Structured Matrix Computations in non-Euclidean geometries: Algorithms and Applications

ABSTRACTS

CIRM, Luminy, October 8-12, 2012.

Minimization principles of the linear response eigenvalue problem

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Abstract

The linear response (LR) eigenvalue problem

$$\begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} x \\ y \end{bmatrix}$$

arises from excitation state (energies) caluclations in the study of collective motion of many particle systems, where $A - B$ and $A + B$ are symmetric positive semi-definite matrices and one of them is definite. There are a great deal of interests in developing efficient simulation techniques for excitation state calculations of molecules for materials design in energy science.

The first part of this talk is to present theoretical results for the LR eigenvalue problem, which include a minimization principle for the sum of the smallest positive eigenvalues and Cauchy-like interlacing inequalities. Although the LR eigenvalue problem is a nonsymmetric eigenvalue problem, these results mirror the well-known trace minimization principle and Cauchy's inequalities for the symmetric eigenvalue problem.

The second part of the talk is to present the best approximation of the few smallest postive eigenvalues via a structure-preserving projection, and a four-dimensional subspace search conjugate gradient-like algorithms for simultaneously computing these eigenvalues and their associated eigenvectors. We will also present numerical examples to illustrate convergence behaviors of the proposed methods with and without preconditioning.

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Symplectic Information Geometry of Toeplitz and Toeplitz-Block-Toeplitz Hermitian Positive Definite Matrices: Busemann Barycenter & Frechet Median by Berger/Mostow Fibration

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Abstract

The median of a set of Toeplitz and Toeplitz-Block-Toeplitz Hermitian Positive Definite Matrices (THPD and TBTHPD matrices) is addressed in this paper [6]. Obviously "mean" computation is also solved but is of less interest due to its lack of robustness to outliers. As there is no "Total Order" for THPD/TBTHPD matrices, median could only be defined geometrically by Frechet's median in metric space [1] and solved by Weiszfeld/Karcher flow [2,3,7].

In a first step, the problem is solved for HPD matrices. In order to introduce with no arbitrary, the "good" metric, we prove that metrics deduced from Information Geometry (Fisher metric that is invariant by all changes of parameterization) and from Cartan-Siegel Homogenous Bounded Domains [4,5] Symplectic geometry (Siegel metric, deduced from Symplectic geometry , that is invariant by all automorphisms of these bounded domains) are exactly the same. Unfortunately, the Weiszfeld/Karcher flow will not preserve Toeplitz structure of HPD matrices.

To solve this drawback, we use the Trench theorem [8] proving that all THPD could be inverted by a new parameterization using the matrix block structure. By analogy, if we consider this THPD, as a covariance matrix of a stationary signal, this parameterization could be exactly identified with Complex Auto-Regressive (CAR) model of this signal. All THPD matrices are then diffeomorphic to $(r_0, \mu_1, \ldots, \mu_n) \in R^+ x D^n$ (r_0 is a real "scale" parameter, μ_k are called reflection/Verblunsky coefficients of CAR model in D the complex unit Poincare disk, and are "shape" parameters). This result has been found previously by Samul Verblunsky in 1936 [9,10]. We have observed that this CAR parameterization of the THPD matrix could be also interpreted as Partial Iwasawa decomposition of the matrix in Lie Group Theory [21,6]. At this step, to introduce the "natural" metric of this model, we used jointly Burbea/Rao [14] results in Information Geometry and Koszul [13] results in Hessian geometry, where the conformal metric is given by the Hessian of the Entropy of the CAR model. This metric has all good properties of invariances. Median of N THPD matrices is then easily computed by classical median for r_0 on R^+, and Weiszfeld/Karcher flow for μ_k in D^n Poincare unit polydisk. To regularize the CAR inverse problem, we have used a "regularized" Burg reflection coefficient [11] avoiding prior selection of AR model order.

To extend the problem for TBTHPD matrices, we have introduced the notion of Berger Fibration/Mostow Decomposition and modify the Weiszfeld/Karcher flow. The point driven by the flow is fixed at the origin of the unit disk and then others points are moved from Weiszfeld/Karcher drift through unit disk automorphism. Inverse automorphism of this drift at each step provides the median point in unit disk coordinates. This is done by using the polar decomposition of points in the unit disk where at each step, the drift is only deduced from the polar phases. For TBTHPD matrices, we used matrix extension of Verblunsky theorem [12] (given the diffeomorphism of TBTHPD matrix with $(R_0, M_1, \ldots, M_n) \in Herm(n)^+ x SD^n$) and Matrix-Burg like algorithm [15,16,17] to compute a Matrix CAR model, where Verblunsky coefficients M_k are no longer in unit Poincare disk but in unit Siegel disk SD. As Siegel disk SD can be fibered by associating geodesically to each point, one point on its Shilov Boundary, this Fibration, given by Mostow Decomposition [18] can be interpreted as matrix extension of Poincare disk polar decomposition for the Siegel disk.

Finally, we make the remark that respectively the Frechet's median in unit Poincare disk/Siegel disk is equivalent to conformal Douady-Earle[19]/Busemann[20] Barycenters of same points geodesically pushed on their Shilov's boundaries.

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Rational Krylov revisited

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Abstract

Since his PhD thesis in 1970 [1], Axel Ruhe has investigated efficient algorithms for solving the algebraic eigenvalue problem. In particular, he was advocating the use of rational Krylov spaces [2, 3, 4, 5, 6], and pointed out the usefulness in model reduction [6]. Further work along these lines include [9, 12]. Over the last ten years, extended Krylov spaces and more generally rational Krylov spaces have regained interest for approaching matrix functions times a vector. This includes both efficient algorithms [8, 13], and new error estimates [7, 11], see for instance the recent summary [10]. In this talk we intend to intend to give a summary of these developments, and present some new results.

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Blind image deconvolution via Hankel based method for computing the GCD of polynomials

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Abstract

This paper is devoted to present an algorithm that permits to solve the problem of blind image deconvolution by computing approximate greatest common divisors (GCD) of polynomials. Specifically, we design a specialized algorithm for computing the GCD of bivariate polynomials of blurred images which corresponding to z-tansforms to recover the original image. The new algorithm is based on the fast GCD algorithm for univariate polynomials in which the successive transformation matrices are upper triangular Toeplitz matrices. The complexity of our algorithm is $O(n^2 \log(n))$ where the size of blurred images is $n \times n$. All algorithms have been implemented in Matlab and experimental results with synthetically blurred images are included to illustrate the effectiveness of our approach.

A step towards a symplectic exponential integrator

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Abstract

Based on the Hamiltonian Lanczos process and the eponentially fitted Euler method, we construct an almost symplectic exponential integrator. For computing the exponential of the projected Hamiltonian matrix, we derive a structure-preserving variant of the scaling-and-squaring approach, that can also be used to compute phi-functions. Though the resulting method cannot be proven to be exactly symplectic yet, numerical results demonstrate that the Hamiltonian is preserved with high accuracy while implementations based on a standard Arnoldi process fail completely in preserving the Hamiltonian.

Structured matrix geometric means: theory and algorithms

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Abstract

The geometric mean of a set of positive definite matrices $A_1, \ldots, A_p$ is usually identified with the Karcher mean G which verifies most of the desirable properties of the scalar geometric mean. Unfortunately, the Karcher mean does not generally preserve the structure of the input matrices. Say, if A_i, $i = 1, \ldots, p$ are Toeplitz, then G is not Toeplitz. In this talk we introduce a definition of geometric mean which preserves the structure of the input matrices, satisfies most of the Ando-Li-Mathias properties and is easily computable. The definition relies on the Riemannian geometry of the cone of positive definite matrices and the algorithms for its computation are obtained by using optimization techniques. Numerical experiments which show the effectiveness of the algorithms are presented.

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A fast structured QZ method for colleague matrix pencils

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Abstract

We present a fast structured version of the QZ algorithm designed to compute the generalized eigenvalues of a class of matrix pencils. This class includes colleague pencils arising from the rootfinding problem for polynomials expressed in the Chebyshev basis.

The method relies on quasiseparable matrix structure and it is based on the representation of the relevant matrices as low rank perturbations of Hermitian or unitary matrices. The complexity for an $N \times N$ pencil is $\mathcal{O}(N^2)$ flops, with $\mathcal{O}(N)$ memory.

Numerical experiments performed using a Matlab implementation confirm the effectiveness and practical stability of the method.

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P. Boito, Y. Eidelman, L. Gemignani, *Implicit QR for rank-structured matrix pencils*, submitted (2012).

A new procedure to compute analytic polar decompositions

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Abstract

Polar decomposition of time-varying matrices has proved to be useful in several contexts. Thus, for instance, it appears in numerical methods for computing singular value decompositions [4] and inversion of time dependent nonsingular square matrices [1]. It is also used in computer graphics and in the study of stress and strain in continuous media [3]. Since both factors possess best approximation properties, polar decomposition can be applied in optimal orthogonalization problems [2]. It has been generalized to abstract Lie groups and even to semigroups. In this setting, the polar decomposition is equivalent to expressing a group element as the product of a term in a symmetric subspace and a term in a subgroup of the given Lie group [5].

In this work we propose a new constructive procedure to compute the polar decomposition of the fundamental real matrix of the linear system $dU/dt = A(t)U$ in the form $U(t) = \exp(X(t))\exp(Y(t))$, where $X(t)$ is a symmetric matrix and $Y(t)$ is skew-symmetric. Both matrices are explicitly constructed as series of the form $X(t) = \sum_{i\geq 1} X_i(t)$, $Y(t) = \sum_{i\geq 1} Y_i(t)$, where each term X_i, Y_i is computed recursively. The procedure is shown to converge for times $t < t_c$, with $\int_0^{t_c} \|A(t)\|dt \leq \mathrm{Si}(\pi)/2 \simeq 0.9259$. An additional advantage of the algorithm proposed here is that, if $A(t)$ belongs to a certain Lie algebra, it provides approximations to the fundamental matrix in the corresponding Lie group, and thus it preserves important qualitative properties of the exact solution.

The procedure can be easily implemented in a symbolic algebra package and is extended without difficulty to get convergent approximations to the analytic polar decomposition of a more general class of nonsingular time dependent matrices and also of the exponential of constant matrices.

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On geometric integrators for polynomial Hamiltonian systems.

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Abstract

There has been a fair amount of work in the last two decades characterizing one step integration methods having certain geometric properties when applied to general Hamiltonian systems: symplectic integrators; energy/integral-preserving integrators; conjugate-to-symplectic integrators.

A different point of view arises if we restrict the class of problems from the case of general Hamiltonian functions to the case of polynomial Hamiltonian functions and polynomial Hamiltonian vector fields. Then, it becomes often easier to preserve geometric properties. For example while for general Hamiltonian systems no Runge-Kutta method can preserve exactly the Hamiltionan, this becomes possible if we restrict to polynomial Hamiltonians. I will discuss the example of the Kahan's method which is a method defined originally for quadratic vector fields. This method has remarkable geometric properties when applied for example to cubic Hamiltonians. Such properties can be explained by studing the B-series of a Runge-Kutta method which reduces to the Kahan's method when applied to quadratic vector fields. This is joint work with R.I. McLachlan, B. Owren, G.W.R. Quispel and Ya Juan Sun.

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Refining estimates of invariant and deflating subspaces for large and sparse matrices and pencils

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Abstract

We consider the refinement of the estimates of invariant (or deflating) subspaces for a large and sparse matrix A (or pencil $A - \lambda B$) in $\mathbb{R}^n$, through some (generalized) nonsymmetric algebraic Riccati equations or their associated (generalized) Sylvester equations [1, 2, 3, 4, 5]. The crux of the method is the inversion of the dense matrix $P_2^\top A P_2 - \gamma I_{n-m}$ (or $P_{l2}^\top (A - \gamma B) P_{r2}$), for some unitary projection P_2 (or unitary projections P_{l2}, P_{r2}) in $\mathbb{R}^{n \times (n-m)}$, via the efficient inversion of $A - \gamma I_n$ (or $A - \gamma B$). All computations have an $O(n)$ complexity. Some numerical examples are given.

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The unwinding matrix

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Abstract

We introduce the *unwinding matrix*: the primary matrix function corresponding to the unwinding number introduced by Corless and Jeffrey in 1996. We show that the unwinding matrix is a valuable tool for deriving correct identities involving the matrix logarithm, matrix fractional powers, and other multivalued functions f and their inverses. We use it to derive new results as well as simple proofs of known results.

Exponential integrators: linear algebra aspects

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Abstract

In this talk we present a short overview about exponential integrators for evolution equations. We discuss different options for constructing such integrators and explain some convergence results.

For practical applications it is crucial to approximate the products of certain matrix functions related to the matrix exponential with vectors efficiently. We will thus also present some recent advances on the linear algebra aspects arising in exponential integrators.

On a generalization of inverse iteration for eigenvector nonlinearities

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Abstract

Let $A : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ be a given, sufficiently smooth function mapping a vector to a symmetric matrix. We will consider the corresponding nonlinear eigenvalue problem where the parameter $v \in \mathbb{R}^n$ equals an eigenvector of the symmetric matrix $A(v)$. That is, we wish to find $(\lambda, v) \in \mathbb{R} \times \mathbb{R}^n\backslash\{0\}$ such that

$$A(v)v = \lambda v,$$

where we also assume that A is invariant of scaling in the sense that $A(\alpha v) = A(v)$ for any $\alpha \in \mathbb{R}\backslash\{0\}$. We will study the following generalization of inverse iteration

$$v_{k+1} = \alpha_k (J(v_k) - \sigma I)^{-1} v_k$$

where $J(v)$ is the Jacobian of $A(v)v$ and $\alpha_k = 1/\|(J(v_k) - \sigma I)^{-1} v_k\|$.

We characterize the convergence of this iteration in several ways. If the shift σ is kept constant then the convergence factor to a simple eigenvalue λ_* with eigenvector v_* is given by $\rho = \frac{|\sigma-\lambda_*|}{|\lambda_{*,2}-\lambda_*|}$ where $\lambda_{*,2} \neq \lambda_*$ is the eigenvalue of $J(v_*)$ which is closest to λ_*. The convergence factor is hence proportional to the distance between the shift and the eigenvalue problem, consistent with inverse iteration for standard eigenvalue problems.

We also show that the iteration can be interpreted as a discretization of the differential equation

$$y'(t) = p(y(t))y(t) - A(y(t))y(t) \quad \text{where} \quad p(y) := \frac{y^T A(y) y}{y^T y},$$

whose stationary points are solutions to $A(y)y = \lambda y$. In particular, the algorithm is equivalent to implicit time-stepping of the differential equation for a particular choice of the step-length and discretization. The trajectories $y(t)$ automatically satisfy $\|y(t)\| = 1$ if $\|y(0)\| = 1$. The implicit time-stepping takes this into account by the standard projection approach. In several examples, we observe that an appropriate choice of the step-length often leads to convergence to the left-most eigenvalue.

Subspace methods for computing the numerical range and associated quantities

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Abstract

For a matrix $A \in \mathbb{C}^{n\times n}$ the *numerical range* (also called *field of values*) is defined as the set of all Rayleigh quotients:

$$W(A) := \left\{ \frac{x^*Ax}{x^*x} : x \in \mathbb{C}^n, x \neq 0 \right\}. \tag{1}$$

It is well known that the real parts of $W(A)$ are contained in the interval

$$\left[\lambda_{\min}\big(H(A)\big), \lambda_{\max}\big(H(A)\big)\right],$$

where $H(A) = (A + A^*)/2$ denotes the Hermitian part of A. By rotation, the intervals

$$\left[\lambda_{\min}\big(H(e^{\mathrm{i}\theta}A)\big), \lambda_{\max}\big(H(e^{\mathrm{i}\theta}A)\big)\right],$$

with $\theta \in [0, \pi]$, completely determine $W(A)$. Essentially all algorithms for computing the numerical range are based on this idea and approximate $W(A)$ by solving a number of parameter-dependent eigenvalue problems. In this talk, we propose to accelerate these algorithms by (implicitly) exploiting the piecewise smoothness of the eigenvalues of $H(e^{\mathrm{i}\theta}A)$. Our algorithm subsequently constructs an orthonormal basis U for a k-dimensional subspace containing samples of the eigenvectors belonging to the extremal eigenvalues of $H(e^{\mathrm{i}\theta}A)$, very much in the spirit of the methods from [1]. It turns out that $W(U^*AU)$ often gives an excellent approximation to $W(A)$ already for very small values of k. This algorithm can be easily adapted to only compute certain quantities associated with $W(A)$, such as the Crawford number. In ongoing joint work with Timo Betcke from UC London, this algorithm is used for the computation of coercivitiy constants in 2D and 3D wave propagation problems.

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The construction and analysis of variational integrators

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Abstract

Variational integrators are a class of geometric structure-preserving numerical methods that are based on a discrete Hamilton's variational principle, and are automatically symplectic and momentum preserving.

We will review the role of Jacobi's solution of the Hamilton–Jacobi equation in the variational error analysis of variational integrators, and demonstrate how it leads to two systematic methods for constructing variational integrators. In particular, Jacobi's solution can be characterized either in terms of a boundary-value problem or variationally, and these lead to shooting-based variational integrators and Galerkin variational integrators, respectively.

Computable discrete Lagrangians can be obtained by choosing a numerical quadrature formula, and either a finite-dimensional function space or an underlying one-step method. We prove that the resulting variational integrator is order-optimal, in that the order of the resulting variational integrator is only limited by the order of accuracy of the numerical quadrature formula, and either the approximation properties of the finite-dimensional function space or the order of accuracy of the underlying one-step method. Furthermore, when spectral basis elements are used in the Galerkin formulation, one obtains geometrically convergent variational integrators.

We will also discuss generalizations of variational integrators to Lie groups and homogeneous spaces. Time permitting, we will also describe efforts to generalize the error analysis to the setting of Lagrangian PDEs.

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Differential equations for Hamiltonian and symplectic matrix nearness problems

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Abstract

We propose and study algorithms for structured matrix optimization problems such as the following:

(A) *Given a Hamiltonian matrix with no eigenvalues on the imaginary axis, find a nearest Hamiltonian matrix having some purely imaginary eigenvalue.*

(B) *Given a Hamiltonian matrix with all eigenvalues on the imaginary axis, find a nearest Hamiltonian matrix such that arbitrarily close to that matrix there exist Hamiltonian matrices with eigenvalues off the imaginary axis.*

The notion of "nearest" depends on the choice of norm, for which we consider the matrix 2-norm in this talk. The Hamiltonian matrices can be allowed to be complex or restricted to be real. Both problems (A) and (B) are closely related to the problem of finding extremal (leftmost or rightmost) points of the structured pseudospectrum of a given matrix with respect to perturbed matrices on a given matrix manifold. We follow up on earlier work by Guglielmi and Lubich on computing extremal points of unstructured pseudospectra, where we used rank-1 differential equations for the perturbations that lead monotonically to the desired extremal points. In the Hamiltonian and symplectic cases we obtain rank-2 differential equations in the complex case, and rank-4 differential equations in the real case, to compute extremal points of the structured pseudospectrum. Combined with an iteration for the perturbation size this gives us algorithms for matrix nearness problems such as (A) and (B) and their symplectic analogues. We conclude the talk with an application to a stability problem of symplectic integrators for Hamiltonian differential equations. The talk is based on joint work with Nicola Guglielmi and Daniel Kressner.

What are the "natural" classes of scalar products?

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Abstract

Many important types of structured matrices, such as symplectic, Hamiltonian, and orthogonal matrices, are associated with an underlying scalar product. Any scalar product is defined by a nonsingular matrix M via $x^T My$ (or $x^* My$), but historically only restricted classes of matrices M have been considered, e.g., M symmetric, Hermitian, or skew-symmetric. Are there compelling *mathematical* reasons to focus attention on just these few scalar product classes, or is it just a matter of convenience? Are there other scalar products worthy of serious study? We consider an extensive list of useful properties that a scalar product may or may not possess, and investigate the logical relations between them. From a careful analysis of these relationships, two classes of scalar products naturally emerge as the ones of primary interest.

Computing the distance to the nearest unstable quadratic pencil

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Abstract

A bisection method for computing the distance of a discrete (continuous)-time stable quadratic pencil to the set of unstable quadratic pencils is described. It amounts to finding the nearest palindromic (even) quadratic pencil with an eigenvalue on the unit circle (the imaginary axis). This task is accomplished by several structure preserving eigensolvers. Their advantages and disadvantages are highlighted.

Joint work with M. Sadkane (Brest).

On solving indefinite least squares–type problems via anti–triangular factorization

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Abstract

The indefinite least squares problem and the equality constrained indefinite least squares problem are modifications of the least squares problem and the equality constrained least squares problem, respectively, involving the minimization of a certain type of indefinite quadratic form. Such problems arise in the solution of Total Least Squares problems [3], in parameter estimation and in H_∞ smoothing [4, 5]. Algorithms for computing the numerical solution of indefinite least squares and indefinite least squares with equality constraint are described in [1, 3] and [2], respectively.

The indefinite least squares problem and the equality constrained indefinite least squares problem can be expressed in an equivalent fashion as augmented square linear systems. Exploiting the particular structures of the coefficient matrices of such systems, new algorithms for computing the solution of such problems are proposed relying on the anti–triangular factorization of the coefficient matrix [6, 7]. Some results on their stability are shown together with some numerical examples.

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Structured backward errors for eigenvalues of Hermitian pencils

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Abstract

In this talk we consider the structured backward errors for eigenvalues of Hermitian pencils or, in other words, the following question:

Given a value $\lambda \in \mathbb{C}$ and two Hermitian matrices $A_1, A_2 \in \mathbb{C}^{n\times n}$, what is the smallest perturbation (Δ_1, Δ_2) with Δ_1, Δ_2 being Hermitian such that λ is an eigenvalue of the Hermitian pencil $(A_1 + \Delta_1) + \varrho(A_2 + \Delta_2)$?

The answer is well known for the case that the eigenvalue λ is real, but not for the case $\lambda \in \mathbb{C} \setminus \mathbb{R}$. In this case, only the structured backward error for *eigenpairs* (λ, v) has been considered so far, i.e., the question of finding the smallest structured perturbation that makes the given pair an eigenpair of the perturbed Hermitian pencil.

In this talk, we give a complete answer to the question by reducing the problem to an eigenvalue minimization problem of Hermitian matrices depending on two real parameters. We will show that the structured backward error of complex nonreal eigenvalues may be significatly different from the corresponding unstructured backward error - which is in conrast to the case of real eigenvalues where the structured and unstructured backward errors coincide.

The Newton polygon and structured eigenvalue perturbation

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Abstract

The Newton polygon, an elementary geometric construction first devised by Sir Isaac Newton, has been often used in the context of perturbation theory as a tool for deriving explicit first-order eigenvalue perturbation expansions. On one hand, this usually gives useful information on the directions in which perturbed eigenvalues move, something which is crucial in practical situations when eigenvalues need to be pushed in certain specific directions, or must be moved as fast as possible away from a critical (or dangerous) region by a perturbation, which is typically small. On the other hand, these asymptotic expansions often lead to sharp bounds on the condition number of eigenvalues.

When the matrix or operator under study belongs to a specific class of structured operators, it makes sense, of course, to consider only perturbations having the same structure, thereby restricting the admissible Newton polygons. So far, it seems that the structures most amenable to such a structured perturbation analysis via the Newton polygon are those defined via indefinite scalar products for which structured canonical forms are available.

In this talk we will both survey classic results for unstructured perturbation, as well as show some more recent, specific results for structured ones. Taking as a guide a specific example, involving zero eigenvalues of complex skew-symmetric matrices, we will illustrate the interplay between matrix structure and the Newton polygon.

Matrix functions for exponential integrators via interpolation at Leja points

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Abstract

Exponential integrators constitute a class of competitive integration schemes for stiff systems of differential equations. In contrast to standard Runge–Kutta methods, which require the solution of large systems of linear equations, exponential integrators are based on the matrix exponential (and related matrix functions) of the Jacobian of the problem. More precisely, the action of such matrix functions on certain vectors is required. There are various methods for carrying out this task; among those are Krylov subspace methods and interpolation methods.

In this talk we will concentrate on interpolation methods based on Leja points. Leja points are defined recursively which makes them attractive for interpolation where the degree of the interpolation polynomial is not known a priory. Moreover, they guarantee superlinear convergence of the interpolant. Recent progress consists in new a priory and a posteriory error estimates for determining the optimal degree of the interpolation polynomial. The main computational task in interpolation methods are matrix-vector multiplications. They can be implemented quite efficiently on graphics processing units (GPUs).

This is joint work with Peter Kandolf and Stefan Rainer, University of Innsbruck, and Marco Caliari, University of Verona.

Integral preserving Lie group integrators

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Abstract

We present a general method for constructing integral preserving numerical schemes on Lie groups, a sort of generalization of the discrete gradient method of Gonzalez. In our setting the discrete gradient will be replaced by the trivialized discrete differential (TDD), a map from GxG into the dual of the Lie algebra of the Lie group G. We give a general definition and show a few examples of TDDs, each of them can be chosen to be symmetric. The differential equation to be solved is expressed by means of a dual two-form on the Lie group, and the corresponding numerical object is a trivialized approximation to this, an exterior two-form on the dual of the Lie algebra. We present methods which preserve arbitrary first integrals in this setting, and show examples of symmetric schemes. We briefly discuss how the approach can be generalized to preserve more than one first integral. Numerical experiments show excellent behavior on some mechanical systems.

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MATRIX POWER MEANS AS THE ONLY AFFINE FAMILY

MIKLÓS PÁLFIA

Means of two positive definite matrices are characterized by Kubo-Ando theory by relating each 2-variable matrix mean function to an operator monotone function. Since every operator monotone function admits an integral characterization due to Loewner's theory, this provides us strong properties which are fulfilled by 2-variable matrix means.

There are several different ways to extend a 2-variable matrix mean to several variables. Most of the extension methods build on analogies from metric geometry. Recently a one-parameter family of means were considered and generalized to several variables by Lim and Pálfia, these are the matrix power means. The extension builds on an idea following from differential geometry. The applicability of the construction is due to the special and unique affine geometric structures related to power means. We will study various properties of this one-parameter family of multivariable means and their corresponding affine geometric structures. One of the most important property of this one-parameter family is that as we take the limit of the chraracterizing parameter $t \to 0$, we end up with the geometric mean (Riemannian mean or center of mass) of several positive definite matrices.

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Eigenvalue perturbation theory of classes of structured matrices under generic structured rank one perturbations

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Abstract

In this talk the perturbation theory of structured matrices under structured rank one perturbations will be discussed. Let $J = -J^T$ be an invertible skew-symmetric matrix, and let $H = H^*$ be a hermitian matrix. We consider the following classes of matrices: a complex matrix A is called J-Hamiltonian when $JA = -A^T J$, and A is called H-selfadjoint when $HA = A^* H$, and finally, A is called H-skew-symmetric if $HA + A^* H = 0$.

We shall discuss the behaviour of the eigenvalues under generic structured rank one perturbations; that is, the eigenvalues of $B = A + uu^T J$ in the case where A is J-Hamiltonian, and of $B = A \pm uu^* H$ in the case where A is H-selfadjoint. Here the vector u is generic.

Generic Jordan structures of perturbed matrices are identified. It is shown in [2] that the perturbation behavior of the Jordan structures in the case of J-Hamiltonian matrices is substantially different from the corresponding theory for unstructured generic rank one perturbation as it has been studied in [1, 4, 5, 6].

Related perturbation results for H-selfadjoint matrices are given in [3]. In that case the result concerning the Jordan structure is less surprising, as it is in line with the result for unstructured generic perturbations. However, there the relation between the sign characteristic of the pair (A, H) and that of the pair $(A + uu^* H, H)$ is of interest.

Finally, we shall discuss recent work on H-skew-symmetric matrices. A rank one perturbation of the form $B = A + uu^* H$ is not in the class of H-skew-symmetric matrices, however, it is a so-called H-positive real matrix. It will be shown that a-typical behaviour similar to the J-Hamiltonian case occurs also in this case. In addition, it will be shown that the eigenvalues of B which are not also eigenvalues of A are necessarily off the imaginary axis. These results arise as a special case of the study of low rank perturbations of H-positive real matrices. This is joint work (in preparation) with D.B. Janse van Rensburg, J.H. Fourie and G.J. Groenewald, NWU, Potchefstroom, South Africa.

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Structured matrices in the rational Lanczos method

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Abstract

The need to evaluate expressions of the form $f(A)v$ or $u^T f(A)v$, where A is a large symmetric, sparse or structured matrix, v is a vector, and f is a nonlinear function arises in many applications. The rational Lanczos method can be an attractive scheme for computing approximations of such expressions. This method projects the approximation problem onto a rational Krylov subspace of fairly small dimension, and then solves the small approximation problem so obtained. We pay particular attention to the case when approximants with few distinct poles are determined. Then an orthonormal basis for the rational Krylov subspace can be generated with short recursion formulas. We discuss the structure of the recursion formulas.

Gram-Schmidt process: from the standard to the non-standard inner product

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Abstract

In this contribution we consider the most important schemes used for orthogonalization with respect to the standard and non-standard inner product and review the main results on their behavior in finite recision arithmetic. Although all the schemes are mathematically equivalent, their numerical behavior can be significantly different. We treat separately the particular case of the standard inner product and show that similar results hold also for the case when the inner product is induced by a positive diagonal matrix. We will show that in the case of general inner product the orthogonality between computed vectors besides the linear independence of initial vectors depends also on the condition number of the matrix that induces the non-standard inner product. Finally we discuss the possible extension of this theory to some bilinear forms used in the context of various structure-preserving transformations.

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Rational Krylov – further developments and yet unsolved problems

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Abstract

The rational Krylov algorithm is a development of the spectral transformation, or more properly shift invert, Lanczos or Arnoldi algorithm, where several shifts are used in one run. It could also be regarded as a Rayleigh quotient iteration where an orthogonal basis is formed by the iterates. It was described nearly 30 years ago, and in the talk I will review some of the developments since then, and list some questions that still wait for an answer.

The first application is model reduction for linear dynamic systems, where it is now a part of standard tools in VLSI circuit simulation. Rational Krylov has been extended to problems with a nonlinear eigenvalue parameter. It is used to compute a nonlinear matrix function acting on a vector.

The traditional, linear Krylov methods can be analyzed with the well established theory of polynomial approximation. The variant of rational approximation, that describes the behavior of rational Krylov, is a current research subject.

There are issues of implementation that are not yet clarified. How can we use iterative algorithms, when solving the systems that make up the denominator in the rational function? Some better test, than just tracking the norm of the residual, must be developed. A detail still waiting for its complete solution, is how to implement rational Krylov in real arithmetic for real matrix pencils. The Francis double shift is still waiting in the sidelines.

Modified symplectic Gram-Schmidt, Householder SR algorithm and structured matrices

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Abstract

In this talk, we show that the SR factorization of a matrix A via the modified symplectic Gram-Schmidt (MSGS) algorithm is mathematically equivalent to Householder SR algorithm applied to an embedded matrix obtained from A by adding two blocks of zeros in the top of the first half and in the top of the second half of the matrix A. Also, due to the special structures of the involved matrices, we demonstrate that the Householder SR algorithm can be performed via 'simplified' Householder transformations which are not only symplectic but also skew-Hamiltonian. Throughout the computations, we stress that MSGS is also numerically equivalent to Householder SR algorithm applied the mentioned embedded matrix.

Structured matrix polynomials and their sign characteristic

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Abstract

Matrix polynomials $P(\lambda) = \lambda^m A_m + \cdots + \lambda A_1 + A_0$ with Hermitian or symmetric matrix coefficients A_i or with coefficients which alternate between Hermitian and skew-Hermitian matrices, or even with coefficient matrices appearing in a palindromic way, commonly arise in applications (see the matrix collection NLEVP [4]).

Standard and Jordan triples (X, J, Y) play a central role in the theory of matrix polynomials with nonsingular leading coefficient. They extend to matrix polynomials the notion of Jordan pairs (X, J) for a single matrix A, where $A = X^{-1}JX$. Indeed, each matrix coefficient A_i of $P(\lambda)$ can be expressed in terms of X, J and Y. We show that standard triples of structured $P(\lambda)$ have extra properties [3]. In particular there is a nonsingular matrix M such that $MY = v_{\mathcal{S}}(J)X^*$, where $v_{\mathcal{S}}(J)$ depends on the structure $\mathcal{S}$ of $P(\lambda)$ and J is M-selfadjoint when $\mathcal{S} \in \{\text{Hermitian, skew-Hermitian}\}$, M-skew-adjoint when $\mathcal{S} \in \{*\text{-even}, *\text{-odd}\}$ and M-unitary when $\mathcal{S} \in \{\text{palindromic, antipalindromic}\}$. The underlying indefinite scalar product is orthosymmetric [6] except for palindromic structures.

The property of J implies that its eigenvalues and therefore those of $P(\lambda)$ occur in pairs $(\lambda, f(\lambda))$ when $\lambda \neq f(\lambda)$, where

$$f(\lambda) = \begin{cases} \overline{\lambda} & \text{for } M\text{-self-adjoint } J, \\ -\overline{\lambda} & \text{for } M\text{-skew-adjoint } J, \\ 1/\overline{\lambda} & \text{for } M\text{-unitary } J. \end{cases}$$

The eigenvalues for which $\lambda = f(\lambda)$, that is, those that are not paired, have a sign $+1$ or -1 attached to them forming the *sign characteristic of* $P(\lambda)$. We define the sign characteristic of $P(\lambda)$ as that of the pair (J, M), show how to compute it and study its properties [1]. We discuss applications of the sign characteristic in control systems, in the solution of structured inverse polynomial eigenvalue problems and in the characterizatio of special structured matrix polynomials such as overdamped quadratics, hyperbolic and quasidefinite matrix polynomials [2].

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Structured matrices and multivariate orthogonal polynomials

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Abstract

For polynomials orthogonal on the real line, the three term recurrence relation can be written in a compact way using a tridiagonal (Jacobi) matrix. In this talk, the structure of the matrices connected to the recurrence relation for multivariate orthogonal polynomials is described. When the inner product is discrete, computing these generalized Hessenberg matrices is equivalent to solving an inverse eigenvalue problem. When looking for "good points" for multivariate polynomial interpolation, we will indicate that these generalized Hessenberg matrices could play an important role.

An extension of the multi-shift QZ-algorithm beyond the Hessenberg-upper triangular pencil

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Abstract

Recently an extension of the class of matrices admitting a Francis type of multishift QR algorithm was proposed by the authors. These so-called condensed matrices admit a storage cost identical to that of the Hessenberg matrix and share all of the properties essential for the development of an effective implicit QR type method. This talk continues along this trajectory by discussing the generalized eigenvalue problem. The novelty does not lie in the almost trivial extension of replacing the Hessenberg matrix in the pencil by a condensed matrix, but in the fact that both pencil matrices can be partially of condensed form. Again, the storage cost and crucial features of the Hessenberg–upper triangular pencil are retained, giving rise to an equally viable QZ like method. The associated implicit algorithm also relies on bulge chasing and exhibits a sort of bulge hopping from one to the other matrix. This talk presents the reduction to a condensed pencil form and an extension of the QZ algorithm. Relationships between these new ideas and some known algorithms are also discussed.

The error in the product QR decomposition and applications

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Abstract

The QR decomposition is applied to sequences of matrices in many circumstances including the approximation of eigenvalues of a matrix and the approximation of stability spectra (Lyapunov exponents, etc.) for dynamical systems. In this talk we present an error analysis for the product QR based upon the recent works [2, 1]. The technique involves application of the classical Newton-Kantorovich Theorem to an appropriate zero finding problem. The theory is shown to be useful under certain conditions that are central to the perturbation theory for Lypapunov exponents. Time permitting, applications of the theory will be presented for the approximation of stability spectra for linear retarded delay differential equations, differential-algebraic equations, and linear Hamiltonian differential equations. This talk represents joint work with M. Badawy (Kansas), D. Breda (Udine), V. Linh (Hanoi), and V. Mehrmann (Berlin).

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Computational methods based on structured pseudospectra

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Abstract

Controllability and observability are important properties of dynamical systems. These are related to the perturbability of the poles of the transfer function under structured perturbations. Therefore we consider structured pseudospectra to analyze the behavior of dynamical systems. The focus of this talk is the computation of the $\mathcal{H}_\infty$-norm for large-scale descriptor systems. It can be shown that for this purpose one has to find the pseudospectrum that touches the imaginary axis, i.e., the right-most pseudopole is on the imaginary axis. A fast iterative scheme that converges to the right-most pseudopole together with a root finder is used to efficiently find this particular pseudospectrum.

Another aspect of this talk will be the fast computation of structured pseudospectral plots, including a comparison of performance and quality of the plots.

Fast computation of eigenvalues of companion, comrade, and related matrices

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Abstract

The usual method for computing the zeros of a polynomial is to form the companion matrix and compute its eigenvalues. In recent years several methods that do this computation in $O(n^2)$ time with $O(n)$ memory by exploiting the structure of the companion matrix have been proposed. We propose a new class of methods of this type that utilizes a factorization of the comrade (or similar) matrix into a product of essentially 2×2 matrices times a banded upper-triangular matrix. Our algorithm is a non-unitary variant of Francis's implicitly shifted QR algorithm that preserves this factored form. We will present numerical results and compare our method with other methods.

Convergence of QR algorithm for normal matrices

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Abstract

The QR algorithm is considered as one of the top 10 algorithms in the 20th century. Yet, its convergence behavior has not been fully understood even in then Hermitian matrix case.

The QR algorithm with both the Rayleigh-quotient shift and Wilkinson's shift is considered but limited to the normal matrix case. A complete characterization about its convergence behavior is provided. Besides the well-known convergence properties, the results also give all other possibilities. Another feature is that the results also show how the eigenvalue location and the vector for the initial Hessenberg reduction govern the convergence of the QR algorithm.

The results may give a better understanding about the QR algorithm, and may help to improve the QR and QR-type algorithms, particularly those developed for structured matrices normally having eigenvalues with special patterns.

Symmetric spaces and Lie triple systems in numerical analysis

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Abstract

A remarkable number of different numerical algorithms can be understood and analyzed using the concepts of symmetric spaces and Lie triple systems, which are well known in differential geometry from the study of spaces of constant curvature and their tangents. In numerical analysis there exist numerous examples of objects forming a *group*, i.e. object that compose in an associative manner, have an inverse and identity element. *Semigroups*, sets of objects close under composition but not inversion, are also well studied in literature. However, there are important examples of objects that are neither a group nor a semigroup. One important case is the class of objects closed under a 'sandwich-type' product, $(a, b) \mapsto aba$. Spaces closed under the algebraically nicer product $(a, b) \mapsto ab^{-1}a$, are called symmetric spaces. For example, the collection of all symmetric positive definite matrices and all selfadjoint Runge–Kutta methods. The theory of symmetric spaces unifies a range of different topics, such as polar-type matrix decompositions, splitting methods for computation of the matrix exponential, generalized polar coordinates for the decompositions of flows in control theory, composition of self-adjoint numerical integrators, the Scovel projection and dynamical systems with reversing symmetries, the Thue–Morse technique and dynamical with symmetries, just to name a few. We also consider a new composition technique for systems with symmetries. The new technique allows to increase the order of preservation of symmetries by two units, with an appropriate choice of stepsize. Since all the time-steps are positive, the technique is particularly suited to stiff problems, where a negative time-step can cause instabilities.

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