

BOOK OF ABSTRACT

IWASEP 8

8th International Workshop on Accurate Solution of Eigenvalue Problems

Berlin, June 28 – July 1, 2010

Organizers:

Jesse Barlow, Zlatko Drmač, Volker Mehrmann (Chair),
Ivan Slapničar, Kresimir Veselić

Local Organizing Committee:

Michael Karow, Christian Mehl, Volker Mehrmann

	Monday	Tuesday	Wednesday	Thursday
	MA 043	MA 043	MA 042	MA 043
8:45-9:00	Opening	————	————	————
9:00-9:25	Demmel	Lin	Tyrtysnikov	Alam
9:25-9:50				
9:50-10:15	Zemke	Watkins	Wachsmuth	Bora

C O F F E E B R E A K

	MA 043	MA 043	MA 042	MA 043
10:45-11:10	Stewart	Komzsik	Moro	Karow
11:10-11:35				Brüll
11:35-12:00	Hochstenbach	Howell	Mengi	Jarlebring

L U N C H B R E A K

	MA 043	MA 043	E X - C U R - S I O N	MA 042
14:00-14:25	Benner	Simoncini		Van Barel
14:25-14:50				Trefethen
14:50-15:15	Parlett	Beyn		C O F F E E
15:15-15:40	Drmač	Miedlar		
C O F F E E B R E A K				
	MA 043	MA 043		
16:10-16:35	Barlow	Subramanian		
16:35-17:00	Muhič	Tomljanović		
17:00-17:25	Ralha	Dax		
17:25-17:50	Molera	Grinfeld		
17:50-18:15	Poster Session in MA 313	Heuveline		
18:15-18:40		————		

19:00-22:00

Conference Dinner

Posters are presented by: Hari, Kürschner, Löchel, Mach, Singer, Slapničar, Veselić, Voigt

The conference dinner will take place in Café Campus behind the Mathematics Building on the campus of TU Berlin.

Rafikul Alam
Department of Mathematics
Indian Institute of Technology Guwahati
Guwahati-781 039
INDIA

rafikiitg.ernet.in
www.iitg.ernet.in/math

Sensitivity and Perturbation analysis of Polynomial Eigenvalue problem

Rafikul Alam

We discuss a general framework for sensitivity and perturbation analysis of polynomial eigenvalue problem. More specifically, we discuss first order variations of simple eigenvalues of matrix polynomials, determine the gradients and present a general definition of condition number of a simple eigenvalue. We show that our treatment unifies various condition numbers of simple eigenvalues of matrix pencils and matrix polynomials proposed in the literature. We present an alternative expression of condition number of a simple eigenvalue that does not involve left and right eigenvectors associated with the eigenvalue. We show that the sensitivity of a simple eigenvalue is inversely proportional to the absolute value of the derivative of the characteristic polynomial at the eigenvalue. We also construct fast perturbations for moving simple eigenvalues of matrix polynomials and discuss perturbation bounds for approximate eigenvalues.

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Jesse Barlow
 Department of Computer Science and Engi-
 neering
 The Pennsylvania State University
 University Park, PA
 16802-6822 USA

barlow@cse.psu.edu
 www.cse.psu.edu/~barlow

The Impact of Reorthogonalization in the Golub–Kahan–Lanczos Bidiagonal Reduction

Jesse L. Barlow

The Golub–Kahan–Lanczos bidiagonal reduction generates a factorization of a matrix $X \in \mathbf{R}^{m \times n}$, $m \geq n$, such that

$$X = UBV^T$$

where $U \in \mathbf{R}^{m \times n}$ is left orthogonal, $V \in \mathbf{R}^{n \times n}$ is orthogonal, and $B \in \mathbf{R}^{n \times n}$ is bidiagonal. Since, in the Lanczos recurrence, the columns of U and V tend to lose orthogonality, a reorthogonalization strategy is necessary to preserve convergence of the singular values of the leading $k \times k$ submatrix $B_k = B(1:k, 1:k)$ to those of B . the computation of matrix functions, it is essential

It is shown that if

$$\text{orth}(V) = \|I - V^T V\|_2,$$

then the singular values of B and those of X satisfy

$$\left(\sum_{j=1}^n (\sigma_j(X) - \sigma_j(B))^2 \right)^{1/2} \leq \mathcal{O}(\varepsilon_M + \text{orth}(V)) \|X\|_2$$

where ε_M is machine precision.

Also, a new approach to computing the left singular vectors is introduced resulting in two improvements to the algorithm. The first is that the computed left and right singular vectors satisfy smaller residual bounds than previous implementations of Lanczos bidiagonalization. The second is that if

$$\Theta_j = \text{diag}(\theta_1, \dots, \theta_j)$$

are the leading j singular values of B_k , then the corresponding approximate left singular vectors of X in the matrix P_j satisfy

$$\|I - P_j^T P_j\|_F \leq \mathcal{O}([\varepsilon_M + \text{orth}(V)] \|X\|_2 / \theta_j]^2).$$

These are stronger than previous published results for any version of the Lanczos bidiagonalization algorithm. Thus regulation of the orthogonality of the columns of V , even if there is no attempt to reorthogonalize the columns of U , serves to preserve accuracy in the singular values, orthogonality in the leading approximate left singular vectors, and smaller residual bounds for computed singular triplets.

Peter Benner
TU Chemnitz
Fakultät für Mathematik
D-09107 Chemnitz
Germany

benner@mathematik.tu-chemnitz.de
<http://www-user.tu-chemnitz.de/~benner/>

Moving the Frontiers in Model Reduction Using Numerical Linear Algebra Peter Benner

Model reduction has become an ubiquitous tool in numerous areas of engineering and the sciences, including analysis and simulation of dynamical systems, control design, circuit simulation, structural dynamics, CFD, process engineering, systems biology, computational electromagnetics, etc. In the past decades many approaches have been developed for reducing the order of a given dynamical system. We will describe how two main approaches in this area have been inspired or pushed forward by Numerical Linear Algebra in a way believed to be impossible just a few years ago. We will see that the system-theoretic method of balanced truncation, believed to be applicable only to small systems with several hundreds of degrees of freedom, can now be applied to linear systems with state-space dimensions in the millions. We will also demonstrate how Krylov subspace methods are now able to reduce certain nonlinear systems so that important features of dynamical systems like limit cycles can be recovered from the reduced-order model. The performance of the discussed approaches will be demonstrated using real-world examples from several disciplines.

Acknowledgements. This work is based on the results of several of my Ph.D. students, including (in alphabetical order) Ulrike Baur, Tobias Breiten, Jens Saak, André Schneider. The work has been supported by grants of the *Deutsche Forschungsgemeinschaft* as well as the German Federal Ministry of Education and Research (BMBF).

Wolf-Juergen Beyn
Department of Mathematics
Bielefeld University
Postfach 100131
33501 Bielefeld

beyn@math.uni-bielefeld.de

An Integral Method for Solving Nonlinear Eigenvalue Problems

Wolf-Juergen Beyn

We propose a numerical method for computing all eigenvalues (and the corresponding eigenvectors) of a nonlinear holomorphic eigenvalue problem that lie within a given contour in the complex plane. The method uses complex integrals of the resolvent operator, applied to at least k column vectors, where k is the number of eigenvalues inside the contour. The theorem of Keldysh is employed to show that the original nonlinear eigenvalue problem reduces to a linear eigenvalue problem of dimension k . No initial approximations of eigenvalues and eigenvectors are needed. The method is particularly suitable for moderately large eigenvalue problems where k is much smaller than the matrix dimension. We also give an extension of the method to the case where k is larger than the matrix dimension. The quadrature errors caused by the trapezoid sum are discussed for the case of analytic closed contours. Using well known techniques it is shown that the error decays exponentially with an exponent given by the product of the number of quadrature points and the minimal distance of the eigenvalues to the contour.

Shreemayee Bora
Department of Mathematics
Indian Institute of Technology Guwahati
Guwahati 781039, Assam, INDIA

shbora@iitg.ac.in
www.iitg.ernet.in/shbora

Nearest Defective Matrices and Geometry of ϵ -Pseudospectra

Shreemayee Bora
Rafikul Alam
Ralph Byers
Michael L. Overton

Given a n -by- n matrix A with distinct eigenvalues, the distance $w(A)$ with respect to the 2-norm to the nearest matrix with multiple eigenvalues was established to be the smallest value ϵ_0 of ϵ for which the 2-norm ϵ -pseudospectrum $\Lambda_\epsilon(A)$ of A has less than n components in [1]. The same work also constructed a matrix B with multiple eigenvalues which attains this distance. From these results it followed that B is also a nearest defective matrix to A in both the 2 and Frobenius norms provided the smallest singular value $\sigma_n(A - z_0I)$ of $A - z_0I$ at a point of coalescence z_0 of two components of $\Lambda_{\epsilon_0}(A)$ is simple. We extend this work to show that there exist defective matrices that attain the distance even if $\sigma_n(A - z_0I)$ is multiple.

One of the key results is that if $\sigma_n(A - z_0I)$ is multiple and z_0 is the common limit of sequences $\{\hat{z}_k\}$ and $\{\tilde{z}_k\}$ from the coalescing components $\Delta_1(\epsilon_0)$ and $\Delta_2(\epsilon_0)$ of $\Lambda_{\epsilon_0}(A)$ respectively along analytic paths, then the corresponding sequences of left and right singular vectors $\{\hat{u}_k\}, \{\hat{v}_k\}, \{\tilde{u}_k\}$ and $\{\tilde{v}_k\}$ satisfying

$$(A - \hat{z}_kI)\hat{v}_k = \sigma_n(A - \hat{z}_kI)\hat{u}_k, (A - \tilde{z}_kI)\tilde{v}_k = \sigma_n(A - \tilde{z}_kI)\tilde{u}_k$$

have limiting vectors $\lim_{k \rightarrow \infty} \hat{v}_k = \hat{v}$, $\lim_{k \rightarrow \infty} \hat{u}_k = \hat{u}$, $\lim_{k \rightarrow \infty} \tilde{v}_k = \tilde{v}$, $\lim_{k \rightarrow \infty} \tilde{u}_k = \tilde{u}$ for which $u^*v = 0$ where $u = c\hat{u} + s\hat{v}$ and $v = c\tilde{u} + s\tilde{v}$ for complex numbers c and s satisfying $|c|^2 + |s|^2 = 1$.

The local geometry of the ϵ -pseudospectrum at coalescence points plays a crucial role in the solution of the distance problem. Our approach generalizes the notion of saddle points to establish that z_0 is a lowest saddle point of the minimum singular value function $f(z) = \sigma_n(A - zI)$ even if f is not differentiable at z_0 . The results lead to a better understanding of the geometry of the pseudospectra surface in the neighbourhood of z_0 and brings up some interesting open problems.

Computing the distance to the nearest matrix with a multiple eigenvalue has been the topic of recent work done in [3] and [4]. Among these, the latter is based on the result in [1]. We briefly outline an algorithm based on our results which computes the distance to a nearest defective matrix and produces a nearest defective matrix which attains this distance.

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Tobias Brüll
Technische Universität Berlin
Sekretariat MA 4-5
Straße des 17. Juni 136
D-10623 Berlin

bruell@math.tu-berlin.de
<http://www.math.tu-berlin.de/~bruell/>

Passivation of Linear Systems through Perturbation of para-Hermitian Matrix Pencils
Tobias Brüll

We will briefly look at some results that link certain problems in linear-quadratic control theory to a special para-Hermitian matrix polynomial N . The spectrum of para-Hermitian matrix polynomials is symmetric with respect to the imaginary axis.

From this we will suggest that a (close to) minimal perturbation, which makes a linear system passive (or more general, dissipative) can be obtained by perturbing all purely imaginary eigenvalues of N away from the imaginary axis.

An algorithm will be presented to efficiently compute a (close to) minimal perturbation of a first-order para-Hermitian matrix polynomial. This algorithm works by turning the original problem into a Hamiltonian eigenvalue problem.

Achiya Dax
Hydrological Service, P.O.B. 36118,
Jerusalem 91360, ISRAEL

dax20@water.gov.il

Orthogonalization via Deflation: The use of Lanczos methods
Achiya Dax

Orthogonalization via Deflation is a new orthogonalization method. Given a real $m \times n$ matrix A , the new method constructs an SVD-type decomposition of the form $A = U\Sigma V^T$. The columns of U and V are orthogonal, or nearly orthogonal, while Σ is a diagonal matrix whose diagonal entries approximate the singular values of A . The method has three versions. In “left-side” orthogonalization the columns of U constitute an orthonormal basis of $\text{Range}(A)$. In “right-side” orthogonalization the columns of V constitute an orthonormal basis of $\text{Range}(A^T)$. In the third version both U and V have orthonormal columns, but the decomposition is not exact. Starting from $A_1 = A$ the deflation process generates a sequence of matrices A_1, A_2, A_3, \dots , by the rule

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

where $\{\sigma_k, \mathbf{u}_k, \mathbf{v}_k\}$ denotes a computed estimate of a dominant singular triplet of A_k . The matrix

$$B_k = \sum_{i=1}^k \sigma_i \mathbf{u}_i (\mathbf{v}_i)^T$$

serves as a low-rank approximation of A . In this talk we consider the use of Lanczos methods for calculating a dominant singular vector of A_k . One advantage of this approach is that the second Ritz vector provides a good starting point for the Lanczos process on A_{k+1} .

James Demmel
Computer Science Division
University of California
Berkeley, CA 94720

demmel@cs.berkeley.edu
www.cs.berkeley.edu/~demmel

Minimizing Communication in Linear Algebra

James Demmel

Algorithms have two kinds of costs: arithmetic and communication, by which we mean moving data either between levels of a memory hierarchy (in the sequential case) or between processors over a network (in the parallel case). Communication costs can already exceed arithmetic costs by orders of magnitude, and the gap is growing exponentially over time, so our goal is to design linear algebra algorithms that minimize communication. First, we show how to extend known communication lower bounds for $O(n^3)$ dense matrix multiplication to all direct linear algebra, i.e. for solving linear systems, least squares problems, eigenproblems and the SVD, for dense or sparse matrices, and for sequential or parallel machines. We also describe dense algorithms that attain these lower bounds; some implementations attain large speed ups over conventional algorithms. Second, we show how to minimize communication in Krylov-subspace methods for solving sparse linear system and eigenproblems, and again demonstrate new algorithms with significant speedups.

A global convergence proof for cyclic Jacobi methods with block rotations
Zlatko Drmač

We present a globally convergent block (column- and row-) cyclic Jacobi method for diagonalization of Hermitian matrices and for computation of the singular value decomposition of general matrices. It is shown that a block rotation (generalization of the Jacobi's 2×2 rotation) can be computed and implemented in a particular way to guarantee global convergence. The proof includes the convergence of the eigenspaces in the general case of multiple eigenvalues. This solves a long standing open problem of convergence of block cyclic Jacobi methods.

Our approach is based on a new class of unitary block-transformations and on a novel technique to study the convergence to a diagonal matrix in a framework of the polyhedral set of all diagonals of the matrices from the adjoint orbit of the given Hermitian H . The proof of global convergence covers the general case of multiple eigenvalues, including the convergence of eigenvectors and eigenspaces, and it is, to our best knowledge, the first result of this kind in the theory of Jacobi methods. The convergence of the eigenspaces is obtained from a Grassmann manifold setting, by using perturbation theory, in particular, the $\sin \Theta$ theorem.

Other important issues will be addressed, in particular how to ensure numerical convergence, how to apply the block-transformations efficiently, and how to preserve the superior numerical accuracy of the Jacobi method. We give a theoretical framework for provable accuracy of block methods (in the case of positive definite H , and for the SVD computation) and discuss some problems that indicate a need for further research.

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Pavel Grinfeld
Drexel University

pg@freeboundaries.com
<http://www.math.drexel.edu/~pg/>

The Calculus of Moving Surfaces and Solution of Near-Symmetrical Eigenvalue Problems

Pavel Grinfeld

The calculus of moving surfaces (CMS) is a powerful technique for analyzing boundary variation problems. The pioneering work belongs to J. Hadamard who discovered the equation for the first order correction of the Laplace and biharmonic eigenvalues with respect to change in shape. Our goal is to generalize Hadamard's analysis to higher orders. We introduce the key elements of the CMS with an eye towards boundary variations of spectral problems. We show how to obtain highly accurate eigenvalues for near-spherical and other near-symmetrical shapes. In particular, we give the first few terms of the series for the eigenvalues of a low-eccentricity ellipse and for a regular polygon with a large number of sides.

Vjeran Hari
Department of Mathematics
University of Zagreb
Bijenička cesta 30
10000 Zagreb
Croatia

hari@math.hr

On Block J -Jacobi Methods

Vjeran Hari, Sanja Singer, Saša Singer

We consider two ways how to make the J -Jacobi method of Veselić an efficient BLAS3 method. The J -Jacobi method solves the definite eigenproblem $Ax = \lambda Jx$, where A is Hermitian and J is the matrix of signs, usually in the form $J = \text{diag}(I_\nu, -I_{n-\nu})$. The most important application of the method is to serve as the second part of the compound method for accurate solving the Hermitian eigenproblem $Hx = \lambda x$, with indefinite H . After the Bunch–Parlett like decomposition of H , $H = GJG^*$, one defines $A = G^*G$ and probably the best way to solve the eigenproblem for (A, J) is to compute the hyperbolic SVD of G , $G = U\Sigma V^{-1}$ with J -unitary V . An efficient and accurate eigensolver for this problem is the one-sided version of the J -Jacobi method. We have modified that method to become a “block-oriented” or a “full-block” method.

In the first approach the algorithm only partially diagonalizes each block-pivot submatrix. We consider the case when at each block step k , only one sweep of simple J -unitary rotations is applied to the pivot block $A_{ij}^{(k)}$ in the row-or column-wise fashion. The pivot blocks are chosen according to three classes of pivot strategies. The first class consists of the wavefront cyclic strategies which includes all strategies which are equivalent to the serial strategies. The second and third classes are the quasi-cyclic strategies which have been advocated by Drmač and Veselić recently, and by Mascarenhas in 1990. We provide the global convergence proofs for all these strategies. We also comment the asymptotic convergence issues. The relative accuracy of these methods is ensured by the known results of Slapničar and by our accuracy result for one step of the one-sided block method. Special attention is paid to numerical implementation and comparison tests. The tests show that the reduction in computational time for the block-oriented algorithms increases up to 40% for the block dimensions of order 32–256, provided that initially the QR factorization with column pivoting of G is used.

In the second approach the algorithm makes the full diagonalization of each block-pivot submatrix. This method is a proper BLAS3 generalization of the one-sided J -Jacobi method, which optimally uses the cache memory. Applying the recent result of Hari on convergence to diagonal form of general block Jacobi-type processes, we have proved, under standard conditions, the convergence of the off-norm of the iteration matrix $A^{(k)}$ to zero for every cyclic strategy which is weakly convergent to the row-cyclic one. We have also proved the relative accuracy of one step of the full block method. Finally, numerical tests have shown that the full block method is most efficient for matrices of dimension larger than 4000. Say, for matrices of order 5000, the speedup with respect to the original non-block method is better than 50%.

Prof. Dr. Vincent Heuveline
 Karlsruhe Institute of Technology (KIT)
 Inst. für Angew. & Num. Mathematik IV
 76128 Karlsruhe

vincent.heuveline@kit.edu
<http://numhpc.math.kit.edu>

Efficient computation of pseudospectra for complex fluid flow problems
 Vincent Heuveline, Chandramowli Subramanian

Stability is a crucial question in most applications since instability means in particular, a computed solution might not be observable in experiments or the control of a procedure in industrial production is just impossible.

Classical methods to investigate how flow processes deal with perturbations stem from the times of Reynolds (experimentally), Rayleigh, Kelvin and Stokes (analytically). But no question which tool we choose, just some aspects of the complex flow behavior which is observed are reflected by available theoretical results - mostly for very simple configurations. In the fields of hydrodynamic stability there are two main approaches: the energy method (or nonlinear stability) and the linear method, where eigenvalues play a key role.

Considering the Navier-Stokes equations

$$\begin{aligned} \partial_t u - Re^{-1} \Delta u + u \cdot \nabla u + \nabla p &= f, & \text{in } \Omega, \\ \nabla \cdot u &= 0, & \text{in } \Omega, \end{aligned} \tag{1}$$

on a bounded domain Ω assuming adequate boundary conditions, we are interested if a small perturbation to a steady solution (U, P) will grow or decay in time. The linear stability theory deals with the eigenvalue problem of the linearization of (1) around (U, P) which seeks for nontrivial u, p and a complex λ such that

$$\begin{aligned} Re^{-1} \Delta u - u \cdot \nabla U - U \cdot \nabla u - \nabla p &= \lambda u, & \text{in } \Omega, \\ \nabla \cdot u &= 0, & \text{in } \Omega, \end{aligned} \tag{2}$$

with appropriate zero boundary conditions. If $\text{Re } \lambda < 0$ for all eigenvalues λ of (2), then the basic flow is said to be *linear stable* and it is said to be *linear unstable* if $\text{Re } \lambda > 0$ for at least one eigenvalue (see e.g. [1]).

However in studying hydrodynamic stability of non-normal problems, eigenvalues can be misleading (see e.g. [4]). Instead of only considering the spectrum of a linear operator A , a promising approach to gain more information about the stability behaviour is by investigating its *pseudospectrum*

$$\sigma_\varepsilon(A) = \{z \in \mathbb{C} : \|(zI - A)^{-1}\| > \varepsilon^{-1}\}.$$

The pseudospectrum of a bounded linear operator A gives information about its exponential behaviour $\|e^{tA}\|$ and therefore especially about its short-time behaviour (see [3]).

Discretizing (2) by using finite element methods we gain the finite dimensional eigenvalue problem

$$A_h u_h = \lambda_h M_h u_h, \tag{3}$$

where A_h denotes the stiffness matrix and M_h the (singular, positive semi-definite) mass matrix. Defining the pseudospectrum of a matrix pencil as

$$\sigma_\varepsilon(A_h, M_h) = \{z \in \mathbb{C} : \|(zM_h - A_h)^{-1}\| > \varepsilon^{-1}\},$$

we carried out numerical computations with our software *HiFlow* (www.hiflow.de).

The used algorithm for computing pseudospectra is based on the computation of the singular values of the resolvent $(zM_h - A_h)^{-1}$ for different z on a grid in a complex domain. Therefore we used a preconditioned version of Davidson's method. Since this problem entails high computational costs we exploited parallelism on two levels. Due to large problem sizes, the use of a parallel linear algebra is virtually mandatory. On the other hand, the computation of singular values for different z needs no communication, which allows us a second level of parallelism.

In this paper, we present numerical results of pseudospectra for the *backflow problem* as well as the associated challenges. The analysis and interpretation of the results related to pseudospectra in the framework of CFD are further being addressed.

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Michiel Hochstenbach
Dept. of Mathematics and Computer Science
TU Eindhoven
PO Box 513
NL-5600 MB Eindhoven
The Netherlands

<http://www.win.tue.nl/~hochsten/>

Fields of Values and Inclusion Regions for Generalized Eigenproblems

Michiel E. Hochstenbach

We are interested in (approximate) eigenvalue inclusion regions for matrix pencils (A, B) , in particular of large dimension, based on certain fields of values. We show how the usual field of values may be efficiently approximated for large Hermitian positive definite B , but also point out limitations of this set. We introduce four field of values based inclusion regions, which may effectively be approximated, also for large pencils. Furthermore, we show that these four sets are special members of two families of inclusion regions, of which we study several properties. Connections with the usual harmonic Rayleigh–Ritz method and a new variant are shown, and we propose an automated algorithm which gives an approximated inclusion region. The results are illustrated by several numerical examples.

When time allows we will also report some other recent progress relating fields of values.

Gary Howell
512 Farmington Woods Dr.
Cary, North Carolina 27511
USA

`gary_howell@ncsu.edu`

Block Householder Computation of Sparse Matrix Singular Values

Gary Howell

This talk introduces block Householder reduction of a rectangular sparse matrix to small band upper triangular form. The computation accesses a sparse matrix only for sparse matrix dense matrix (SMDM) multiplications and for “just in time” extractions of row and column blocks. For a bandwidth of $k + 1$, the dense matrices are the k rows or columns of a block Householder transformation. Other than the SMDM, computations are BLAS-3.

Because Householder transformations have condition number very near one, run time computations of Frobenius norms can give an accurate idea of how much of the matrix has been captured after elimination of l rows and columns. The number of rows and columns eliminated is limited by the amount of available random access memory (RAM) to store the dense blocks used to eliminate rows and columns. Because RAM is plentiful and cheap, the algorithm makes more sense now than was previously the case.

Using an initial random block Householder transformation allows reliable computation of a collection of largest singular values. Tests on the Tim Davis UF collection of matrices indicate that the block Householder reduction is numerically stable and scalable.

The results to be presented show the algorithm to work well with a non-uniform access shared memory machine. Using OpenMP with initialization loops in the same pattern as computation loops allows efficient BLAS-3 computations with “long skinny” matrices. Using 64 GBytes of RAM with 16 cores often allows determination of a moderate number of singular values for matrices of size to about a million. In contrast, a SCALAPACK Householder based SVD computation for a million by million matrix requires about 8 TBytes for matrix storage and $O(1000)$ processors.

Tradeoffs involved in the bandwidth k and some guidelines as to which matrices are “difficult” are discussed.

Block Householder reduction also has good potential for scalable distributed memory parallelization. Some applications other than computing singular values are proposed.

Elias Jarlebring
 K.U. Leuven, Dept. comp. science
 Celestijnenlaan 200 A
 B-3001 Heverlee
 Belgium

elias.jarlebring@cs.kuleuven.be
<http://www.cs.kuleuven.be/~elias>

Infinite Chebyshev Arnoldi for Nonlinear Eigenvalue Problems

Elias Jarlebring, Karl Meerbergen, Wim Michiels

Let B be a matrix depending on a scalar parameter, i.e., $B : C \rightarrow C^{n \times n}$, such that each element is an entire function of the parameter λ . Consider the problem of finding $\lambda \in C$ and $x \in C^n \setminus \{0\}$ such that

$$\lambda B(\lambda)x = x. \quad (4)$$

This is a nonlinear eigenvalue problem written in a form which is suitable for our purposes. In literature on nonlinear eigenvalue problems (e.g. [Vos04]) we typically find the formulation $M(\lambda)x = 0$. Note that if we let $B(\lambda) := \frac{I - M(0)^{-1}M(\lambda)}{\lambda}$ for $\lambda \neq 0$ and $B(0) := -M(0)^{-1}M'(0)$, then the formulations are equivalent, except from possibly $\lambda = 0$.

We will here present a method for (4) which is mathematically equivalent to the *Arnoldi method*. Note that the Arnoldi-type method in [Vos04] reduces to standard Arnoldi if $M(\lambda) = A - \lambda I$. Although very successful in practice, there appears to be no known interpretation of [Vos04] as a true Arnoldi scheme for the general nonlinear eigenvalue problem.

The derivation here starts with a reformulation of (4) as an infinite-dimensional eigenvalue problem corresponding to an operator acting on a function. Consider the operator \mathcal{B} defined by the action,

$$(\mathcal{B}\varphi)(\theta) = C(\varphi) + \int_0^\theta \varphi(\theta) d\theta,$$

with

$$C(\varphi) = \left(B\left(\frac{d}{d\theta}\right)\varphi \right)(0), \quad (5)$$

and the domain $D(\mathcal{B})$, which can be taken as the set of all smooth functions φ for which $C(\varphi)$ exists. The functional $B(\frac{d}{d\theta})$ is defined by the power series expansion of B . Our first important result is that the nonlinear eigenvalue problem (4) is fully equivalent to the infinite-dimensional eigenvalue problem,

$$\lambda \mathcal{B}\varphi = \varphi. \quad (6)$$

The power method applied to a matrix is expected to converge to the largest eigenvalue of the matrix. Hence, we expect the power method (in a function setting) applied to the operator \mathcal{B} to first converge to $1/\lambda \in \sigma(\mathcal{B})$ corresponding to λ close to the origin. Note that \mathcal{B} is an integration operator and that if ψ is a vector of polynomials then $\mathcal{B}\psi$ is a vector of polynomials of one degree higher than degree of ψ . Hence, all iterates in the power method for \mathcal{B} started with a constant vector, will be vectors of polynomials.

The coefficients in the Chebyshev basis is generally accepted as a good way to represent polynomials from a numerical stability point of view. For this reason, let

$$\psi(\theta) = \sum_{k=0}^N y_k T_k(\theta)$$

with $y_0 \dots, y_N \in C^m$ and the corresponding image after applying \mathcal{B} ,

$$(\mathcal{B}\psi)(\theta) =: \sum_{k=0}^{N+1} z_k T_k(\theta)$$

with $z_0 \dots, z_{N+1} \in C^m$. Note that z_1, \dots, z_{N+1} are linear combinations of y_0, \dots, y_N , following from the recurrence relations of Chebyshev polynomials.. The coefficient z_0 is computed using the formula $z_0 = \sum_{k=0}^N (B(\frac{d}{d\theta})T_k)(0)y_k$. The expression $(B(\frac{d}{d\theta})T_k)(0)$ can often be simplified and computed analytically, e.g., the corresponding operation for the quadratic eigenvalue problem $M(\lambda) = \lambda^2 M + \lambda C + K$, is $(B(\frac{d}{d\theta})T_k)(0) = -K^{-1}MkU_{k-1}(0) - K^{-1}CT_k(0)$ for $k > 0$, where U_k is the Chebyshev polynomial of the second kind. Hence, the operation of \mathcal{B} on a vector of polynomials represented as the coefficients in the Chebyshev basis can be implemented as a mapping expressed in terms of linear algebra operations applied to the coefficients in the Chebyshev expansion. This construction allows us to compute the iterates in the power method for \mathcal{B} in a successive manner.

Arnoldi is (in exact arithmetic) equivalent to the eigenvalue problem corresponding to the orthogonal projection onto the space spanned by the iterates of the power method. Note that the orthogonalization in Arnoldi (in our function setting) preserves the degree of the polynomial since the functions are always orthogonalized against the previous iterates. Hence, the orthogonalization in a function setting can also be implemented as a mapping of the coefficients. The projection is defined by an orthogonality condition here induced by a scalar product. There are several natural ways to define scalar products in a function setting. We will here use the scalar product for which the Chebyshev polynomials are orthonormal. This yields simple formulas. Moreover, for the *delay eigenvalue problem*, the iteration reduces to the method in [JMM10] which has an interpretation as a spectral discretization with exponential convergence.

Finally, we show by examples that the presented method posses many of the attractive properties of standard Arnoldi, including efficiency and robustness.

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Michael Karow
Institut für Mathematik
Technische Universität Berlin
Straße des 17. Juni 136
10623 Berlin, Germany

karow@math.tu-berlin.de
<http://www.math.tu-berlin.de/~karow/>

A Perturbation Bound for Invariant Subspaces.

Michael Karow

Let X be a simple invariant subspaces of the square matrix A . If the matrix E is sufficiently small then $\tilde{A} = A + E$ has invariant subspaces \tilde{X} which is close to X . We provide a (hopefully) new bound for the maximum canonical angle between X and \tilde{X} . Furthermore, we compare our estimate with the classical results by Chatelin, Demmel and Stewart.

Louis Komzisk
10824 Hope Street
Cypress, Ca 90630
USA

louis.komzisk@siemens.com
<http://www.siam.org/visiting/speakers/komzisk.php>

Complex model order reduction in industrial rotor dynamics

Louis Komzisk, Siemens PLM

The ever widening use of finite element analysis in the industry produces increasingly difficult eigenvalue problems. The high fidelity requirements of industrial analyses demand accuracy and the very large models necessitate efficiency in the solutions of such problems.

A particular area of high importance in the industry, especially in the energy sector, is the analysis of rotating structures. Such analyses bring forth un-symmetric matrices whose terms are function of the rotational velocity. Since the usual operational range of the rotational structures analyzed in the industry is wide, a sequence of eigenvalue problems must be solved.

The direct solution of a sequence of large un-symmetric eigenvalue problems is impractical due its cost. The alternative solution of a real model order reduction is inaccurate for complex practical problems. To achieve both the accuracy and efficiency goals simultaneously, we use a complex model order reduction approach.

The presentation will briefly review some fundamentals of rotational physics and dynamics. It will discuss the complex model order reduction technique implemented into NX NASTRAN, the world leader in the area of structural finite element analysis. Industrial rotor dynamics application results will be used to demonstrate the merits of the technology. Finally, further improvement possibilities will also be shown.

Patrick Kürschner
TU Chemnitz
Fakultät für Mathematik
D-09107 Chemnitz
Germany

kupa@hrz.tu-chemnitz.de

Modal Approximation of Large Scale Dynamical Systems using Jacobi-Davidson Methods

Peter Benner
Michiel Hochstenbach
Patrick Kürschner

Large scale dynamical systems arise in many physical and technical application areas. An approximation, e.g. with model order reduction techniques, of these large systems is crucial for a cost efficient simulation.

On this poster we restrict ourselves to linear time invariant (LTI) systems and present a model order reduction approach based on modal truncation, where the original system is projected onto the left and right eigenspaces corresponding to the dominant poles of the system. The dominant poles form a small subset of the poles of the systems transfer function and have a significant influence on the system's behavior. The computation of the dominant poles can be a formidable task, since they can lie anywhere inside the spectrum and the corresponding right and left eigenvectors have to be approximated as well.

For this purpose we investigate the two-sided and alternating Jacobi-Davidson method for the efficient solution of the underlying generalized eigenvalue problem in this modal truncation framework. Some numerical examples for practically relevant LTI systems will be presented as well.

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Wen-Wei Lin
National Chiao Tung University
Dept. of Applied Math.
No. 1001 University Road
Hsinchu 300
Taiwan

wwlin@math.nctu.edu.tw
<http://www.math.nctu.edu.tw/~wwlin/>

Solving a structured quadratic eigenvalue problem by a structure-preserving doubling algorithm

Chun-Hua Guo, Wen-Wei Lin

In studying the vibration of fast trains, we encounter a palindromic quadratic eigenvalue problem (QEP) $(\lambda^2 A^T + \lambda Q + A)z = 0$, where $A, Q \in \mathbb{C}^{n \times n}$ and $Q^T = Q$. Moreover, the matrix Q is block tridiagonal and block Toeplitz, and the matrix A has only one nonzero block in the upper-right corner. So most of the eigenvalues of the QEP are zero or infinity. In a linearization approach, one typically starts with deflating these known eigenvalues, for the sake of efficiency. However, this initial deflation process involves the inverses of two potentially ill-conditioned matrices. As a result, large error may be introduced into the data for the reduced problem. In this paper we propose using the solvent approach directly on the original QEP, without any deflation process. We apply a structure-preserving doubling algorithm to compute the stabilizing solution of the matrix equation $X + A^T X^{-1} A = Q$, whose existence is guaranteed by a result on the Wiener–Hopf factorization of rational matrix functions associated with semi-infinite block Toeplitz matrices and a generalization of Bendixson’s theorem to bounded linear operators on Hilbert spaces. The doubling algorithm is shown to be well defined and quadratically convergent. The complexity of the doubling algorithm is drastically reduced by using the Sherman–Morrison–Woodbury formula and the special structures of the problem. Once the stabilizing solution is obtained, all nonzero finite eigenvalues of the QEP can be found efficiently and with the automatic reciprocal relationship, while the known eigenvalues at zero or infinity remain intact.

Chun-Hua Guo:

Department of Mathematics and Statistics, University of Regina, Regina, Canada

Wen-Wei Lin:

Department of Applied Mathematics, National Chiao Tung University, Taiwan

Dominik Löchel
Institute for Applied and Numerical Mathematics
Karlsruhe Institute of Technology (KIT)
D-76128 Karlsruhe

dominik.loechel@kit.edu
<http://www.math.kit.edu/ianm1/>

A multilevel Jacobi-Davidson method for polynomial and rational pde eigenvalue problems

Dominik Löchel

The simulation of drift instabilities in the plasma edge leads to a rational pde eigenvalue problem with parameter dependent coefficients. The aim is to determine the wave number which leads to the maximum growth rate of the amplitude of the wave. This requires the solution of a large number of pde eigenvalue problems. Since we are only interested in a smooth eigenfunction corresponding to the eigenvalue with largest imaginary part, the Jacobi-Davidson method can be applied. Unfortunately, a naive implementation of this method is much too expensive for the large number of problems that have to be solved.

In a first step the rational eigenvalue problem was reformulated as a cubic eigenvalue polynomial and the multilevel Jacobi-Davidson strategy was developed. The basis idea is as follows. On a coarse grid the dimension of the discretized eigenvalue problem is small and a standard solver like the *QZ* algorithm applied to the linearized problem. Among all eigenpairs, the approximation to the desired eigenpair is selected. The eigenvector is prolonged to a finer grid and used as the initial search space in the Jacobi-Davidson algorithm. Within the Jacobi-Davidson cycle the selection of the right Ritz pair is done by an appropriate similarity measure. The correction equation is solved efficiently via the one-step-approximation, where the derivative terms are approximated by finite differences, while spectral methods are used in the projected eigenvalue equation to gain a high level of accuracy. The process is repeated until the final resolution is reached.

The multilevel Jacobi-Davidson method comes with additional advantages. At the beginning of each Jacobi-Davidson procedure, an approximation of the desired eigenpair is known and can be used for scaling. Further, it can be extended to two-sided Rayleigh quotients for a better approximation of the Ritz values. In our physical example, the multilevel strategy achieves, that the Jacobi-Davidson algorithm is in the regime of quadratic convergence since the first cycle and explains its high efficiency.

In a more advanced physical scenario it turned out, that the condition number of the polynomial formulation rises with the number of grid points and becomes too large with respect to the floating point precision. The condition of the original rational formulation, however, stays on a moderate level and is almost independent of the spatial resolution. Therefore, the multilevel Jacobi-Davidson algorithm was extended to rational eigenvalue equations. The projected eigenvalue equation is now solved by inverse iteration.

This is joint work with Marlis Hochbruck, Karlsruhe. The physical example was elaborated in collaboration with Mikhail Tokar and Dirk Reiser, Jülich. This work has been supported by the Deutsche Forschungsgemeinschaft through the research training group GRK 1203.

Thomas Mach
 Technische Universität Chemnitz
 Fakultät für Mathematik
 09107 Chemnitz

thomas.mach@mathematik.tu-chemnitz.de
<http://www-user.tu-chemnitz.de/~tmac>

Slicing the Spectrum of \mathcal{H}_ℓ -Matrices

Peter Benner
 Thomas Mach

We will present an algorithm which computes the eigenvalues of a symmetric \mathcal{H}_ℓ -matrix. The \mathcal{H}_ℓ -matrices are a subclass of the hierarchical (\mathcal{H} -) matrices, which were both introduced by W. Hackbusch in 1998 [Hac99]. Hierarchical matrices are data-sparse and require only $\mathcal{O}(nk \log n)$ storage. The \mathcal{H}_ℓ -matrices are \mathcal{H} -matrices with a simple structure. They are defined by the following recursion: a matrix M is called an \mathcal{H}_ℓ -matrix of maximal block-wise rank k , short $M \in \mathcal{H}_\ell(k)$, if

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix},$$

with $M_{11}, M_{22} \in \mathcal{H}_{\ell-1}(k)$, $M_{12} = A_1 B_1^T$ and $M_{21} = B_2 A_2^T$, where $A_i, B_i \in \mathbf{R}^{n/2 \times k'}$ and $k' \leq k$. For symmetric M we have $A_1 = A_2$ and $B_1 = B_2$. On the lowest level we demand that an $\mathcal{H}_0(k)$ -matrix is a dense matrix of size $n_{\min} \times n_{\min}$. The number ℓ denotes the number of levels. For constant n_{\min} the number of levels ℓ grows like $\log n$.

Like for hierarchical (\mathcal{H} -) matrices, there are a lot of arithmetic operations of linear-polylogarithmic complexity for \mathcal{H}_ℓ -matrices. The need for truncation in order to close the class of \mathcal{H} -matrices under addition, multiplication and inversion makes formal \mathcal{H} -arithmetic an approximative arithmetic. The same is true for \mathcal{H}_ℓ -matrices. But we will show that the exact LDL^T factorisation of an $\mathcal{H}_\ell(k)$ -matrix is in $\mathcal{H}_\ell(k\ell)$. So truncation is not necessary if we allow a small increase of the maximal block-wise rank from k to $k\ell$. The simple structure of \mathcal{H}_ℓ -matrices simplifies the arithmetic operations.

In “The Symmetric Eigenvalue Problem” [Par80, p. 51] Beresford N. Parlett described a bisection method to find the eigenvalues of a symmetric matrix $M \in \mathbf{R}^{n \times n}$. The spectrum Λ of a real, symmetric matrix is contained in \mathbf{R} . We will call the number of eigenvalues $\lambda_i \in \Lambda$ smaller than μ $\nu(\mu)$ or $\nu(M - \mu I)$. Obviously, ν is a function $\mathbf{R} \rightarrow \{0, \dots, n\} \subset \mathbf{N}$. If the function $\nu(\cdot)$ is known, one can find the m th eigenvalue as the limit of the following process:

- a:** Start with an interval $[a, b]$ with $\nu(a) < m \leq \nu(b)$.
- b:** Determine, $\nu_m := \nu(\frac{a+b}{2})$. If $\nu_m > m$, then continue with the interval $[a, \frac{a+b}{2}]$, else with $[\frac{a+b}{2}, b]$.
- c:** Repeat the bisection (step b) until the interval is small enough.

If $M - \mu I$ has an LDL^T factorisation $M - \mu I = \text{LDL}^T$ with L invertible, then D and $M - \mu I$ are congruent. Since D is diagonal we can count easily the number of negative eigenvalues.

Sylvester's inertia law tells us that the number of negative diagonal entries in D is equal to the number of negative eigenvalues of $M - \mu I$, $\nu(D) = \nu(\mu)$.

Since we need an LDL^T factorisation in each step this process is prohibitively expensive for dense matrices. But for \mathcal{H}_ℓ -matrices we have a cheap exact LDL^T factorisation of linear-polylogarithmic complexity.

There are other eigenvalue algorithms for symmetric \mathcal{H}_ℓ -matrices, too. J. Gördes described in her diploma thesis [Gör09] an eigenvalue algorithm for $\mathcal{H}_\ell(1)$ -matrices based on Divide-and-Conquer. This algorithm has a total complexity of $\mathcal{O}(n^2 (\log n)^\beta)$.

Further M. Van Barel et al. present in [DFV08] a transformation of \mathcal{H}_ℓ - and the related HSS-matrices into semi-separable matrices. For semi-separable matrices there is a QR-algorithm [VVM05]. Both steps have quadratic or quadratic-polylogarithmic complexity.

We have a complexity analysis for the LDL^T slicing algorithm which shows that the complexity for the computation of the whole spectrum is comparable to that of both existing algorithms. Further we will show, that if we compute only some few interior eigenvalues, then the LDL^T slicing algorithm is superior to the other algorithms.

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Emre Mengi
 Koç University
 Rumelifeneri Yolu, 34450
 Sariyer, Istanbul
 Turkey

emengi@ku.edu.tr
<http://home.ku.edu.tr/~emengi>

Nearest Linear Systems with Highly Deficient Reachable Subspaces Emre Mengi

Given a linear time-invariant dynamical system

$$\dot{x}(t) = Ax(t) + Bu(t), \quad (7)$$

where $A \in \mathbf{R}^{n \times n}$, $B \in \mathbf{R}^{n \times m}$. We consider the distance [1]

$$\tau_r(A, B) = \inf\{\|\Delta A \ \Delta B\| : \text{rank}(\mathcal{C}(A + \Delta A, B + \Delta B)) \leq r\} \quad (8)$$

with

$$\mathcal{C}(A, B) = [B \ AB \ A^2B \ \dots \ A^{n-1}B]$$

denoting the controllability matrix, whose rank gives the dimension of the reachable subspace of (7). In (8) and elsewhere $\|\cdot\|$ denotes the matrix 2-norm unless otherwise stated.

The quantity $\tau_r(A, B)$ can be considered as a generalization of the distance to uncontrollability

$$\tau(A, B) = \inf\{\|\Delta A \ \Delta B\| : \text{rank}(\mathcal{C}(A + \Delta A, B + \Delta B)) \leq n - 1\}$$

for which the singular value characterization

$$\tau(A, B) = \inf_{\lambda \in \mathbf{C}} \sigma_n([A - \lambda I \ B])$$

is derived by Eising, where $\sigma_j(C)$ denotes the j th largest singular value of C . Eising's characterization is a simple consequence of the PBH test, which establishes the equivalence of rank-deficiency of $\mathcal{C}(A, B)$ and the condition

$$\exists \lambda \in \mathbf{C} \ \text{rank}([A - \lambda I \ B]) < n. \quad (9)$$

In this work we first generalize the PBH test. Let

$$P_d^\Lambda(A) = (A - \lambda_1 I)(A - \lambda_2 I) \dots (A - \lambda_d I)$$

denote the monic matrix polynomial with roots $\Lambda = [\lambda_1 \ \lambda_2 \ \dots \ \lambda_d]^T$. In particular we deduce that

$$\text{rank}(\mathcal{C}(A, B)) \leq r \iff \exists \Lambda \in \mathbf{C}^{n-r} \ \text{s.t.} \ \text{rank}([P_{n-r}^\Lambda(A) \ B]) = r$$

under the assumption that A has distinct eigenvalues. Then we linearize this generalized PBH test. By exploiting the linearized PBH test we derive the singular value optimization characterization

$$\tau_r(A, B) = \inf_{\Lambda} \sup_{\Gamma} \sigma_{k+1} \left(\mathcal{A}_{n-r}^{\Gamma, \Lambda}(A, B) \right)$$

where $k := (n-r)(n-1)$,

$$\mathcal{A}_{n-r}^{\Gamma, \Lambda}(A, B) := \begin{bmatrix} A - \lambda_1 I & B & 0 & 0 & 0 & 0 & 0 & 0 \\ \gamma_{2,1} I & 0 & A - \lambda_2 I & B & 0 & 0 & 0 & 0 \\ \gamma_{3,1} I & 0 & \gamma_{3,2} I & 0 & A - \lambda_3 I & B & 0 & 0 \\ & & & & \ddots & & & \\ & & & & & \ddots & & \\ \gamma_{n-r,1} I & 0 & \gamma_{n-r,2} I & 0 & & & A - \lambda_{n-r} I & B \end{bmatrix},$$

and

$$\Gamma = [\gamma_{2,1} \ \gamma_{3,1} \ \dots \ \gamma_{n-r,1} \ \gamma_{3,2} \ \gamma_{4,2} \ \dots \ \gamma_{n-r,2} \ \dots \ \gamma_{n-r,n-r-1}]^T \in \mathbf{C}^{(n-r-1)(n-r)/2}.$$

The singular value optimization characterization holds under a mild multiplicity assumption regarding the optimal singular value and a linear independence assumption concerning the optimal singular vectors.

We suggest a numerical technique to solve the derived singular value optimization problems. In theory the inner maximization problem is neither unimodal nor convex, however it turns out that it is easy to check whether a local maximizer is a global maximizer or not. Therefore we use BFGS to perform inner maximization. In practice we typically observe that a converged local maximizer is a global maximizer. The outer problem is a Lipschitz minimization problem. More precisely define

$$f(\Lambda) := \sup_{\Gamma} \sigma_{k+1} \left(\mathcal{A}_{n-r}^{\Gamma, \Lambda}(A, B) \right).$$

The Lipschitz continuity of $f(\Lambda)$,

$$|f(\Lambda + \delta\Lambda) - f(\Lambda)| \leq \|\delta\Lambda\|,$$

is a simple consequence of the Weyl's theorem. Numerically we exploit the Lipschitz continuity of $f(\Lambda)$ to solve the outer minimization problem. We utilize the Piyavskii-Shubert algorithm, or more precisely a sophisticated version of the Piyavskii-Shubert algorithm called DIRECT attempting to estimate the Lipschitz constant locally, for the outer Lipschitz optimization problem. The numerical technique is meant for low precision. We illustrate the significance of the singular value optimization characterization and effectiveness of the numerical technique on numerical examples. Without the singular value characterization it is not clear how one can compute $\tau_r(A, B)$ even to a few-digits precision.

The problem that we consider (provide a singular value optimization characterization and numerically solve) is in essence a special case of the problem of finding the smallest perturbation

to a rectangular $k \times n$ pencil with $k > n$ so that it has ℓ finite eigenvalues [2]. More precisely in [2] for a given $k \times n$ pencil $\tilde{A} - \lambda\tilde{B}$ the distance problem

$$\inf \left\{ \left\| \begin{bmatrix} \Delta\tilde{A} & \Delta\tilde{B} \end{bmatrix} \right\|_F : \exists \lambda_j \in \mathbf{C}, v_j \in \mathbf{C}^n \text{ s.t. } \left((\tilde{A} + \Delta\tilde{A}) - \lambda_j(\tilde{B} + \Delta\tilde{B}) \right) v_j = 0 \text{ for } j = 1, \dots, \ell \right\}$$

where $\{v_1, \dots, v_\ell\}$ is linearly independent is discussed. The quantity $\tau_r(A, B)$ turns out to be the distance above with

$$\tilde{A} = \begin{bmatrix} A^* \\ B^* \end{bmatrix}, \quad \tilde{B} = \begin{bmatrix} I \\ 0 \end{bmatrix}$$

and the Frobenius norm above replaced by the 2-norm. A singular value characterization for the general problem was given in [2] when $\ell = 1$. Otherwise, the general problem is open for $\ell > 1$.

Furthermore, $\tau_r(A, B)$ is a measure of degree of reducibility to order r for the system

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) \\ y(t) &= Cx(t) + Du(t) \end{aligned}$$

with zero initial conditions, and $A \in \mathbf{C}^{n \times n}$, $B \in \mathbf{C}^{n \times m}$, $C \in \mathbf{C}^{p \times n}$ and $D \in \mathbf{C}^{p \times m}$. Let us use the shorthand notation (A, B, C, D) for the system above and pose the problem

$$\tau_r(A, B, C) = \inf \left\{ \left\| \begin{bmatrix} \Delta A & \Delta B \\ \Delta C & 0 \end{bmatrix} \right\| : \exists A_r \in \mathbf{C}^{r \times r}, B_r \in \mathbf{C}^{r \times m}, C_r \in \mathbf{C}^{p \times r} \right. \\ \left. (A + \Delta A, B + \Delta B, C + \Delta C, D) \equiv (A_r, B_r, C_r, D) \right\}$$

where we use $(A + \Delta A, B + \Delta B, C + \Delta C, D) \equiv (A_r, B_r, C_r, D)$ to denote that the left-hand and right-hand arguments are equivalent systems. It is well-known that when the reachable subspace of the system (A, B, C, D) is r , there is an equivalent system of order r implying

$$\tau_r(A, B, C) \leq \tau_r(A, B).$$

In words if there is a nearby system whose reachable subspace has dimension r , then there is also a nearby system that is equivalent to a system of order r .

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Agnieszka Miedlar
Technische Universität Berlin
Sekretariat MA 4-5
Strasse des 17. Juni 136
D-10623 Berlin

miedlar@math.tu-berlin.de
<http://www.math.tu-berlin.de/~miedlar/>

Inexact adaptive finite element algorithms for PDE eigenvalue problems

Agnieszka Miedlar
(joint work with Volker Mehrmann)

Recently, adaptive finite element methods (AFEM) entered the new area of solving partial differential eigenvalue problems [Lar00, HR01, Ney02, DPR03, CG08, GMZ08]. However, in most AFEM approaches it is assumed that the resulting finite dimensional algebraic problem (linear system or eigenvalue problem) is solved exactly and the computational costs for this part of the method as well as the fact that this problem is solved in finite precision arithmetic are typically ignored. Both a priori and a posteriori error estimates derived for PDE eigenvalue problems do not consider iteration errors (errors connected to solving algebraic eigenvalue problems using iterative methods). Iterative eigensolvers, i.e. Krylov subspace methods, used for solving algebraic problems are used as a 'black box' often wasting computational time and resources. In particular, the contribution of the complexity of algebraic solvers into the total AFEM complexity is ignored and even not analyzed. This is acceptable if the costs for the algebraic problems are small and the problem is well-conditioned, so that the solution of these problems to full accuracy is possible. Unfortunately, nowadays, 'large-scale' means solving problems of dimension few millions, the costs for a very accurate solution of the corresponding algebraic eigenvalue problem start to dominate over the total costs. On the other hand ignoring computational error may lead to incorrect results since a poor approximation influence the error estimator, mesh refinement and quality of the final solution [AGL09].

In [JSV07] Jiranek, Strakos and Vohralik derived fully computable a posteriori error estimates which take into account an inexact solution of the linear algebraic system and constructed efficient stopping criteria for iterative solvers in the context of a second-order elliptic pure diffusion model problem. Some a posteriori error estimates based on eigenvalue perturbation results was obtained in [MM09]. Inspired by the work of Arioli et al. [ANR01, ALW05] for linear systems arising from finite element discretization, we discuss the backward error analysis and stopping criteria for iterative eigensolvers in the context of adaptive finite element algorithm.

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Juan M. Molera
Avda. Universidad 30
28911 Leganés
Spain

molera@math.uc3m.es
http://gauss.uc3m.es/web/personal_web/molera/molera.html

High Relative Accuracy Implicit Jacobi Algorithm for the SVD

Juan M. Molera
Johan Ceballos
Froilán M. Dopico

We prove that a Jacobi-like algorithm applied implicitly on a decomposition $A = XDY^T$ of a matrix A , where D is diagonal, and X, Y are well conditioned, computes all singular values of A to high relative accuracy. The relative error in every eigenvalue is bounded by $O(\epsilon \max[\kappa(X), \kappa(Y)])$, where ϵ is the machine precision and $\kappa(X) = \|X\|_2 \|X^{-1}\|_2$, $\kappa(Y) = \|Y\|_2 \|Y^{-1}\|_2$ are, respectively, the spectral condition number of X and Y . The singular vectors are also computed accurately in the appropriate sense. We compare it with previous algorithms for the same problem [J. Demmel et al. Linear Algebra and its Applications, 299 (1999) 21-80] and see that the new algorithm is faster and more accurate.

Julio Moro
Universidad Carlos III de Madrid
Departamento de Matemáticas jmoro@math.uc3m.es
Avenida de la Universidad, 30 http://gauss.uc3m.es/web/personal_web/jmoro/jmoro.html
28911, Leganés, Madrid
Spain

Directional perturbation in structured eigenproblems

Julio Moro

The design and analysis of structure-preserving algorithms to solve structured eigenproblems has led in the last decades to a steady interest in *structured* eigenvalue perturbation theory, i.e. in determining the behavior of eigenvalues and other spectral objects (e.g., invariant subspaces, sign characteristics,...) when a matrix or operator is subject to perturbations which belong to the same class of operators as the unperturbed one. It is well known that this behavior is usually quite different from the behavior under arbitrary, nonstructured perturbations. In this talk we give an overview of *first order* structured perturbation theory, i.e. of results involving the local variation of eigenvalues as expressed by their directional derivatives, and its interaction with the fact that perturbations are restricted within the class of interest. Such results are relevant in many practical situations when eigenvalues need to be pushed in certain specific directions, or must be moved as fast as possible away from a critical (or dangerous) region by a small, usually structured, perturbation. Special emphasis is made on classes of matrices and matrix pencils with symmetries in some indefinite scalar product, which often arise in several applications in Control and Systems Theory.

Andrej Muhič
Institute for Mathematics, Physics and Me-
chanics (IMFM)
Jadranska 19, SI-1000 Ljubljana

andrej.muhic@fmf.uni-lj.si
<http://www.fmf.uni-lj.si/~muhic/en/>

On linearizations of the quadratic two-parameter eigenvalue problems

Andrej Muhič
Bor Plestenjak
Michiel E. Hochstenbach

We present several transformations that can be used to solve the quadratic two-parameter eigenvalue problem (QMEP), which has a general form

$$\begin{aligned} Q_1(\lambda, \mu) x_1 &:= (A_{00} + \lambda A_{10} + \mu A_{01} + \lambda^2 A_{20} + \lambda \mu A_{11} + \mu^2 A_{02}) x_1 = 0, \\ Q_2(\lambda, \mu) x_2 &:= (B_{00} + \lambda B_{10} + \mu B_{01} + \lambda^2 B_{20} + \lambda \mu B_{11} + \mu^2 B_{02}) x_2 = 0, \end{aligned} \tag{10}$$

where A_{ij}, B_{ij} are given $n_i \times n_i$ complex matrices, $x_i \in \mathbf{C}^{n_i}$ is a nonzero vector for $i = 1, 2$, and $\lambda, \mu \in \mathbf{C}$, by formulating an associated linear multiparameter eigenvalue problem. Two of these transformations are generalizations of the well-known linearization of the quadratic eigenvalue problem and linearize the QMEP as a singular two-parameter eigenvalue problem. The third one introduces a new approach, substituting all nonlinear terms with new variables and adding new equations for their relations. The QMEP is thus transformed into a nonsingular five-parameter eigenvalue problem. The advantage of these transformations is that they enable one to solve the QMEP using the existing numerical methods for the multiparameter eigenvalue problems. We also consider several special cases of the QMEP, where some of the quadratic terms are missing.

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Beresford Parlett

parlett@math.berkeley.edu
<http://math.berkeley.edu/~parlett/>

The contributions of Paul Willems to the MRRR algorithm
Beresford Parlett

Although the MRRR algorithm contributed some practical seminal ideas to the computation of mutually orthogonal eigenvectors of symmetric tridiagonal matrices there were some blemishes in the implementation. The recent dissertation of Paul Willems takes a fresh look at the algorithm and makes improvements in the representations, the proofs and the blocked representations thereby removing the blemishes.

Rui Ralha
Dep. de Matematica
Universidade do Minho
Campus de Gualtar
4710-057 Braga
Portugal

`r_ralha@math.uminho.pt`

Reliable Eigenvalues of Tridiagonals

Rui Ralha

We present a method to improve or just guarantee the accuracy of the approximations delivered by any fast method for the eigenvalues of symmetric tridiagonal matrices. The motivation for this approach is two-folded: 1) the fastest state-of-the-art algorithms do not always deliver eigenvalues as accurate as they are defined by the data; 2) in some cases it is difficult to estimate the number of correct digits in the computed approximations for the eigenvalues of smaller size. We tackle both issues in the following way: starting with the computed approximation $\tilde{\lambda}_k$ (for some k), our method finds an interval that is guaranteed to contain the exact eigenvalue λ_k . The relative gap of the bounds of this interval depends solely on how well the matrix entries define λ_k . Therefore, for eigenvalues defined to high relative accuracy, the computed intervals are very tight in the relative sense. In other cases, λ_k may not be defined to high relative accuracy but still have many significant digits correct which are difficult to predict through the use of perturbation theory results. We show that our method can be extended to the computation of real eigenvalues of unsymmetric matrices. Numerical examples are given.

Valeria Simoncini
Dipartimento di Matematica
Università di Bologna
Bologna
Italy

valeria@dm.unibo.it
<http://www.dm.unibo.it/~simoncin/>

An Implicitly-Restarted Krylov Subspace Method for Real Symmetric/Skew-Symmetric Eigenproblem

Valeria Simoncini

In this talk we will describe a recently developed implicitly-restarted Krylov subspace method for real symmetric/skew-symmetric generalized eigenvalue problems. The new method improves and generalizes the SHIRA method of V. Mehrmann and D. Watkins, “Structure-preserving methods for computing eigenpairs of large sparse skew-Hamiltonian/Hamiltonian pencils”, *SIAM J. Sci. Comput.*, 22:1905–1925, 2001, to the case where the skew symmetric matrix is singular. We will show that the new algorithm can accurately compute a few eigenvalues and eigenvectors of the matrix pencil close to a given target point. Several applications from control theory will be presented and the properties of the new method will be illustrated by benchmark examples.

This is joint work with V. Mehrmann and C. Schröder, both at TU Berlin, Germany.

Sanja Singer
Faculty of Mechanical Engineering
and Naval Architecture
University of Zagreb
Ivana Lučića 5
10000 Zagreb
Croatia

ssinger@fsb.hr
<http://www.fsb.hr/ssinger>

A GPU-based hyperbolic SVD algorithm

Vedran Novaković
Sanja Singer

Given a factorization G^*JG of an indefinite matrix A , with G^*G positive definite matrix and J diagonal matrix holding the inertia of A , we aim at computing the hyperbolic SVD of the factor G , or – in other terms – at solving the eigenproblem for the matrix A .

Our method of choice for such a problem is the one-sided hyperbolic Jacobi algorithm, which has been much studied in the recent years, due to its high relative accuracy and various possibilities of the efficient blocking and parallelization in the scope of the conventional CPU computing.

We will show that the same algorithm is elegantly parallelizable on the modern GPUs, not utilizing them as a mere coprocessor for the offload of the simple computations, but as a primary target for the algorithm execution. The numerical experiments will demonstrate the beneficence of such an approach, compared to the standard, multi-process parallel implementation.

Ivan Slapničar
University of Split
FESB, R. Boškovića b.b.
HR-21000 Split, Croatia

ivan.slapnicar@fesb.hr
www.fesb.hr/~slap

Jacobi-type algorithms for Hamiltonian matrices

Ivan Slapničar

We present recent results on Jacobi-type algorithms for real and complex Hamiltonian matrices. The algorithms use orthogonal (unitary) and non-orthogonal shear transformations. Convergence and accuracy properties of the algorithms are discussed.

G. W. (Pete) Stewart
Department of Computer Science
University of Maryland
College Park MD 20742
USA

stewart@cs.umd.edu
www.cs.umd.edu/~stewart/

On Oblique Projectors

G. W. Stewart

An oblique projector is an idempotent matrix whose spectral norm is greater than one. Oblique projectors arise in a number of application, in particular in the orthogonalization of Krylov sequences with respect to a positive definite matrix B . In this talk we will consider various representations of projectors and their numerical properties. We will also consider the problem of complementation—the oblique generalization of orthogonalization—and show that the “twice is enough” rule of thumb for Gram–Schmidt orthogonalization continues to hold in a certain sense for complementation. We will also discuss some potential problems with bases generated by B -orthogonalization.

Chandramowli Subramanian
 Karlsruhe Institute of Technology (KIT)
 Inst. für Angew. & Num. Mathematik IV
 76128 Karlsruhe

chandramowli.subramanian@kit.edu
<http://numhpc.math.kit.edu>

Estimates and calculations for the Poincaré constant in an annulus based on eigenvalue problems

Vincent Heuveline, Arianna Passerini, Chandramowli Subramanian, Gudrun Thäter

In the study of a variety of subjects such as thermal energy storage systems, aircraft cabin insulation, cooling of electronic components, electrical power cable as well as thin films, one has to understand the fluid flow between two horizontal coaxial cylinders. Depending on the material properties (encoded in the Rayleigh and Prandtl number) as well as the actual relation of the radii $R_i < R_o$ or more precisely, the non-dimensional *inverse relative gap width*

$$\mathcal{A} := \frac{2R_i}{R_o - R_i}$$

the problem is very complex and allows for very different possible behavior of the flow. Up to now it was mostly investigated by numerical experiments (see, e.g. [4] and references therein). To find bifurcations in this way is a very delicate task. For that we started to use mathematical analysis (see [3] and references therein) to narrow down possible regions for bifurcation.

To gain a first insight a twodimensional geometry is helpful, i.e. we consider $\Omega = \{(r, \varphi): R_i < r < R_o, 0 \leq \varphi < 2\pi\}$ and its nondimensional version $\Omega_{\mathcal{A}} := \{(\hat{r}, \varphi): \mathcal{A}/2 < \hat{r} < 1 + \mathcal{A}/2\}$, respectively, with $\hat{r} := r/(R_o - R_i)$.

A special role for the qualitative and quantitative description of the flow and especially for the determination of critical values for stability plays the *Poincaré constant* k_p , i.e. the constant in the inequality

$$\|f\|_2 \leq k_p \|\nabla f\|_2, \quad (11)$$

which holds of all $f \in H_0^1$ (i.e. $f, \nabla f \in L_2$ with zero trace) if the domain under consideration is bounded in at least one dimension (see e.g., [1, Prop. 1.2]). To find analytical estimates for the existence, regularity and stability of solutions it is necessary to have good bounds for k_p . Usually, they depend on the diameter of the domain.

To find those bounds one can use the well-known fact that $k_p = \lambda^{-1}$ for λ being the smallest eigenvalue of the Laplace problem

$$-\Delta u = \lambda u \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega. \quad (12)$$

Up to the moment (see, e.g. [3]) the best available result has been

$$k_p = k_p(\mathcal{A}) \leq \min \left\{ \frac{1}{2} \sqrt{1 + \frac{2}{\mathcal{A}}}, \frac{\sqrt{2}}{\pi} \left(1 + \frac{\mathcal{A}}{2} \right) \right\}, \quad (13)$$

which is far from being optimal. To get an idea how far, a numerical determination of the smallest eigenvalue of problem (3) as a function of \mathcal{A} has been carried out with our software.

Unfortunately, such plot is not directly useful for analytical purposes. Nevertheless, at the same moment a result of [2] showed us the way to a better estimate, namely

$$k_p \leq \frac{1}{\pi}. \quad (14)$$

Now, our results shows that the analytical bound (4) is almost sharp.

This will directly improve our bounds for the critical Rayleigh number in the above described flow problems.

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Zoran Tomljanović
Department of Mathematics,
J.J. Strossmayer University of Osijek
Trg Ljudevita Gaja 6
31000 Osijek
Croatia

ztomljan@mathos.hr
<http://www.mathos.hr/~ztomljan/>

Optimal Damping of Partial Spectra Using Dimension Reduction

Peter Benner¹, Zoran Tomljanović, Ninoslav Truhar²

We will consider a mathematical model of a linear vibrational system described with second-order differential equation

$$M\ddot{x} + D\dot{x} + Kx = 0,$$

where M and K are positive definite matrices of order n , called mass and stiffness, respectively. The damping matrix is $D = C_u + C$, where C_u represents the internal damping and C is the external damping which is positive semidefinite matrix. The problem of determination of optimal damping is equivalent to minimization of the trace of the solution of the Lyapunov equation

$$AX + XA^T = -GG^T,$$

where A is the $2n \times 2n$ matrix obtained from linearizing the second-order differential equation. The matrix G depends on the part of the eigenfrequencies which has to be damped. Usually, G has small rank which corresponds with the damping of the some part of the eigenfrequencies.

Finding the optimal C_0 , such that $\text{trace}X(C)$ is minimal, is a very demanding problem, caused by the large number of trace calculations which can be required for bigger matrix dimensions.

We propose a dimension reduction to accelerate the optimization process. Also, we present corresponding error bound for the approximation the trace of the solution of the Lyapunov equation obtained by this reduction, which includes the influence of the right-hand side GG^T and allow us to control accuracy of the trace approximation.

¹Mathematics in Industry and Technology, Department of Mathematics, Chemnitz University of Technology, Chemnitz, Germany, benner@mathematik.tu-chemnitz.de

²Department of Mathematics, J.J. Strossmayer University of Osijek, Croatia, ntruhar@mathos.hr

Lloyd N. Trefethen
Mathematical Institute
24-29 St. Giles'
Oxford OX1 3LB, UK

trefethen@maths.ox.ac.uk
<http://www.maths.ox.ac.uk/~trefethen>

The EIGS Command in Chebfun

Toby A. Driscoll
Lloyd N. Trefethen

In chebfun computing, users work with functions instead of vectors, operators instead of matrices. Both differential and integral operators acting on an interval $[a, b]$ are available, and the underlying algorithms come from the field of Chebyshev spectral collocation methods. Now what if we want the eigenvalues and eigenvectors of an operator? We can't ask for all of them, as they will be infinite in number, so the right Matlab program to overload is `eigs`, not `eig`. How do we pick out the required finite set from an infinite collection? Is it best to solve and then discretize, or discretize and then solve? This talk will present the algorithms for this task that are encoded in the chebfun `eigs` command, which with surprising speed and reliability compute eigenvalues and eigenvectors of many operators to ten digits of accuracy or more.

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Eugene Tyrtyshnikov
Russian Academy of Sciences
Gubkin Street 8
Moscow 119333
Russia

tee@bach.inm.ras.ru

Eigenvalue solvers with tensor-train data

Eugene Tyrtyshnikov

In many applications (multi-parametric optimization, quantum molecular dynamics, etc.) eigenvalue problems arise for symmetric operators on d -dimensional cubes and with separated variables in the eigenfunctions. The latter implies an exact or approximate tensor structure in the eigenvectors. We suggest to represent the eigenvectors by tensor trains (TT-decompositions), in other contexts also called linear tensor networks or matrix-product networks. The name "tensor trains" (TT) is recently used to indicate efficient algorithms (appeared in 2009) for approximate arithmetics and interpolation in the TT-format. Some standard eigensolvers can be modified so that all the data is kept in the TT-format. This leads to algorithms with the complexity linear in d . In particular, we consider tensor-train modifications of iterative methods of minimization of the Raleigh quotient in the scalar or block form.

Marc Van Barel
Department of Computer Science
Katholieke Universiteit Leuven
Celestijnenlaan 200A
B-3001 Leuven (Heverlee)
Belgium

marc.vanbarel@cs.kuleuven.be
<http://people.cs.kuleuven.be/~marc.vanbarel/>

An Efficient Implicit Double Shift QR -Algorithm for Companion Matrices

Marc Van Barel
Raf Vandebril
Paul Van Dooren
Katrijn Frederix

In this talk an implicit (double) shift QR -method for computing the eigenvalues of companion matrices will be presented. Companion matrices are Hessenberg matrices, that can be decomposed into the sum of a unitary and a rank 1 matrix. The Hessenberg, the unitary as well as the rank 1 structures are preserved under a step of the QR -method. This makes these matrices suitable for the design of a fast QR -method.

Several techniques already exist for performing a QR -step. The implementation of these methods is highly dependent on the representation used. Unfortunately for most of the methods compression is needed since one is not able to maintain all three, unitary, Hessenberg, rank 1 structures.

In this talk an implicit algorithm will be designed for performing a step of the QR -method onto the companion matrix based on a representation consisting of Givens transformations. Moreover, no compression is needed as the specific representation of the involved matrices is maintained. Finally also a double shift version of the implicit method is presented. Numerical experiments will show the robustness of the new method with respect to scaling of the polynomial coefficients in comparison with other existing methods.

Kresimir Veselić
Fernuniversität Hagen

kresimir.veselic@FernUni-Hagen.de

Condition in block diagonalising J -Hermitian matrices

Kresimir Veselić

Given a (generally not J -unitary) transformation matrix S block diagonalising a given J -Hermitian matrix a method is designed to convert S to a J -unitary one, which is shown always to improve the condition number.

Matthias Voigt
TU Chemnitz
Fakultät für Mathematik
D-09107 Chemnitz
Germany

`mattv@hrz.tu-chemnitz.de`

Computation of the Eigenvalues of Skew-Hamiltonian/Hamiltonian Pencils in SLICOT

Peter Benner
Vasile Sima
Matthias Voigt

Skew-Hamiltonian/Hamiltonian pencils appear in many applications, including linear quadratic optimal control problems, \mathcal{H}_∞ optimization, certain multi-body systems and many other areas in applied mathematics, physics, and chemistry. On this poster we present a structure-preserving method for accurately computing the eigenvalues of such pencils. This method is based on the embedding of the pencils into larger skew-Hamiltonian/Hamiltonian pencils in order to ensure the existence of a particular condensed form. We show some details of the implementation of the algorithm in the Subroutine Library In COntrol Theory (SLICOT) and present some numerical results. Finally, we illustrate how skew-Hamiltonian/Hamiltonian pencils can be applied to compute the \mathcal{L}_∞ -norm of linear time-invariant descriptor systems.

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Daniel Wachsmuth
Johann Radon Institute (RICAM)
Austrian Academy of Sciences
Altenbergerstraße 69
A-4040 Linz, Austria

daniel.wachsmuth@oeaw.ac.at

Error analysis for eigenvalues of Hessians for optimal control problems

Daniel Wachsmuth
Saheed Akindeinde

Many technical processes are described by partial differential equations. Here, it is important to optimize these processes. For many applications, the optimization criterion is not a convex function, and the underlying partial differential equation is non-linear. Then two types of optimality conditions become equally important. First-order necessary optimality conditions help to find critical points, while sufficient second-order conditions can ensure the local optimality of such a point. Moreover, the convergence analysis of fast optimization methods as well as of approximation techniques is based on sufficient optimality conditions. Hence, it is desirable to check whether these conditions are satisfied for a given solution candidate.

In the talk, we will investigate an optimization problem subject to an elliptic partial differential equation with a finite number of control parameters. Then the sufficient optimality condition is equivalent to positive definiteness of an underlying Hessian matrix. However, the entries of the matrix cannot be computed exactly, since they depend on solutions of partial differential equations. Hence, we will compute approximations of the entries by means of a finite element discretization of the elliptic equation. With the help of a-posteriori error representations the error in the entries can be estimated. Applying results from matrix perturbation theory, we obtain error bounds for the eigenvalues, which enables to check whether the Hessian matrix is positive definite.

The talk ends with a discussion of the following open problem: if the space of controls is infinite-dimensional then the sufficient optimality condition is equivalent to a generalized eigenvalue problem of the form

$$\begin{pmatrix} A & B^* \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ x \end{pmatrix} = \lambda \begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} u \\ x \end{pmatrix}.$$

Here, none of the operators is positive definite, and any linear combination of both operators is indefinite. Thus, this eigenvalue problem cannot be treated with standard methods. Any suggestions on how to obtain lower eigenvalue bounds are welcome.

David S Watkins
Department of Mathematics
Washington State University
Pullman, WA 99164-3113
USA

watkins@math.wsu.edu
<http://www.math.wsu.edu/faculty/watkins/>

Francis's Algorithm

David S Watkins

Francis's implicitly-shifted QR algorithm has for many years been the most widely used algorithm for computing eigenvalues of matrices, especially in the nonsymmetric case. The standard (and time-honored) method of justifying Francis's algorithm is to show that each iteration is equivalent to a step (or several steps) of the explicitly-shifted QR algorithm. In this talk we will argue that the standard approach is unduly complicated. Instead one should argue directly that Francis's algorithm performs nested subspace iterations with a change of coordinate system at each step. This is done by bringing to light the role of the nested Krylov subspaces that lurk in the transforming matrices.

Jens-Peter M. Zemke
Institut für Numerische Simulation E-10
Technische Universität Hamburg-Harburg
Schwarzenbergstraße 95
D-21073 Hamburg
Germany

zemke@tu-harburg.de
<http://www.tu-harburg.de/~matjz/>

Relations between Rayleigh Quotient Iteration and the Opitz-Larkin Method

Jens-Peter M. Zemke

We show that different members of Rayleigh Quotient Iteration (RQI) and related methods like inverse iteration exactly correspond to different members of the Opitz-Larkin method applied to certain meromorphic scalar functions. These meromorphic functions are related to the characteristic polynomial and have only roots at eigenvalues. Well-known results like the speed of convergence are re-phrased in the framework of the Opitz-Larkin method. More recently suggested choices of shifts in the QR algorithm are placed into this framework.

List of participants

Rafikul Alam, Indian Institute of Technology Guwahati, India
Branimir Anić, Karlsruhe Institute of Technology, Germany
Jesse Barlow, Penn State University, USA
Peter Benner, TU Chemnitz, Germany
Wolf-Jürgen Beyn, University of Bielefeld, Germany
Shreemayee Bora, Indian Institute of Technology Guwahati, India
Tobias Brüll, TU Berlin, Germany
Shu-Ming Chang, National Chiao Tung University, Taiwan
Achiya Dax, Hydrological Service of Israel, Israel
James Demmel, University of California Berkeley, USA
Zlatko Drmač, University of Zagreb, Croatia
Heike Faßbender, TU Braunschweig, Germany
Pavel Grinfeld, Drexel University, USA
Vjieran Hari, University of Zagreb, Croatia
Vincent Heuveline, Karlsruhe Institute of Technology, Germany
Michiel Hochstenbach, TU Eindhoven, The Netherlands
Gary Howell, North Carolina State University, USA
Tsung-Ming Huang, National Taiwan Normal University, Taiwan
Elias Jarlebring, Katholieke Universiteit Leuven, Belgium
Michael Karow, TU Berlin, Germany
Louis Komzsik, Siemens PLM, USA
Yueh-Cheng Kuo, National University of Kaohsiung, Taiwan
Patrick Kürschner, TU Chemnitz, Germany
Jörg Liesen, TU Berlin, Germany
Wen-Wei Lin, National Chiao Tung University, Taiwan
Dominik Löchel, Karlsruhe Institute of Technology, Germany
Philip Losse, TU Berlin, Germany
Thomas Mach, TU Chemnitz, Germany
Christian Mehl, TU Berlin, Germany
Volker Mehrmann, TU Berlin, Germany
Emre Mengi, Koc University, Turkey
Agnieszka Miedlar, TU Berlin, Germany
Juan Molera, Universidad Carlos III de Madrid, Spain
Julio Moro, Universidad Carlos III de Madrid, Spain
Andrej Muhič, Institute for Mathematics, Physics and Mechanics (IMFM), Slovenia
Reinhard Nabben, TU Berlin, Germany
Vedran Novakovic, University of Zagreb, Croatia
Beresford Parlett, University of California Berkeley, USA
Rui Ralha, Universidade de Minho, Portugal
Miloud Sadkane, University of Brest, France
Christian Schröder, TU Berlin, Germany
Valeria Simoncini, Università di Bologna, Italy

Sanja Singer, University of Zagreb, Croatia
Sasa Singer, University of Zagreb, Croatia
Ivan Slapničar, University of Split, Croatia
G.W. (Pete) Stewart, University of Maryland, USA
Tatjana Stykel, TU Berlin, Germany
Chandramowli Subramanian, Karlsruhe Institute of Technology, Germany
Zoran Tomljanović, University of Osijek, Croatia
Nick Trefethen, Oxford University, UK
Ninoslav Truhar, University of Osijek, Croatia
Eugene Tyrtysnikov, Russian Academy of Sciences, Russia
Aleksandar Ušćumlić, University of Zagreb, Croatia
Marc Van Barel, Katholieke Universiteit Leuven, Belgium
Kresimir Veselić, FernUniversität Hagen, Germany
Matthias Voigt, TU Chemnitz, Germany
Daniel Wachsmuth, RICAM Linz, Austria
David Watkins, Washington State University, USA
Jens-Peter Zemke, TU Hamburg-Harburg, Germany