Numerical Linear Algebra with Applications (NL2A)

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Topics:

The meeting will take place at CIRM (Luminy, Marseille). The main topics of the conference are:

- Large-scale matrix equations, Eigenvalue problems and Preconditioning.
- Ill-posed problems, Image restoration.
- Model reduction methods.
- Numerical methods for PDEs.
- Applications: Image processing, Optimal control,...

List of abstracts

Accelerating convergence in sparse least squares iterative solvers using LU factorization

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Abstract

We study how to use an LU factorization as a right-preconditioner of standard iterative methods (e.g., `lsqr` [1] or `lsmr` [2]) for solving overdetermined sparse least squares problems. Usually L is much better conditioned than A, so iterating with lower trapezoidal L instead of A gives a faster convergence. In previous work [3], we showed that when L is not sufficiently well-conditioned, we could use a partial orthogonalization of L to accelerate convergence. In this talk, we illustrate that, alternatively to partial orthogonalization, convergence can be improved by iterating with LL_1^{-1} where L_1 is the square upper triangular part of L, resulting in a cheaper algorithm. Mixed precision techniques [4] can be also used to reduce execution time.

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On the numerical rank of positive definite Hankel matrices

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Abstract

Matrices with displacement structure such as Pick, Vandermonde, and Hankel matrices appear in a diverse range of applications. In this talk, we use an extremal problem for rational functions to derive explicit bounds on the singular values of such matrices. For example, we show that the kth singular value of a real $n \times n$ positive semidefinite Hankel matrix, H, with $n \geq 2$, is bounded by $Ce^{-\alpha k/\log n}\|H\|_2$ with explicitly given constants C and $\alpha > 0$, where $\|H\|_2$ is the spectral norm. This means that any positive semidefinite Hankel matrix can be approximated, up to an accuracy of $\epsilon\|H\|_2$ with $0 < \epsilon < 1$, by a rank $R = \mathcal{O}(\log n \log(1/\epsilon))$ matrix. Analogous results are obtained for Pick, Cauchy, real Vandermonde, and Löwner matrices.

References

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An Iterative method for computing a symplectic SVD-Like decomposition

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Abstract

We present in this paper a constructive iterative method to compute symplectic SVD-like decomposition for a $2n$-by-m rectangular real matrix A. The main purpose is based on using a block power iterative method and R^JR decomposition in order to compute a k-block $J-SVD$ decomposition, namely $A_k = S_k\Sigma_k V_k^T$ where $S_k \in \mathbb{R}^{2n\times 2s}$ is symplectic and $V_k \in \mathbb{R}^{m\times 2s}$ is orthogonal. This method allows us to compute eigenvalues of structured matrices.

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Generalized matrix functions: properties, algorithms, and applications

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Abstract

Generalized matrix functions were introduced in 1973 by Hawkins and Ben-Israel as a way to extend the notion of a matrix function to rectangular matrices [2]. If A is a matrix of rank r and $A = U_r \Sigma_r V_r^*$ is a compact singular value decomposition of A, then one can define a function of A as $f(A) := U_r f(\Sigma_r) V_r^*$ for any scalar function f defined on the singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$ of A. (Note that, generally speaking, this kind of matrix function does not reduce to the usual one when A is square.) While the paper by Hawkins and Ben-Israel attracted little attention, generalized matrix functions arise naturally in various applications, and over the course of time several authors have made use of them without recognizing them as such. In this talk I will review the basic properties of generalized matrix functions and discuss some applications and numerical methods for their approximation.

The talk is based on joint work with Francesca Arrigo and Caterina Fenu [1].

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Computing matrix functions of infinite quasi-Toeplitz matrices

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Abstract

In certain applications concerning stochastic processes, like the analysis of a random walk in the quarter plane, one encounters semi-infinite matrices $P = (p_{i,j})_{i,j\in\mathbb{Z}^+}$ which can be written in the form $P = T(a) + F$, where $T(a) = (t_{i,j})_{i,j\in\mathbb{Z}^+}$ is a Toeplitz matrix associated with the symbol $a(z) = \sum_{k\in\mathbb{Z}} a_k z^k$, i.e., $t_{i,j} = a_{j-i}$, moreover $a(z)$ and $F = (f_{i,j})_{i,j\in\mathbb{Z}}$ are such that $\sum_{k\in\mathbb{Z}} |a_k| < +\infty$, and $\sum_{i,j\in\mathbb{Z}^+} |f_{i,j}| < +\infty$. We call a matrix P of this form a semi-infinite quasi-Toeplitz matrix.

In this talk we present some results concerning this class of matrices together with some related computations. More specifically, we show that quasi-Toeplitz matrices associated with a symbol $a(z)$ which is analytic over an annulus $\mathbb{A}(r, R) = \{z \in \mathbb{C} : \quad r < |z| < R\}$, where $0 < r < 1 < R$, form a matrix algebra endowed with a sub-multiplicative norm. As a consequence, we prove that the matrix exponential $Y = \exp(X)$ of a quasi-Toeplitz matrix X is well defined and is still a quasi-Toeplitz matrix. We also provide efficient algorithms for its computation. These results are extended to the case of general matrix functions under suitable mild conditions.

We also prove that matrix equations of the kind $AX^2 + BX + C = 0$, which model infinite random walks where the coefficients A, B, C are semi-infinite quasi-Toeplitz matrices, have a nonnegative solution G which is still semi-infinite quasi-Toeplitz. We also provide effective algorithms, for the computation of G, based on the cyclic reduction iteration.

Finally we present a Matlab implementation of the matrix arithmetic in the algebra of semi-infinite quasi-Toeplitz matrices where $T(a)$ is represented by means of the numerical truncation of $a(z)$ and F is represented as the product $F = UV^T$ where U and V have a finite number of columns and their entries $u_{i,j}$ and $v_{i,j}$ are zero for i sufficiently large. This toolbox enables one to easily implement algorithms for the computation of certain matrix functions $f(X)$ of a semi-infinite quasi-Toeplitz matrix X, and to solve quadratic matrix equations where coefficients and unknown are semi-infinite quasi-Toeplitz matrices. Numerical experiments are presented.

References

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[2] D.A. Bini, S. Massei, B. Meini, Quasi-Toeplitz infinite matrix arithmetic with applications. In preparation (2016)

Anderson Acceleration and the Reduced Rank Extrapolation

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Abstract

In this talk, we compare two well-known schemes for accelerating sequences of vectors. The first is Anderson mixing [1] which has been widely used in physics and the second is the Reduced Rank Extrapolation (RRE) algorithm [2, 3] which is a standard 'general' technique designed for accelerating arbitrary sequences. It is known that the two methods are mathematically equivalent in the linear case. This paper establishes their equivalence in the nonlinear case.

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Point-spread function reconstruction in ground-based astronomy

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Abstract

Because of atmospheric turbulence, images of objects in outer space acquired via ground-based telescopes are usually blurry. One way to estimate the blurring kernel or point spread function (PSF) is to make use of the aberration of wavefront received at the telescope, i.e., the phase. However only the low-resolution wavefront gradients can be collected by wavefront sensors. In this talk, I will discuss how to use regularization methods to reconstruct high-resolution phase gradients and then use them to recover the phase and the PSF in high accuracy.

Stabilized Time Marching Schemes for High Accurate Finite Differences Solutions of Nonlinear Parabolic Equations

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Abstract

The present work deals with the stabilization of explicit time marching schemes for parabolic equations, with a special attention to the high order finite differences discretization in space. These type of stabilized schemes, have been introduced independently in [1] and [4] (but in a spectral point of view) as a backward Euler's method with a simplified implicit part for the solution of parabolic problems, the simplification is realized by using proper pre-conditioners of the implicit part. We propose here a unified framework and derive general stability properties in the linear and in the nonlinear case. Practical implementations and extensions are proposed for the long time simulation of nonlinear parabolic problems when discretized by using high order finite differences compact schemes. Numerical simulations of Phase Fields problems in image processing as well as in fluid dynamics (2D incompressible Navier-Stokes Equations) are presented [2].

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Uniqueness of solution of systems of generalized Sylvester and $\star$-Sylvester equations

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Abstract

The *generalized Sylvester equation*

$$AXB - CXD = E$$

has been a subject of interest since, at least, the early 20th century. Recently, the $\star$*-generalized Sylvester equation*

$$AXB - CX^{\star}D = E,$$

with $\star$ being either the transpose or the conjugate transpose, has attracted some attention within the linear algebra community.

In this talk, we provide necessary and sufficient conditions for the uniqueness of solution of homogeneous systems of generalized Sylvester and $\star$-Sylvester equations, namely

$$A_i X_{\alpha_i}^{s_i} B_i - C_i X_{\beta_i}^{t_i} D_i = 0, \qquad i = 1, \ldots, r,$$

with $s_i, t_i \in \{1, \star\}$.

We focus on the case where the system has the same number of equations and unknowns (namely, r), and where all coefficient matrices (and unknowns) are square and with the same size.

Spectral analysis and numerical methods for fractional diffusion equations

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Abstract

Fractional partial diffusion equations (FDEs) are a generalization of classical partial differential equations, used to model anomalous diffusion phenomena. Several discretization schemes (finite differences, finite volumes, etc.) combined with (semi)-implicit methods leads to a Toeplitz-like matrix-sequence.

In the constant diffusion coefficients case such a matrix-sequence reduces to a Toeplitz one, then exploiting well-known results on Toeplitz sequences, we are able to describe its asymptotic eigenvalue distribution. In the case of nonconstant diffusion coefficients, we show that the resulting matrix-sequence is a generalized locally Toeplitz (GLT) and then we use the GLT machinery to study its singular value/eigenvalue distribution as the matrix size diverges (see [4]).

The new spectral information is employed for analyzing preconditioned Krylov and multigrid methods recently appeared in the literature [2, 3], with both positive and negative results. Moreover, such spectral analysis guides the design of new preconditioning and multigrid strategies. We propose new structure preserving preconditioners with minimal bandwidth (and so with efficient computational cost) and multigrid methods for 1D and 2D problems (see [1] for the 1D case). Some numerical results confirm the theoretical analysis and the quality of the new proposals.

References

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Strong linearizations of rational matrices: theory and explicit constructions

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Abstract

Rational eigenvalue problems (REPs) $G(\lambda)x = 0$, where $G(\lambda)$ is a regular matrix whose entries are rational functions of the variable λ, arise in interesting applications [3] [4] and their numerical solution is a challenging problem [3]. Recently, a new method for solving REPs was proposed in [4]. This method is based on constructing first a linear pencil whose finite eigenvalues are the finite eigenvalues of $G(\lambda)$, i.e., those finite zeros of $G(\lambda)$ which are not poles, and then on applying a standard algorithm for the generalized eigenvalue problem to such linear pencil. This linear pencil is called a *linearization* of the *rational matrix* $G(\lambda)$. The method introduced in [4] has been formalized and generalized in [1], where a formal definition of a linerization of a square rational matrix is introduced, which indeed guarantees that the finite eigenvalues of the linearization are the finite eigenvalues of the rational matrix. In addition, many examples of linearizations are explicitly constructed in [1] based on the well known Fiedler linearizations of matrix polynomials. However, apart from other technical drawbacks, the definition of linearization in [1] does not guarantee that such pencils reflect the structure at infinity of the rational matrix. In this talk, we introduce the new concept of *strong linearization* of an arbitrary rational matrix that may be square or rectangular, regular or singular, and prove rigorously that such pencils reflect the complete finite and infinite zero and pole structures of the rational matrix. Moreover, we construct explicitly infinitely many examples of strong linearizations. These constructions take as inputs a minimal state-space realization of the strictly proper part of $G(\lambda)$ and any strong block minimal bases linearization [2] of its polynomial part.

References

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Direct nonlinear imaging via data-driven discrete-time ROMs of large-scale wave propagation

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Abstract

The inverse coefficient problems for large scale PDEs are notoriously computationally extensive. They are normally solved by nonlinear (often nonconvex) data fitting via multiple PDE solves. A popular approach to address computational complexity is to use reduced order models (ROMs) for data simulation as proxies for expensive PDE solvers. Instead, here we directly image the unknown coefficient distributions from ROMs obtained by interpolating measured data. We focus on the time-domain problem of seismic exploration, which is possibly the most difficult inverse problem for linear time-invariant dynamic systems due to huge sizes of PDE grids and Jacobians, resulting in weeks and even months of processing time.

We consider multidimensional inverse problems for acoustic wave equation with an array of m receivers (outputs). The shots are fired by moving the transmitter (input) consequently at the receiver positions, so the data are the elements of the MIMO transfer function $F(t) = F(t)^* \in \mathbb{R}^{m\times m}$, sampled at $t = j\tau$, $j = 0, \dots, 2n-1$. The imaging algorithm is outlined below.

1. Compute discrete-time ROM on data with stiffness and mass matrices as sums of block Toeplitz and Hankel matrices of data [2].
2. Transform the above ROM to block-tridiagonal form via block-QR transform computed with the help of block-Cholesky decomposition of the mass matrix [1].
3. Image unknown coefficient (reflectivity distribution) via approximate Galerkin approximation of the true (unknown) PDE operator with the help of the above block-tridiagonal matrix and global basis functions for some known (e.g., constant coefficient) problem.

Steps 1 and 3 are linear and step 3 is not, and it suppresses nonlinear data artifacts such as multiple reflections and de-focusing of the wave package. The success of our algorithm is based on *week dependence* of the QR-reorthogonolized ROM basis on the PDE coefficient distribution, which sets it (the algorithm) favorably apart from other known MOR approaches.

We present 2D numerical examples for geophysical (seismic, sonic) and medical (ultrasound) applications.

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Block Lanczos Algorithm for Digital Colour Images

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Abstract

In this work we present an efficient algorithm for solving a Tikhonov regularization problem for multichannel image deblurring when the model is described by a linear system of equations with multiple right-hand sides contaminated by errors. The proposed method is based on the symmetric block Lanczos algorithm, in connection with block Gauss quadrature rules [1] to inexpensively determine a value of the regularization parameter when using the discrepancy principle and an associated approximate solution of colour images degraded by within- and cross-channel blurs, as well as additive Gaussian noise [2].

References

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Varying the s in s-step GMRES

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Abstract

Krylov methods are commonly used iterative methods for solving large sparse linear systems, however they suffer communication bottlenecks on parallel computers. Therefore, s-step methods have been developed where the Krylov subspace is built block by block, with a fixed block size s. We develop an adaptive s-step GMRES algorithm, where the block size is variable and increases gradually. We give lower bounds for the condition numbers of each block. In our numerical experiments, we compare our variable approach to a fixed one. Results show that our strategy allows a faster convergence in most cases.

References

[1] D. IMBERTI AND J. ERHEL, *Vary the s in Your s-step GMRES*, preprint, submitted (2016). https://hal.inria.fr/hal-01299652.

Iterative regularization in variable exponent Lebesgue spaces

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Abstract

Let us consider a functional equation $Af = g$ characterized by an ill-posed linear operator $A : X \longrightarrow Y$ between two Banach spaces X and Y. In this talk, we propose an extension of the Tikhonov regularization approach to the (unconventional) setting where X and Y are both two variable exponent Lebesgue spaces. Basically, a variable exponent Lebesgue space $L^{p(\cdot)}$ is a (non-Hilbertian) Banach space where the exponent $1 \leq p(\cdot) \leq +\infty$ used in the definition of the norm is not constant, but rather is a function $p(\cdot)$ of the domain [1]. This way, instead of $\int |f(x)|^p dx$ with p constant, to measure a function f in such a $L^{p(\cdot)}$ Banach spaces we have to compute

$$\int |f(x)|^{p(x)} dx \, .$$

Inside the general framework of the regularization theory in Banach spaces [2], we develop an iterative regularization method in variable exponent Lebesgue spaces $L^{p(\cdot)}$ based on duality maps, which is able to adaptively and automatically set up pointwise different regularization levels. Indeed, the formulation of the ill-posed problem in a variable exponent Lebesgue space $L^{p(\cdot)}$ allows us to assign different regularization parameters, related to different values of the function parameter $p(\cdot)$, on different regions of the domain.

In the case of image deblurring problems, different pointwise regularization is useful because background, low intensity, and high intensity values of the image to restore require different filtering (i.e., regularization) levels [3]. This way, the proposed iterative algorithm represents a natural and continuous extension of early procedures based on image segmentation techniques, developed to vary the "amount" of regularization depending on the "local" signal to noise ratios in all the different portions of the image domain. A numerical evidence of the proposal will be also discussed.

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Block Matrix Formulations for Evolving Networks

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Abstract

Many types of pairwise interaction take the form of a fixed set of nodes with edges that appear and disappear over time.

In the case of discrete-time evolution, the resulting evolving network may be represented by a time-ordered sequence of adjacency matrices. More precisely, let $\{G^{[k]}\}_{k=1}^{M} = \left(V, \{E^{[k]}\}_{k=1}^{M}\right)$ be a sequence of unweighted graphs evolving in discrete time, that is, the set of nodes V, with $|V| = n$, is fixed and the dynamism is given by the change in the set of the arcs. With this notation, given the ordered sequence of time points $\{t_k\}_{k=1}^{M}$, the network at time t_k is represented by its $n \times n$ adjacency matrix $A^{[k]}$. As usual for unweighted networks, the (i, j)th entry of $A^{[k]}$ equals 1 if there in an edge from node i to node j at time t_k, and 0 otherwise. This type of connectivity structure arises naturally in many types of human interaction. For example, within a given population, we may record physical interactions, phone calls, text messages, emails, social media contacts or correlations between behavior such as energy usage or on-line shopping [1].

Although we may regard $\{A^{[k]}\}_{k=1}^{M}$ as a three dimensional tensor, we emphasize that, in this context, the third dimension is very different from the first two. Typical quantities of interest are invariant to the ordering the nodes—we may consistently permute the rows and columns of each $A^{[k]}$, or, equivalently, we may relabel the nodes, without affecting our conclusions. However, for most purposes, it is not appropriate to reorder the time points.

We consider here the issue of representing the system as a single, higher dimensional block matrix, built from the individual time-slices. We focus on the task of computing network centrality measures, and present a particular block formulation that allows us to recover dynamic centrality measures [2, 3] respecting times arrow.

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Fast nonnegative least squares through flexible Krylov subspaces

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Abstract

Constrained linear least squares problems arise in a variety of applications, and many iterative methods are already available to compute their solutions. This talk proposes a new efficient approach to solve nonnegative linear least squares problems. The starting points of the new method, dubbed MFCGLS, are the KKT conditions associated to the nonnegativity constraints. The original problem is thus reformulated as a nonlinear system, which is then solved using a CGLS scheme with adaptive diagonal preconditioning. Since the preconditioner is updated at each iteration, MFCGLS belongs to the framework of flexible Krylov subspace methods. Some properties of MFCGLS are illustrated. MFCGLS can be easily applied to image restoration and reconstruction problems, where the components of the solution represent nonnegative intensities. Data affected by both Gaussian and Poisson noise are considered. Many numerical experiments and comparisons are provided in order to validate MFCGLS, which delivers results of equal or better quality than many state-of-the-art solvers for nonnegative least squares, with a significant speedup.

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Low rank approximate solutions to large-scale differential matrix Riccati equations

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Abstract

Differential Riccati equations play a fundamental role in many areas such as control, filter design theory, model reduction problems, differential equations and robust control problems. In our presentation, we consider large-scale continuous-time differential algebraic Riccati equations having low rank right-hand sides. These equations are generally solved by Backward Differentiation Formula (BDF) or Rosenbrock methods leading to a large scale algebraic Riccati equation which has to be solved for each timestep. A new approach, based on the reduction of the problem dimension prior to integration will be discussed. We project the initial problem onto an extended block Krylov subspace and get a low-dimentional differential algebraic Riccati equation. The latter matrix differential problem is then solved by Backward Differentiation Formula (BDF) method and the obtained solution is used to reconstruct an approximate solution of the original problem. We give some theoretical results and a simple expression of the residual allowing the implementation of a stop test in order to limit the dimension of the projection space. Some numerical experiments will be given.

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Column-Action Methods in CT

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Abstract

Filtered back projection, FDK and similar "direct" reconstruction methods in computed tomography (CT) give excellent results when we have plenty of data and when the noise in the data is low. But for situations with high noise and/or limited data, or when it is desirable to incorporate constraints, an algebraic approach is often preferred.

Row-action methods is a specific class of algebraic iterative methods. It includes Kaczmarz's algorithm, which was independently suggested under the name "ART" to solve tomographic reconstruction problems. It is also known how to base an algebraic iterative reconstruction algorithm on *columns* rather than on rows. The main advantage of the column version is that it does not exhibit the cyclic convergence of the row version, but converges to a least squares solution. Another advantage is the possibility for saving computational work during the iterations, as demonstrated by numerical examples in this talk.

Column-oriented algorithms have not been explored much in the literature. An exception is Watt [3] who derives a column-based reconstruction method and compares it with ART (also using nonnegativity constraints). A more recent paper is [1] where a two-parameter algorithm based on a block-column partitioning is studied.

The row and column methods seek to solve different problems. The row methods aim to compute a minimum-norm solution to a consistent system of equations, while the column methods aim to compute a least squares solution. Hence, for inconsistent problems the asymptotic behavior of the methods is different. The row-action methods exhibit cyclic convergence but not in general to a least squares solution. The column methods, on the other hand, converge to a least squares solution but not in general to the minimum norm solution.

This talk presents recent work related to [2]. We set the stage by briefly summarizing the well-known row action methods, and then we introduce the column versions and derive and discuss the associated convergence properties. We also demonstrate how computational work can be reduced by not performing small updates, typically of solution elements that have converged.

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An Alternating Modulus Nonnegative Least-Squares Method for Nonnegative Matrix Factorization

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Abstract

Consider the nonnegative matrix factorization (NMF) [1]: $\min_{W,H} \|V - WH\|_{\mathrm{F}}$, where $V \in \mathbf{R}^{m\times n}$ is a given nonnegative matrix, $W \in \mathbf{R}^{m\times r}$ and $H \in \mathbf{R}^{r\times n}$ are unknown nonnegative matrices, and $\|\cdot\|_{\mathrm{F}}$ represents the Frobenius norm of the corresponding matrix. Here, $r \ll \min(m,n)$ is assumed. Therefore, the NMF problem seeks a nonnegative low rank approximation of a given nonnegative matrix.

NMF arises in many scientific computing and engineering applications, e.g., image processing, spectral data analysis, audio signal separation, text mining, document clustering, recommender system, etc.

For the solution of NMF, we propose a new alternating nonnegative least squares method by utilizing the modulus method [2, 3] for solving the nonnegative constrained least squares (NNLS) problems in each iteration. The method employs the modulus transform $H = Z + |Z|$ and $W = Y + |Y|$ for each subproblem to transform the NNLS problem to a sequence of unconstrained least squares problems, which can be solved by a CGLS method for matrix variables. Numerical experiments on random problems and ORL face image problems show the efficiency of the proposed method compared to the multiplicative update method [4] and gradient-type methods.

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On applying the block Arnoldi process to the solution of a particular Sylvester-observer equation

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Abstract

In this talk, we describe a new block method for solving multi-input Sylvester-observer equations that arise in the construction of the well known Luenberger observer. More precisely, we follow the ideas developed in [1, 2] and show how to use the block Arnoldi process in order to generalize, to the multi-input case, the method proposed by Datta and Saad for the single input Sylvester-observer equation [1]. By using matrix valued polynomials which were used in [3, 4] for describing some blok Krylov methods, we give some new algebraic properties and show how to construct the Luenberger observer by solving a special large Sylvester equation for which two unknowns are to be computed. The numerical tests show that the proposed approach is very effective and can be used for large-scale Luenberger observer.

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Fast computation of the matrix exponential for a Toeplitz matrix

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Abstract

The computation of the matrix exponential is a ubiquitous operation in numerical mathematics, and for a general, unstructured $n \times n$ matrix it can be computed in $\mathcal{O}(n^3)$ operations. An interesting problem arises if the input matrix is a *Toeplitz matrix*, for example as the result of discretizing integral equations with a time invariant kernel. In this case it is not obvious how to take advantage of the Toeplitz structure, as the exponential of a Toeplitz matrix is, in general, not a Toeplitz matrix itself. In this talk, we present an algorithm of *quadratic complexity* for the computation of the Toeplitz matrix exponential. It is based on the scaling and squaring framework, and connects classical results from rational approximation theory to matrices of low displacement rank. As an example, the developed methods are applied to Merton's jump-diffusion model for option pricing.

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Bidiagonalization with Parallel Tiled Algorithms

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Abstract

We consider algorithms for going from a "full" matrix to a condensed "band bidiagonal" form using orthogonal transformations. We use the framework of "algorithms by tiles". Within this framework, we study (1) the tiled bidiagonalization algorithm (`bidiag`) which is a tiled version of the standard scalar bidiagonalization algorithm [3] and (2) the R-bidiagonalization algorithm (`R-bidiag`) which is a tiled version of the algorithm which consists in first performing the QR factorization of the initial matrix, then performing the band-bidiagonalization of the R-factor [1]. For both bidiagonalization algorithms (`bidiag` and `R-bidiag`), we use HQR-based reduction trees [2]. We consider a variety of reduction trees, so called (A) Flat TS, (B) Flat TT or (C) Greedy TT and more. Previous work on band bidiagonalization [4] has only focused on (1A), that is a standard bidiagonalization algorithm with Flat TS tree. We provide a study of critical path length for these algorithms and we provide an extensive set of experiments on a shared memory system to show the superiority of the new algorithms for tall and skinny matrices.

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Doubling Algorithms, General Theory, and Applications

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Abstract

Iterative methods are widely and indispensably used in numerical approximations. Basically, any iterative method is a rule that produces a sequence of approximations and with a reasonable expectation that newer approximations in the sequence are better. The goal of a doubling algorithm is to significantly speed up the approximation process by seeking ways to skip computing most of the approximations in the sequence but sporadically few, in fact, extremely very few: only the 2^i-th approximations in the sequence, kind of like computing α^{2^i} via repeatedly squaring. However, this idea is only worthwhile if there is a much cheaper way to directly obtain the 2^i-th approximation from the 2^{i-1}-th one than simply following the rule to generate every approximation between the 2^{i-1}-th and 2^i-th approximations in order to obtain the 2^i-th approximation. Anderson (1978) had sought the idea to speed up the simple fixed point iteration for solving the discrete-time algebraic Riccati equation via repeatedly compositions of the fixed point iterative function. As can be imagined, under repeatedly compositions, even a simple function can usually and quickly turn into nonetheless a complicated and unworkable one. In the last 20 years or so in large part due to an extremely elegant way of formulation and analysis, the researches in doubling algorithms thrived and continues to be very active, leading to numerical effective and robust algorithms not only for the continuous-time and discrete-time algebraic Riccati equations from optimal control that motivated the researches in the first place but also for M-matrix algebraic Riccati equations (MARE), structured eigenvalue problems, and other nonlinear matrix equations. But the resulting theory is somewhat fragmented and sometimes ad hoc. In this talk, we will seek to provide a general and coherent theory, discuss new highly accurate doubling algorithm for MARE, and look at several important applications.

Adaptive cross approximation for ill-posed problems

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Abstract

Integral equations of the first kind with a smooth kernel and perturbed right-hand side, which represents available contaminated data, arise in many applications. Discretization gives rise to linear systems of equations with a matrix whose singular values cluster at the origin. The solution of these systems of equations requires regularization, which has the effect that components in the computed solution connected to singular vectors associated with small singular values are damped or ignored. In order to compute a useful approximate solution typically approximations of only a fairly small number of the largest singular values and associated singular vectors of the matrix are required. The presentation will explore the possibility of determining these approximate singular values and vectors by adaptive cross approximation. This approach is particularly useful when a fine discretization of the integral equation is required and the resulting linear system of equations is of large dimensions, because adaptive cross approximation makes it possible to compute only fairly few of the matrix entries.

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Computing the Jordan structure of an eigenvalue

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Abstract

In this talk we revisit the problem of finding an orthogonal similarity transformation that puts an $n \times n$ matrix A in a block upper-triangular form that reveals its Jordan structure at a particular eigenvalue λ_0. The obtained form in fact reveals the dimensions of the null spaces of $(A - \lambda_0 I)^i$ at that eigenvalue via the sizes of the leading diagonal blocks, and from this the Jordan structure at λ_0 is then easily recovered. The method starts from a Hessenberg form that already reveals several properties of the Jordan structure of A. It then updates the Hessenberg form in an efficient way to transform it to a block-triangular form in $\mathcal{O}(mn^2)$ floating point operations, where m is the total multiplicity of the eigenvalue. The method only uses orthogonal transformations and is backward stable. We illustrate the method with a number of numerical examples.

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Recursive Interpolation Algorithm for Polynomials: RIAP

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Abstract

Let $x_0, x_1, \cdots, x_n$ be a set of n+1 distinct real numbers (i.e., $x_i \neq x_j$, for $i \neq j$) and $y_0, y_1, \cdots, y_n$, be real numbers, we know that there exist a unique polynomial $p_n(x)$ of degree n such that $p_n(x_i) = y_i$, for $i = 0, 1, \cdots, n$, p_n is the Lagrange interpolation polynomial for the set $\{(x_i, y_i),\ i = 0, 1, \cdots, n\}$. The polynomial $p_n(x)$ can be computed by using the Lagrange method or the Newton method. This paper presents a new method for computing interpolation polynomials. We will reformulate the interpolation polynomial problem and give a new algorithm for giving the solution of this problem, the Recursive Interpolation Algorithm for Polynomials (RIAP). Some properties of this algorithm will be studied and some numerical examples will also be given.

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An optimal Q-OR Krylov subspace method for solving linear systems

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Abstract

In [2] it is shown that most Krylov methods for solving linear systems with nonsymmetric matrices can be described as so-called quasi-orthogonal (Q-OR) or quasi-minimum (Q-MR) residual methods. There exist many pairs of Q-OR/Q-MR methods. Well-known examples are FOM/GMRES, BiCG/QMR and Hessenberg/CMRH. These pairs mainly differ by the different bases of the Krylov subspace they used.

In this lecture we will first recall the generic properties of the Q-OR methods that were studied in [1]. Then, we will show how to construct a non-orthogonal basis of the Krylov subspace for which the Q-OR method yields the same residual norms as GMRES up to the final stagnation phase. Therefore, for a given Krylov subspace, this is the optimal Q-OR method. We will also established some properties of this new basis that will help us simplifying the implementation of the proposed algorithm.

We will illustrate the performances of the new algorithm with numerical experiments. In particular, for many linear systems, this new method gives a better attainable accuracy than GMRES using the modified Gram-Schmidt algorithm as well as GMRES using Householder reflections.

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Computing the Least Common Multiple of Polynomial Sets

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Abstract

In the present work, we present a numerical method for the computation of the Approximate Least Common Multiple (ALCM) of univariate polynomial sets. The basic characteristic of the proposed method is that it avoids root finding algorithms and computations involving the Greatest Common Divisor (GCD) The main tool is the algebraic construction of a special matrix containing key data from the original polynomial set. From this matrix is formulated a linear system which provides the degree and the coefficients of the ALCM using low-rank approximation techniques and numerical optimization tools particularly in the presence of inaccurate data. The stability and complexity of the method is analysed. Furthermore, we present several numerical examples to illustrate the effectiveness of the method and a comparison with other methods is provided as well.

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Identification of hydraulic conductivity for saltwater intrusion problem in free aquifers

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Abstract

In this talk, we focus on the identification of the hydraulic conductivity K for saltwater intrusion problem for a nonhomogeneous, isotropic and free aquifer. The estimation of this parameter is based on observations or field measurements made on the depth of the freshwater/saltwater interface and on the depth of the water table. We note that concretely, we only have specific observations (in space and in time) corresponding to the number of monitoring wells. In addition the seawater intrusion phenomenon is often transient and the study of sensitivity shows that the form of freshwater/saltwater interface depends mainly on the hydraulic conductivity, the other parameters such as especially porosity, have an impact mainly on the time taken to reach the steady state. We formulate this identification problem by an optimization problem whose cost function measures the squared difference between experimental hydraulic heads and those given by the model. Then, thanks to the regularity and the uniqueness of the exact solution, we can establish the existence of the control problem. Considering the exact problem as a constraint for the optimization problem and introducing the Lagrangian associated with the cost function, we prove that the optimality system has at least one solution.
Then we use the adjoint method to calculate the gradient of the cost function. Numerically, we write an algorithm based on the method of descent direction, and we use the line search method with the Wolf conditions to determine the step length. Finally, we present some numerical results.

Approximated structured pseudospectra

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Abstract

Many applications in science and engineering require knowledge of the location of some or all eigenvalues of a matrix and the sensitivity of the eigenvalues to perturbations of the matrix. The sensitivity can be studied with the aid of the eigenvalue condition number, based on particular rank-one perturbations of the matrix, as described by Wilkinson [2, Chapter 2], or by computing pseudospectra. Let $\Lambda(A)$ denote the spectrum of the matrix $A \in \mathbb{C}^{n\times n}$. The ε-pseudospectrum of the matrix A is defined as

$$\Lambda_\varepsilon(A) := \left\{\lambda \in \mathbb{C}\colon \lambda \in \Lambda(A+E),\ \ E \in \mathbb{C}^{n\times n},\ \ \|E\| \le \varepsilon\right\} \tag{1}$$

for some $\varepsilon > 0$. An insightful discussion of the ε-pseudospectrum and many applications are presented by Trefethen and Embree [1].

Algorithms for eigenvalue computations that respect the matrix structure may yield higher accuracy and require less computing time than structure-ignoring methods. They also may preserve eigenvalue symmetries in finite-precision arithmetic. The structured ε-pseudospectrum can be applied to measure the sensitivity of the eigenvalues of a structured matrix to similarly structured perturbations. Let $\mathcal{S}$ denote the subset of matrices in $\mathbb{C}^{n\times n}$ with a particular structure, such as bandedness, Toeplitz, Hankel, or Hamiltonian. Then, for some $\varepsilon > 0$, the structured ε-pseudospectrum of a matrix $A \in \mathcal{S}$ is given by

$$\Lambda_\varepsilon^{\mathcal{S}}(A) := \{\lambda \in \mathbb{C}\colon \lambda \in \Lambda(A+E),\ \ E \in \mathcal{S},\ \ \|E\| \le \varepsilon\}\,; \tag{2}$$

see, e.g., [3] for discussions and illustrations.

The computation of pseudospectra and structured pseudospectra, however, can be very demanding for all but small matrices. In fact, there are few methods available for computing the structured ε-pseudospectrum besides plotting the spectra of structured random perturbations. A new approach, based on determining the spectra of many suitably chosen rank-one or projected rank-one perturbations of the given matrix is proposed. The choice of rank-one or projected rank-one perturbations is inspired by Wilkinson's analysis of eigenvalue sensitivity.

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Gauss quadrature for quasi-definite linear functionals

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Abstract

The Gauss quadrature can be formulated as a method for approximating positive definite linear functionals. Its mathematical context is extremely rich, with orthogonal polynomials, continued fractions and Padé approximation on one (functional analytic or approximation theory) side, and with the method of moments, (real) Jacobi matrices, spectral decompositions, and the Lanczos method on the other (algebraic) side. The quadrature concept can therefore be developed using many different ways. This talk investigates the question of a meaningful generalization of the Gauss quadrature for approximation of linear functionals which are not positive definite. For that purpose we use the algebraic approach. As the main result we present the form of the generalized Gauss quadrature and prove that the quasi-definiteness of the underlying linear functional represents the necessary and sufficient condition for its existence. The connections with Padé approximants and (complex) Jacobi matrices are pointed out.

Applications of the simplified topological ε–algorithms

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Abstract

Let $(\mathbf{S}_n)$ be a sequence of elements of a vector space E on a field $\mathbb{K}$ ($\mathbb{R}$ or $\mathbb{C}$) which converges to a limit $\mathbf{S}$. If the convergence is slow, it can be transformed, by a *sequence transformation*, into a new sequence or a set of new sequences which, under some assumptions, converges faster to the same limit. When E is $\mathbb{R}$ or $\mathbb{C}$, a well known such transformation is due to Shanks, and it can be implemented by the scalar ε–algorithm of Wynn.

This transformation was generalized in several different ways to sequences of elements of a vector space E. When E is $\mathbb{R}^p$ or $\mathbb{C}^p$, this generalization leads to the *Reduced Rank Extrapolation* (RRE) and to the *Minimal Polynomial Extrapolation* (MPE). For a general vector space E, the *Modified Minimal Polynomial Extrapolation* (MMPE) and the *topological Shanks transformations* are obtained. The interest of these last two generalizations is that they can treat sequences or matrices or even tensors, and that they can be recursively implemented, the first one by the $S\beta$ algorithm of Jbilou [3] and the second ones by the topological ε–algorithms of Brezinski [1].

However, the topological ε–algorithms are quite complicated since they possess two rules, they require the storage of many elements of E, and the duality product with an element $\mathbf{y}$ is recursively used in their rules. Recently, simplified versions of these algorithms were obtained and called the *simplified topological ε–algorithms* [2]. They have only one recursive rule instead of two, they require less storage than the initial algorithms, elements of the dual vector space E^* of E no longer have to be used in the recursive rules but only in their initializations, the numerical stability is improved, and it was possible to prove theoretical results on them.

In this talk, we present several results obtained by using the simplified topological ε–algorithms for accelerating the convergence of sequences of elements of a vector space: solution of linear and nonlinear systems of vector and matrix equations, and computation of matrix functions. The solution of nonlinear Fredholm integral equations of the second kind will also be evocated.

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Generalized Krylov subspace methods for ℓ_p-ℓ_q minimization

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Abstract

This talk presents new efficient approaches for the solution of ℓ_p-ℓ_q minimization problems based on the application of successive orthogonal projections onto generalized Krylov subspaces of increasing dimension. The subspaces are generated according to the iteratively reweighted least-squares strategy for the approximation of ℓ_p/ℓ_q-norms by weighted ℓ_2-norms. Computed image restoration examples illustrate the performance of the methods discussed. The combination of a fairly low iteration count and a modest storage requirement makes the proposed methods attractive.

Fast and backward stable computation of the eigenvalues of matrix polynomials

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Abstract

The computation of matrix polynomials eigenvalues has gained some interest in the last decades, especially the search for adequate linearizations and good scaling techniques.

The approach which is most often used to approximate the eigenvalues of a $k \times k$ matrix polynomial of degree d is to construct a linearization, which is a $kd \times kd$ pencil, whose eigenvalues coincide with the ones of the matrix polynomial and can be approximated using the QZ method. The pencil $A - \lambda B$ typically built in this context is endowed with a particular structure: Both A and B are rank k perturbations of $kd \times kd$ unitary matrices. However, all the available structured methods for this problem are effective only when $k \ll d$ [2, 3].

We present a new structured method that allows to compute the eigenvalues of $k \times k$ matrix polynomials of degree d in $O(d^2k^3)$ flops, which is always asymptotically faster than the $O(d^3k^3)$ complexity obtained computing the eigenvalues of $A - \lambda B$ with an unstructured QZ. The result is obtained by rephrasing the unitary plus rank k structure as the product of k unitary plus rank 1 matrices. This factorization can be obtained at (almost) no cost starting from the original structure, but is much more convenient from the numerical perspective. In particular, we can develop a structured method by re-using some tools developed in [1]. Several choices for this initial factorization and for the subsequent reduction to upper Hessenberg-triangular form are presented. We show that some choices are more favorable from the numerical point of view.

We prove that the presented method is backward stable on A and B, and that it reaches the same accuracy of the QZ iteration. Several numerical experiments confirm that the method is fast and accurate.

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Regularized inversion of frequency domain electromagnetic geophysical data

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Abstract

Electromagnetic (EM) induction is a non-invasive technique used to characterize the spatial variability of soil properties, which has widespread use in archaeological, hydrological, and geotechnical applications. The inversion of EM data can be accomplished by a nonlinear model which is dominated by error propagation. The ill-conditioning of the problem is further amplified in the presence of strongly conductive materials in the subsoil. We will describe an extension of a regularization algorithm originally described in [1, 2]. In particular, we will show that the knowledge of the exact Jacobian matrix of the nonlinear model, coupled to suitable updating techniques, allows one to improve both computing time and accuracy with respect to the standard approach, based on finite difference approximation. We will also show that fast and accurate linear algebra tools are needed in order to process in real time the large amount of complex valued data produced by recent measuring devices. At the same time, the lack of information on the noise level in real-world applications calls for an efficient strategy for estimating the regularization parameter.

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Vector estimates for the action of matrix functions on vectors

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Abstract

Let $A \in \mathbb{R}^{p\times p}$ be a diagonalizable matrix, $b \in \mathbb{R}^p$ a vector and f a smooth function. We are interested in estimating the action of $f(A)$ on a vector b, i.e. $f(A)b$, without computing $f(A)$, by using an extrapolation procedure. In the present work, we derive families of one-term and two-term vector estimates for the quantity $f(A)b$ and we connect them with the estimates for the corresponding matrix functionals of a given diagonalizable matrix A. The quantity $f(A)b$ arises in many applications, especially those with a large, sparse matrix A, in which it is not feasible to compute explicitly the whole matrix $f(A)$ and those originating from partial differential equations [3]. We present several numerical examples to illustrate the effectiveness of the derived families for several functions f for the quantity $f(A)b$.

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Divide and conquer algorithms and software for large Hermitian eigenvalue problems

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Abstract

Divide-and-conquer paradigms can lead to efficient and flexible techniques for solving large Hermitian eigenvalue problems. This talk will discuss how these techniques can be put to work to implement 'spectrum slicing' strategies, i.e., strategies that extract slices of the spectrum independently. The presentation will begin with an overview of polynomial filtering, a general approach that can be quite efficient in the situation where the matrix-vector product operation is inexpensive and when a large number of eigenvalues is sought. We will present a few algorithms that combine the Lanczos algorithm with and without restarts, as well as subspace iteration. An alternative to polynomial filtering that is generating a growing interest is a class of methods that exploit filtering by rational functions. Good representatives of this general approach are the FEAST eigensolver and the Sakurai-Sugiura algorithm. Here we will argue that the standard Cauchy integral–based approach can be substantially improved upon – especially when iterative solvers are involved. Finally, the talk will discuss our ongoing work to develop a code named EVSL (for eigenvalues slicing library) that implements these ideas.

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Analysis of the rational Krylov subspace method for large-scale algebraic Riccati equations

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Abstract

In the numerical solution of the algebraic Riccati equation $A^*X + XA - XBB^*X + C^*C = 0$, where A is large, sparse and stable, and B, C have low rank, projection methods have recently emerged as a possible alternative to the more established Newton-Kleinman iteration [3]. In spite of convincing numerical experiments, a systematic matrix analysis of this class of methods has been lacking. We derive new relations for the approximate solution, the residual and the error matrices, giving new insights into the role of the matrix $A - BB^*X$ and of its approximations in the numerical procedure. In the context of linear-quadratic regulator problems, we show that the Riccati approximate solution is related to the optimal value of the reduced cost functional, thus completely justifying the projection method from a model order reduction point of view [2]. The new results provide theoretical ground for recently proposed modifications of projection methods onto rational Krylov subspaces [1].

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Stagnation of block GMRES and its relationship to block FOM

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Abstract

We analyze the the convergence behavior of block GMRES and characterize the phenomenon of stagnation which is then related to the behavior of the block FOM method. We generalize the block FOM method to generate well-defined approximations in the case that block FOM would normally break down, and these generalized solutions are used in our analysis. This behavior is also related to the principal angles between the column-space of the previous block GMRES residual and the current minimum residual constraint space. At iteration j, it is shown that the proper generalization of GMRES stagnation to the block setting relates to the columnspace of the jth block Arnoldi vector. Our analysis covers both the cases of normal iterations as well as block Arnoldi breakdown wherein dependent basis vectors are replaced with random ones. Numerical examples are given to illustrate what we have proven, including one constructed (artificially) from small application problem to demonstrate the validity of the analysis in a less pathological case.

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Block Krylov subspace methods for matrix functions

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Abstract

Block Krylov subspace methods have been successfully developed for linear systems and matrix equations. When it comes to functions of matrices, their application has been less established. In this talk, we present a general setting for block Krylov subspaces for functions of matrices with several right hand sides. We focus in particular on methods analogous to the full orthogonalization method (FOM) for linear systems, and therefore refer to these methods as B(FOM)^2: block FOM for functions of matrices. We prove error bounds, and present numerical experiments illustrating the behavior of versions of B(FOM)^2 with restarts on practical examples.

The roots of GMRES polynomials need not influence GMRES residual norms

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Abstract

The convergence behavior of Krylov subspace methods has been linked to the convergence of Ritz values, in particular for the CG method, see, e.g., [4]. For the GMRES method, some results suggest that the convergence of Ritz values often goes hand in hand with an acceleration of residual norm convergence and may in fact be the cause of superlinear convergence [5]. However, mathematically, any residual norm history is possible with any set of Ritz values in the individual iterations of the GMRES process [1]. This result can be regarded as a generalization of the fact that any residual norm history is possible with any set of final Ritz values, i.e., of eigenvalues [2]. It also shows that the Arnoldi method for eigenvalues can exhibit arbitrary convergence behavior.

However surprising this may seem, the Ritz values are not the roots of GMRES polynomials and this makes it more credible that GMRES residual norms can be completely independent from Ritz values. The roots of the GMRES polynomials are the *harmonic* Ritz values [3]. In our talk we show that not even harmonic Ritz values need have any influence on the residual norm history of GMRES (provided the stagnation case is treated correctly). In other words, any residual norm history is possible with any set of harmonic Ritz values in the individual iterations of the GMRES process.

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Block Kronecker Linearizations of Matrix Polynomials and their Backward Errors

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Abstract

We introduce a new family of strong linearizations of matrix polynomials, which we call "block Kronecker pencils", and perform a backward stability analysis of complete polynomial eigenproblems. These problems are solved by applying any backward stable algorithm to a block Kronecker pencil, such as the staircase algorithm for singular pencils or the QZ algorithm for regular pencils. This stability analysis allows us to identify those block Kronecker pencils that yield a computed complete eigenstructure which is exactly that of a slightly perturbed matrix polynomial. These favorable pencils include the famous Fiedler linearizations, which are just a very particular case of block Kronecker pencils. Thus, our analysis offers the first proof available in the literature of global backward stability for Fiedler pencils. In addition, the theory developed for block Kronecker pencils is much simpler than the theory available for Fiedler pencils, especially in the case of rectangular matrix polynomials. The global backward error analysis in this work presents for the first time the following key properties: it is a rigurous analysis valid for finite perturbations (i.e., it is not a first order analysis), it provides precise bounds, it is valid simultaneously for a large class of linearizations, and it establishes a framework that may be generalized to other classes of linearizations.

Tropical scaling of a Lagrange-type linearization for matrix polynomial eigenvalue problems

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Abstract

Let $P(z)$ be a $s \times s$ matrix polynomial of degree d. The *polynomial eigenvalue problem* (PEP) is to look for nonzero vectors v (right eigenvectors) and corresponding eigenvalues λ such that $P(\lambda)v = 0$.

The standard way of solving the PEP is via *linearization*, that is, by constructing a $ds \times ds$ matrix polynomial $L(z)$ of degree one such that

$$E(z)L(z)F(z) = \begin{bmatrix} P(z) & 0 \\ 0 & I_{(d-1)s} \end{bmatrix}$$

with $E(z)$ and $F(z)$ unimodular matrix polynomials. Then clearly $P(z)$ and $L(z)$ have the same eigenvalues. Many linearizations have been proposed in the literature based on the basis in which $P(z)$ is represented, e.g., degree graded bases such as the monomial basis, the Chebyshev basis, ..., or interpolation bases, such as the Lagrange polynomials. Companion linearizations are commonly used in practice for matrix polynomials expressed in the monomial basis but these are known to affect the sensitivity of eigenvalues and, when used with numerically stable eigensolvers for generalized eigenproblems, they can compute eigenpairs for P with large backward errors unless the linear problem is solved several times with different scalings of the eigenvalue parameter.

The matrix polynomial $P(z)$ is uniquely determined by its values P_i in d points σ_i, $i = 1, 2, \ldots, d$ and its highest degree coefficient P_d. A Lagrange-type linearization based on this representation is

$$L(z) = \left[\begin{array}{c|ccc} P_d & \beta_1 P(\sigma_1) & \cdots & \beta_d P(\sigma_d) \\ \hline -I_s & (z-\sigma_1)I_s & & \\ \vdots & & \ddots & \\ -I_n & & & (z-\sigma_d)I_n \end{array}\right],$$

where the β_i are the so-called barycentric weights.

We show numerically that the (well-conditioned) eigenvalues of a PEP can be computed with high relative precision using only one run of the QZ algorithm even when the eigenvalues have a large variation in magnitude. To this end a particular choice of the interpolation points σ_i, i.e., well-separated tropical roots, is taken in the Lagrange-type linearization as defined above together with an appropriate scaling. Also the QZ algorithm has to be slightly adapted such that the QZ iteration does not stop too early for eigenvalues with a large difference in magnitude. This is connected to the fact that for certain matrix pencils the QZ algorithm exhibits a structured backward error as we will illustrate by numerical experiments.

A Framework for Structured Linearizations of Matrix Polynomials in Various Bases

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Abstract

We present a framework for the construction of linearizations for scalar and matrix polynomials based on dual bases which, in the case of orthogonal polynomials, can be described by the associated recurrence relations. The framework provides an extension of the classical linearization theory for polynomials expressed in non-monomial bases and allows to represent polynomials expressed in product families, that is as a linear combination of elements of the form $\phi_i(x)\psi_j(x)$, where $\{\phi_i(x)\}$ and $\{\psi_j(x)\}$ can either be polynomial bases or polynomial families which satisfy some mild assumptions.

We show that this general construction can be used for many different purposes. Among them, we show how to linearize sums of polynomials and rational functions expressed in different bases. As an example, this allows to look for intersections of functions interpolated on different nodes without converting them to the same basis.

A fast contour-integral eigensolver for non-Hermitian matrices and the approximation accuracy

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Abstract

We design a fast contour-integral eigensolver for finding selected or all the eigenpairs of a non-Hermitian matrix, and study the eigenvalue accuracy when some approximations are involved. The design is based on a series of analytical and computational techniques, such as the analysis of filter functions, quick and reliable eigenvalue count via low-accuracy matrix approximations, and fast shifted factorization update. The quality of some quadrature rules for approximating a relevant contour integral is analyzed. We show that a filter function based on the Trapezoidal rule has nearly optimal decay in the complex plane away from the unit circle (as the mapped contour), and is superior to the Gauss-Legendre rule. The eigensolver needs to count the eigenvalues inside a contour. We justify the feasibility of using low-accuracy matrix approximations for the quick and reliable count. Both deterministic and probabilistic studies are given. With high probabilities, the matrix approximations give counts very close to the exact one. Our eigensolver is built upon an accelerated FEAST algorithm. Both the eigenvalue count and the FEAST eigenvalue solution need to solve linear systems with multiple shifts and right-hand sides. For this purpose and also to conveniently control the approximation accuracy, we use a type of rank structured approximations and show how to control the accuracy. The structured approximations also allow the fast update of the factorization for varying shifts. The eigensolver may be used to find a large number of eigenvalues, where a search region is then partitioned into subregions. We give an optimal threshold for the number of eigenvalues inside each bottom level subregion so as to minimize the complexity, which is $\mathcal{O}(rn^2) + \mathcal{O}(r^2n)$ to find all the eigenpairs of an order-n matrix with maximum off-diagonal rank or numerical rank r.

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Weighted Golub-Kahan-Lanczos Algorithms

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Abstract

For any real symmetric positive definite matrices K and M there exist an M-orthogonal matrix X and a K-orthogonal matrix Y such that

$$KY = XB, \quad MX = YB^T,$$

where B is bidiagonal. Two versions of Lanczos-type iterative method are constructed based on the factorizations, depending on whether B is upper or lower bidiagonal. In the upper bidiagonal case, with an initial y_1 as the first column of Y, a k-step of Lanczos-type iteration produces the matrices Y_k and X_k that consist of the first k columns of Y and X, respectively, as well as B_k, the leading $k \times k$ principal matrix B, such that

$$KY_k = X_k B_k, \quad MX_k = Y_k B_k^T + \beta_k y_{k+1} e_k^T.$$

The proposed methods are the weighted versions of the standard Golub-Kahan-Lanczos (GKL) algorithms given in [4, 5]. They are also the special case of the more generalized GKL algorithms developed in [1]. The proposed methods provide a simple and straightforward way for solving the eigenvalue problem or a linear system associated with a matrix of the form KM, MK, or $\mathbf{H} := \begin{bmatrix} 0 & M \\ K & 0 \end{bmatrix}$. The eigenvalue problem of $\mathbf{H}$ arises from linear response theory ([2, 3]). Another interesting fact is that they give a simple connection with the classical CG method.

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Multi-scale S-fraction reduced-order models for massive wavefield simulations

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Abstract

We present a reduced-order multi-scale method for solving large time-domain wavefield simulation problems. The algorithm consists of two main stages. During the first "off-line" stage the computational domain is split into multiple subdomains. Then projection-type multi-scale reduced order models (ROMs) are computed for the partitioned operators at each subdomain. The off-line stage is "embarrassingly" parallel as ROM computations for the subdomains are independent of each other. It also does not depend on the number of simulated right-hand sides and it is performed just once before the entire time-domain simulation. At the second "on-line" stage the time-domain simulation is performed within the obtained multi-scale ROM framework. The crucial feature of our formulation is the representation of the ROMs in terms of matrix Stieltjes continued fractions (S-fractions). This allows us to sparsify the obtained multi-scale subdomain operator ROMs and to reduce both the computational cost and communications which is highly beneficial for serial as well as parallel implementations of the on-line stage. The performance of the method is illustrated on $3D$ composite anisotropic elastic problems.

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Phase-preconditioned Rational Krylov Subspaces for model reduction of large-scale wave propagation

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Abstract

Rational Krylov Subspaces (RKS) is a powerful tool for interpolatory model-reduction of large-scale dynamical systems. However, it is fundamentally limited by the Nyquist-Shanon sampling rate for the transfer function of such a system. More specifically, at least two interpolation points per period of the cut-off frequency of the transfer function are required, which can lead to thousands of interpolation points for large-scale wave propagation and thus prohibitively large RKS as these interpolation points need to be solved for every right hand side. We suggest to precondition the RKS via the phase term of the WKB approximation, easily obtainable from the eikonal equation.

The advantage of the proposed formulation is threefold, as it allows reduction in frequency-domain sampling, number of right hand sides, and spatial sampling. First, the preconditioning method factors out the main part of the dependence of the RKS on the interpolation frequency. This allows a reduction of the frequency domain sampling rate with respect to the Nyquist-Shanon sampling rate. Secondly, after this factorization, the RKS basis is only weakly dependent on the right hand side, which allows us to significantly reduce the complexity of MIMO problems. Third, our approach also factors out the dominant part of the spatial dependence of the solution. This allows us to reduce the spatial sampling required for the accurate computation of the RKS. The latter is of special importance for three-dimensional problems.

We show large-scale numerical examples with dramatically model reduction for the acoustic Marmousi model, a seismic exploration benchmark problem.

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