and Pasciak introduced a Conjugate Gradient method which is widely used to solve saddle point problems of the form

$$\mathcal{A} = \begin{bmatrix} A & B^T \\ B & -C \end{bmatrix}$$

where the preconditioner

$$P = \begin{bmatrix} A_0 & 0 \\ B & -I \end{bmatrix}$$

is incorporated. The preconditioned matrix $\mathcal{A} = P^{-1}\mathcal{A}$ is symmetric and positive definite in the inner product defined by G. Therefore, the inner product matrix

$$G = \begin{bmatrix} A - A_0 & \\ & I \end{bmatrix}$$

is needed to be symmetric positive definite as does the preconditioner A_0 for A. An improved variant was given by Meyer and Steidten in 2001. Our goal is to relax some of these conditions. We analyze alternative solvers and their behaviour for different situations. We investigate a MINRES implementation with a G-inner product and also the use of the ideal transpose-free Quasi Minimal Residual method proposed by Freund in 1992. Numerical results coming from the IFISS package will be given.

ON THE MARKOV CHAIN SAFETY MODELS

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Keywords: Markov Chain, tolerable hazard rate, safety assessment, lumpability, random failures, quantitative safety target

Abstract

European norms for the railway industry require proof that the system or equipment meets given quantitative safety target. It is specifically written in the norm that a quantified assessment of random failure integrity shall be carried out, by means of probabilistic calculations. The purpose of these calculations is to ensure that the hazardous failure rate during the life cycle of the equipment doesn't exceed given value of tolerable hazard rate (THR).

Values given for the THR are usually very low (e.g. 10^{-8}). Therefore probabilistic calculation using mathematical model is the only way for the quantitative safety assessment of the equipment. An approach to the computation of some dependability parameters of complex systems was mentioned in [1].

This paper deals with the basic problems connected to the assessment of quantitative safety targets using Markov chains. Some basic relations between hazard rate and characteristics evaluated from the Markov model are observed and impact of eigenvalues on the required parameter hazard rate is discussed.

Since the evaluation of required parameter hazard rate is often a so-called stiff problem we would like to discuss also substitution of Continuous Time Markov Chains by Discrete Time Markov Chains using formulas mentioned in [2] for the evaluation of the required parameter. Impact of this substitution and its advantages and disadvantages will be mentioned.

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NEW CONDITIONS FOR NON-STAGNATION OF GMRES, AND CORRESPONDING CONVERGENCE BOUNDS

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Keywords: GMRES, non-stagnation, convergence bounds

Abstract

A well-established condition guaranteeing that GMRES makes some progress, i.e., that it does not stagnate, is that the symmetric part of the coefficient matrix, $(A+A^T)/2$, be positive definite [1]. This condition results in a bound of the convergence rate for the iterative method which depends on the minimum eigenvalue of $(A + A^T)/2$ and of the norm of A. This bound is usually very pessimistic. Nevertheless, it has been extensively used, e.g., to show that certain preconditioned problems have a convergence bound for GMRES which is independent of the underlying mesh size of the discretized partial differential equation. In this talk we discuss new and more general conditions on the coefficient matrix so that one can guarantee that there is no stagnation of GMRES. These conditions do not require the symmetric part of the coefficient matrix to be positive definite. Thus, we enlarge the class of matrices for which a bound of the convergence rate for GMRES is available.

(joint work with Valeria Simonicini, Universitá di Bologna)

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SOME NUMERICAL SIMULATIONS OF MULTI-PHASE PROBLEMS BY AN ENERGY-STABLE FINITE ELEMENT SCHEME

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Keywords: finite element method, two-fluid flow problems, energy-stability, Navier-Stokes equations, surface tension

Abstract

Multifluid and multiphase flows occur in many scientific and engineering problems. Two key issues in analyzing those flows are to find the position of interfaces separating fluids and to handle the surface tension on the interfaces. Many numerical schemes have been developed and applied to those flow problems, but it is not an easy task to construct numerical schemes, stable and convergent. To the best of our knowledge, there are no numerical schemes whose solutions are proved to converge to the exact one. There are very little discussion even for the stability of schemes.

Recently we have developed a finite element scheme based on energy-stable approximation [1], [2]. In the case of no surface tension, the scheme is unconditionally stable in the energy-sense. When there exists surface tension, they are proved to be stable if a quantity corresponding to L^2-norm of the curvature remains bounded in the computation. Since we do not use the maximum norm, the computation proceeds stably while the squared integral value is bounded even if the value becomes very large at a point.

By using this scheme, some numerical simulations are performed for rising bubble problems and hourglass problems, where the fluids are governed by the incompressible Navier-Stokes equations and surface tension is exerted on the interface. On the boundary both slip and non-slip boundary conditions are considered. Numerical results show the robustness and the applicability of these schemes.

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SYMMETRIC DIFFERENTIAL MATRIX RICCATI EQUATIONS

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Keywords: Riccati differential equation, ODE, boundary value problem, transfer of boundary conditions, self-adjoint differential equation

Abstract

We concerned on matrix differential Riccati equations with square matrix. It has been proved, that if these equations fulfill some special conditions for matrix coefficients and initial conditions than these equations possess a unique solution on tho whole interval and, moreover, that this solution is represented by symmetric matrix whose eigenvalues lie in $\langle -1, 1\rangle$.

Considered type of Ricatti equations has a strong application in to the field of study of boundary value problem for self-adjoint differential equations.

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UPDATING OF PRECONDITIONERS FOR LARGE, SPARSE, NONSYMMETRIC LINEAR SYSTEMS

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Keywords: nonsymmetric preconditioning, preconditioner updates, sequences of linear systems, permutations

Abstract

Many applications such as computational fluid dynamics, structural mechanics or numerical optimization lead to sequences of linear systems. If efficient preconditioners for the individual linear systems of the sequences are computationally demanding, updates of previous preconditioners can be advantageous alternatives. Updating of large and sparse preconditioners has been done, among others, with small rank updates in case of applying Quasi-Newton methods [2], by recycling subspaces in the context of Krylov subspace methods [4], or by means of diagonal updates for SPD systems arising from parabolic PDE's [1].

In this contribution we explain our extension of the approach from [1] to general nonsymmetric systems which was proposed in [3]. In addition, we address several issues that cannot be found in [3], including theoretical results about the influence of diagonal dominance on the quality of our updates, permutation strategies, quantification of the superiority of updated over frozen preconditioners for some types of incomplete factorizations.

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BACKWARD PERTURBATION ANALYSIS OF THE SCALED TOTAL LEAST SQUARES PROBLEM

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Keywords: backward perturbation analysis, scaled total least squares

Abstract

Given $A \in \mathbb{R}^{m\times n}$ with $m \geq n$, $b \in \mathbb{R}^m$, and $\gamma \in (0, \infty)$, the scaled total least squares (STLS) problem can be defined as follows:

$$\min_{E,f,x}\{\|[E, \gamma f]\|_F\} \quad \text{subject to} \quad (A + E)x = b + f.$$

The STLS problem reduces to the ordinary least squares (LS) and data least squares (DLS) problems as $\gamma \to 0$ and $\gamma \to \infty$, respectively.

Given an approximate solution $y \in \mathbb{R}^n$ to the STLS problem, we derive a formula for a lower bound on the corresponding backward error. When $\gamma \to 0$ the lower bound reduces to the backward error obtained in [2] for the LS problem. When $\gamma \to \infty$ it becomes the lower bound on the backward error of the DLS problem obtained in [1].

Numerical experiments suggest that when y is a reasonable approximation to the exact STLS solution, this lower bound is in fact the backward error.

We also provide an easily computable lower bound and an asymptotic estimate for the above lower bound, and discuss how these could be useful for the design of stopping criteria for iterative solution methods.

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NUMERICAL-SYMBOLICAL METHODS COMPUTING THE RANK OF BLOCK BIDIAGONAL TOEPLITZ MATRICES

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Keywords: rank, block Toeplitz, QR, SVD, numerical-symbolical methods

Abstract

The computation of the Rank of a matrix is an interesting problem with applications in many computational fields of science such as control theory, numerical linear algebra etc. In the present paper we study the computation of the Rank [1], [2], [4] of a block bidiagonal sequence of matrices called PAPS sequence, which appears in the computation of the Weierstrass Canonical form of regular Matrix Pencils [3]. We propose matrix-based, numerical and symbolical, updating and direct methods computing the Rank (or the Nullity) of block bidiagonal Toeplitz matrices and compare them with classical procedures. Methods such as QR factorization [1], [2] and Singular Value Decomposition are stable but non-efficient because of the big size of our initial matrix. Updating methods exploit the special structure of the PAPS matrix. We present new algorithms and modifications of the classical which deploy the special form of our matrix reducing significant the required flops and lead to fast and efficient algorithms. The numerical implementation of the algorithms leads to serious problems such as the computation of the numerical Rank in contrast with the symbolical implementation which guarantees the computation of the exact Rank of the matrix. The combination of numerical and symbolical operations suggest a new approach in software mathematical computations denoted as hybrid computations. For some of the above methods their hybrid nature is presented. An overall comparison of the behavior of the methods according to their error analysis and useful remarks about their stability are concluded. All methods are tested and the results are summarized in tables.

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TENSOR APPROXIMATION BY MATRIX TECHNIQUES

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Keywords: tensor approximation, low rank, singular value decomposition

Abstract

Tensor approximation is a rapidly developing topic due to many applications in data analysis and high-dimensional problems. Moreover, tensor is a very useful kind of nonlinear structure that can be successfully used in addition and in combination with conventional types of linear structure in matrices. We consider new approaches involving classical matrix techniques and demonstrate some applications to large-scale numerical problems. In particular, we present a sub-linear complexity algorithm for the approximate inversion of a two-level Toeplitz matrix of a small tensor rank.

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SOLVERS FOR LARGE LINEAR SYSTEMS ARISING IN THE STOCHASTIC FINITE ELEMENT METHOD

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Keywords: stochastic finite element method, recycling MINRES, simultaneous diagonalization, structured matrix

Abstract

The discretization of stochastic elliptic boundary value problems by means of the stochastic finite element method [1] requires the solution of a large linear system of equations. Firstly, we discuss the structure of the stiffness matrix that strongly depends on the representation of the stochastic input data. Based on this examination we give an overview of recent solvers for SFEM discretizations.

For stochastic coefficients linear in a finite set of independent random variables we employ Krylov subspace recycling techniques [3] after decoupling the SFEM stiffness matrix [2] by simultaneous diagonalization of certain mass matrices related to the stochastic part of the discretization.

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A NEW FAMILY OF ITERATIVE METHODS FOR SOLVING NONSYMMETRIC SYSTEMS OF LINEAR EQUATIONS

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Keywords: iterative methods, Krylov subspace methods, nonsymmetric linear systems, limited memory techniques

Abstract

In the talk we present a new family of iterative methods for solving nonsymmetric systems of linear equations. Our technique uses a limited amount of memory: only a modest (fixed) number of vectors is needed to carry out the iterative process.

We will present the theoretical framework of the new technique, and illustrate the efficiency of the methods with numerical experiments using both academic and realistic test problems. The realistic examples include a 2D convection-diffusion problem from oceanography and a 3D Helmholtz problem from acoustics.

Comparison with Bi-CGSTAB [1], CGS [2] and other state-of-the-art techniques shows that for our test cases our new technique outperforms the other methods, both with respect to the number of matrix-vector products and with respect to the overall number of operations.

Acknowledgement: Part of this research has been funded by the Dutch BSIK/BRICKS project.

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TENSOR-BASED BIOSIGNAL PROCESSING

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Keywords: tensor, PARAFAC, biomedicine, signal processing, multilinear algebra

Abstract

This contribution deals with tensor decompositions and their benefits in biomedical signal processing. After a brief introduction of tensors and their differences with matrices, different decompositions are described and their computational algorithms are introduced as generalizations of matrix-based counterparts. In particular, we will focus on 'Parallel Factor Analysis' (Parafac, also known as Candecomp or the CP model), the most popular tensor decomposition, and overview its mathematical properties. The CP model decomposes in a unique way a higher-order tensor in a minimal sum of rank-1 'atoms'.

Furthermore, we will give an overview of biomedical applications, in which tensors are useful. In particular, we will focus on the presurgical evaluation of refractory partial epilepsy for the delineation of the irritative and ictal onset zones using long-term electroencephalographic (EEG) recordings. We will extract the potential distribution of the ictal activity using the higher-order CP model and show that only one atom is related to the seizure activity.

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HIGHER ORDER DISCRETE MAXIMUM PRINCIPLE FOR A PROBLEM WITH ABSOLUTE TERM

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Keywords: elliptic problems, *hp*-FEM, discrete maximum principle

Abstract

This contribution discusses the discrete maximum principle (DMP) for the one-dimensional problem $-u'' + \kappa^2 u = f$ discretized by higher-order finite element method. The problems of DMP are studied almost exclusively in the context of the lowest order approximations. This presentation shows techniques suitable for higher-order finite elements.

Moreover, it is easy to infer that for linear finite elements the above problem leads to a linear algebraic system with M-matrix if and only if $\kappa h_i \leq \sqrt{6}$ holds for all elements (here h_i denotes the length of the i-th element). We show that this condition can be weakened for higher order elements. This is non-trivial because the straightforward application of higher-order elements *does not* lead to M-matrices in general. We present a technique that leads to M-matrices (and hence to DMP) even in the case of higher order elements.

The results about DMP for higher-order approximations are scarce. This work extends the original results of the author and his co-workers [1]–[3].

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NEW CLASS OF LIMITED-MEMORY VARIATIONALLY-DERIVED VARIABLE METRIC METHODS

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Keywords: unconstrained minimization, variable metric methods, limited-memory methods, quadratic termination property, invariance property, numerical results

Abstract

A new family of limited-memory variationally-derived variable metric or quasi-Newton methods for unconstrained minimization is given. The methods have quadratic termination property and use updates, invariant under linear transformations. Since the resulting variable metric matrices are singular, the corrected matrices are used to calculate the direction vectors. Some encouraging numerical experience is reported.

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ROBUST ALGORITHMS FOR CHEBYSHEV POLYNOMIAL APPROXIMATION

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Abstract

A polynomial approximation in Chebyshev sense appears in various applications (antennas, digital signal processing, etc.) The recursive algorithms for such polynomials, Zolotarev polynomials and their relatives are presented. A nonlinear first order differential equation is usually used for parametric representation of these polynomials. We show that the second order differential equation can be derived correspondingly, which is linear and possess iterative solution. The recursive algorithm are found for Chebysev expansion of each polynomial and its numerical robustness is demonstrated.

SOLVING REGULARIZED TOTAL LEAST SQUARES PROBLEMS

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Abstract

Many problems in data estimation are governed by overdetermined linear systems

$$Ax \approx b, \quad A \in \mathbb{R}^{m\times n},\ b \in \mathbb{R}^m, m \geq n \tag{1}$$

where both the matrix A and the right hand side b are contaminated by some noise. This may happen for instance if the matrix A is obtained by measurements.

A possible approach to this problem is the total least squares (TLS) method which determines perturbations $\Delta A \in \mathbb{R}^{m\times n}$ to the coefficient matrix and $\Delta b \in \mathbb{R}^m$ to the vector b such that

$$\|[\Delta A, \Delta b]\|_F^2 = \text{min!} \quad \text{subject to } (A + \Delta A)x = b + \Delta b \tag{2}$$

where $\|\cdot\|_F$ denotes the Frobenius norm of a matrix.

In practical situations the linear system is often ill-conditioned. In these cases the TLS solution can be physically meaningless, and regularization is necessary for stabilizing the solution.

In this talk we consider regularization by adding a quadratic constraint, and we discuss methods for regularized total least squares problems which are based on sequences of eigenvalue problems. Methods of this type were considered by Renaut and Guo [3], and by Sima, Van Huffel and Golub [4]. Both types of methods can be improved considerably taking advantage of thick initial bases and early updates [1], [2].

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MULTIGRID METHODS FOR VARIATIONAL MOTION COMPUTATION IN VIDEOS

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Keywords: multigrid methods, variational techniques, image analysis

Abstract

Analysing motion in image sequences is a key problem in computer vision, and its applications range from robot navigation over driver assistance systems to video coding. The most accurate methods for computing the apparent motion (optic flow field) in image sequences are based on variational models. Finite difference discretisations of their corresponding Euler-Lagrange equations lead to very large linear or nonlinear systems of equations. In order to apply variational optic flow models to many real-world problems, these systems must be solved in a highly efficient way on standard PCs. In this talk we will show how multigrid methods can be adapted such that they become suitable to address this problem. A real-time demo on a laptop demonstrates the practicability of these concepts.

Acknowledgement: This research was partly funded by the German Research Foundation (DFG).

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STRUCTURED MATRIX METHODS FOR THE COMPUTATION OF MULTIPLE ROOTS OF UNIVARIATE POLYNOMIALS

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Keywords: polynomials, structured matrices, Sylvester resultant matrix, approximate greatest common divisors

Abstract

Significant effort has been devoted to the development of numerically reliable algorithms for the computation of the roots of a polynomial, but problems persist. For example, computations with the Wilkinson polynomial show that the accurate determination of the simple roots of a polynomial may not be trivial. Furthermore, these problems are compounded as the degree of the polynomial increases and/or the polynomial has multiple roots.

This paper describes a radically new method for the computation of the roots of a univariate polynomial. In particular, computations that involve the Sylvester resultant matrix of the polynomial and its derivative are used to calculate the multiplicities of the roots. The Sylvester matrix has a well-defined structure, and thus structured matrix methods are used to obtain improved results to the resulting least squares equality problem. The multiplicities are then used as constraints when the roots are calculated, and the method of non-linear least squares is used to improve the initial estimates of the roots.

Interesting problems occur when the coefficients of the polynomials are inexact, in which case there exists a (potentially infinite) family of solutions. In this case, it may be required to compute the roots that have a particular multiplicity structure, and it is therefore necessary to compute the smallest perturbation of the given inexact polynomial, such that the roots of the perturbed polynomial satisfy the given constraints on their multiplicities. These computations are very similar to those that are required for the computation of an approximate greatest common divisor of two inexact polynomials. The algorithm requires an estimate the rank of a noisy matrix, and it is shown that the *minimum description length* (MDL) can be used to obtain this quantity. The fundamental idea of the principle of MDL, which is closely related to Occam's razor, is that any regularity that is present in a given set of data can be used to compress the data. Since it is desired to select the hypothesis that captures the most regularity in the data, the hypothesis that achieves maximum compression is selected.

The talk will contain several computational examples in order to illustrate the theoretical ideas.

INTERVALS, TRIDIAGONAL MATRICES AND THE LANCZOS METHOD

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Keywords: Lanczos method, tridiagonal matrix, eigenvalues, Ritz values, Riemann-Stieltjes integral, Gauss approximations

Abstract

Consider the eigenvalue problem $Au = \lambda u$, where A is a large, real symmetric and sparse matrix. The Lanczos method (or any of its variants) is the method of choice if one is to seek approximations to a few eigenpairs (λ, u) of A. Due to rounding errors in finite precision computations the Lanczos vectors may lose their orthogonality even for a small number of iterations. Consequently, it can be numerically observed that clusters of Ritz values are generated: multiple copies of Ritz values all approximating a single eigenvalue of A.

In this contribution we will work on two conjectures posed by Zdeněk Strakoš and Anne Greenbaum in [1] on the clustering of Ritz values.

The first conjecture is as follows: Has any Ritz value in a tight, well separated cluster stabilized to within a small quantity δ which is proportional to the square root of the length of the cluster interval and the gap in the spectrum?

The second conjecture is concerned with the concept of *stabilization of weights*. Any nonzero vector together with the eigenvectors and eigenvalues of A defines a weight function and hence a Riemann-Stieltjes integral. The Lanczos method implicitly computes a sequence of Gauss quadrature approximations. This situation leads to the following question: If a cluster of Ritz values closely approximates an eigenvalue λ of A, does the sum of weights corresponding to the clustered Ritz values closely approximate the original weight belonging to the eigenvalue λ?

We will briefly present our solutions in this talk.

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NUMERICAL RANGE, RESOLVENTS AND BOUNDED SEMIGROUPS

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Abstract

We intend to discuss various characterizations of the boundedness of operator powers and their Cesaro means, in terms of the resolvent and numerical range. A number of open questions will be mentioned.

EIGENPAIR EXTRACTION USING KRYLOV SUBSPACES

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Keywords: Krylov subspace, eigenpair approximation, QOR methods, QMR methods, harmonic extraction, refined extraction

Abstract

This contribution deals with the various extraction methods to compute eigenpair approximations using Krylov subspaces. We present some of the known methods, like those based on

- Ritz pairs,
- zeros of (quasi-)kernel polynomials, and
- refinement of eigenvector approximations

in a common framework focusing on the assets and drawbacks. We give a glimpse of what might be beyond. This understanding helps to better rate the already known methods.

MULTI-GRID METHOD FOR INTEGRAL EQUATIONS OF FIRST KIND AND IT'S APPLICATIONS

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Keywords: first-kind Fredholm integral equation, multi-grid method, Tikhonov regularization

Abstract

The generic form of a first kind Fredholm integral equation is not a new problem:

$$\int_a^b K(x,s)u(s)ds = f(x)\,, \qquad a \le x \le b\,, \tag{1}$$

where the kernel function K is a known function, and the right-hand function f is also given, while u is the unknown function. The underlying theory of first-kind integral equations is well developed, and we know there are three main methods to solve them: (a) the truncated Singular Value Decomposition (SVD) [2]; (b) Tikhonov regularization [3]; (c) Iterative methods [2]. However none of them can solve large-scale problems efficiently, in our work, we propose some techniques so that we can solve the integral equation of the first kind (1) by the powerful multi-grid methods [1]. The first kind integral equation – an inverse process – is expected to amplify the high-frequency components and it is unusual "desmoothing process", which is contradict with the context of multi-grid methods. By introducing some transforms, we reverse pairing between eigenvalues and eigenvectors in order to adopt multi-grid algorithms.

We can also employ the same idea combined with Bézier parameterizations to a linear model – shape reconstruction problem, and a nonlinear model problem – RAE2822 airfoil.

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MATRIX SECTOR FUNCTION – PROPERTIES AND ALGORITHMS

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Keywords: matrix sector function, Newton's and Halley's methods, Padé approximation

Abstract

Matrix functions arise in numerous applications in science and engineering. This talk is concerned with the matrix sector function, introduced by Shieh, Tsay and Wang as a generalization of the matrix sign function (see L.S. Shieh, Y.T. Tsay, C.T. Wang, Matrix sector functions and their applications to system theory, IEEE Proceedings 131(5): 171–181, 1984.). Our goal is to review properties and applications of the matrix sector function, and analyze some known algorithms.

For a positive integer p and a matrix $A \in \mathbb{C}^{n\times n}$ having no eigenvalues with argument $(2k+1)\pi/p$ for $k = 0, 1, \ldots, p-1$, the matrix sector function is defined by $\mathrm{sect}_p(A) = A(\sqrt[p]{A^p})^{-1}$, where $\sqrt[p]{X}$ denotes the principal pth root of X. If $A = Z\mathrm{diag}(J_1, \ldots, J_m)Z^{-1}$ is a Jordan cannonical form, where J_l is the Jordan block of order r_l corresponding to the eigenvalue λ_l, then

$$\mathrm{sect}_p(A) = Z\mathrm{diag}\big(s_p(\lambda_1)I_{r_1}, \ldots, s_p(\lambda_m)I_{r_m}\big)Z^{-1},$$

where $s_p(\lambda)$ is the scalar sector function. Let

$$\lambda = |\lambda|e^{\theta i} \in \mathbb{C}, \quad \theta \in \left(\frac{2\pi}{p}(k-\frac{1}{2}), \frac{2\pi}{p}(k+\frac{1}{2})\right) \quad k = 0, 1, \ldots, p-1.$$

Then $s_p(\lambda) = e^{i2\pi k/p}$. The matrix sign function is a particular case for $p = 2$.

Although the matrix sector function can be computed directly from the spectral decomposition of A, an alternative approach based on iterative methods is useful. Numerical experiments comparing Newton's and Halley's methods, and the Padé recursions for computing the matrix sector function are presented. Our attention is drawn to the convergence and stability of the algorithms. We also deal with conditioning of the matrix sector function.

CONVERGENCE OF A RESTARTED AND AUGMENTED GMRES METHOD

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Keywords: restarted GMRES, augmented Krylov subspace, convergence of restarted GMRES

Abstract

The symbol GMRES(m, k) denotes the restarted GMRES with restart m, where to the standard Krylov subspace of dimension m the additional subspace of dimension k is added. This subspace usually approximates an invariant subspace of the matrix A. The GMRES(m, k) method is used for the solution of a linear system $Ax = b$. The behaviour of residual bounds is described and discussed for various choices of vectors generating the additional k-dimensional subspace.

The obtained estimates are independent of the choice of an initial approximation and yield sufficient conditions for convergence of GMRES(m, k). It will be illustrated in the discussion that the augmentation technique can remove stagnation or slow convergence of restarted GMRES in many cases.

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