

S16. Linear Algebra: Algorithms and Applications

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Tuned preconditioners for iterative SPD eigensolvers

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To compute a few of the leftmost eigenpairs of a large and sparse SPD matrix A , iterative eigensolvers require the solution of a number of *inner* linear systems where the system matrix is either A or $A - \theta I$ with θ a suitable shift parameter. We are focussing on the tuned preconditioners for such linear systems. A tuned preconditioner is defined as an initial inverse approximation of A plus a low-rank matrix. We present both theoretical and experimental results of the efficiency of such preconditioners in the acceleration of the Implicitly Restarted Lanczos Method (IRLM) [4] as well as of Newton's method in the unit sphere [2, 1]. In particular we will discuss a new update formula [3] for IRLM which reveals more efficient than the preconditioner presented in [4]. We will present results with realistic matrices (with size up to 10^6 unknowns and 4×10^7 nonzeros) arising from 3D Finite Element discretizations of flow and structural PDEs as well as from the laplacian of graphs.

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Preconditioners based on the ISM factorization

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In this work we study preconditioners based on the ISM factorization [1], which computes the LDU factorization of a matrix A using recursion formulas derived from the Sherman-Morrison formula. In the first part, we study preconditioners which have been constructed successfully when there is no breakdown in the LDU factorization [2, 3, 4]. In the second part, we present a modification in the recursion formulas of the ISM factorization that allows pivoting and so the construction of preconditioners for any nonsingular matrix. The ISM algorithm computes a vector at each step, by contrast the new pivoting algorithm in the k th step modifies all the vectors from k to n . Thus, it can be seen as a right-looking version with pivoting of the ISM factorization.

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Polynomial rootfinding using Fiedler companion matrices

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Computing roots of scalar polynomials as the eigenvalues of Frobenius companion matrices using backward stable eigenvalue algorithms is a classical approach. The introduction of new families of companion matrices allows for the use of other matrices in the root-finding problem. In this talk, we analyze the backward stability of polynomial root-finding algorithms via Fiedler companion matrices. In other words, given a polynomial $p(z)$, the question is to determine whether the whole set of computed eigenvalues of the companion matrix, obtained with a backward stable algorithm for the standard eigenvalue problem, are the set of roots of a nearby polynomial or not. We show that, if the coefficients of $p(z)$ are bounded in absolute value by a moderate number, then algorithms for polynomial root-finding using Fiedler matrices are backward stable, and Fiedler matrices are as good as the Frobenius companion matrices. This allows us to use Fiedler companion matrices with favorable structures in the polynomial root-finding problem. However, when some of the coefficients of the polynomial is large, companion Fiedler matrices may produce larger backward errors than Frobenius companion matrices, although in this case neither Frobenius nor Fiedler matrices lead to backward stable computations. To prove this we obtain explicit expressions for the change, to first order, of the characteristic polynomial coefficients of Fiedler matrices under small perturbations. We will show that, for all Fiedler matrices except the Frobenius ones, this change involves quadratic terms in the coefficients of the characteristic polynomial of the original matrix, while for the Frobenius matrices it only involves linear terms. We present extensive numerical experiments that support these theoretical results. The effect of balancing these matrices will be also investigated.

Updating constraint preconditioners for KKT systems via low-rank correction and scaling techniques

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We are interested in preconditioning sequences of KKT systems such as those arising in interior point methods for convex quadratic programming. Constraint Preconditioners (CPs) have proved to be very effective in this case; nevertheless, their factorization may still be too expensive for large-scale problems, and resorting to cheaper approximations of CPs appears to be a viable alternative. In this talk we present a procedure for building inexact CPs for KKT matrices of the sequence, by updating a block LDL^T factorization of a “seed” CP available for a preceding KKT matrix [1, 2]. This procedure consists of two steps: first, the seed CP is updated by performing a low-rank correction of the Schur complement of its (1,1) block; second, if the (2,2) block of the KKT matrix to be preconditioned is nonzero, a low-cost technique based on diagonal modification and matrix scaling is applied to the updated Schur complement, in order to recover information associated with the (2,2) block that has been neglected in the previous step. Theoretical results and numerical experiments show that these inexact CPs can speed up iterative procedures for solving sequences of large-scale KKT systems, thus enhancing the overall efficiency of interior point methods.

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Algorithms for matrix functions arising from matrix equations

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Several matrix functions of interest are defined implicitly through a matrix equation of the type $F(X) = A$. This will lead to a possibly multivalued function in the scalar case with an even more complicated situation in the matrix case [1].

The simplest examples are given by matrix roots which are defined through the equation $X^p = A$ and by matrix logarithms which are obtained through $e^X = A$. Different equations may give rise to less known special functions.

We discuss about algorithms for matrix functions arising from matrix equations. In particular, we focus on matrix roots algorithms, making a comparison of the features and the numerical performance of some existing algorithms [3, 4, 2], with some recent updates, also in view of the practical applications. We consider also the twin problem of computing the action of the Fréchet derivative of the root functions in one matrix direction.

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On solving KKT linear systems arising in Model Predictive Control via recursive anti-triangular factorization

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The solution of Model Predictive Control problems [1, 2, 3] is often computed in an iterative fashion, requiring to compute, at each iteration, the solution of a quadratic optimization problem. The most expensive part of the latter problem is the solution of symmetric indefinite KKT systems, where the involved matrices are highly structured.

Recently, an algorithm for computing a block anti-triangular factorization of symmetric indefinite matrices, based on orthogonal transformations, has been proposed [4]. The aim of this talk is to show that such a factorization, implemented in a recursive way, can be efficiently used for solving the mentioned KKT linear systems.

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CORK: A compact Rational Krylov method for solving the nonlinear eigenvalue problem

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The solution of the nonlinear eigenvalue problem, in its most general form, written as

$$A(\lambda)x = 0 \quad , \quad x \neq 0$$

where λ is the eigenvalue, is appearing more and more often in applications arising from PDEs. We consider matrices of the form

$$A(\lambda) = A_0 + \lambda A_1 + \sum_{i=1}^m f_i(\lambda) B_i$$

with f_i a scalar function in the complex plane, and A_i, B_i constant matrices.

In this talk, we discuss methods that lie in between local and global search methods. The Newton method and the residual inverse iteration method can be seen as methods that approximate $A(\lambda)$ by a polynomial of degree one. We build an interpolating polynomial of degree k for $A(\lambda)$ in the points $\sigma_0, \dots, \sigma_k \in \mathbb{C}$ and then perform k iterations of the rational Krylov method on the linearization of the resulting polynomial eigenvalue problem. When we use Newton polynomials and choose the poles of the rational Krylov method equal to the nodes of the Newton interpolation, then the algorithm can be organized in such a way that the nodes need not be determined in advance. This allows for tuning these parameters during the execution of the algorithm. In this way, we obtain a method that can converge in less iterations than, e.g, the Newton method. The method thus behaves like a local search method, but can be used for building a global approximation, but in a dynamic way.

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Computing the exponential of a large block triangular block Toeplitz matrix

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The Erlangian approximation of Markovian fluid queues leads to the problem of computing the exponential e^U of an upper block triangular, block Toeplitz (BTBT) matrix U [2]. The block size ℓ of U may be huge, while the size m of the blocks is generally small. The matrix exponential $A = e^U$ is still an upper BTBT matrix; moreover, since U is a subgenerator, the matrix A is substochastic.

We propose some numerical methods for computing e^U , that exploit the BTBT structure and allow to deal with very large sizes. Two numerical methods rely on the property that a block z -circulant matrix can be block diagonalized by means of Fast Fourier Transforms [1]. Therefore the computation of the exponential of an $n \times n$ block z -circulant matrix with $m \times m$ blocks can be reduced to the computation of n exponentials of $m \times m$ matrices. The idea of the first method is to approximate $A = e^U$ by the exponential of a block ϵ -circulant matrix where $\epsilon \in \mathbb{C}$ and $|\epsilon|$ is sufficiently small. In the second approach the matrix U is embedded into a $K \times K$ block circulant matrix C_K , where K is sufficiently large, and an approximation of e^U is obtained from a suitable submatrix of e^{C_K} . Another numerical method consists in specializing the shifting and Taylor series method of [3]. The BTBT structure is exploited in the FFT-based matrix multiplications involved in the algorithm, leading to a reduction of the computational cost.

Theoretical and numerical comparisons among the three numerical methods are presented.

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First order expansions for eigenvalues of multiplicatively perturbed matrices

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Given a square matrix A and one of its eigenvalues λ_0 , first order eigenvalue perturbation theory is usually applied to *additive* perturbations $A(\varepsilon) = A + \varepsilon B$, where ε is a small real parameter and B is any perturbation matrix, either structured or unstructured. Fractional expansions in ε are typically obtained for the eigenvalues $\lambda(\varepsilon)$ of $A(\varepsilon)$ such that $\lambda(0) = \lambda_0$. In this talk we consider *multiplicative* perturbations $\hat{A}(\varepsilon) = (I + \varepsilon B)A(I + \varepsilon C)$ instead, which are more natural when analyzing perturbations for families of matrices with an underlying multiplicative structure. Any Jordan structure is allowed for A . We use the Newton Polygon technique to derive first order expansions for the splitting of an eigenvalue λ_0 of A under such perturbations. Explicit formulas for both the leading exponents and coefficients are obtained, involving the perturbation matrices B and C and appropriately normalized eigenvectors of A . If $\lambda_0 \neq 0$ corresponds to a Jordan block of size n , the expansions are shown to be generically of the order of $\varepsilon^{1/n}$, very much like those for additive perturbations. If $\lambda = 0$, the situation is quite different, due in part to the fact that rank is preserved by multiplicative perturbations: in that case, the perturbed eigenvalues are generically of order $\varepsilon^{1/(n-1)}$, and the formulas are valid only for blocks of dimension $n > 2$.

Tropical roots as approximations of eigenvalues of regular matrix polynomials

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Let $P(x) = \sum_{j=0}^k A_j x^j$, $A_j \in \mathbb{C}^{n \times n}$, be a regular matrix polynomial and let $\|\cdot\| : \mathbb{C}^{n \times n} \rightarrow \mathbb{R}_{\geq 0}$ be any operator norm. The tropical roots of the associated max-times polynomials $t : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}_{\geq 0}, x \mapsto \max_j \|A_j\| x^j$ are the points of nondifferentiability of t contained in its domain of definition. Recently, for the spectral norm, it was showed in [1] that if all the coefficients A_j have 2-norm condition number equal to 1 then, under some assumptions on $\|A_j\|_2$, the tropical roots of t define localization annuli that contain all the eigenvalues of $P(x)$. We extend this result to any induced norm and, importantly, we relax the hypothesis that all the coefficients are perfectly conditioned. We obtain localization results depending on (1) the shape of the Newton polygon associated with t and (2) the condition number of those coefficients A_j corresponding to vertices of the Newton polygon. Hence, we discuss when the tropical roots of t yield good order-of-magnitude approximations for the eigenvalues of $P(x)$. Finally, we clarify the mutual relations between the tropical localization results and those coming from the generalized Pellet theorem both in the version given in [1] and the one appeared in [2]. In particular, we show that the generalized Pellet theorem of [1] always provides the tightest bounds. On the other hand, the tropical roots are extremely cheap and easy to compute, and our analysis provides sufficient conditions for their reliability as estimators for the moduli of the eigenvalues of a matrix polynomial.

This talk is based on joint work with Meisam Sharify and Françoise Tisseur (both from the University of Manchester).

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Accurate computations for subclasses and superclasses of totally positive matrices

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A matrix is totally positive if all its minors are nonnegative. Sign regular matrices and SBD matrices (matrices with signed bidiagonal decompositions) contain the class of totally positive matrices. For some subclasses of nonsingular totally positive matrices, accurate methods for computing their singular values, eigenvalues or inverses have been obtained, assuming that adequate natural parameters related to their bidiagonal decompositions are provided. We present some recent results in this field and some extensions of these methods to other related classes of matrices such as sign regular matrices and SBD matrices, assuming that adequate natural parameters related to their bidiagonal decompositions are provided.

Multivariate time series estimation via projections and matrix equations

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The Exponentially Weighted Moving Average model is a stochastic time series model that takes the form

$$x_t = u_t - \Theta u_{t-1},$$

where $u_t \in \mathbf{R}^n$ is a white noise random variable (zero mean and fixed variance Σ), and $\Theta \in \mathbf{R}^{n \times n}$. Its scalar version is widely used in economics and production planning; in the multivariate case, though, the main difficulty is its estimation, i.e., reconstructing the (unknown) value of the parameter Θ given only a number of observation x_1, x_2, \dots, x_T . The cost of Maximum Likelihood (ML) estimation grows badly with the dimension n , and convergence problems are often encountered. We focus first on a special version of the problem coming from a random-walk-plus-noise model, and propose a new estimator that uses the following strategy, using a combination of applied linear algebra and statistics/econometrics techniques:

1. Given vectors $w_1, w_2, \dots, w_k \in \mathbf{R}^n$, take each of the series $y_t^{(j)} := w_j^T x_t$ and estimate it using a “tamer” scalar Maximum Likelihood.
2. Use the obtained results to estimate of the original time series, by solving a Riccati-type matrix equation for the autocovariance function of the time series.

The resulting estimator has good performance compared to ML and is cheaper to compute. We discuss its properties and possible generalizations to other models.

Robust Preconditioners for Optimal Control problems with State and Control Constraints

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We address the problem of preconditioning a sequence of saddle-point linear systems arising in the solution of PDE-constrained optimal control problems via Primal-Dual Active-Set methods. Specifically, we consider problems with control and (regularized) state constraints; these yield nonlinear optimality systems with saddle-point Jacobian matrices with variable dimension blocks containing information on the current active-set. We present two new preconditioners based on a full block-matrix factorization of the Schur complement of the Jacobian matrices where the active-set blocks are merged into the constraint blocks. The first preconditioner is block-diagonal and positive definite and the second one is symmetric and indefinite. We show the robustness of the new preconditioners with respect to the parameters of the continuous problem, e.g. the mesh-size and the regularization coefficient. We also discuss the spectral properties of the preconditioned matrix. Numerical experiments on 3D problems are presented together with comparisons with existing approaches based on PCG in a nonstandard inner product.

Recent advances in the numerical solution of dense polynomial eigenvalue problems

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The most widely used approach for solving dense, small to medium size polynomial eigenvalue problems (PEPs) $P(\lambda)x = 0$, $y^*P(\lambda) = 0$, where

$$P(\lambda) = \lambda^d P_d + \lambda^{d-1} P_{d-1} + \cdots + \lambda P_1 + P_0, \quad P_i \in \mathbb{C}^{n \times n}, \quad P_d \neq 0,$$

is to linearize to produce a larger order pencil $L(\lambda) = A - \lambda B$, whose eigensystem is then found by the QZ algorithm. There is currently no linearization-based eigensolver for dense matrix polynomials of degree $d > 2$ with guaranteed backward stability. Indeed solving the PEP by applying a backward stable algorithm to a linearization $L(\lambda)$ can be backward unstable for the PEP. Also, the conditioning of the solutions of the larger linear problem can be worse than that for the original polynomial, since the class of admissible perturbations is larger. Now the exponential of the roots of the max-times scalar polynomial

$$\text{tp}(x) = \max_{0 \leq k \leq d} (\|P_k\| + kx)$$

are known to be good order of magnitude approximations to the eigenvalues of $P(\lambda)$ [2]. These roots are interesting from the numerical point of view since they are cheap to compute and can be used to define a family of eigenvalue parameter scalings for $P(\lambda)$ [1]. We show that these scalings improve both the backward stability of polynomial eigensolvers based on linearizations and do not increase the eigenvalue condition numbers of the linearized problem.

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Roots of polynomials: a new fast QR algorithm

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In this lecture we will propose a new fast and stable manner of computing roots of polynomials. Roots of polynomials are typically computed by putting the coefficients of the polynomial in the companion matrix and then computing the eigenvalues of this matrix. Exploiting the available *low-rank* structure leads to an algorithm of quadratic instead of cubic complexity.

Several low-cost algorithms have already been proposed. Either they fully exploit the low-rank properties of the involved matrices by representing them for instance via quasiseparable factors, or they write the companion matrix as the sum of a unitary plus low rank matrix and exploit this structure.

In this lecture we will use the second manner. However, only few QR steps (deflation of a single eigenvalue) require the use of the low rank part. After that we can put the low rank term aside and continue only with the unitary matrix, translating the problem thereby to a unitary eigenvalue problem. Only in the end the low rank matrix is reconstructed to retrieve the eigenvalues.

Numerical experiments validate the approach, illustrate its reliability and speed. The algorithm is compared against other available methods.

This research is joint work with David S. Watkins and Jared L. Aurentz from Washington State University, USA and Thomas Mach from the KU Leuven, Belgium.

Coprime Rational Matrix Functions and Equivalence

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Strict system equivalence of polynomial system matrices was introduced by Rosenbrock to classify linear control systems with the same transfer function matrix. Rosenbrock's equivalence heavily relies on the Smith equivalence of matrix polynomials and so, on the use of unimodular matrices. Fuhrmann discovered that unimodular matrices can be replaced by more general matrices provided that some coprimeness constraints are satisfied. Since then these coprimeness conditions have been consistently present in numerous papers dealing with the problem of providing an equivalence relation in closing form (i.e., using elementary operations) that classifies the matrix polynomials according to their finite and infinite elementary divisors.

Coprimeness is a natural concept for matrices defined on rings but polynomials are not elements of the ring at infinity. As a consequence, in order to characterize when two matrix polynomials have the same infinite elementary divisors using Fuhrmann's approach, the concept of coprimeness must be extended to cover matrix polynomials which are coprime at infinity. Several attempts have been made in this respect. It will be shown in this contribution that the concept of coprimeness can be extended to matrices of rational functions, that it is a local property and a new characterization of equivalence of matrix polynomials at infinity will be given in terms of coprime matrices at infinity.