

MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

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Numerical Linear Algebra with Applications

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The conference, organized by Gene H. Golub (Stanford), Wilhelm Niethammer (Karlsruhe) and Richard S. Varga (Kent), was attended by 43 individuals from 13 countries. The 38 contributed lectures at this meeting offered a broad view of actual topics in numerical linear algebra. One major topic was the iterative solution of large linear systems of equations and — to some extent — eigenvalue problems. In addition, developments in other areas were included, where tools from linear algebra were used.

In connection with iterative methods, theoretical problems, such as the stability of different cg-like and Krylov subspace methods, were examined. Several talks considered iterative methods for the Navier-Stokes, the Helmholtz and the Maxwell equations. Substructuring and multisplitting techniques were also discussed.

Numerical methods from linear algebra in control theory and signal processing were considered. Other applications discussed were the use of matrix least squares for adjusting deformable mirrors in telescopes, and the simulation, via matrix theory, of material properties of plating devices. Several talks were devoted to inverse problems and corresponding regularizing methods. Finally, some theoretical questions, such as the minimization of condition numbers and the stability of matrix norms, were treated.

As a result of the wide variety of related topics and the good mixture of experts from theory and applications, the intimate atmosphere of the conference led to many fruitful discussions and initiated forthcoming joint projects.





Vortragsauszüge

G. S. Ammar:

Computing the zeros of Szegő polynomials

The zeros of Szegő polynomials arise in time series and signal processing applications as the poles of autorcgressive processes. We present a new procedure for computing these zeros, based on the fact that a Szegő polynomial is the characteristic polynomial of a Hessenberg matrix determined by the associated Schur parameters (reflection coefficients). The procedure first computes the eigenvalues of a unitary Hessenberg matrix, using a of several eigenvalue algorithms for this problem. These eigenvalues are then used as starting points for a continuation (path-following) procedure, which terminates at the desired eigenvalues of a particular "sub-unitary" matrix. In this way we can exploit the special structure of the Hessenberg matrix. The procedure is efficient and parallelizable, and may therefore be suitable for real-time implementation.

This is joint work with D. Calvetti and L. Reichel.

Z. Bai:

Parallel solution of nonsymmetric eigenvalue problems and its applications

With the growing demands from a large number of disciplines and interdisciplines of science and engineering for the numerical solution of the nonsymmetric eigenvalue problem, competitive new techniques have been developed for solving the problem over the past decade. In this talk, we examine the state of the art of the algorithmic techniques and the software scene for the problem. A design of a nonsymmetric eigenroutine tool box will be proposed.

Part of this work is joint with James Demmel at University of California at Berkeley.

A. Björck:

Lanczos methods for ill-posed linear systems

The conjugate gradient method is among the most efficient iterative methods for ill-posed linear systems. However, it is essential that the iterations are terminated after the optimal number of steps. Methods based on Lanczos bidiagonalization can be combined with regularization in a Kryov subspace. This avoids problems with semi-convergence. If performed with full reorthogonalization generalized cross validation generally provides a reliable rule for chosing the regularization parameter. Finally it is discussed how the implicit shift Lanczos method of Sorensen can be used to achieve regularization.

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D. Bolev:

A block nonsymmetric Lanczos algorithm with multiple starting vectors

We propose a nonsymmetric Lanczos algorithm for multiple starting vectors. This is motivated by applications in control. We will formulate the method to include look-ahead by combining the two-sided Gram-Schmidt process of Parlett with a process to generate the two Krylov sequences (left and right). We discuss the generalization of the single starting vector algorithm from the viewpoint of the structure of control models, and give an example involving the eigenvalues of a matrix.

A. Bunse-Gerstener:

Unitary Hessenberg methods for signal processing problems

A basic problem in signal processing is to find an approximation to an observed signal by a sum of weighted sinusoids or exponentials. Methods for solving this problem are often based on the idea of approximating the Toeplitz matrix of autocorrelation lags of a certain dimension by a singular Toeplitz matrix T and receiving from its kernel approximations to the desired frequencies. To any Hermitian positive semidefinite Toeplitz matrix we can associate a unitary Hessenberg matrix H and the eigenvalues of H and the first components of its eigenvectors give the information about the frequencies and weights, respectively. Efficient eigenvalue methods especially developed for unitary matrices can thus be employed to compute the desired qualities. Making use of the relation between Toeplitz matrices and unitary Hessenberg matrices we can solve the Toeplitz approximation problem posed by Kung under a mild restriction. In particular for real signals this solution turns out to be a generalization of the composite sinusoidal wave method and has an interpretation as an isometric Arnoldi process applied to the downshift operator and the observed signal.

This is joint work with C. He.

D. Calvetti:

An adaptive Richardson iteration method for indefinite linear systems

An adaptive Richardson iteration method is presented for the solution of large linear systems of equations with a sparse, symmetric, nonsingular, indefinite matrix. The relaxation parameters for Richardson iteration are chosen to be reciprocal values of Leja points for a compact set $K = [a, b] \cup [c, d]$, where [a, b] is an interval on the negative real axis and [c, d] is an interval on the positive real axis. Endpoints of these intervals are determined adaptively by computing certain modified moments during the iterations. Computed examples are presented to show that this adaptive Richardson algorithm can be competitive with SYMMLQ and CR.



This is joint work with L. Reichel.

T. F. Chan:

Analysis of a CG-based method for solving linear systems with multiple right hand sides

We analyze the conjugate gradient method proposed by Smith, Petrson and Mittra to solve the linear system AX = B where A is SPD and B is a multiple of right hand sides. This method generates a Krylov subspace from a set of direction vectors obtained by solving one of the systems (the seed) by the CG method and then project the residual of the other systems to get an approximate solution. The whole process is repeated with another unsolved system as a seed until all the systems are solved. We observe practice a sperconvergence behavior of the CG process. We also observe that only a few restarts a required to solve all the systems if the right hand sides are close to each other. These two features together make the method particularly effective. We give theoretical proof to justify these two obervations. Furthermore, we propose a block extension of this method.

L. Elden:

Accurate least squares solutions for Toepliz matrices

We present a new algorithm for triangularizing an $m \times n$ Toeplitz matrix. The algorithm is a modification of a previous algorithm that exploits the Toeplitz structure and computes each row of the triangular factor by updating and downdating steps. Due to ill-conditioned downdating transformations, the previous algorithm gives inaccurate results for certain problems. We show that it is possible to postpone such ill-conditioned downdates, and perform them at the end using a more accurate downdating method based on corrected seminormal equations. Numerical examples are presented, which show that the new algorithm improves the accuracy significantly, while the complexity remains only O(mn).

T. Elfing:

A constrained Procrustes problem

The following constrained matrix problem is studied. Find the matrix X which minimizes the Frobenius norm of AX - B, with A and B given matrices and where X is restricted to a closed convex cone. In particular, we consider the cone of symmetric positive semidefinite matrices and the cone of (symmetric) elementwise nonnegative matrices. The optimal matrix is characterized and the result is specialized to the two cases above. Further we report from a numerical study of some projection type algorithms.

This is joint work with Lars-Erik Andersson.

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H. Ehman:

Preconditioned iterative methods for the discrete Navier-Stokes equations

Discretization of the steady state Navier-Stokes equations

$$-\nu\Delta u + u \cdot \nabla u + \nabla p = f$$
$$-\operatorname{div} u = 0$$

gives rise to asystem of nonlinear algebraic equations for discretized velocities (u) and pressures (p). Linearization using a Picard iteration leads to a matrix equation of the form

$$\left[\begin{array}{cc} A & B^T \\ B & 0 \end{array}\right] \left[\begin{array}{c} u \\ p \end{array}\right] \left[\begin{array}{c} f \\ 0 \end{array}\right].$$

We present several preconditioning strategies for this system that produce eigenvalue distributions that are independent of the mesh size used in the discretization. Numerical experiments with GMRES and QMR iterative solvers confirm this mesh independence of convergence rates on the viscosity μ .

This is joint work with David Silvester.

L. Elsner:

Minimizing condition numbers by completion

There are applications, for example when solving block tridiagonal systems, where in a matrix a rectangular block X has to be specified so that the condition is moderate. The question of an optimal choice is unsolved. Here we give the solution in an important special case, where

$$W(X) = \begin{bmatrix} A & B \\ B^H & X \end{bmatrix}, \qquad A = A^H, X = X^H.$$

A is positive definite and X is restricted to the set of all $X = X^H$, such that W(X) > 0. The problem

$$\min\{||W(X)||\cdot||W^{-1}(X)||: X=X^H, W(X)>0\}$$

can be reduced to the problem of finding the minimum of a strictly convex function on an interval.

This is joint work with C. He and V. Mehrmann.

O. Ernst:

An iterative imbedding algorithm for exterior Helmholtz problems

We introduce a variational formulation for an exterior boundary value problem for the



Helmholtz equation as they typically arise in scattering problems. It is shown how an FFT-based fast solver can be used to solve this problem for special domains taking into account even an exact radiation boundary condition. An imbedding method is then used to treat arbitrary domains. These methods require the solution of a small dense linear system of equations. Using the theory of integral equations, we show that Krylov subspace methods converge mesh-independently when used to solve this systems.

B. Fischer:

Practical use of Bernstein-Szegő polynomials in matrix computations

In this talk we investigate the use of Bernstein-Szegő (BS) polynomials in matrix compatitions. These polynomials may be viewed as weighted Chebyshev polynomials. The basidea is to model the associated weight function after the (unknown) eigenvalue distribution of a given large symmetric matrix.

Beside the actual computation of the weight function and the corresponding BS polynomials we will outline two problem classes where these polynomials may used to advantage.

First, we consider the problem of computing a few eigenvalues of a given matrix using the Lanczos process. Here the BS polynomials serve as so-called polynomial filters for either the initial vector or the matrix itself. Second, we discuss polynomial iteration methods for the solution of large linear systems of equations (with possibly multiple right hand sides). We will show that the BS polynomials define a powerful polynomial preconditioner and may be used as kernel for a competitive semi-iterative method.

The effectiveness of the proposed applications will be demonstrated in a variety of numerical examples.

This is joint work with Roland W. Freund.

R. W. Freund:

Efficient circuit analysis by Padé approximation via the Lanczos process

Recently, a new approach, called asymptotic waveform evaluation (AWE), for the simulation of large linear networks has been proposed. The AWE method is often considerably faster than traditional circuit-simulation techniques such as SPICE. However, AWE sufferom a number of serious numerical difficulties. In this talk, we show that AWE is actually numerically unstable. We propose a new implementation of the Padé approximation, on which AWE is based, via the look-ahead Lanczos process. The resulting algorithm, called Padé via the Lanczos process (PVL), is numerically stable. We present results of numerical experiments with PVL for a variety of circuits. Finally, we discuss extension of PVL to the multi-input, multi-output case that is based on a new general block Lanczos process.

This is joint work with Peter Feldmann (AT&T Bell Labs).



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S. K. Godunov:

Stability of the Krylov basis and subspaces

The problems of numerical analysis with large sparse matrices involve often a projection of this matrix on a Krylov subspace to obtain a smaller matrix which is used to solve the initial problem. The subspace depends on the matrix and on an arbitrary vector. We consider, in this paper, a method to study the stability of the Krylov subspace through a matrix perturbation. This method includes a definition of the condition numbes for the computation of the Krylov basis and the Krylov subspace. A practical method for estimating these numbers is provided. It is based on the solution of a large triangular system.

This is joint work with J. F. Carpeaux and S. V. Kuznetsov.

M. Goldberg:

Matrix norms: multiplicativity, quadrativity, and stability

Let $||\cdot||$ be a norm or a seminorm on $\mathbb{C}^{n\times n}$, the algebra of $n\times n$ complex matrices. A constant $\mu>0$ is called a multiplicativity factor for $||\cdot||$ if $||AB||\leq \mu||A||\cdot||B||$ for all A,B in $\mathbb{C}^{n\times n}$. Similarly, $\lambda>0$ is a quadrativity factor for $||\cdot||$ if $||A^2||\leq \lambda||A||^2$ for all A in $\mathbb{C}^{n\times n}$. Further we say that $||\cdot||$ is stable if for some $\sigma>0$ we have $||A^k||\leq \sigma||A||^k$ for all A in $\mathbb{C}^{n\times n}$ and all positive integers k. In particular, we call $||\cdot||$ strongly stable if $||\cdot||$ is stable with $\sigma=1$.

We begin this talk by discussing the existence of multiplicativity and quadrativity factors for arbitrary seminorms and norm on $\mathbb{C}^{n\times n}$. We exhibit the best (least) factors for certain well-known norms; and then proceed to show that while norms always have such factors, proper seminorms do not. The second part of the talk is devoted to stability. Our main objective here is to prove that not all stable norms on $\mathbb{C}^{n\times n}$ are strongly stable.

A. Greenbaum:

Accuracy of computed solutions from conjugate gradient-like methods

A framework is established for determing the accuracy of computed solutions from conjugate gradient-like methods for solving linear systems. It is shown that the difference between the actual residual vectors generated by such a method depends on the machine precision ε and on the maximum growth in norm of the iterates over their initial value and the norm of the true solution. To estimate the size of the smallest actual residual one should: 1) show that the updated approximate residual vectors converge to zero, and 2) bound the growth in norm of the iterates.

Using this technique, it is shown that the steepest descent method and the conjugate



gradient method for SPD problems generate approximate solutions with relative residuals of order ε . This is also the case for the CGNE method for nonsymmetric problems, and it is conjectured to be the case for the CR method applied to symmetric indefinite problems. It is shown that the ORTHODIR method for nonsymmetric problems generates an approximate solution with relative residual bounded by $\kappa O(\varepsilon)$, where κ is the condition number of the matrix. It is argued that the smallest residual vector for stationary iterative methods, as well as some other methods that do not minimize any standard error norm, cannot be bounded, in general, and that occasionally these methods may fail to produce an accurate approximate solution to even a well-conditioned linear system.

M. H. Gutknecht:

Local minimum residual smoothing

Schönauer (1987) introduced a smoothing process suitable for nonmonotonically (or even "erratically") converging iterative methods for solving linear systems, such as, in particular, BiCG. Here, we first generalize this smoothing process (LMR1) by replacing the one-dimensional local minimum residual computation of each step by a two (LMR2) or even higher dimensional (LMR(l)) minimization process. Numerical results exhibit that LMR1 and LMR2 are very effective in smoothing the residual norm history of BiCG and (Bi)CGS, and LMR2 is, in general, somewhat superior to LMR1.

An alternate idea is to integrate the LMR principle directly into a transpose-free Lanczos-type product method. BiCGStab can be understood as such a product method with the second factor being determined by LMR1. However, integrating LMR2 does not lead to BiCGStab2, but to a more effective method, BiCG*LMR2.

M. Hanke:

Stopping rules for conjugate gradient regularization based on error estimation

The conjugate gradient iteration is one of the most powerful methods for computing regularized approximations of linear and structured 2D or 3D inverse problems. Here, the regularization effect stems from early stopping of the iteration, since the iteration index takes the role of a regularization parameter. As a consequence, the development of reliable stopping rules is one of the major demands in this context. In the talk, we present a new "heuristic stopping rule" (i.e., a rule which avoids any information about the noise level in the right-hand side data): it is based on the theoretical analysis of the discrepancy principle as given by Nemirovskii. The method is shown to perform better than the so-called L-curve criterion. The new stopping rule can also be generalized to a particular minimal residual type method for selfadjoint indefinite problems.



C. He:

The matrix sign function method and the computation of invariant subspaces

The matrix sign function method is discussed as a method to split the eigenspace of a matrix A into two invariant subspaces corresponding to its stable and unstable eigenvalues, respectively. A new perturbation theorem for the matrix sign function is presented which shows that the method is competitive to the conventional methods for computing invariant subspaces, provided a numerically stable method for computing the sign function is given. We will analyze the properties of the Newton iteration in this context.

This is joint work with Ralph Beyers and Volker Mehrmann.

N. J. Higham:

From the matrix sign function to the polar decomposition

We show that it is useful to regard the matrix sign function as being part of a matrix sign decomposition. This leads to a new representation for sign(A) and reveals analysis with the polar decomposition. We derive a parallel method for computing the polar decomposition from a corresponding method of Kenney and Laub for the matrix sign function, and describe its implementation on the Kendall Square KSRI computer.

M. Hochbruck:

A Chebyshev-like semiiteration for inconsistent linear systems

Semiiterative methods are known as a powerful tool for the iterative solution of nonsingular linear systems of equations. For singular but consistent linear systems with coefficient matrix of index one, one can still apply the methods designed for the nonsingular case. However, if the system is inconsistent, the approximations usually fail to converge. Nevertheless, it is still possible to modify classical methods like the Chebyshev semiiterative method in order to fulfill the additional convergence requirements caused by the inconsistency. These modifications may suffer from instabilities since they are based on the computation of the diverging Chebyshev iterates. In this talk we present an alternative algorithm which allows to construct more stable approximations. This algorithm can be efficiently implemented with short recurrences. There are several reasons indicating that the new algorithm is the most natural generalization of the Chebyshev semiiteration to inconsistent linear systems.

In addition, we show that this framework can also be applied to cg-type methods. Here, different choices for the underlying inner product lead to the stabilized OD method, a minimal residual method, and a new algorithm which minimizes the error in the energy norm.

This is joint work with Martin Hanke, Universität Karlsruhe,



T. A. Manteutfel:

FOSLS: A methodology for solving systems of PDEs

The process of modeling a physical system involve creating a mathematical model, forming a discrete approximation, and solving the resulting linear or nonlinear system. As numerical linear algebraists, we are most interested in the last step. Too often, however, we are handed matrix equations that possess properties that make them difficult to solve, for example, nonsymmetry and indefiniteness. Too often, the solution, when found, is a poor approximation to the solution of the model. In this talk I will outline a methodology for rearranging the mathematical model in a way that naturally leads to accurate discretizations that are especially amenable to numerical solution. In particular, we will examine general second-order elliptic partial differential equations. The methodology in volves expanding the original equation as a system of first-order equations by introducing new variables, adding extra constraints, and constructing a least squares functional. The bilinear form associated with the functional will be shown to be elliptic with respect to the H^1 norm in each variable. This guarantees that a discrete system based on simple finite element subspaces will possess particularly nice properties; for example, they will be symmetric positive definite with condition $O(h^{-2})$. Moreover, multilevel techniques yield rapid convergence.

G. Mayer:

Multisplitting methods

Multisplitting methods are parallel iterative methods for linear systems Ax = b, where A is a non-singular $n \times n$ matrix and b is a vector with n components. They are based on p splittings $A = M_l - N_l$, M_l non-singular, $l = 1, \ldots, p$, and some averaging process. More exactly, the new iterate x^{k+1} is defined by

$$x^{k+1} := \sum_{l=1}^{p} E_{l} M_{l}^{-1} (N_{l} x^{k} + b),$$

where the weighting matrices E_l are non-negative diagonal matrices of which the sum is the identity matrix.

In our talk we will consider particular multisplitting methods for band matrices. We will present new comparison results which we illustrate by numerical examples.

V. Mehrmann:

Staircase like forms for the computation of invariants of descriptor systems

This talk concerns the structure that can be achieved by feedback in descriptor systems





that lack certain controllability and/or observability conditions. Staircase and double stair case condensed forms obtained through a sequence of orthogonal state transformations are used to determine the invariants of the system and display when and how feedback can be used to achieve minimal index. Furthermore, they reveal that the modes that are uncontrollable and unobservable at infinity have a fixed minimal index that can not be reduced by feedback. However, this fixed higher index part of the control system is constrained to be zero. The remainder is a reduced order system that is controllable and observable at infinity which can be made to have index one by feedback.

G. Meurant:

Solving the Maxwell equations using conforming finite elements. Lagrange multipliers and iterative methods

In this talk, we consider solving the harmonic Maxwell equations using conforming finite elements in three dimensions. The aim of this work is to compute the scattering of an impinging electro-magnetic wave on a three dimensional perfectly conducting body. First, a variational formulation is described with usual Sobolev spaces. Then, the boundary condition $E \times n = g$ on the body is handled via a Lagrange multiplier. At this point usual conforming finite element approximations can be used. This leads to a large sparse linear systems of the form

 $\left[\begin{array}{cc} A & B^T \\ B & 0 \end{array}\right] x = b,$

where A is complex symmetric. This systems is solved with iterative methods. We used GMRES and Bi-CGSTAB as candidates. Of course, a preconditioner has to be used to improve the convergence rate. The one we chose is

$$M = \left[\begin{array}{cc} A & B^T \\ B & -\epsilon I \end{array} \right].$$

The preconditioned system at each iteration is also solved with an iterative method (actually GMRES or Bi-CGSTAB), so we have nested iterations.

We describe numerical experiments both on this difficult problem and also for the Helmholtz equation. It turns out that Maxwell equations are more difficult to solve and that the inner iterations have also to be preconditioned. This is done by an incomplete LU decomposition where we keep some fill ins according to their size. The experiments show that this leads to an efficient method for solving the Maxwell equations while retaining the simplicity of implementation of usual conforming elements.



R. Nabben:

Ultrametric matrices

Recently, Martinez, Michon. and San Martín introduced the new class of (symmetric) strictly ultrametric matrices. They proved that the inverse of a strictly ultrametric matrix is a strictly row and strictly column diagonally dominant Stieltjes matrix. Here, we generalize this result by introducing a class of nonsymmetric matrices, called generalized ultrametric matrices. We give a necessary and sufficient condition for the regularity of these matrices and prove that the inverse of a nonsingular generalized ultrametric matrix is a row and column diagonally dominant M-matrix. We establish that a nonnegative matrix is a generalized ultrametric matrix if and only if the matrix is a certain sum of at most rank-two matrices. Moreover, we give a characterization of generalized ultrametric matrices, based on weighted trees. The entries of generalized ultrametric matrices the arise as certain "distances" between the leaves and the root of the tree.

N. M. Nachtigal:

First principles simulation of material properties

In recent years, as the available computing power has increased, the capability to predict material properties from first principles based models has also increased. As a result, more and more emphasis is placed on predictive computer models that can assist experimental designers in their work.

The talk will present an overview of the material sciences effort at Oak Ridge National Lab, with an emphasis on the linear algebra and computation issues that arise.

A. Neumaier:

Iterative regularization for large-scale ill-conditioned linear systems

To solve a constraint regularization problem

$$Ax \approx b$$
, $x \geq 0$, Jx not large

we propose methods which are based on the convex envelope of a finite set of approximate solutions \tilde{x}_l , represented as a 2d plot of $(q(\tilde{x}_l), r(\tilde{x}_l))$, where

$$q(x) = ||Jx||_2^2, \quad r(x) = ||Ax - b||_2^2.$$

The envelope is updated after each iteration of a CG method with preconditioning for $f_{\lambda}(x) = r(x) + \lambda q(x)$, and λ is updated depending on the geometry of the envelope.

When the noise is small, an alternative method applies CG to the compromise function

$$f(x) = \sqrt{q(x)r(x)^6}.$$



whose interior local minimum typically gives a close match to simulated problems with a known designed solution.

The technique is applied to a linear system arising in tomography (PET), and the resolution of the reconstructed image is much better than for other iterative methods, while the amount of work is moderate (~ 20 matrix-vector products).

This is joint work with Linda Kaufman.

M. Neumann:

Convergence of infinite products of matrices and inner-outer iteration schemes

We develop conditions under which a product $\prod_{k=0}^{\infty} T_k$ of matrices chosen from a possibly infinite set of matrices $S = \{T_j | j \in J\}$ converges. We obtain the following conditions which are sufficient for the convergence of the product: There exists a vector norm such that all matrices in S are nonexpansive with respect to this norm and there exists a subsequence $\{i_k\}_{k=0}^{\infty}$ of the sequence of the nonnegative integers such that the corresponding sequence of operators $\{T_k\}_{k=0}^{\infty}$ converges to an operator which is paracontracting with respect to this norm. We deduce the continuity of the limit of the product of matrices as a function of the sequence $\{i_k\}_{k=0}^{\infty}$. But more importantly, we apply our results to the question of the convergence of inner-outer iteration schemes for solving singular consistent linear systems of equations, where the outer splitting is regular and the inner splitting is weak regular.

N. Nichols:

Computation of smooth singular value decompositions with an application to the regularization of time-varying differential-algebraic control systems

Smooth singular value decompositions are used to reduce a time-varying descriptor system, governed by the equations

$$E(t)\frac{dx}{dt} = A(t)x + B(t)u, \qquad y = C(t)x,$$

to a condensed form that reveals controllability and observability properties. Under suitable conditions derivate and proportional output feedback controls are then constructed to ensure that the systems is index one and pointwise regular. Initial experiments show that the feedback can also be selected so that the closed loop matrix E + BGC has constant rank over the interval of interest and is "near optimally" conditioned.

The smooth singular value decompositions are determined from the solutions to a system of ordinary differential matrix equations. A novel "orthogonality-preserving" numerical integration scheme is used to compute the right and left singular factors. A form of deferred correction leads to results of unusually high order of accuracy.



R. J. Plemmons:

A trace maximization problem in control

This problem involves the control of a set of very fast-acting deformable mirrors designed for atmospheric turbulence compensation in atmospheric imaging. Here the control model reduces to the maximization of the functional f(U) given by

$$f(U) = \sum_{j=1}^{R} \max\{(U^{T} M_{j} U)_{ii}\}$$

over unitary matrices U, where the M_j are the mirror matrices associated with the adaptive optics control problem. Various algorithms are suggested for partial solution to this problem and several open problems are discussed.

This is joint work with B. Ellenbroek, C. Van Loan and N. Pitsianis.

L. Reichel:

Incomplete partial fractions for parallel evaluation of rational matrix functions

Frequently one needs to evaluate expressions of the form $(p(A))^{-1}q(A)b$ where $A \in \mathbb{R}^{N \times N}$, $b \in \mathbb{R}^N$ and p and q are polynomials with $\partial q \leq \partial p$ and such that no zero of p is an eigenvalue of A. Algorithms based on the partial fraction representation of q/p when evaluating $(p(A))^{-1}q(A)b$ lend themselves well to implementation on parallel computers, but might yield poor accuracy. We discuss how to determine an incomplete partial fraction representation of q/p which allows parallel computation while retaining high accuracy.

This is joint work with D. Calvetti and E. Gallopoulos.

G. Starke:

Subspace orthogonalization and substructuring for nonsymmetric linear systems

We consider substructuring preconditioners in combination with various Krylov subspace methods for the solution of nonsymmetric systems of linear equations. In particular, we propose modifications of optimal iterative methods like GMRES by restricting the computation of inner products and storage of basis elements to a subset of the unknowns. This allows us to run the optimal iterative methods for much longer and produce an accurate approximation at these unknowns. If the subspace is chosen such that it constitutes a separator set, dividing the original problem into smaller pieces, these subproblems can then be solved independently in a final extension phase. The effectiveness of this approach will be illustrated by numerical experiments for non-self-adjoint elliptic boundary value problems.



G. W. Stewart:

On graded QR decompositions of products of matrices

This paper is concerned with the singular values and vectors of a product of the form $C_m = A_1A_2 + A_m$. The chief computational problem is that with increasing m the ratios of the smaller to the larger singular values of C_m may fall below the rounbding unit, so that the former are computed inaccurately. The solution presented here is to factor $C_m = QRP^T$, where Q is orthogonal, R is upper triangular, and P is a permutation. The matrix R is graded, with its ith row being approximately the size of the ith singular value. This means that even the small singular values can be computed accurately. The heart of the method is an algorithm for updating a graded QRP factorization of A to a graded QRP factorization of the product C = AB.

Z. Strakos:

On the numerical stability of the Krylov space methods for solving nonsymmetric systems

We will base our analysis on the basic recurrence formula for the basis of the Krylov space (or the Krylov residual space)

$$AV_k = V_{k+1}H_{k+1,k} + F_k (1)$$

where V_k is the matrix of the basis vectors v_j as its columns, $H_{k+1,k}$ is the upper Hessenberg matrix and F_k characterizes the rounding errors. $||F_k||$ is of the order $o(N,\epsilon)||A||$, where $o(N,\epsilon)$ denotes terms involving the product of the machine precision ϵ with a small power of N and a constant. Using the recurrence, the original problem for the matrix A is transformed in the Krylov methods to the more feasible problem for the matrix $H_{k+1,k}$. When the matrix A is highly nonnormal, then, using the bound $||A^*A - AA^*|| \leq 2||A||^2$, the matrix F_k may have large entries. Therefore, any method based on the matrix $H_{k+1,k}$ can be very inefficient or can even fail. For ||A|| reasonable bounded, the actual size of $||F_k||$ does not play an important role in our analysis. Then, a key question in the analysis and designing method based on (1) is "How to construct the efficient recurrence preserving the nonsingularity of the matrices V_{k+1} and $H_{k+1,k}$ " (well preserved nonsingularity of $H_{k+1,k}$ guarantees, e.g., that the norm of the residual of the transformed least squares problem (Arnoldi residual) is sufficiently close to the norm of the residual computed directly).

We will examine different approaches using both long and short term recurrences. We will present an error analysis of the GMRES method - including its newly proposed variants - and try to give a quantitative theoretical explanation of the experimental results reported in the literature.



H. van der Vorst:

A Jacobi-Davidson iteration method for linear eigenvalue problems

Davidson has proposed a method for the iterative computation of a few extremal eigenvalues of a symmetric matrix. The method is reported to be quite successful, especially for some applications in chemistry. Success of the method seems to depend quite heavily on strong (diagonal) dominance of the given matrix.

The method of Davidson is commonly seen as an extension to Lanczos' method. In spite of this the method is not well understood.

As we will show, Davidson's method has an interesting connection with an old method of Jacobi. This leads to another view on the method of Davidson, that may help to explain and to improve the method. It turns out that the method can be easily generalized non-diagonal dominant and nonsymmetric matrices as well.

P. van Dooren:

Computing the SVD of a product/quotient of several matrices

We present an implicit bidiagonalization method of a product or quotient of two or more matrices. The method applies only orthogonal transformations on the matrices of the product/quotient and implicitly bidiagonalizes the product/quotient. We analyze the complexity and accuracy of this approach and discuss its advantages over the current PSVD, QSVD code. We also show via numerical examples its high relative accuracy for expressions with regular values of large dynamical range.

Joint work with G. H. Golub and K. Solna.

Berichterstatter: Marlis Hochbruck und Gerhard Starke





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