IWASEP 10

International Workshop on Accurate Solution of Eigenvalue Problems X

CAAS, Dubrovnik, June 2-5, 2014

organized by
University of Split
Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture
and
University of Zagreb
Department of Mathematics

In cooperation with
SIAM Activity Group on Linear Algebra (SIAG/LA)

Abstracts

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State-space linearization method for solution of rational eigenvalue problem

Rafikul Alam

Let $G(\lambda)$ be an n-by-n rational matrix function. We wish to solve the rational eigenvalue problem (REP) $G(\lambda)u = 0$ for $(\lambda, u) \in \mathbb{C} \times \mathbb{C}^n$ with $u \neq 0$. The REP $G(\lambda)u = 0$ can be solved by employing general nonlinear eigensolvers such as the Newton method and nonlinear Rayleigh-Ritz methods. However, the convergence analysis of a general nonlinear eigensolver is a challenging task. Alternatively, the REP can be converted into a polynomial eigenvalue problem by clearing out the denominators in $G(\lambda)$ and then "linearizing" the resulting polynomial eigenvalue problem to obtain a generalized eigenvalue problem. A downside of this brute-force approach is that the resulting generalized eigenvalue problem may be of very large dimension especially when $G(\lambda)$ has a large number of poles. On the other hand, we can consider a state-space realization of $G(\lambda)$, that is, view $G(\lambda)$ as a transfer function of a linear time invariant (LTI) state-space system Σ :

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t) \\ y(t) &= Cx(t) + P(\tfrac{d}{dt})u(t) \end{aligned}$$

and then compute "transmission zeros" of Σ, where $P(\lambda)$ is an n-by-n matrix polynomial and A, E, C, B are constant matrices of appropriate dimensions with E being nonsingular. Note that an eigenvalue of $G(\lambda)$ is a transmission zero of Σ. Consequently, the eigenvalues and eigenvectors of $G(\lambda)$ can be obtained from the transmission zeros and zero directions of the state-space system Σ.

We describe a framework for computing transmission zeros of the state-space Σ by introducing a family of Fiedlier-like linearizations of the Rosenbrock system matrix $\mathcal{S}(\lambda)$ associated with Σ. We show that the linearizations of the Rosenbrock system matrix $\mathcal{S}(\lambda)$ are in a sense "linearizations" of $G(\lambda)$ when Σ is both controllable and observable, that is, when Σ is a minimal state-space realization of $G(\lambda)$. Schematically, our strategy for numerical solution of a rational eigenvalue problem is as follows:

$$\text{Rational matrix function} \longrightarrow \text{State-space realization} \longrightarrow \text{Linearization} \longrightarrow \text{Solution}.$$

There are efficient methods for computing a (minimal) state-space realization of a rational matrix function. We, therefore, focus on the construction of Fiedler-like linearizations of the Rosenbrock system matrix $\mathcal{S}(\lambda)$ so that the resulting generalized eigenvalue problems can be solved for computing eigenvalues and eigenvectors of $G(\lambda)$ as well as the transmission zeros and zero directions of the state-space system Σ.

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A Restarted Induced Dimension Reduction method to approximate eigenpairs of large unsymmetric matrices

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1 Introduction

In a variety of applications it is required to solve the eigenvalue problem, i.e., to find a subset of pairs (λ, x) of a matrix $A \in \mathbb{C}^{n\times n}$, such that

$$Ax = \lambda x, \tag{1}$$

where $\lambda \in \mathbb{C}$ is called eigenvalue, and the nonzero vector $x \in \mathbb{C}^n$ is its corresponding eigenvector. When the matrix A is large and unsymmetric, solving the eigenvalue problem becomes computationally challenging.

Usually the methods to approximate a subset of eigenpairs of large unsymmetric matrices are based on the construction of a Hessenberg relation, i.e.

$$AU_m = U_m B_m + u_{m+1} b^T \tag{2}$$

where $U_m \in \mathbb{C}^{n\times m}$, $B_m \in \mathbb{C}^{m\times m}$, $u_{m+1} \in \mathbb{C}^n$, and $b \in \mathbb{C}^m$ with m typically much smaller than n. Under mild conditions the eigenvalues of the matrix B_m approximate a subset of eigenvalues of A. The Arnoldi method [1] builds a Hessenberg relation where U_m is a matrix with orthogonal columns, B_m is an upper Hessenberg matrix and $b = e_m$ the m-th canonical vector. This method is widely used to approximate a subset of the eigenpairs of A, however, its computational and memory cost increases rapidly.

In 2008 the Induced Dimension Reduction (IDR(s)) was introduced for solving linear systems [5]. IDR(s) is a short recurrences method and it has obtained attention for its rapid convergence and efficiency. IDR(s) as a method to compute eigenvalues was first studied by M. H. Gutknecht and J.-P. M. Zemke in [3]. The work we present here is a a continuation of [2]. We describe how to obtain an underlying Hessenberg relation of the form (2) from IDR(s), and, we combine it with the implicitly restarting technique introduced by D.C. Sorensen [6] for Arnoldi in order to approximate eigenpairs of interest. Additionally, we suggest a parameter selection for our proposed method which defines a filter polynomial for the spectrum.

2 A Hessenberg relation based on the IDR(s) method

The IDR(s) method is based on the following theorem:

Theorem 1. *Let $P = [p_1, p_2, p_3, \ldots, p_s]$ be an $n \times s$ matrix, I the identity matrix of size n, and let $\{\mu_j\}$ be a sequence in $\mathbb{C}$. With $\mathcal{G}_0 \equiv \mathbb{C}^n$, define*

$$\mathcal{G}_{j+1} \equiv (A - \mu_{j+1} I)(\mathcal{G}_j \cap P^{\perp}) \quad j = 0, 1, 2 \ldots$$

If $P^{\perp}$ does not contain an eigenvector of A, then, for all $j = 0, 1, 2 \ldots$ we have that:

$$\mathcal{G}_{j+1} \subset \mathcal{G}_j, \text{ and dimension}(\mathcal{G}_{j+1}) < \text{dimension}(\mathcal{G}_j) \text{ unless } \mathcal{G}_j = \{0\}.$$

(See proof in [5].)

In order to solve a linear system, IDR(s) forces the residual vector $r_k = b - Ax_k$ to be in the nested and shrinking spaces $\mathcal{G}_j$, and then extracts the approximate solution x_k. Every vector w_{i+1} in $\mathcal{G}_{j+1}$ can be written as:

$$w_{i+1} = (A - \mu_{j+1} I) \left(w_i - \sum_{l=1}^{s} c_l w_{i-l} \right), \tag{3}$$

where the $s+1$ vectors $w_{i-s}, w_{i-s-1}, \ldots, w_i$ belong to $\mathcal{G}_j$, and the constants c_l are obtained from the solution of the $s \times s$ linear system:

$$(P^T [w_{i-s}, w_{i-s+1}, \ldots, w_{i-1}])c = P^T w_i$$

Using Eq. (3), we have:

$$Aw_i = w_{i+1} + \mu_{j+1} w_i - \mu_{j+1} \sum_{l=1}^{s} c_l w_{i-l} + \sum_{l=1}^{s} c_l A w_{i-l}$$

Setting $W_k = [w_1, w_2, \ldots, w_k]$, and assuming that Aw_{i-l} can be written as a linear combination of the vectors $w_1, w_2, w_{i-l}, w_{i-l+1}$, for $i = 1, 2, \ldots, i-1$, this is: $Aw_{i-l} = W_{i-l+1} H_{i-l}$, we obtain:

$$Aw_i = W_{i+1} \left(\begin{bmatrix} \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} \\ -\mu_{j+1} \begin{bmatrix} c \end{bmatrix} \\ \begin{matrix} \mu_{j+1} \\ 1 \end{matrix} \end{bmatrix} + \sum_{l=1}^{s} c_l H_{i-l} \right) = W_{i+1} H_{i+1} \tag{4}$$

Applying Eq. (4) for $i = 1, 2, \ldots, m$, we obtain a Hessenberg relation that we call the **IDR factorization**:

$$AW_m = W_{m+1} \bar{H}_m \tag{5}$$

$$= W_m H_m + w_{m+1} e_m^*. \tag{6}$$

3 Implicit Restarting and selection of the parameter μ_j

In some applications it is important to find eigenvalues and its corresponding eigenvectors in a specific region of the complex plane. For example, the eigenvalues with largest real part for stability analysis, or the nearest eigenvalues to a given point for vibrational analysis, for this reason, We implement two techniques to refine the spectral information obtained from the Hessenberg relation described in the previous section. The first technique is the implicitly restarting proposed by D.C. Sorensen. The idea is to remove the unwanted Ritz values applying the QR method over the matrix H_m using the unwanted Ritz values as shifts, and then, update the Hessenberg relation (for further details see [6]).
The second technique to remove the spectral unwanted information, is based on an observation made in [5], that each vector w_k in the subspace $\mathcal{G}_j$ satisfies:

$$w_k = \Omega_j(A)\Psi_{m-j}(A)w_1$$

where:

$$\Omega_j(t) = (1-\omega_1 t)(1-\omega_2 t)\dots(1-\omega_j t), \tag{7}$$

and $\Psi_{m-j}(A)$ is a polynomial of degree $m-j$ and its coefficient are fully determined by the IDR(s) procedure. We exploit this fact by selecting the parameters μ_i in (7) to minimize the norm of the polynomial Ω_j in area where the unwanted eigenvalues are localized. This is achieved by choosing μ_i as the Chebyshev nodes on the interval $[l,\, u]$, where l and u are the foci of the ellipse that encloses the unwanted portion spectrum of the matrix H_m (see [4] for more details).

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Solving a Parameterized Eigenvalue Problem from Regularized Total Least Squares

Geunseop Lee
Jesse Barlow
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The solution of an ill-conditioned total least squares (TLS) problem from high–resolution imaging by regularization approach of Golub et al. [SIAM J. Matrix Anal. Appl. 21(1):185-194,1999] is considered. The problem can be viewed as a parameterized eigenvalue problem. The approach given here is a Newton method that iterates for the parameter and the associated eigenvalue problem. The two nonlinear equations are formulated from a standard regularization bound constraint and a spectral function from the paramterized eigenvalue problem. The Jacobian of the system can be computed inexpensively and can be proven to be nonsingular under certain reasonable assumptions. A basic Newton method is presented as well two approximate Newton methods based upon projections. The resulting algorithm is applied to a problem from high-resolution image reconstruction that is appropriately modeled by total least squares.

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Relative Variational Principles for Eigenvalues of Self-adjoint Operators

Christopher Beattie

The Courant-Fischer-Weyl min-max characterization of the eigenvalues in the lower spectrum of self-adjoint operators has long been an important tool in spectral analysis, providing a critical mechanism for establishing upper bounds and proving existence of lower eigenvalues. While there is a dual max-min characterization for eigenvalues in the lower spectrum that could provide complementary lower bounds in principle, this is far less useful in practice since for unbounded operators the maximum must occur over a class of infinite dimensional subspaces. The results discussed here provide a max-min characterization of the eigenvalues of self-adjoint operators involving a maximum over a class of *finite*-dimensional subspaces. Among other consequences, this leads to a computationally tractable procedure for calculating lower bounds to the eigenvalues of self-adjoint operators with only modest requirements for *a priori* information. Sums and restrictions of operators are considered and these may be defined with respect to the associated quadratic forms. Furthermore, the operators of interest need only be symmetric with some weakening of conclusions.

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Fast Algorithm for Computing the Condensed Form of Four Matrices for the VZ Algorithm

Nela Bosner

Charles F. Van Loan in [3] proposes a general QR-type process called the VZ algorithm for the solution of the general matrix eigenvalue problem $ACx = \lambda BDx$, where $A, B \in R^{m\times n}$, $C, D \in R^{m\times n}$, and $m \geq n$. Especially, this algorithm is suitable for solving the generalized singular value problem $A^TAx = \mu^2 B^TBx$. The main point of the discussion presented in this article is that transforming the general eigenvalue problem to the standard form $(BD)^{-1}(AC)x = \lambda x$ represents a possible numerical danger. The formation of the products AC and BD, as well as the formation of the inverse $(BD)^{-1}$ can produce a result with a large backward error. Thus, the VZ algorithm attempts to solve the general eigenvalue problem without forming these products and inverse. This approach transforms each of the four matrices separately into a desired form. Actually, the algorithm computes orthogonal matrices $Q, U \in R^{n\times n}$ and $V, Z \in R^{m\times m}$ such that QAZ is upper quasi-triangular, and QBV, Z^TCU and V^TDU are upper triangular. The VZ algorithm begins by reducing the matrices A, B, C, and D to an equivalent condensed form by the finite step initial reduction. This reduction finds orthogonal matrices Q_0, U_0, V_0 and Z_0, such that Q_0AZ_0 is upper Hessenberg, and Q_0BV_0, $Z_0^TCU_0$ and $V_0^TDU_0$ are upper triangular. Then, the VZ iterations are applied to the matrices in the condensed form. As Van Loan pointed out, while the VZ algorithm can successfully solve the generalized singular value problem, even in pathological situations, it does have the drawback of being very inefficient. In the initial reduction, A is reduced to the upper Hessenberg form, while simultaneously preserving triangularity of the other three matrices. This is done by the Givens rotations, annihilating one by one element of A, and by generating three more rotations applied to the other matrices per each annihilation. Such an algorithm is quite inefficient. In our work, we propose a blocked algorithm for the initial reduction, which is a generalization of the blocked algorithm for the m-Hessenberg–triangular–triangular reduction proposed in [1], and the blocked algorithm for the Hessenberg–triangular reduction proposed in [2]. These blocked algorithms are based on the aggregated Givens rotations, which are applied in the outer loop updates. The blocked algorithm for the initial reduction has another level of blocking, exploited in the inner loop updates, since there is a larger number of matrices involved in these updates. Preliminary tests confirmed, that our blocked algorithm is up to 2.7 times faster than the original algorithm for the initial reduction when orthogonal factors are not computed, and over 4 times faster when orthogonal factors are accumulated. This way the efficiency of the whole VZ algorithm is increased. In the future work, we plan to generalize the efficient version of the QR iterations proposed in [4]

to the VZ iterations, which will produce an efficient and accurate algorithm for solving general eigenvalue problem.

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On the invariant subspace approach to solving the Riccati equation

Zvonimir Bujanović
Peter Benner

Finding the solution of the continuous algebraic Riccati equation $A^*X + XA + Q - XGX = 0$ is of great interest to the control theory community, and current applications require efficient algorithms in cases where A is a large sparse matrix and $Q = C^*C$, $G = BB^*$ are positive semidefinite low-rank matrices. In particular, one is interested in obtaining the stabilizing solution X_+, which is the unique positive semidefinite solution that makes the closed-loop matrix $A - GX$ stable.

There are several competitive methods to tackle this problem, designed to exploit the expected low-rank structure of the solution. These methods include the Newton-ADI (Alternate Direction Implicit) and the various projection-type methods, usually based on approximations using the Krylov or rational Krylov subspaces generated by the matrices A^* and A^{-*} and the initial (block-)vector C^*.

In this talk, we follow up on the approach introduced in [1, 2]. They suggested computing a low-dimensional stable invariant subspace of the Hamiltonian matrix $H = \begin{bmatrix} A & G \\ Q & -A^* \end{bmatrix}$ via a symplectic Lanczos procedure and using it for approximating the stabilizing solution of the Riccati equation. We discuss the properties of the Riccati equation that imply the rapid decay in the singular values of its solution, and justify the existence of a low-rank invariant subspace of H that yields a good approximation. We address the questions on how to construct such an approximation, and which are the eigenvalues the Lanczos procedure should be steered towards.

Finally, we relate the Krylov methods for computing Hamiltonian eigenspaces to the aforementioned projection-type methods for solving the Riccati equation. This gives some new insights on the latter, in particular on the shift selection in the rational Krylov method.

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On implicit restarting of the Arnoldi and the Krylov-Schur algorithms

Zlatko Drmač
Zvonimir Bujanović

This contribution introduces a new framework for implicit restarting of the Krylov-Schur algorithm. It is shown that restarting with arbitrary polynomial filter is possible by reassigning some of the eigenvalues of the Rayleigh quotient through a rank-one correction, implemented using only the elementary transformations (translation and similarity) of the Krylov decomposition. This framework includes the implicitly restarted Arnoldi algorithm (IRA), and the Krylov-Schur algorithm with implicit harmonic restart as special cases. Further, it reveals that the IRA algorithm can be turned into an eigenvalue assignment method.

Since eigenvalue assignment is notoriously ill-conditioned procedure, this revealed connection opens many interesting numerical issues related to implicit restarting. We will discuss some of them.

The new framework is used to tackle the problems of implicit restarting of the second order Arnoldi type algorithms (such as e.g. SOAR), which is challenging task with many open problems.

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The Fiedler Matrix and the LR Transform

Beresford Parlett
Carla Ferreira

This pentadiagonal rival to the (Frobenius) companion matrix was introduced only in 2003 but has since received much attention. We show how it relates to several larger classes such as CMV matrices and banded matrices with banded inverses. Our interest is in the iterates of this matrix, its transpose and its inverse under the LR transform. In particular, they all share the semiseparable property. The Rayleigh quotient iteration turns out to be identical to Newton's iteration on the polynomial.

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Probabilistic bounds for the matrix condition number
with extended Lanczos bidiagonalization

Sarah W. Gaaf
Michiel E. Hochstenbach

Reliable estimates for the condition number of a large (sparse) matrix A are important in many applications. To get an upper bound for the condition number $\kappa(A)$, a lower bound for the smallest singular value is needed. Krylov subspaces are usually unsuitable for finding a good approximation to the smallest singular value. Therefore, we study extended Krylov subspaces which turn out to be ideal for the simultaneous approximation of both the smallest and largest singular value of a matrix. First, we develop a new extended Lanczos bidiagonalization method. With this method we obtain a guaranteed lower bound for the condition number. Moreover, the method also yields a probabilistic upper bound for $\kappa(A)$. This probabilistic upper bound holds with a user-chosen probability.

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Residual estimates for eigenvalue/vector approximations of nonlinear eigenvalue problems by higher order finite elements

Christian Engstrom
Stefano Giani
Luka Grubišić

This talk is about a posteriori analysis of the accuracy of adaptive higher order finite element methods for approximations of nonlinear eigenvalue problems for Fredholm valued operator functions. We are particularly interested in problems which appear in the modeling of periodic optical structures.

We construct and prove reliability and local efficiency of a residual type estimator for higher order conforming finite element methods.

Several model problems from the modeling of photonic crystal fibers are used for numerical testing of the accuracy of the constructed method. The performed tests indicate robustness of this residual estimator.

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Efficient and Reliable Matrix Algorithms for Data Analysis

Ming Gu

We develop novel matrix algorithms for computing the CX decomposition and for sparse principle component analysis. Our matrix analysis confirms the robustness of our approaches, and our numerical analysis on synthetic and large real application data confirms their efficiency.

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On the Convergence of the Cyclic and Quasi-cyclic Block Jacobi Methods

Erna Begović
Vjeran Hari

Jacobi-type eigenvalue methods are known for their relative accuracy and inherent parallelism. Recent research of Drmač, Veselić and others has shown that some of these methods can be efficiently implemented on standard computers. The natural way to enhance efficiency of these methods on contemporary computers is by modifying them to use BLAS 3 routines. The obtained methods are known by the common name block diagonalization (or block Jacobi-type) methods.

In the recent paper [1] we have proved simple conditions under which a general block Jacobi-type method converges to diagonal form. The result is proved for the cyclic pivot strategies which are weakly equivalent to the serial strategies (weak wavefront strategies). Here we develop tools for proving the same kind of convergence results under several other classes of cyclic and quasi-cyclic strategies. The new results can be applied to Jacobi-type processes for ordinary and generalized eigenvalue problems.

The main tool used in [1] was the theory of cyclic Jacobi operators introduced by Henrici and Zimmermann and later generalized in several papers by Hari. In [1] Jacobi operators are generalized to deal with block diagonalization methods. The theory from [1] shows that, for the given class of cyclic strategies, it is important that the spectral norm of the associated Jacobi operators is not larger than a constant smaller than one.

Let J be a Jacobi operator associated with some cyclic block Jacobi method for Hermitian matrices. Then applying J to a vector a, i.e. the relation $a' = Ja$, can be interpreted as a special block Jacobi method of the form $A^{(k+1)} = U_k^* A^{(k)} U_k$, $k \geq 0$, $A^{(0)} = A$, where the initial matrix A and the final matrix $A' = A^{(N_m)}$ are associated with the vectors a and a', respectively. Here, $N_m = m(m-1)/2$, where m is number of diagonal blocks in the block-matrix partition. The matrices U_k are unitary elementary block matrices, which differ from the identity matrix I_n in four blocks, two diagonal and the two corresponding off-diagonal blocks. These matrices are extracted from J. It appears that showing $\|J\|_2 \leq c_n < 1$ is equivalent to showing $\mathrm{off}(A') \leq c_n \,\mathrm{off}(A)$, where, generally, $\mathrm{off}(X) = \|X - \mathrm{diag}(X)\|_F$ is the off-norm of X. The proof may use only certain bounds for the blocks in each U_k (and should not depend on the elements or blocks of the matrices $A^{(k)}$). The constant c_n may depend just on n.

We prove results of this type for four new classes of the cyclic and two new classes of the quasi-cyclic strategies. Each such strategy is defined by some ordering or by some sequence of pairs

from the set $P_m = \{(i,j);\, 1 \le i < j \le m\}$. The proofs use different techniques including the theory of the Jacobi operators mentioned above. They all hold for the block methods.

As an immediate application of the obtained general results, we show that the standard Jacobi method for Hermitian (or symmetric) matrices is globally convergent if the matrix is of order 4 and the pivot strategy is any cyclic strategy. Note that there are altogether 120 cyclic strategies provided that the first transformation annihilates the element at position $(1,2)$.

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An (subjective) introduction to randomized matrix algorithms

Ilse Ipsen

The emergence of massive data sets, over the past fifteen or so years, has lead to the development of a new class of matrix algorithms, so-called randomized algorithms. They are being designed for matrix multiplication, solution of least squares problems, canonical correlations, and low-rank approximations. Randomized algorithms have been used effectively in applications like machine learning, population genomics, astronomy and nuclear engineering.

We give a flavour of randomized algorithms via a Monte-Carlo algorithm for approximating a Gram product, that is, the product of a short and wide matrix with its transpose. Along the way we discuss key concepts, including sampling methods, matrix concentration, coherence and leverage scores.

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Accurate eigenvalue decomposition of arrowhead matrices, rank-one modifications of diagonal matrices and applications

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We present a novel class of forward stable algorithms for solving eigenvalue problems for $n \times n$ real symmetric arrowhead matrices and rank-one modifications of diagonal matrices. The algorithms compute all eigenvalues and all components of the corresponding eigenvectors with high relative accuracy in $O(n)$ operations per eigenvalue/eigenvector. The algorithms are based on a shift-and-invert approach. Only a single element of the inverse of the respective shifted matrix eventually needs to be computed with double the working precision. Each eigenvalue and the corresponding eigenvector can be computed separately, which makes the algorithms adaptable for parallel computing. Our results can also be applied to Hermitian matrices and singular value decompositions. The methods can be used as a part of divide-and conquer methods for tridiagonal problems.

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Nonsymmetric Preconditioning for Symmetric Linear Equations and Eigenvalue Problems

Andrew Knayzev

We numerically analyze the possibility of turning off post-smoothing (relaxation) in geometric multigrid when used as a preconditioner in conjugate gradient linear and eigenvalue solvers for the 3D Laplacian. We solve linear systems using two variants (standard and flexible) of the preconditioned conjugate gradient (PCG) and preconditioned steepest descent (PSD) methods. The eigenvalue problems are solved using the locally optimal block preconditioned conjugate gradient (LOBPCG) method available in hypre through BLOPEX software. We observe that turning off the post-smoothing dramatically slows down the standard PCG. For the flexible PCG and LOBPCG, our numerical results show that post-smoothing can be avoided, resulting in overall acceleration, due to the high costs of smoothing and relatively insignificant decrease in convergence speed. We numerically demonstrate for linear systems that PSD converges nearly identical to flexible PCG if SMG post-smoothing is off. A theoretical justification is provided. [See arxiv.org/abs/1212.6680]

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Variational characterisations of real eigenvalues for Gyroscopically stabilized systems

Aleksandra Kostić
Heinrich Voss

Voss and Kostić have previously proven that several extreme eigenvaluesfor gyroscopically stabilized systems can be variationally characterized This paper presents a further basis for the variational characterization of the.eigenvalues for gyroscopically stabilized systems.For $\lambda > 0$ the idea is constructed in transformation of the eigenvalue problems for gyroscopically stabilized systems of the form

$\lambda^2 Ix + \lambda Bx + Cx = 0$, where $B = \begin{pmatrix} B_1 & 0 \\ 0 & -B_2 \end{pmatrix}$, $C = \begin{pmatrix} C_{11} & C_{12} \\ C_{12}^T & C_{22} \end{pmatrix}$, $B_1, B_2, C > 0$ and $x = \begin{pmatrix} z \\ y \end{pmatrix} \neq 0$ in the form of

$\lambda^2 y^T y - \lambda y^T B_2 y + y^T C_{22} y - y^T C_{12}^T \left(\lambda^2 I + \lambda B_1 y + C_{11}\right) C_{12} y = 0$, $y \neq 0$ from which conclusions simply follow.

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Pietzsch algorithm for diagonalization of skew-symmetric matrices on GPUs

Neven Krajina

In his dissertation, Pietzsch described a one-sided algorithm for diagonalization of skew-symmetric matrices which calculates the eigenvalues to high relative accuracy by using only real arithmetic. While there are algorithms for the same purpose, like QR method of Ward and Gray or Jacobi-like method of Paardekooper, they compute the eigenvalues of a skew-symmetric matrix A up to an absolute error bound of $f(n)\|A\|_2\varepsilon$, where $f(n)$ is some slowly growing function of the matrix order n and ε is the machine precision. Thus, eigenvalues of larger module are computed with high relative accuracy, while the smaller ones may not be relatively accurate at all. On the other hand, we can also reduce our matrix to tridiagonal skew-symmetric matrix and compute the eigenvalues by the bidiagonal QR method (without shifts) with high relative accuracy. Although both of the above arguments give the method of Pietzsch a substantial advantage, its disadvantage is speed, since Jacobi-like methods are known to be quite slow, despite their quadratic convergence.

In this work, we describe implementation of skew-symmetric Cholesky-like factorization of Bunch and Pietzsch method for orthogonalization of factors on graphic processing units. While retaining the same accuracy, our implementation shows substantial speedup in comparisson to sequential algorithm.

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Solving eigenvalue problems with a googol of unknowns

Daniel Kressner

The electronic Schroedinger equation, spin networks, and stochastic automata networks all give rise to huge eigenproblems. In these applications, an exponential growth of the degress of freedom is caused by tensorization, for example when tensorizing physical domains or considering joint probability densities. Standard eigenvalue solvers completely fail to handle such situations, simply because one cannot even afford to store a single vector explicitly. In this talk, we will survey recent developments in mathematics and physics that circumvent this problem by approximately representing vectors in a low-rank tensor format. We will briefly discuss the type of problems for which such a nonlinear approximation can be expected to work well and point out the (very few) existing theoretical results in this direction. Once a low-rank tensor format is set up, the eigenvalue problem is then solved within this format, for example, by applying an optimization procedure. We will demonstrate the power and limitation of this approach with a number of numerical examples.

This talk is based on joint work with Francisco Macedo, Michael Steinlechner, Christine Tobler, and Andre Uschmajew.

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Structured Sylvester and T-Sylvester equations

Ivana Kuzmanović

Sylvester and T-Sylvester equations are matrix equations of the form $AX + XB = E$ and $AX + X^T B = E$, respectively, where A, B and E are given and X is unknown matrix.

Sylvester equations appear frequently in many areas of applied mathematics. For example, Sylvester equations play vital roles in matrix eigen-decompositions, control theory, model reduction, numerical solution of matrix differential Riccati equations and algebraic Riccati equation, image processing, and many more. On the other hand, T-Sylvester matrix equations have recently attracted attention of researchers because of their relationship with palindromic eigenvalue problems.

We present result about structured Sylvester and T-Sylvester equations, especially for structured problems with the system matrices of the form $A = A_0 + U_1 V_1$ and $B = B_0 + U_2 V_2$ where U_1, U_2, V_1, V_2 are small rank update matrices. We give the Sherman-Morrison-Woodbury-type formula for the solutions of this type of equation. The obtained formulas are used for the construction of algorithms which solves the equations of the above form much more efficiently than the standard algorithms. Application of obtained algorithms will be illustrated in several examples.

This is joint work with Ninoslav Truhar.

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On the stability of polynomial eigenvalue problems solved via linearization

Piers W. Lawrence

In this work, we investigate the accuracy and stability of polynomial eigenvalue problems expressed in the Lagrange basis that are solved by linearization [1]. For the scalar case, it has been demonstrated that computing the roots of polynomials via the eigenvalues of a certain arrowhead linearization is backward stable under certain conditions [2]. We extend this analysis to polynomial eigenvalue problems, and show the conditions under which the eigenvalues are computed with small backward errors. We also investigate a generalization of the arrowhead linearization to cover rational and nonlinear eigenvalue problems. We generate linearizations directly from sample values of the underlying problem at distinct nodes, avoiding the often ill-conditioned transformations between different bases. For certain special choices of nodes (real or on the unit circle), we can efficiently reduce the linearizations to block Hessenberg form [3, 4]. The algorithm simultaneously transforms all of the sample values of the polynomial matrix to the coefficients of orthogonal polynomials with respect to a discrete inner product that is based on the interpolation nodes.

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On Deflations in Extended QR Algorithms

Thomas Mach
Raf Vandebril

Deflation procedures are one of the core parts of every iterative eigenvalue algorithm. In this lecture we discuss the deflation criterion used in the extended QR algorithm based on the chasing of rotations. We show that this deflation criterion can be considered to be optimal with respect to absolute and relative perturbation of the eigenvalues.

Further, we present a generalization of aggressive early deflation to the new extended QR algorithms. Aggressive early deflation is the key techniques for the identification and deflation of already converged eigenvalues. We present numerical results illustrating the power of aggressive early deflation in the context of extended QR algorithms.

Preliminary results show that the ideas can be further generalized by the transcription of middle deflations.

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Reliable computation of the distance to discrete-time instability

Alexander Malyshev

In 1988 R. Byers proposed to use structure-preserving algorithms for Hamiltonian eigenvalue problems in order to reliably compute the distance to instability, which is given by the parameter

$$\min_{\omega \in R} \sigma_{\min}(A - i\omega I),$$

where A is a square matrix, $i = \sqrt{-1}$, I is the identity matrix, and $\sigma_{\min}$ is the minimum singular value of a matrix.

In this talk I show how to use structure-preserving algorithms for palindromic matrix pencils in order to reliably compute the distance to the discrete-time instability, which is given by the parameter

$$\min_{\omega \in R} \sigma_{\min}(A - i\omega I).$$

The approach is also valid for computation of the parameter

$$\min_{\omega \in R} \sigma_{\min}(P(e^{i\omega})),$$

where $P(\lambda) = A_0 + A_1\lambda + A_2\lambda^2$ is a quadratic matrix polynomial or higher order matrix polynomial.

By reliable computation we mean availability of strict bounds on the effect of rounding errors during computation.

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On matrix nearness problems: distance to delocalization

Vladimir R. Kostić
Agnieszka Międlar
Jeroen J. Stolwijk

In this talk we will introduce two new matrix nearness problems that are intended to generalize the distance to instability and the distance to stability. They are named the distance to delocalization and the distance to localization due to their applicability in analyzing the robustness of eigenvalues with respect to arbitrary localization sets (domains) in the complex plane. For the open left-half plane or the unit circle, the distance to the nearest unstable/stable matrix is obtained as special case. We will discuss the theoretical framework of Hermitian functions and the Lyapunov-type localization approach, we present a new Newton-type algorithm for the distance to delocalization (D2D). We will illustrate our approach on several practical examples. Furthermore, in the special case when the distance to delocalization becomes the distance to instability, we will validate our algorithms against the state of the art computational methods.

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$\sin 2\Theta$ Theorems for Definite Matrix Pairs

Suzana Miodragović
Luka Grubišić
Ninoslav Truhar

We present new $\sin 2\Theta$ theorems for relative perturbations of Hermitian definite generalized eigenvalue problem $A - \lambda B$, where matrices A and B are Hermitian and B is positive definite. The rotation of eigenspaces is measured in the matrix dependent scalar product. We assess the sharpness of the new estimates in terms of the effectivity quotients (the quotient of the measure of the perturbation and the estimator). The known $\sin 2\Theta$ theorems for relative perturbations of the single matrix Hermitian eigenspace problem are included as special cases in our approach. Our bound is dependent on the norm of the block diagonalizing J-unitary matrix F ($F^*JF = J$) which can be efficiently bounded for the case when the matrix A is *quasi-definite*.

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Scalable computation of document similarity across languages

Andrej Muhič
Jan Rupnik
Primož Škraba

With the rise of the internet, automatic text analysis has been extensively studied over the last few decades. Primarily, methods have been tailored to a single language, English. However, in the last decade, the web has become increasingly multilingual, requiring new tools for analysis and bringing new mathematical challenges. The most common representation of documents for text analysis is the bag-of-words representation, which models the data as a vector space. In this project, we consider multilingual data in this vector space representation. Rather than match dimensions explicitly (through machine translation) we will exploit the underlying latent structure of the data to construct language independent similarity measures. The existence of such similarity functions enables the transformation of multilingual problems into a monolingual setting. For example, we can apply monolingual versions of clustering, information retrieval, classification, and similarity computation directly on multilingual data. This reduces the cost of the required infrastructure as large problems can be handled by one fast machine. By contrast, machine translation tools are prohibitively expensive. Moreover, this can be applied to any two languages given some direct or indirect alignment. For example, Google translation service currently supports 71 languages but our approach can be used on any comparable data of sufficient quality, i.e. for more than 100 top languages on Wikipedia.

This has many concrete applications. One application is tracking information in a language independent way - for example, this would allow the Slovenian press to track their articles and republished content on Internet. Another application is a recommender system which deliver relevant local content for foreign users visiting a news page in English. It also enables the language independent demand prediction which can provide service according to currently hot topics. Lastly, the language independent measure of similarity can be used for plagiarism detection of diplomas, PhDs, etc., detecting translations or content use in other languages without citations.

There are two main approaches to computation of latent information. Using spectral analysis of the data, we can find hidden structure using approaches such as canonical correlation analysis (CCA), principal component analysis (PCA), latent semantic indexing (LSI), and spectral LDA, where the higher order moments – tensors are used to recover the underlying distribution. All spectral approaches use some variant of truncated singular value decomposition (truncated SVD), usually computed using a randomized approach to reduce the dimensionality and the noise in the data. Another popular choice is to consider nonnegative decompositions that are

easily interpretable but much more expensive to compute. Another possibility is to use graphical models to model conditional dependence structure between random variables. Two such examples are both generative models: probabilistic latent semantic indexing (PLSI) and latent Dirichlet allocation (LDA). Lastly there are natural extensions of the spectral and SVD approach to tensors, one concrete application to cross-language retrieval is PARAFAC2.

There are many pitfalls that are encountered when trying to construct language independent similarity measure, many inherent to the structure of data available. The data often has missing alignments between pairs of languages. Furthermore there may be no comparable documents available, but nevertheless we would like to construct the similarity measure. A somewhat related problem is incompatible topic coverage – known as topic drift. For example, data common to English and Slovenian covers wide range of topics but English and Neapolitan may have data only almost exclusively about sports. Moreover, openly available data is noisy and only weakly aligned. While the documents are comparable, they do not consist of direct translations, which must be accounted for. The quantity of monolingual data always exceeds the quantity of available multilingual data which may be used to further improve the similarity measure. We will show some preliminary results how to exploit additional structure when it is available, such as class information and entity data available for all languages, intra language links, etc.

Another key class of problems pertain to the computation itself. The methods often require computing empirical covariance and variance on samples of small size and sometimes even having to using nonaligned data sets for the computation. This can cause instability in the estimation. For example, the computation using spectral LDA is efficient but may lead to negative topic weights which have no meaningful interpretation. Likewise, a large vocabulary size can hurt performance of LDA. These phenomena needs to be further explored; Due to large dimensionality of the data with additional structure, there is a need for new numerical methods that would exploit this availability of additional structure. This is naturally related to structured numerical linear algebra problems such as structured eigenvalue computation.

As we are dealing with large matrices or tensors an efficient implementation must look beyond the theory and consider the appropriate data structures and preprocessing to be able to produce meaningful results. The best known numerical approaches, which build on idea of block Krylov subspace methods and random projections to compute relevant compressions of the data will be used as a basis for the development of novel approaches that also consider structure to improve stability and parallelizability of the computations. We will address how to take advantage of the additional structure of matrices and tensors and perform more efficient and scalable robust optimization, avoiding NP-hard problems to keep the methods as robust as possible. To ensure that the methods used are not the cause of poor performance, we will perform careful numerical analysis of approximation methods to ensure the numerical stability and accuracy of the computations. Approximation of sparse matrices and tensors have been widely studied due to the efficiency of algorithms but we will also consider underlying structure of the problem to improve the stability. Our goal is to make methods that are practical, easy to use and implementable to promote their application in practice. Finally, we will present results of extensive experimentation and evaluation using publicly available data sets with a primary

focus on Wikipedia where alignment information is provided in the form of interlanguage links.

We will also show a preliminary demo of the cross-lingual similarity computation that can be accessed at http://aidemo.ijs.si/xling/wikipedia.html. The authors gratefully acknowledge that the funding for this work was provided by the projects X-LIKE (FP7-ICT-288342-STREP), xLiMe (FP7-ICT-611346), SOPHOCLES (FP7-317534-STREP).

For some initial results from authors see:

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A hierarchically blocked Jacobi SVD algorithm for single and multiple GPU(s)

Vedran Novaković

We present a hierarchically blocked one-sided Jacobi algorithm for the singular value decomposition (SVD), targeting both single and multiple graphics processing units (GPUs). The blocking structure reflects the levels of GPU's memory hierarchy. The algorithm may outperform MAGMA's `dgesvd`, while retaining high relative accuracy. To this end, we developed a family of parallel pivot strategies on GPU's shared address space, but applicable also to inter-GPU communication. Unlike common hybrid approaches, our algorithm in a single GPU setting needs a CPU for the controlling purposes only, while utilizing GPU's resources to the fullest extent permitted by the hardware. When required by the problem size, the algorithm, in principle, scales to an arbitrary number of GPU nodes. The scalability is demonstrated by more than twofold speedup for sufficiently large matrices on a Tesla S2050 system with four GPUs vs. a single Fermi card.

The preprint is available at http://arxiv.org/abs/1401.2720

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Sensitivity of eigenvalues of an unsymmetric tridiagonal matrix

Beresford N. Parlett

The Wilkinson condition number ignores the tridiagonal form and so can be unduly pessimistic. We propose several relative condition numbers that exploit the tridiagonal form. Some of these numbers are derived from different factored forms (or representations) of the (possibly shifted) matrix and so they shed light on which factored forms are best for computation. We show some interesting examples.

This contribution is joint work with Carla Ferreira (University of Minho, Portugal) and Froilán Dopico (Universidad Carlos III de Madrid, Spain).

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On Error Resilience of a Complex Moment-based Eigensolver

Tetsuya Sakurai
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We consider a problem for finding eigenvalues in a domain enclosed by a Jordan curve Γ on the complex plane of the generalized eigenvalue problem $Ax = \lambda Bx$, where A and B are n-by-n matrices. The Sakurai-Sugiura (SS) method [1, 2, 3] is an eigensolver using complex moments obtained by contour integral. In the SS method, a subspace that includes eigenvectors corresponding to eigenvalues located in the given domain is constructed with solutions of systems of linear equations $(z_j B - A)Y_j = BV$, where V is an n-by-L matrix. This method has hierarchical parallelism, and has a good parallel scalability.

In large-scale parallel computing environment, fault tolerant of a method is required since failure ratio increases due to a huge number of cores. Recently, we have proved that the target eigenvectors can be extracted even if a solution Y_s is contaminated by an error caused by a fault. This property suggests an error resilience of the eigensolver without checkpointing or replication techniques. We show the theorem supporting this aspect. Some numerical experiments are also shown to confirm the error resilience in the method.

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New relative pivoting strategies for the LR and Cholesky factorizations

Sanja Singer

It is well–known that the complete and the partial pivoting in the LR factorization need not be effective for all matrices. An example of such a matrix, given by Heinz Rutishauser, is

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 10^{-10} & 0 \\ 1 & 0 & 10^{-10} \end{bmatrix}.$$

Based on this example, Rutishauser has introduced the *relative* complete and the *relative* partial pivoting strategy.

In this work we analyze how to minimize the errors introduced by one step of the LR and Cholesky factorization if they are computed according to the IEEE standard. It turns out that pivoting strategies that minimize errors of computed elements are similar to the relative pivoting strategies introduced by Rutishauser.

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Forward stable computation of roots of real polynomials with only real distinct roots

Ivan Slapničar
Nevena Jakovčević Stor

In [LAA 141 (1990)], Miroslav Fiedler showed that any polynomial can be expressed as a characteristic polynomial of a complex symmetric arrowhead matrix. This expression is not unique. If the polynomial is real with only real distinct roots, the matrix can be chosen real. By using accurate forward stable algorithm for computing eigenvalues of real symmetric arrowhead matrices, we derive a forward stable algorithm for computation of roots of such polynomials in $O(n^2)$ operations. The algorithm computes each root to almost full accuracy. In some cases, the algorithm invokes extended precision routines by Dekker [Num. Math. 18 (1971)], but only in the non-iterative part. Our examples include numerically difficult problems, like the well-known Wilkinson's polynomials.

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A DEIM Induced CUR Factorization

Danny C. Sorensen

I will present a CUR matrix factorization based upon the Discrete Empirical Interpolation Method (DEIM). A CUR factorization provides a low rank approximate factorization of a given matrix $\mathbf{A}$ of the form $\mathbf{A} \approx \mathbf{CUR}$ where $\mathbf{C}$ is a subset of the columns of $\mathbf{A}$ and $\mathbf{R}$ is a subset of the rows of $\mathbf{A}$. The matrix $\mathbf{U}$ is constructed so that $\mathbf{CUR}$ is a good approximation to $\mathbf{A}$. Assuming a low rank SVD $\mathbf{A} \approx \mathbf{VSW}^T$ is available, the DEIM points for $\mathbf{V}$ and $\mathbf{W}$ are used to select the matrices $\mathbf{C}$ and $\mathbf{R}$ respectively. This approximate factorization will satisfy $\|\mathbf{A} - \mathbf{CUR}\|_2 = \mathcal{O}(\sigma_{k+1})$, the first neglected singular value of $\mathbf{A}$ for a certain construction of $\mathbf{U}$.

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An Efficient Algorithm for Computing the Generalized Null Space Decomposition

G. W. Stewart
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The generalized null space decomposition is a unitary reduction of a general matrix A of order n to a block upper triangular form that reveals the structure of the Jordan blocks of A corresponding to a zero eigenvalue. The reduction was introduced by Kublanovskaya. It was extended first by Ruhe and then by Golub and Wilkinson, who based the reduction on the singular value decomposition. Unfortunately, if A has large Jordan blocks, the complexity of this reduction can approach $O(n^4)$. This paper presents an alternative algorithm, based on repeated updates of a QR decomposition of A, that is guaranteed to be of order n^3. Numerical experiments confirm the stability of this algorithm, which turns out to produce essentially the same results as the Golub and Wilkinson algorithm, even when A is perturbed. The effect of errors in A on the ability to recover the the original structure is investigated empirically.

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Repairing the Indefiniteness of a Correlation Matrix with a Fixed Block

Nicholas J. Higham
Nataša Strabić
Vedran Šego

In many applications from bioinformatics, finance and social sciences involving statistical modelling, the first step in the analysis is to estimate a correlation matrix (real symmetric positive semidefinite matrix with unit diagonal) from empirical or experimental data. As a result of data being asynchronous, inconsistent or missing, this approximate correlation matrix often lacks definiteness, in which case it needs to be replaced with a valid correlation matrix.

Additionally, in some applications a positive semidefinite submatrix of an indefinite estimator is known to be exact and needs to be preserved. To achieve this, we propose utilizing an idea from statistics called shrinking, which has been successfully applied to the sample covariance matrix estimation. We, however, use it in a new context: as a means of transforming an indefinite correlation matrix to a positive semidefinite one, while preserving a specified block.

Specifically, let C be a symmetric indefinite matrix with unit diagonal and A its leading principal positive semidefinite submatrix that we wish to preserve. The shrinking method consists of choosing a target matrix T and a parameter $\alpha \in [0,1]$ such that the convex linear combination $S(\alpha) = \alpha T + (1-\alpha)C$ has the desired properties, which in our case means that $S(\alpha)$ is a valid correlation matrix having the upper-left block A.

We discuss the choice of the target matrix $T = \mathrm{diag}(A, I)$ and the shrinking parameter $\alpha_* = \mathrm{argmin}\{\alpha \in [0,1] \colon S(\alpha) \text{ is positive semidefinite}\}$, analyze three different methods for computing the optimal parameter, namely, the bisection method, Newton's iteration and as a specific generalized eigenvalue of the corresponding indefinite matrix pencil $C - \alpha(C - T)$, and present the results of numerical experiments.

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The hyperbolic Schur decomposition and the SVD it implies

Vedran Šego

The Schur decomposition $A = UTU^*$ is a unitary similarity between any given complex square matrix A and some complex upper triangular matrix T of the same order. It is a structure preserving decomposition, i.e., T is complex diagonal if and only if A is normal, real diagonal if and only if A is Hermitian, positive (nonnegative) real diagonal if and only if A is positive (semi)definite and so on.

Closely related to the Schur decomposition of a positive semidefinite matrix is the singular value decomposition (SVD) $A = U\Sigma V^*$: a unitary equivalence of any (not necessarily square) matrix A and a nonnegative real diagonal matrix Σ of the same order. Given an SVD of A, the Schur decomposition of A^*A is obtained directly from it ($A^*A = V^*\Sigma^T\Sigma V$), thus removing the need to compute A^*A.

Both of these decompositions work with unitary matrices, whose defining property is the preservation of the Euclidean scalar product: $\langle Uv, Uw\rangle = \langle v, w\rangle$. However, if our vector space is equipped with a different scalar product, the structures (like unitarity and Hermitianity) are defined with respect to it, and then the question arises of generalizing the Schur decomposition and the SVD to this non-Euclidean scalar product space.

We focus on the hyperbolic scalar products ($[u, v]_J := \langle Ju, v\rangle$ for some signature matrix J), which are among the simplest and the most often used nonstandard scalar products. Working in the hyperbolic space instead of the Euclidean results in some known changes to the matrix structure that will be reflected in the generalized Schur decomposition: triangularity and diagonality need to be replaced with quasitriangularity and quasidiagonality (i.e., we introduce diagonal blocks of order up to 2) and the unitarity property needs to be weakened to preserve only orthonormality (a property which is equivalent to the unitarity in the Euclidean case).

Further, we investigate the structural properties of this generalization and use it to define and discuss the existence of the related SVD, a generalization of several other previously proposed extensions of the SVD to the hyperbolic spaces. We show that Σ has to be defined in a seemingly more complex way, with the expected diagonal blocks of order 1 and 2 just two among several needed forms. However, the rest of the blocks are fairly simple in structure, and they completely reveal the nature of the degeneracy (the drop of rank when computing the hyperbolic equivalent of A^*A) of the decomposed matrix.

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Low-rank Updates of Matrix Functions

Ana Šušnjara
Daniel Kressner

The efficient and reliable update computation of large-scale matrix functions subject to low-rank perturbations is of interest in several applications, such as the analysis of networks. For addressing this problem, Beckermann and Kressner have proposed the use of tensor polynomial and rational Krylov subspace methods. Starting from the exactness property of (rational) Krylov subspaces, convergence bounds for the tensor Krylov subspace method have been derived. In this talk, we discuss how these bounds provide important insight into the choice of poles for setting up the rational Krlyov subspaces. In particular, we discuss $\exp(A)$ and $\operatorname{sign}(A)$. The matrix sign function immediately yields the corresponding spectral projector and we discuss how tensorized Krylov subspace methods can be used in the solution of eigenvalue problems. For the case of the matrix exponential, the error expansion in terms of $\varphi-$ functions as well as the resulting corrected scheme proposed by Saad are extended to the tensor Krylov subspace method. While the corrected scheme itself may not offer advantages, it has been observed useful in deriving stopping criteria.

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Optimal Direct Velocity Feedback

Zoran Tomljanović

We present a novel approach to the problem of Direct Velocity Feedback (DVF) optimization of vibrational structures, which treats simultaneously small as well as large gains.

The first approach is based on the gains optimization using the Lyapunov equation. In the scope of this approach we present a new formula for the optimal gain and we present a relative error for modal approximation. In addition, we present a new formula for the solution of the corresponding Lyapunov equation for the case with multiple undamped eigenfrequencies, which is a generalization of existing formulae.

The second approach studies the behavior of the eigenvalues of the corresponding quadratic eigenvalue problem. Since this approach leads to the parametric eigenvalue problem we consider small and large gains separately. Fort he small gains, which are connected to a modal damping approximation, we present a standard approach based on Gerschgorin discs. For the large gains we present a new approach which allows us to approximate all eigenvalues very accurately and efficiently.

Besides mentioned application the new bounds are also valuable for better understanding of damped vibration systems where eigenvalue behavior plays important role.

Joint work with Ivica Nakić and Ninoslav Truhar.

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Relative Perturbation Theory for Definite Matrix Pairs and Hyperbolic Eigenvalue Problem

Ninoslav Truhar
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We present a new relative perturbation bounds for the eigenvalues as well as for the eigensubspaces of the definite Hermitian matrix pairs and the quadratic hyperbolic eigenvalue problem. First we present relative perturbation bounds for the eigenvalues and the sine θ type theorems for the eigensubspaces of the definite matrix pairs (A, B), where both $A, B \in \mathbb{C}^{m\times m}$ are Hermitian nonsingular matrices. Further we consider the quadratic hyperbolic eigenvalue problem $(\mu^2 M+\mu C+K)x = 0$, where $M, C, K \in \mathbb{C}^{n\times n}$ are given Hermitian matrices. Using a proper linearization and the new relative perturbation bounds for definite matrix pairs (A, B), we develop corresponding relative perturbation bounds for the eigenvalues and the sine θ type theorems for the eigensubspaces for considered quadratic hyperbolic eigenvalue problem. The new bounds are uniform and depend only on matrices M, C, K perturbations δM, δC and δK and the standard relative gaps.

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Nonlinear eigenvalue problems and contour integrals

Marc Van Barel
Peter Kravanja
Laurent Sorber

Nonlinear eigenvalue problems involving analytic matrix functions can be solved via a numerical method that is related to the Sakurai-Sugiura method as well as Polizzi's FEAST algorithm for generalized eigenvalue problems. This method is based on contour integrals. These are approximated numerically by a quadrature formula, which corresponds to a filter function. In this talk the properties of such a filter function as well as its implications on the nonlinear eigenvalue approximation problem will be investigated.

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On spectral gaps for some block matrices

Krešimir Veselić

We estimate the size of the spectral gap at zero for some Hermitian block matrices. Included are quasi-definite matrices, quasi-semidefinite matrices (the closure of the set of the quasi-definite matrices) and some related block matrices which need not belong to either of these classes. Matrices of such structure arise in quantum models of possibly disordered systems with supersymmetry or graphene like symmetry. Some of the results immediately extend to infinite dimension. This is a joint work with I. Veselić, Chemnitz.

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Variational characterization of eigenvalues of a non–symmetric eigenvalue problem governing elastoacoustic vibrations

Markus Stammberger
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In this talk we consider the elastoacoustic vibration problem, which consists of determining the small amplitude vibration modes of an elastic structure coupled with an internal inviscid, homogeneous, compressible fluid.

Different formulations have been proposed to model this problem, the most obvious of which describes the structure by its relative displacement field u and the fluid by its pressure p. Thus one arrives at the following system of homogeneous time-independent partial differential equations

$$\begin{aligned} \text{Div } \sigma(u) + \omega^2 \rho_s u &= 0 \text{ in } \Omega_s, \\ \nabla^2 p + \frac{\omega^2}{c^2} p &= 0 \text{ in } \Omega_f, \\ u &= 0 \text{ on } \Gamma_D, \\ \nabla p \cdot n_f &= 0 \text{ on } \Gamma_N, \\ \sigma(u)\, n - p\, n &= 0 \text{ on } \Gamma_I, \\ \omega^2 \rho_f u \cdot n + \nabla p \cdot n &= 0 \text{ on } \Gamma_I, \end{aligned} \tag{1}$$

where Ω_s and Ω_f denotes the region occupied by the structure and the fluid, respectively. Γ_D and Γ_N are Dirichlet– and Neumann-parts of the outer boundary of the structure, and Γ_I the interface between the fluid and the structure. The interface boundary conditions are a consequence of an equilibrium of acceleration and force densities at the contact interface.

Although this eigenvalue problem is not self–adjoint it shares many important properties with self–adjoint models: It has a countable set of eigenvalues which are real and non–negative, and taking advantage of a Rayleigh functional (which generalizes the Rayleigh quotient for self–adjoint problems) its eigenvalues allow for the variational characterizations known from the symmetric theory [3]. Namely, they can be characterized by Rayleigh's principle, and are minmax and maxmin values of the Rayleigh functional.

Discretizing the elastoacoustic problem with finite elements where the triangulation obeys the geometric partition into the fluid and the structure domain one obtains a non–symmetric matrix

eigenvalue problem which inherits the variational properties.

$$Kx := \begin{bmatrix} K_s & C \\ 0 & K_f \end{bmatrix} \begin{bmatrix} x_s \\ x_f \end{bmatrix} = \lambda \begin{bmatrix} M_s & 0 \\ -C^T & M_f \end{bmatrix} \begin{bmatrix} x_s \\ x_f \end{bmatrix} =: \lambda M x. \tag{2}$$

The following properties can be proved:

- The eigenvalues of the discrete problem (2) are upper bounds of the corresponding eigenvalues of problem (1).
- The standard spectral approximation theory applies to prove convergence results for Galerkin type methods.
- Eigenfunctions (of problem (1) and of its adjoint problem) can be chosen to satisfy an orthogonality property.
- A Krylov–Bogoliubov type eigenvalue bound holds [4].
- For the matrix eigenvalue problem the Rayleigh functional iteration is cubically convergent as is the Rayleigh quotient iteration for linear symmetric problems [1].
- Based on the variational characterization structure preserving iterative projection methods of Jacobi–Davidson type and nonlinear Arnoldi type can be defined [1, 4].
- The automated multi-level sub-structuring method (AMLS) introduced by Bennighof for linear symmetric eigenvalue problems in structural analysis can be generalized to the non–symmetric elastoacoustic problem, and an a priori error bound can be proved using the minmax characterization [2].

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On Quadratic Convergence of the Block Jacobi Method in the Presence of Multiple Eigenvalues

Yusaku Yamamoto

1 Introduction

There has been a renewed interest in Jacobi methods for the symmetric eigenvalue problem in recent years. One of the reasons for that is they are especially suited to modern massively parallel machines. As is well known, the Jacobi methods are inherently parallel and their computational kernels are simple. Moreover, the block Jacobi methods, which are natural extensions of the original point Jacobi methods, have high level of data locality and large grain parallelism. Thanks to these features, block Jacobi methods have advantages when solving a small to medium eigenvalue problems using a large number of processors [1]. Such a situation occurs in quantum chemistry computations and in a certain type of first-principles molecular dynamics. Our recent experiments show that when solving an eigenvalue problem of size $n = 10,000$ on the K computer, the block Jacobi method is more than twice faster than ScaLAPACK.

In this talk, we focus on the local convergence property of the block Jacobi methods. At each step of the block Jacobi method, one picks up four blocks according to some predetermined rule and find an orthogonal matrix (block rotation) $\tilde{P}^{(k)}$ that diagonalizes the 2 by 2 block matrix:

$$\begin{pmatrix} P_{II}^{(k)} & P_{IJ}^{(k)} \\ P_{JI}^{(k)} & P_{JJ}^{(k)} \end{pmatrix}^{\top} \begin{pmatrix} A_{II}^{(k)} & A_{IJ}^{(k)} \\ A_{JI}^{(k)} & A_{JJ}^{(k)} \end{pmatrix} \begin{pmatrix} P_{II}^{(k)} & P_{IJ}^{(k)} \\ P_{JI}^{(k)} & P_{JJ}^{(k)} \end{pmatrix} = \begin{pmatrix} A_{II}^{(k+1)} & O \\ O & A_{JJ}^{(k+1)} \end{pmatrix}. \tag{1}$$

We write this as $(\tilde{P}^{(k)})^{\top} \tilde{A}^{(k)} \tilde{P}^{(k)} = \tilde{A}^{(k+1)}$ for brevity. In a recent paper [2], Drmač shows that the block row (or column) cyclic Jacobi method is globally convergent if the block rotations are computed in a particular way. He also shows that the convergence is asymptotically quadratic if the eigenvalues are simple. However, it seems not straightforward to extend the proof of quadratic convergence to the case of multiple eigenvalues. This is because the $\sin\Theta$ theorem cannot give a valid upper bound on the block rotation angles when $A_{II}^{(k)}$ and $A_{JJ}^{(k)}$ contain diagonal elements that converge to the same eigenvalue. Drmač proposes to adapt block partitioning to the distribution of the eigenvalues in such a case ([2], Remark 3.2). This strategy should work well on a sequential or shared-memory parallel computers, but in the case of distributed memory

parallel computers, one cannot move the block boundary freely, because other factors such as load balancing and inter-processor communication are involved.

2 Modification to the computation of the block rotation and quadratic convergence

We propose an alternative approach to determine the block rotation in the case of multiple eigenvalues. Assume that the final stage of convergence has been reached and all the off-diagonal elements of $A^{(k)}$ have become smaller than a sufficiently small constant δ. So, each diagonal element is within a distance of $O(\delta)$ from some eigenvalue of $A^{(k)}$ and is far from other eigenvalues. Now assume that some of the diagonal elements of $A_{II}^{(k)}$ and $A_{JJ}^{(k)}$ are close to the same eigenvalue λ. We further assume that the diagonal elements of $\tilde{A}^{(k)}$ are sorted, because sorting usually promotes convergence [3]. Thus the diagonal elements close to λ are at the bottom right corner of $A_{II}^{(k)}$ and top left corner of $A_{JJ}^{(k)}$. Then we repartition the matrix $\tilde{A}^{(k)}$ into 3 by 3 blocks as

$$\tilde{A}^{(k)} = \begin{pmatrix} A_{aa}^{(k)} & A_{ab}^{(k)} & A_{ac}^{(k)} \\ A_{ba}^{(k)} & A_{bb}^{(k)} & A_{bc}^{(k)} \\ A_{ca}^{(k)} & A_{cb}^{(k)} & A_{cc}^{(k)} \end{pmatrix}, \tag{2}$$

so that $A_{bb}^{(k)}$ contains diagonal elements close to λ. Note that the norms of off-doagonal blocks such as $A_{bc}^{(k)}$ is $O(\delta)$. Furthermore, as is shown in [4] (Theorem 9.5.1), the off-doagonal elements of $A_{bb}^{(k)}$ is $O(\delta^2/d)$, where d is the smallest distance from λ to other eigenvalues.

Now we repartition the orthogonal matrix $\tilde{P}^{(k)}$ in the same way as Eq. (2). It is easy to show by using the $\sin\Theta$ theorem that the norms of off-diagonal blocks of $\tilde{P}^{(k)}$ is $O(\delta)$. On the other hand, the diagonal block $P_{bb}^{(k)}$ is close to an orthogonal matrix, but might be far from the identity matrix. This causes a problem, because this gives rise to a possibly large rotation between the upper block rows and lower block rows in the original partitioning in (1). This can cause a once eliminated block of norm $O(\delta^2)$ outside $\tilde{A}^{(k)}$ to be violently mixed with a not yet eliminated block of norm $O(\delta)$ and impede quadratic convergence. In the case of cyclic point Jacobi methods, one can solve this problem by skipping the elimination of an off-diagonal element associated with two diagonal elements that are nearly identical [4]. In the block case, this corresponds to replaceing $P_{bb}^{(k)}$ with the identity matrix and $P_{ba}^{(k)}$ and $P_{bc}^{(k)}$ with zero. Unfortunately, this will not work because then $A_{ba}^{(k+1)}$ and $A_{bc}^{(k+1)}$ will remain $O(\delta)$.

To solve this problem, we propose to use the polar decomposition $P_{bb}^{(k)} = Q_{bb}^{(k)} M_{bb}^{(k)}$, where $Q_{bb}^{(k)}$ is orthogonal and $M_{bb}^{(k)}$ is symmetric positive definite. Let $\tilde{Q}^{(k)} = \mathrm{diag}(I_{aa}, Q_{bb}^{(k)}, I_{cc})$, where I_{aa} and I_{cc} are identity matrices of the same size as $A_{aa}^{(k)}$ and $A_{cc}^{(k)}$, respectively. In the proposed procedure, we compute the next iterate as

$$\tilde{A}^{(k+1)} = (\tilde{Q}^{(k)})^\top (\tilde{P}^{(k)})^\top \tilde{A}^{(k)} \tilde{P}^{(k)} \tilde{Q}^{(k)}. \tag{3}$$

Of course, the whole matrix $A^{(k)}$ is transformed accordingly. Clearly, (3) constitutes an orthogonal transformation on $A^{(k)}$. Furthermore, it can be shown that the transformation has the following properties.

- Off-diagonal blocks of $\tilde{A}^{(k+1)}$ (in the sense of new partitioning) become zero.
- Off-diagonal elements of the diagonal block $A_{bb}^{(k+1)}$ remains $O(\delta^2/d)$, as in $A_{bb}^{(k)}$.
- The rotation angle between the upper block rows and lower block rows (in the sense of original partitioning) is $O(\delta/d)$.

Thus we expect that the proposed transformation does not disturb the quadratic convergence. The price to pay is that the off-diagonal elements of $A_{bb}^{(k+1)}$ are not exactly zero. But this should not be a problem, because they are of the same order as other once eliminated off-diagonal elements. Note that this procedure does not need changing the block boundaries, so it is well suited to distributed memory parallel computers.

3 Conclusion

We proposed a modification to the computation of block rotation in the block Jacobi method to retain quadratic convergence in the presence of multiple eigenvalues. In the talk, details of the proposed procedure and some numerical examples will be given. Application of this procedure to other types of block Jacobi methods, such as Bečka et al.'s dynamic ordering parallel block Jacobi method, will also be discussed.

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On Structured Pencils arising in Sonneveld methods

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In [1, 2] we developed the mathematical theory of an eigensolver based on Sonneveld's and van Gijzen's method of induced dimension reduction (IDR) [6, 4]. In [2] we extended the theory to its generalization IDRStab [5, 3]. The arising pencils are banded upper Hessenberg/triangular, a property that is destroyed if we use a standard QZ algorithm. Due to the peculiarities of IDR-based methods, some eigenvalues of the pencils are known in advance. We sketch our ideas to reliably compute the other eigenvalues.

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Matrix Balancing for Field of Values Type Inclusion Regions

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The field of values may be an excellent tool for generating a spectral inclusion region: it is easy to approximate numerically, and for many matrices this region fits relatively tightly around the eigenvalues. However, for some matrices the field of values may be a poor eigenvalue inclusion region: the numerical radius may be much larger than the spectral radius. We show that balancing the matrix may be helpful for generating a quality inclusion region based on the field of values. and introduce a new Krylov based balancing method. We believe that both the (sparse) balancing and the new "Krylov and balance" technique, combined with a projected field of values, render spectral inclusion regions that may be hard to beat in both quality and efficiency.

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