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Abstracts

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A Jacobi–Davidson algorithm for large eigenvalue problems from opto-electronics

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The construction of prototypes of nowadays opto-electronic components during their development is very expensive. Therefore, they are developed and simulated on the computer. This procedure admits to determine and optimize their characteristics, in particular their optical characteristics, in advance. The progressive miniaturization of opto-electronic components leads to numerous quantum-mechanical effects, that cannot be treated by the usual classical models. Quantum-mechanical methods have to be employed. The states of the charge carriers and the dispersion relations are determined by coupled Schrödinger equations. Their discretization by means of the finite element method leads to large sparse generalized complex Hermitian matrix eigenvalue problems. If multiple bands of the electronic band structure are simulated by the $\mathbf{k}\cdot\mathbf{p}$ method the matrix becomes indefinite.

Because of their size the solution of these eigenvalue problems requires sophisticated eigensolvers. We present a variant of the Jacobi–Davidson (JD) algorithm that is based on a real symmetric formulation of the complex Hermitian eigenvalue problem. The correction equations that have to be solved in each step of JD are solved by a conjugate gradient-type algorithm preconditioned by a V-cycle of smoothed aggregation multigrid. In the indefinite case the spectrum is folded to arrive at positive definite problems.

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A Linearization Method for Polynomial Eigenvalue Problems Using a Contour Integral

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We consider a numerical method for solving polynomial eigenvalue problems. The polynomial eigenvalue problem (PEP) [1, 3] involves finding an eigenvalue λ and corresponding nonzero eigenvector $\boldsymbol{x}$ that satisfy $F(\lambda)\boldsymbol{x} = \mathbf{0}$, where $F(\lambda) = \sum_{i=0}^{l} \lambda^i A_i$ with real or complex coefficient matrices. Polynomial eigenvalue problems can be used in a variety of problems in science and engineering. However, its applications are more complicated than standard and generalized eigenvalue problems. We herein propose a linearization scheme, which prevents the inflation of the matrix dimension. Indeed, we can instead reduce the dimension of the problem by focusing on only the eigenvalues of physical interest. The Sakurai-Sugiura (SS) method [2], which solves a generalized eigenvalue problem, finds certain eigenvalues in a given domain. The SS method can deal with non-Hermitian systems and is compatible with modern distributed parallel computers. We show that the SS method is directly applicable to PEP. The proposed method enables us to obtain the eigenvalues of the matrix polynomial by solving the generalized eigenvalue problem, which is derived by solving systems of linear equations. Since these linear systems are independent for each equation, they can be solved in parallel. We discuss the proposed method from a theoretical point of view, and present numerical examples that confirm the theoretical observations.

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On the Convergence of Block Kogbetliantz Methods for Calculating the SVD

Zvonimir Bujanović, Zlatko Drmač

For a given matrix $A \in \mathbf{C}^{n\times n}$, the Kogbetliantz method calculates its singular value decomposition $A = U\Sigma V^\star$. It achieves this goal by applying a series of plane rotations $(U_k)_k$ and $(V_k)_k$ to the initial matrix $A_0 = A$, generating the sequence $A_k = U_k^\star A_{k-1} V_k$. At each step k, the rotations are chosen so that a couple of elements of A_{k-1} at mutually transposed positions is annihilated. Forsythe and Henrici [3] have shown that if elements to be annihilated are chosen in a row-cyclic order, then $(A_k)_k$ converges to Σ under certain conditions and Fernando [2] further refined the proof by loosening the constraints under which the convergence occurs.

In this presentation, we introduce the block Kogbetliantz method. The initial matrix is partitioned into blocks, and instead of annihilating a couple of elements by plane (2 by 2) rotations at each step, we consider annihilating a couple of blocks at mutually transposed positions by more general block rotations.

Following the idea of Drmač [1], we discuss conditions that block rotations have to satisfy in order for a row-cyclic algorithm to converge. We also prove convergence of left and right singular vectors.

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Extremum Properties of Orthogonal Quotients Matrices

Achiya Dax

In this talk we explore extremum properties of Orthogonal Quotients matrices. The Orthogonal Quotient Equality that we prove expresses the Frobenius norm of a difference between two matrices as a difference between the norms of two matrices. This turns the Eckart-Young minimum norm problem into an equivalent maximum norm problem. The symmetric version of this equality involves traces of matrices, and adds new insight into Ky Fan's extremum problems. A comparison of the two cases reveals a surprising similarity between the Eckart-Young minimum principle and Ky Fan's maximum principle. Returning to Orthogonal Quotients matrices, we derive extended extremum principles, which consider maximizing (or minimizing) sums of powers of singular values.

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Implicit standard Jacobi gives high relative accuracy on rank revealing decompositions

Froilán M. Dopico
Joint work with: Plamen Koev and Juan M. Molera

Given the real matrices X, with full column rank, and D, diagonal and nonsingular, we show that the standard cyclic Jacobi algorithm implicitly applied on X computes all the eigenvalues of XDX^T, including the tiniest ones, with relative errors bounded by $O(\epsilon\kappa_2(X))$, where ε is the machine precision and $\kappa_2(X)$ is the condition number of X. The eigenvectors are computed with errors bounded by $O(\epsilon\kappa_2(X))$ divided by the relative gap between eigenvalues. Since accurate rank revealing factorizations XDX^T, with X well conditioned, can be computed for many classes of symmetric matrices, the implicit Jacobi algorithm allows us to compute eigenvalues and eigenvectors with high relative accuracy for many types of symmetric matrices. The algorithm we introduce is the first algorithm that computes eigenvalues and eigenvectors of symmetric factorized matrices XDX^T with high relative accuracy, preserving the symmetry of the problem, and by using only orthogonal transformations. We present in this talk a detailed description of this algorithm, backward and forward error analyses, and a comparison with previously existing algorithms in the literature.

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Spectral Calculations for Quasiperiodic Schrödinger Operators

David Damanik, Mark Embree, Anton Gorodetski, Serguei Tcheremchantsev

One-dimensional discrete Schrödinger operators are among the fundamental objects in mathematical physics, yet aspects of their spectral theory continue to pose significant theoretical and computational challenges. Such a bounded, self-adjoint operator H on $\ell_2(\mathbf{Z})$ can be viewed as a doubly-infinite tridiagonal matrix with ones on the super- and sub-diagonals, and the nth entry of the main diagonal given by the potential $V(n)$ for $n \in \mathbf{Z}$. When $V(n)$ is periodic, the spectrum is absolutely continuous: it is the union of closed real intervals ("bands") whose boundaries can be determined by solving finite-dimensional eigenvalue problems of dimension equal to the length of the period. At the other extreme are random potentials, which give rise to the celebrated phenomenon of *Anderson localization* and allow for almost-sure statements about the spectrum.

Between periodic and random potentials fall a variety of deterministic, non-periodic models, which are of physical interest as models of quasi-crystals. In this talk we shall focus on the quasi-periodic Fibonacci potential, given by

$$V(n) = \begin{cases} 0, & (n/\phi \bmod 1) < 1 - 1/\phi; \\ \lambda, & \text{otherwise,} \end{cases}$$

where $\phi = \frac{1}{2}(1+\sqrt{5})$ is the golden ratio and $\lambda > 0$ is fixed. It is well-known that the spectrum of this operator has zero measure and Cantor-like structure; see [1] for details.

The nature of the spectrum is of substantial physical interest, as it relates to the rate at which solutions to the dynamical system $u_t = -iHu$ spread in time given a perfectly localized initial condition, $u(0) = \delta_j$ (a vector zero everywhere except for one in the jth position). Periodic potentials lead to rapid spreading, while random potentials typically give rise to localized eigenvectors and slow spreading. Knowledge of the spectrum allows for estimates of the spreading in the quasi-periodic case.

Approximations for the Fibonacci potential obtained from the eigenvalues of finite sections of the doubly infinite matrix H provide only a coarse impression of this beautiful spectrum. Finer detail can be obtained using a procedure due to Sütő [4], whereby the quasiperiodic potential is approximated by one that is periodic, and whose spectrum thus comprises the union of finitely many real intervals bands. One might hope to use such approximations to estimate the fractal dimension of the spectrum; however, the number of bands grows combinatorially as the approximation to the potential is refined, thus posing a considerable computational obstacle.

Fortunately, a careful characterization of the manner in which the bands develop from one level of approximation to the next [3] facilitates more precise statements. In particular, we show that the number of bands obey combinatorial formulas related to the coefficients of Chebyshev polynomials; this observation, together with an understanding of the asymptotic properties of the band widths, allows for the explicit characterization of the fractal dimension of the spectrum in the large λ regime: $\dim(\sigma(H)) \log \lambda \to \log(1 + \sqrt{2})$ as $\lambda \to \infty$ [2].

In this talk we shall provide a brief survey of one-dimensional Schrödinger operators, then describe the computational challenges surrounding our calculation of the fractal dimension. Our path to this rigorous result was guided through a variety of computational tools, including MATLAB, Mathematica, the On-Line Encyclopedia of Integer Sequences [5], and finally the Inverse Symbolic Calculator [6].

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Eigenvalues of tridiagonals from triple dqds

Carla Ferreira
Beresford Parlett

We present some aspects of the real unsymmetric tridiagonal eigenproblem and our new algorithm 3dqds which uses only real arithmetic and takes three dqds steps at once. We show some interesting numerical examples.

C. Ferreira. *The Unsymmetric Tridiagonal Eigenproblem*, University of Minho, July 2007, http://hdl.handle.net/1822/6761.

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NLA techniques for efficient, reliable and asymptotically exact eigenvalue estimation

Luka Grubišić

Using the 2D Dirichlet Laplacian on (possibly) non-convex domains as a model problem, we consider an efficient and reliable assessment of finite element approximations of multiple or clustered eigenvalues and their associated invariant subspaces. Using the weakest possible regularity assumptions, we prove the equivalence of our hierarchical estimator—with explicit and reasonable constants—and the true discretization error. Furthermore, we present an abstract framework for establishing asymptotic exactness of a large class of residuum based eigenvalue/vector estimators. To demonstrate the power of our abstract approach we give an example of how to adapt our analysis of the hierarchical error estimator to considerations of estimators which are based on gradient recovery techniques. Our analysis is based on an error representation formulae which originate from Numerical Linear Algebra and we argue that this approach is natural for the error estimation problem at hand. To strengthen this argument we present numerical experiments which demonstrate the effectiveness of the derived practical procedures even on coarse meshes. *This is a joint work with Jeffrey S. Ovall.*

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A quadratic two-parameter eigenvalue problem arising from delay differential equations

Michiel Hochstenbach, Elias Jarlebring

We study critical delays for time-delay systems (differential equations with a delay): the delays for which the system has a purely imaginary eigenvalue. We show that this may lead to a new type of eigenvalue problem: a quadratic two-parameter eigenvalue problem, which combines properties of the quadratic eigenvalue problem and the linear two-parameter eigenvalue problem.

We present some properties of the problem and a subspace approach to numerically approximate critical delays for large matrices.

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Matrix analysis in stability theory

Olga Holtz

I will discuss various theoretical and algorithmic connections between the theory of stable univariate polynomials and matrix theory, including linear algebra of structured matrices, matrix functions, and the theory of moments.

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Accurate Eigenvalues of Random Matrices

Plamen Koev

While the subject of numerically computing the eigenvalues of matrices is quite mature, the problem of computing eigenvalue *distributions* of *random* matrices is still in its infancy. The problem is to compute the distributions of the eigenvalues given the distributions of the matrix entries for certain random matrix classes, e.g., Wishart, Jacobi, etc.

Somewhat surprisingly, explicit formulas for these eigenvalue distributions have been available since the 1960s, but only in terms of the *hypergeometric function of a matrix argument* – a notoriously slowly converging series of multivariate orthogonal polynomials called Jack functions. The accurate and efficient evaluation of such distributions had eluded the researchers for over 40 years even though the matrices involved are sometimes as small as 3×3.

In this talk I will present the basic ideas and connections from combinatorics, representation theory, and Fast Fourier transforms, which make the accurate and efficient eigenvalue computation possible.

The computational aspects quickly revert back to classical numerical linear algebra as one is forced to compute accurate solutions to (block) Toeplitz matrices.

Many computational problems remain open and I will present some of the ideas we have for approaching them.

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Accurate solution of eigenvalue problems in industrial life-cycle simulations

Louis Komzsik

Life-cycle simulations are important components of the virtual product development in the industry. Historically only the structural integrity of a product was the topic of computer simulations, for example the natural vibrations of the cars or airplane wings. That has changed significantly with the concept of the life-cycle simulations.

Life-cycle simulations also consider the environment the structure operates in during the products life. Some operational scenarios involve the structures rotating, containing fluid, or operating in a fluid flow. Other operational interactions are structural impacts and road excitations. The mathematical models describing the dynamic behavior of structures under these considerations involve un-symmetric and sometimes complex matrices.

These challenging simulations require very specific, robust and efficient computational solutions. These solutions, in many cases, are based on modal methods, a technology that is in its renaissance. The physical fidelity of the simulation depends on the completeness of the modal space and may be improved by various dynamic reduction techniques.

The most crucial component of modal solution methods is an accurate solution of eigenvalue problems. These problems in the industry involve very wide frequency ranges and exhibit constantly growing problem sizes. Hence the high performance of the accurate solution is of utmost significance, and to achieve this, industrial solutions undergo a constant evolution.

The presentation will briefly review lifecycle simulations and the role of accurate eigenvalue computations therein. The evolution of eigenvalue solutions in the past three decades of the industry will be demonstrated with problem and solution statistics. The current state of the art industrial solutions of NASTRAN will also be discussed. The presentation will conclude with future requirements and directions.

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Relative Perturbations for s.d.d. Matrices with Applications

Josip Matejaš
Vjeran Hari

Improved relative perturbation bounds for the eigenvalues of scaled diagonally dominant Hermitian matrices and new bounds for the singular values of the symmetrically scaled diagonally dominant square matrices are derived. In the case of definite Hermitian matrices, the new result reduces to the existing one. The result extends to some other classes of scaled diagonally dominant matrices, like skew-Hermitian and "hidden Hermitian" matrices. Using the standard technique with the Wielandt matrix one obtains an appropriate result for the singular values.

A new relative perturbation result for the singular values of a square, symmetrically scaled matrix, which uses the scaled polar factors in the bound, is also presented.

The new results are used to prove the relative accuracy of the standard two-sided Jacobi method on scaled diagonally dominant indefinite Hermitian matrices and also of the Kogbetliantz method for computing the singular value decomposition of triangular matrices. Using a subtle error analysis, very sharp eigenvalue perturbation bounds coming from a single Jacobi step and from a whole Jacobi sweep are derived. As for the Kogbetliantz method, the standard Voevodin formulas for computing the SVD of 2×2 triangular matrices are modified to define a relatively accurate algorithm. Using a subtle error analysis, the appropriate error bounds are derived, which compare favorably to the bounds for the existing *LAEV2 routine from LAPACK, which are also obtained by the same analysis.

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Numerical solution of eigenvalue problems from acoustic field computations

Volker Mehrmann

We present numerical methods for the solution of large scale structured nonlinear eigenvalue problems arising in the context of acoustic field computations in car interiors.

These eigenvalue problems are very ill-conditioned and badly scaled as well. We discuss different numerical solution techniques and their advantages and disadvantages.

We show some real world applications form the project with our industrial partner and present numerical examples.

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On Spectral Bipartite Clustering Algorithm and Automatic Determination of the Number of Clusters

Ivančica Mirošević
Nevena Jakovčević Stor

The main idea of spectral clustering is in modeling of a data set in a form of a simple undirected weighted graph, and observing the graph Laplacian spectrum. Usually, data partition can be reconstructed from dominant eigenvectors.

We introduce several heuristic algorithms for accurate determination of number of clusters. The algorithms are based on properties of coupling matrix introduced in [1]. In this presentation we give several examples of datasets sucessfully clustered by our algorithms, both artificial and real-world ones.

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Numerical Method for Two-Parameter Quadratic Polynomial Eigenvalue Problems

Andrej Muhič
Bor Plestenjak

We consider the *quadratic two-parameter eigenvalue problem*

$$\begin{aligned}(A_1+\lambda B_1+\mu C_1+\lambda^2 D_1+\lambda\mu E_1+\mu^2 F_1)x &= 0\\ (A_2+\lambda B_2+\mu C_2+\lambda^2 D_2+\lambda\mu E_2+\mu^2 F_2)y &= 0,\end{aligned} \tag{1}$$

where $A_i, B_i, \ldots, F_i$ are given $n_i \times n_i$ complex matrices, $x \in \mathbf{C}^{n_1}$, $y \in \mathbf{C}^{n_2}$ nonzero vectors and $\lambda, \mu \in \mathbf{C}$. We say that (λ, μ) is an eigenvalue of (1) and the tensor product $x \otimes y$ is the corresponding eigenvector. In the generic case problem (1) has $4n_1n_2$ eigenvalues.

Linearizing (1) we obtain the *two-parameter eigenvalue problem*

$$\begin{aligned}&\left(\overbrace{\begin{bmatrix}A_1 & B_1 & C_1\\ 0 & I & 0\\ 0 & 0 & I\end{bmatrix}}^{A^{(1)}}+\lambda\overbrace{\begin{bmatrix}0 & D_1 & \frac{1}{2}E_1\\ -I & 0 & 0\\ 0 & 0 & 0\end{bmatrix}}^{B^{(1)}}+\mu\overbrace{\begin{bmatrix}0 & \frac{1}{2}E_1 & F_1\\ 0 & 0 & 0\\ -I & 0 & 0\end{bmatrix}}^{C^{(1)}}\right)\overbrace{\begin{bmatrix}x\\ \lambda x\\ \mu x\end{bmatrix}}^{w_1} = 0\\ &\left(\overbrace{\begin{bmatrix}A_2 & B_2 & C_2\\ 0 & I & 0\\ 0 & 0 & I\end{bmatrix}}^{A^{(2)}}+\lambda\overbrace{\begin{bmatrix}0 & D_2 & \frac{1}{2}E_2\\ -I & 0 & 0\\ 0 & 0 & 0\end{bmatrix}}^{B^{(2)}}+\mu\overbrace{\begin{bmatrix}0 & \frac{1}{2}E_2 & F_2\\ 0 & 0 & 0\\ -I & 0 & 0\end{bmatrix}}^{C^{(2)}}\right)\overbrace{\begin{bmatrix}y\\ \lambda y\\ \mu y\end{bmatrix}}^{w_2} = 0,\end{aligned} \tag{2}$$

where matrices $A^{(i)}, B^{(i)}$, and $C^{(i)}$ are of size $3n_i \times 3n_i$.

The usual approach for two-parameter eigenvalue problems of type

$$\begin{aligned}\left(A^{(1)}+\lambda B^{(1)}+\mu C^{(1)}\right)w_1 &= 0\\ \left(A^{(2)}+\lambda B^{(2)}+\mu C^{(2)}\right)w_2 &= 0\end{aligned} \tag{3}$$

is to define *operator determinants*

$$\begin{aligned}\Delta_0 &= B^{(1)}\otimes C^{(2)} - C^{(1)}\otimes B^{(2)},\\ \Delta_1 &= C^{(1)}\otimes A^{(2)} - A^{(1)}\otimes C^{(2)},\\ \Delta_2 &= A^{(1)}\otimes B^{(2)} - B^{(1)}\otimes A^{(2)}\end{aligned}$$

on the tensor product space $\mathbf{C}^{3n_1} \otimes \mathbf{C}^{3n_2}$ and consider the *coupled generalized eigenvalue problem*

$$\begin{aligned} \Delta_1 z &= \lambda \Delta_0 z \\ \Delta_2 z &= \mu \Delta_0 z, \end{aligned} \tag{4}$$

where $z = w_1 \otimes w_2$.

If $A^{(i)}, B^{(i)}$, and $C^{(i)}$ are generic matrices of size $3n_i \times 3n_i$ for $i = 1, 2$, then Δ_0 is nonsingular. In such case we say that (3) is a nonsingular two-parameter eigenvalue problem. From well known results for nonsingular two-parameter eigenvalues problems [1] it follows that matrices $\Delta_0^{-1}\Delta_1$ and $\Delta_0^{-1}\Delta_2$ commute, and that problem (3) has $9n_1n_2$ eigenvalues (λ, μ) that can be computed from eigenvalues of $\Delta_0^{-1}\Delta_1$ and $\Delta_0^{-1}\Delta_2$.

In our case, where $A^{(i)}, B^{(i)}$, and $C^{(i)}$ are from linearization (2), Δ_0 is singular and (3) is a *singular two-parameter eigenvalue problem*. The theory for singular two-parameter eigenvalue problems is scarce and there are no general results linking eigenvalues of (3) to eigenvalues of (4). For the particular case (2) we are able to prove that eigenvalues of (1) are contained in the common regular part of pencils $\Delta_1 - \lambda\Delta_0$ and $\Delta_2 - \mu\Delta_0$. As we can also show that the regular part of each of the pencils $\Delta_1 - \lambda\Delta_0$ and $\Delta_2 - \mu\Delta_0$ is of size $4n_1n_2$, it turns out that the eigenvalues of (1) are exactly the regular eigenvalues of (4).

In order to solve the singular two-parameter eigenvalue problem we derive an algorithm for the extraction of the common regular part of two matrix pencils. Motivation for the algorithm can be found in [2]. In our case, the algorithm returns matrices Q and U with orthonormal columns that define matrices $\widetilde{\Delta_i} = Q^H \Delta_i U$ of size $4n_1n_2 \times 4n_1n_2$ for $i = 0, 1, 2$, such that $\widetilde{\Delta_0}$ is nonsingular, matrices $\widetilde{\Delta_0}^{-1}\widetilde{\Delta_1}$ and $\widetilde{\Delta_0}^{-1}\widetilde{\Delta_2}$ commute, and the eigenvalues of the quadratic two-parameter eigenvalue problem (1) are exactly the eigenvalues of the projected pencils $\widetilde{\Delta_1} - \lambda\widetilde{\Delta_0}$ and $\widetilde{\Delta_2} - \mu\widetilde{\Delta_0}$.

We were able to apply this algorithm to some other singular two-parameter eigenvalue problems as well, for example to the polynomial two-parameter eigenvalue problem or to problems that appear in model updating.

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The Envelope Method for computing orthogonal eigenvectors belonging to isolated clusters of very close eigenvalues of a symmetric tridiagonal matrix

Beresford Parlett

There is structure in the invariant subspace for a cluster of close eigenvalues that is well separated from the rest of the spectrum. This structure is captured by the cluster's "envelope" which reveals a distinguished sparse basis which, in turn, permits the rapid calculation of both eigenvectors and eigenvalues. Recently we found an inexpensive way to obtain an adequate approximation of this envelope whose justification rests on a simple result that is a complement to Gersgorin's circle theorem.

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Do we need yet another Code for Symmetric Tridiagonals?

Rui Ralha
Carlos Campos

We will give examples of indefinite symmetric tridiagonal matrices which define well their eigenvalues and for which the unique LAPACK code that delivers highly accurate results is DSTEBZ. This routine uses bisection to compute eigenvalues with prescribed accuracy. The bisection method is able to guarantee approximations which are the exact eigenvalues of a matrix which differs from the original one by small relative perturbations in the off-diagonal entries.

Furthermore, the bisection method adapts well to the mixed precision paradigm. This new paradigm is triggered by the arrival to the market of processors that are much faster in single precision than they are in double precision. For example, on the Intel's Pentium IV, floating point operations can be performed up to two times faster in single precision, as compared to double precision, and on the IBM's Cell Broad Engine processor this ratio goes up to ten [1].

A critical issue in the design of a mixed precision bisection algorithm is a good criteria for switching from single to double precision. Perturbation theory of the eigenvalues is at the center of this topic. We will present some results (initiated in [2]) to tackle this problem in the case of matrices with entries and eigenvalues of different orders of magnitude. For these matrices, we also demonstrate the advantages of using, in a combined way, the three pythagorean means to compute iteration points.

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Computing Smallest and Interior Eigenvalues in SLEPc

Jose E. Roman

SLEPc, the Scalable Library for Eigenvalue Problem Computations [1], is a software library for the solution of large, sparse eigenvalue problems on parallel computers. It can be used for the solution of problems formulated in either standard or generalized form, both Hermitian and non-Hermitian, with either real or complex arithmetic, as well as other related problems such as the singular value decomposition (SVD). SLEPc is built on top of PETSc [2], and extends it with all the functionality necessary for the solution of eigenvalue problems. It is publicly available and used in many applications around the world.

The current version provides the following eigensolvers:

- Krylov-Schur (the default).
- Explicitly restarted Arnoldi and Lanczos.
- Subspace iteration and Power/RQI iteration.
- Seamlessly integrated third-party software, including ARPACK, PRIMME, and BLOPEX.

In addition, SLEPc provides built-in support for different types of problems and spectral transformations such as shift-and-invert or Cayley transform. For solving the associated linear systems, the user can select from many different direct and iterative solvers and preconditioners, provided by PETSc.

A partial SVD of a rectangular matrix can be computed either by making use of one of the above eigensolvers or via specific solvers such as restarted Lanczos bidiagonalization.

Although SLEPc is being successfully used in many application areas, it still has important limitations. The most remarkable one is arguably the difficulty of computing eigenvalues (or singular values) that have smallest magnitude or are located in the interior of the spectrum. In this talk, we will discuss SLEPc's current ability to handle these cases, as well as ongoing developments for improving the functionality. These developments are based on the well-established concepts of harmonic projection [3] and refined extraction [4]. We analyze how these techniques fit in the different available eigensolvers and SVD solvers, and illustrate the performance with a set of test cases.

Finally, we mention preliminary work related to preconditioned eigensolvers in SLEPc, as well as other potential research lines for the future.

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An Inner/Outer Loop Free Parallel Method for Interior Eigenvalue Problems

Tetsuya Sakurai
Hiroto Tadano

We present a method for finding a limited set of eigenpairs in a given domain of the generalized eigenvalue problem $A\boldsymbol{x} = \lambda B\boldsymbol{x}$, where A is real symmetric, and B is symmetric positive definite. When matrices A and B are large-scale and sparse, iterative methods are often employed. Most of iterative subspace methods require two nested loops, an inner loop to construct an approximate subspace, and an outer loop to update approximate eigenvectors. Since these loops are recurrently repeated, the parallel performance is limited.

Our method is based on contour integral presented in [2]. The major advantage of this method is that the iterative processes for constructing subspaces and updating approximate eigenvectors are not required. We recently proposed a Rayleigh-Ritz type method[3] and a block variant of the method[1] in order to improve numerical stability.

The numerical accuracy of the presented method depends on some parameters, i.e. the dimension of the projected pencil, the number of nodes for numerical integration, and the block size. In this paper, we discuss the influence of these parameters, and show some numerical properties of the method. The computation at each contour involves linear system solutions where the coefficient matrices are derived from A and B. These systems can be solved independently, allowing a variety of parallel programming model. Some experimental results applied for large-scale molecular orbital computations in a parallel computing environment are also included.

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Parallel Implementations of the One–Sided Indefinite Block Jacobi Methods

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The indefinite one-sided Jacobi algorithm for computing the hyperbolic singular value decomposition of a rectangular matrix is known to be accurate in the relative sense. However, it is far too slow for serial computation, when compared with some other accurate algorithms. On the other hand, Jacobi-type methods are considered to be ideal for parallelization, when properly implemented to achieve data independency that is required by simple models of parallel computing.

Modern computer clusters have a more complex architecture than such simple models. This is due to a multi-level memory hierarchy, which includes a local cache memory inside each cluster member.

This memory hierarchy structure can be efficiently exploited by blocking of the algorithm. First, we describe two different approaches for obtaining block generalizations of the simple indefinite Jacobi algorithm: a *block oriented* and a *full block* approach.

Then we construct a parallel, locally fast Jacobi algorithm which respects a three-level memory hierarchy consisting of: distant data, locally stored data, and local cache memory. This is done by using two levels of blocking:

- The "outer" level of blocking uses the modulus block strategy for data independence to achieve proper load balancing between different processors.
- The "inner" level of blocking uses the cyclic block strategy to reuse data that is already in the local cache memory of each processor.

Since both of the above approaches can be used for blocking at each level, we obtain many variants of the algorithm.

We will also describe various implementation details that affect the speedup, and present a series of numerical results that show an almost ideal speedup of properly implemented versions of the indefinite block Jacobi algorithm.

Finally, it can be shown that all proposed block modifications preserve the relative accuracy of the original unblocked algorithm. With regards to theory, the work in progress includes proving the global convergence for some important variants, and block partitioning that ensures the asymptotic quadratic convergence.

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Fast computation of QR factorisation and eigenvalue decomposition via one-sided plane rotations

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By using one-sided Givens rotations and adequate block strategy in choosing pivot elements, it is possible to attain the speed comparable to the LAPACK implementation of the QR factorisation which uses BLAS 3 routines. The advantage of the new approach is simpler implementation. Similar approach also gives very good results in computing eigenvalues and eigenvectors of symmteric matrices, where one-sided Jacobi-type rotations are applied to a symmetric factorization obtained in double of the working precision.

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A Quadratically Constrained Eigenvalue Minimization Problem Arising from PDE of Monge-Ampère Type

D.C. Sorensen
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This talk concerns the development and analysis of a solution technique for a quadratically constrained eigenvalue minimization problem. This class of problems arises in the numerical solution of fully-nonlinear boundary value problems of Monge-Ampère type. Though it is most important in the three dimensional case, the solution method is directly applicable to systems of arbitrary dimension.

The focus here shall be on solving the minimization subproblem which is part of a methodology to numerically solve a Monge-Ampère type equation. These subproblems must be evaluated many times in this numerical solution technique and thus efficiency is of utmost importance.

A novelty of the minimization algorithm is that the method is finite with the exception of solving a very simple rational function of one variable. This function is essentially the same for any dimension. This result is quite surprising given the nature of the minimization problem.

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On B-Orthogonalization

G. W. Stewart

Orthogonalization in the inner product generated by a positive definite matrix B is used in some algorithms for solving the generalized eigenvalue problem $Ax = \lambda Bx$. This talk (which reports ongoing research) will consider three related topics. First, given a projector P, we characterize the positive definite matrices B whose inner product generates P. Second, we present a rounding error analysis of the B-Gram–Schmidt step in which a vector x is B-orthogonalized against a B-orthonormal matrix U. The error is shown to depend primarily on the spectral norm of U. Finally, we consider the problem of semi-definite B. The problem here is that the B-Gram–Schmidt step cannot purge vectors in the null space of B. For ordinary B-orthogonalization, this appears not to be a serious problem. When it is a Krylov sequence that is being B-orthogonalized, however, the null space errors can grow dramatically. Reasons are given for believing that this phenomenon is associated with the convergence or Ritz vectors.

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Modal approximation to linear damped systems

Krešimir Veselić

Proportional and modal damping is a common approximation when dealimg with damped linear systems. Practitioners often leave aside the assessment of it, while it is known that it may lead to catastophically false predictions. We study these approximations by means of the perturbation theory. The results give rigorous meaning to some known asymptotic estimates.

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Quasi-Minimal Residual Eigenpairs

Jens-Peter M. Zemke

We motivate a new type of eigenpair extraction from a Krylov subspace entitled quasi-minimal residual eigenpairs (QMR eigenpairs). This approach is obtained by extending the quasi-minimal residual approach of Roland Freund et al. for the approximation of the solution of a linear system using Krylov subspace methods to eigenpair approximation. The defining relation for a *QMR eigenpair* $(\grave{\theta}, \grave{v})$, where $\grave{\theta} \in \mathbf{C}$ is called a *QMR eigenvalue* and $\grave{v} \in \mathbf{C}^k$ is called a *QMR eigenvector*, is

$$\frac{\|(\grave{\theta}\underline{I}_k - \underline{C}_k)\grave{v}\|}{\|\grave{v}\|} = \min_{z\in\mathbf{C}, v\in\mathbf{C}^k} \frac{\|(z\underline{I}_k - \underline{C}_k)v\|}{\|v\|}. \tag{5}$$

Here, $\mathbf{C}$ denotes the field of complex numbers, $\underline{I}_k$ is a $k+1$ by k identity matrix, $\underline{C}_k$ is an unreduced extended $k+1$ by k Hessenberg matrix, and the minimization is a local minimization with respect to both parameters. The relation (5) appears in several contexts, some of them fairly new and still developing.

By analyzing relation (5), we extend the work of N. J. Lehmann on optimal eigenvalue inclusions to general complex square matrices, the price to pay is the replacement of the forward error bounds directly related to the accuracy of the eigenvalues by backward error bounds. Whereas Lehmann was interested in theoretical bounds, we shift the focus to the numerical computation of "best" or "optimal" bounds.

Our results and the connections to various other eigenpair extraction methods used in the Krylov subspace method setting, e.g., Ritz-Galërkin, shifted harmonic Ritz, ρ-values, and Jia's refinement of approximate eigenvectors are described. The links between these methods are used to highlight certain peculiar assets and drawbacks of particular methods. These theoretical aspects are linked to easy-to-understand pictures capturing the main information, which are suitable for a classroom introduction of eigenpair extraction based on Krylov subspace methods.

The theory behind QMR eigenpairs roots in Grassmannian optimization, minimization of real-analytic complex functions including Wirtinger derivatives, and complex SVD perturbation theory, which is related to the non-analytic perturbation theory of Hermitean matrices. There are intimate connections to pseudospectra, eigenvalues of rectangular matrices and rectangular pencils, and the distance of a controllable pair of matrices to the nearest uncontrollable pair.

We give a few examples that are intended to highlight some more or less surprising aspects of the QMR eigenvalues (and eigenvectors), many of them already noted in other related contexts.

A special example is the analytic solution of the QMR eigenproblem for an extended Jordan block, which is related to the distinct properties of finite and infinite Toeplitz operators, the field of values of a Jordan block, and to the distance to uncontrollability.

We state a few of the many possible algorithms and briefly compare the accuracy and speed of the computations when carried out in IEEE 754 arithmetic using known building blocks, e.g., BLAS and LAPACK. Our main aim is to work out the relations between the choice of the extraction method and the applications.

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