

Due giorni di Algebra Lineare Numerica e Applicazioni

Book of Abstracts

8th-9th February 2018, Padua

Department of Mathematics “Tullio Levi-Civita”



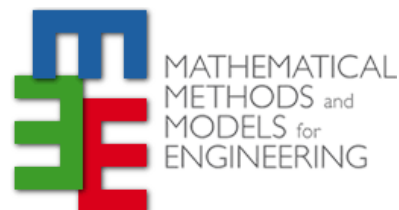
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Sponsors



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8:45 → 9:00 Opening Remarks	
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09.00 → 09.25 E. Tyrtysnikov	08.45 → 09.10 A. Wathen
09.25 → 09.50 B. Iannazzo	09.10 → 09.35 D. di Serafino
09.50 → 10.15 S. Massei	09.35 → 10.00 F. Durastante
10.15 → 10.40 L. Aceto	10.00 → 10.25 C. Janna
10.40 → 11.05 R. Zanotto	10.25 → 10.50 M. Tani
11:05 → 11:30 Coffee Break	10.50 → 11.20 Coffee break
11.30 → 13.10 Chair: V. Simoncini	11.20 → 13.00 Chair: D. Bertaccini
11.30 → 11.55 P. Dell'Acqua	11.20 → 11.45 E. Perracchione
11.55 → 12.20 B. Carpentieri	11.45 → 12.10 D. Palitta
12.20 → 12.45 L. Fermo	12.10 → 12.35 S. Maset
12.45 → 13.10 N. Caruso	12.35 → 13.00 A. Fazzi
13:10 → 14:50 Lunch	13.00 → 14.30 Lunch
14:50 → 16.30 Chair: D. Di Serafino	14.30 → 16.35 Chair: N. Mastronardi
14.50 → 15.15 S. Pozza	14.30 → 14.55 A. Cicone
15.15 → 15.40 D. Fasino	14.55 → 15.20 D. Bianchi
15.40 → 16.05 F. Tudisco	15.20 → 15.45 M. Dessole
16.05 → 16.30 F. Poloni	15.45 → 16.10 A. Franceschini
	16.10 → 16.35 S. Cipolla
16.30 → 17.00 Coffee break	
	16.35 → 17.00 Closing + Coffee Break
17.00 → 18.40 Chair: S. Serra-Capizzano	
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17.25 → 17.50 C. Garoni	
17.50 → 18.15 G. Barbarino	
18.15 → 18.40 I. Furci	
20.30 → Dinner at "Ristorante Zairo"	
Prato della Valle 51	

Abstracts

Rational approximations of fractional powers of matrices

Lidia Aceto¹, Paolo Novati²

8 Feb
10:15

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Fractional powers of matrices can be used to construct numerical methods for the solution of problems involving fractional derivatives. For instance, denoting by A the approximation of the standard Laplacian with homogeneous Dirichlet boundary conditions obtained by using any finite difference method, the so-called *matrix transfer technique* introduced by Ilić et al. in [4, 5] approximates the fractional Laplacian operator of order 2α , $\alpha \in (1/2, 1]$, by A^α . The idea can be extended to other kind of fractional derivatives whenever A represents the discretization of the corresponding integer order one [1].

In this view, any numerical scheme able to compute the matrix fractional powers can be potentially used to define a method for fractional equations. Nevertheless, when working with fractional powers, it must be kept in mind that raising to a fractional number destroys the sparsity structure of the underlying integer order approximation. As a consequence, the corresponding solver may be extremely expensive for large size matrices. In order to tackle this problem, in [2, 3] we have studied a rational approximation to A^α , that is,

$$A^\alpha \approx [q_k(A)]^{-1} p_k(A), \quad (1)$$

where $p_k, q_k \in \Pi_k$, the set of polynomials of degree k and smaller. Considering that good accuracy is attainable for values of the bandwidth k much less than the size of A^α , the action of A^α is then approximated through the action of sparse matrices. However, the condition number of $p_k(A)$ and $q_k(A)$ becomes (with respect to k) quickly very large.

In this talk, we first recall the basic features about this rational approximation, that is essentially a scaled Padé form, and then we present a simple but reliable strategy that allows to keep the conditioning under control.

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Perturbations of Hermitian Matrices and Applications to Spectral Symbols

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It is often observed in practice that matrix sequences $\{A_n\}_n$ generated by discretization methods applied to linear differential equations, possess a *Spectral Symbol*, that is a measurable function describing the asymptotic distribution of the eigenvalues of A_n . Sequences composed by Hermitian matrices own real spectral symbols, that can be derived through the axioms of *Generalized Locally Toeplitz* sequences [1].

The spectral analysis of matrix-sequences which can be written as a non-Hermitian perturbation of a given Hermitian matrix-sequence has been performed in a previous work by Leonid Golinskii and the second author [2]. A result was proven but under the technical restrictive assumption that the involved matrix-sequences are uniformly bounded in spectral norm. Nevertheless that result had a remarkable impact in the analysis of spectral distribution and clustering of matrix-sequences coming from various applications, mainly in the context of the numerical approximation of partial differential equations (PDEs) and related preconditioned matrix-sequences.

In this presentation, we propose a new result that does not require the boundedness of the sequences and permits to enlarge substantially the class of problems, such as variable-coefficient PDEs and preconditioned matrix-sequences with unbounded coefficients.

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Regularization preconditioners for frame-based image deblurring

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We are interested in fast and stable iterative regularization methods for image deblurring problems with space invariant blur. The associated coefficient matrix has a Block Toeplitz Toeplitz Blocks (BTTB) like structure depending on the boundary conditions imposed on the imaging model. In the literature, several strategies have been proposed in the attempt to define proper preconditioner for iterative regularization methods that involve such linear systems. Usually, the structure of the preconditioner is chosen Block Circulant with Circulant Blocks (BCCB) because it can be efficiently exploited by Fast Fourier Transform (FFT). Nevertheless, for ill-conditioned problems, it is well known that BCCB preconditioners cannot provide a strong clustering of the eigenvalues. Moreover, in order to get an effective preconditioner, it is crucial to preserve the structure of the coefficient matrix.

On the other hand, thresholding iterative methods are recently successfully applied to image deblurring problems, exploiting the sparsity of the image in a proper wavelet domain. Motivated by the results of recent papers [2, 3], we combine a nonstationary preconditioned iteration [1] with the modified linearized Bregman algorithm (MLBA) and proper regularization operators.

We prove that our algorithms are regularizing and convergent. Finally, several numerical experiments shows the consistency of our methods in terms of speed and quality of the restorations.

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-

Preconditioning Boundary Integral Equations with Application to High-Frequency Wave Propagation Analysis

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8 Feb
11:55

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Boundary integral equations are integral equations defined on the boundary of the domain of interest. The price that one pays for replacing a three-dimensional model with a two-dimensional model is that upon discretization a sparse problem in $\mathcal{O}(n^3)$ variables is replaced by a dense problem in $\mathcal{O}(n^2)$. Most truly dense linear systems arising from scientific applications come from the solution of boundary integral equations. Their size can be extremely large in applications. The scattering of a plane wave by a perfectly electrically conducting spherical geometry with a diameter of 1800 wavelengths modelled using surface integral equations would give rise to a fully populated matrix with more than three billion unknowns. Direct methods, both in-core and out-of-core, are not affordable to solve problems of this size even on modern parallel computers due to the large memory requirements. Iterative Krylov methods can solve the problems of space of direct methods, but they need fast matrix-vector products and robust preconditioners to achieve almost linear complexity.

In this talk, we present our recent advances in the design of preconditioned Krylov methods for solving dense linear systems arising from boundary element discretization of high-frequency cavity scattering problems. We discuss various numerical linear algebra aspects, such as the choice of the iterative method, the characteristics and performance of fast integral equation solvers for the matrix-vector product operation, and the design of algebraic preconditioners based on multilevel incomplete LU factorization, sparse approximate inverses and inner-outer methods combined with fast solvers. We also consider symmetry-preserving strategies both for the iterative method and for the preconditioner. These numerical linear algebra tools have enabled us the solution of large scattering applications efficiently on a moderate number of processors.

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In this work we study the behaviour of the LSQR algorithm in the solution of the linear equation $Ax = b$ where A is a compact operator between two separable Hilbert spaces and $b \in \mathcal{R}(A)$ the range of A . We present a rigorous analysis concerning the existence of a Krylov solution, and new results on the rate of convergence in terms of an ℓ_p sequence where p depends on the summability of the singular values of the operator. We also study the approximation of the singular values of the operator obtained by the bidiagonal matrices derived from the Lanczos bidiagonalisation algorithm.

On the numerical convergence and properties of the Iterative Filtering method for the analysis of nonlinear and nonstationary signals

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The decomposition and analysis of nonstationary and nonlinear signals are of great interest both from a theoretical and an applied standpoint. Among possible applications we mention, for instance, the refining of nondestructive techniques for the identification of faults in buildings or machineries; the identification of hidden quasiperiodicities and long term behaviors in a time series like the average troposphere temperature, a financial index, or the terrestrial magnetic field driven by the solar wind [3].

Standard techniques like Fourier or wavelet Transform are unable to properly capture nonlinear and nonstationary phenomena. For this very reason in the last two decades several ad hoc methods have been proposed in the literature. Among them there is the so called Iterative Filtering method [1, 2, 4], whose numerical convergence and stability was not completely understood so far.

In this talk we quickly overview previously developed methods, we introduce a complete numerical convergence of Iterative Filtering, we provide details about its properties and show some numerical examples.

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A Markov Chain is a discrete stochastic process $\{X_t\}_{t=0}^{\infty}$ over a finite state space where the probability distribution of X_{t+1} depends on the previous X_t, \dots, X_0 . However, the classic “Markov property” specifies that the transition probability to the next state only depends on the probability of the current state, i.e. $\mathbb{P}(X_{t+1}|X_t, \dots, X_0) = \mathbb{P}(X_{t+1}|X_t)$. Nevertheless, there are situations where it is important to keep track of what happens further in the past, leading to what we call *Higher Order Markov Chain*.

Given a random walk on a directed graph, the PageRank modification [1] builds a new Markov chain that always has a unique stationary distribution. Recently this idea has been extended to Higher Order Markov Chains [2]. Although this extension has attractive theoretical properties, it is computationally intractable for problems of large size; hence an approximation of the ideal Higher Order PageRank vector is introduced, called Multilinear PageRank. The Multilinear PageRank vector can be interpreted as the stationary distribution of a non-Markovian stochastic process called the “spacey random surfer”.

In this talk, after a short survey on results about the existence/uniqueness of the solution and on the state-of-the-art of computational techniques for the Multilinear PageRank vector, we will show how its computation can be considerably sped-up using extrapolation techniques. In particular we will show how the sequence generated by two fixed point-type techniques as the SS-HOPM [3] and the Inner-Outer Method [2], are accelerated using the The Simplified Topological ϵ -Algorithm (STEA) [4] in the restarted form [5]. The considerable improvement of the rate of convergence in the accelerated version, obtained at the cost of a fixed number of scalar products per step, suggests that the sequences generated by the considered methods are particularly close to the Shanks Kernel and hence encourages further theoretical investigation.

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8 Feb
11:30

A general framework for ADMM acceleration

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The Alternating Direction Multipliers Method (ADMM) is a very popular algorithm for addressing the problem of minimizing a convex function subject to some constraints. Such problem is important from the application point of view, since it occurs in many fields of science and engineering. ADMM is a good numerical tool, but unfortunately it has the drawback that it can exhibit slow convergence. Thus, several approaches for accelerating it have been proposed. In this talk we present a general framework for acceleration of ADMM algorithm. In particular, we describe an algorithm in which it is possible to insert any acceleration step and still having convergence guarantee, thanks to a guard condition. Numerical results, in which we consider several acceleration strategies, show that this framework leads to an improvement with respect to the state of the art.

9 Feb
15:20 **On the approximate solution of triangular systems for massively parallel machines**

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Parallel solution of sparse triangular linear systems is indeed a challenging task due to its inherently sequential nature. Many classical techniques are based on level scheduling rows that are independent [1], but depending on the sparsity pattern there may be a very large number of levels with a small amount of work to efficiently use massively-parallel architectures like GPUs. In the present talk we show other possibilities for the case of a Krylov subspace method coupled with a LU-type preconditioner. In particular, we introduce an hybrid direct/iterative two steps method and we present a numerical application to a CFD model problem [4] that shows performance gains of this approach over cuSPARSE direct solver.

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Designing constraint-preconditioned Krylov methods for the solution of regularized saddle-point systems

9 Feb
09:10

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We are interested in the iterative solution of regularized saddle-point systems where the leading block of the matrix can be either symmetric or non-symmetric. These systems arise in many areas of scientific computing, such as interior point and augmented Lagrangian methods for constrained optimization, and stabilized finite-element discretizations of incompressible flow problems [1, 2].

When the leading block is symmetric and satisfies additional conditions, e.g., accounting for the local convexity of an associated minimization problem, the system can be solved by using the conjugate gradient method coupled with a constraint preconditioner, a choice that has proved to be very effective, especially in optimization applications. In this work, we consider more general leading blocks and investigate the design of constraint-preconditioned variants of other Krylov methods, by focusing on the underlying basis-generation processes.

We build upon [3] to provide general guidelines that allow us to specialize any Krylov method to regularized saddle-point systems. In particular, we obtain constraint-preconditioned variants of Lanczos and Arnoldi-based methods, including MINRES, SYMMLQ, GMRES(m) and DQGMRES. A numerical illustration of their behaviour is provided, using systems arising in constrained optimization and fluid-flow simulation.

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Fast Solution of Time-Dependent Fractional PDEs: Sparse and Limited Memory Block Preconditioners

9 Feb
09:35

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In our talk, we propose an innovative algorithm for the large (dense) linear systems of time-dependent partial fractional differential equations discretized in time with linear multistep formulas, both in classical [1] and in boundary value form [2]. We use, in both cases, the short-memory principle to ensure the decay of the entries of sparse approximations of the discretized operator and its inverse.

Standard Krylov methods with preconditioners based on short-memory principle as well are then used to solve the underlying sequence of linear systems, while FGMRES method is used for the systems in boundary value form. The sparse approximate inverse preconditioners for linear multistep formulas in classical form are implemented on GPU devices by means of the techniques proposed in [3]. Notes on recent tests for some nonlinear time-fractional problems will be also presented.

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Spectral Preconditioner for the numerical solution of Branched Transport model

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We present the efficient strategy described in [2] for the solution of sequences of linear systems arising in the numerical solution of a Branched Transport model, extension of the Dynamical Monge-Kantorovich equations introduced in [1]. The linear systems are characterized by large sparse very ill conditioned symmetric positive definite (SPD) matrix A . These linear systems are generated by a combination of Galerkin Finite Element discretization and explicit Euler time stepping yield a linear system to be solved at each time step. Extreme cases even prevent the convergence of PCG with standard preconditioners such as an IC (with partial fill-in) factorization of A , which can not always be computed.

We present several preconditioning strategies that incorporate partial approximated spectral information of the matrix A . In our approach, we compute a number of approximated eigenvectors for a given coefficient matrix in the sequence of linear systems to be solved (i.e. the first one). Then, we used these spectral informations to obtain an efficient preconditioner for the subsequent systems in the sequence. We present numerical evidence showing the efficiency of the proposed techniques, in terms of reduction of the condition number of the preconditioned systems, and thus decreasing the number of PCG iterations and the overall CPU time.

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The *tensor train decomposition* is a representation technique which allows compact storage and efficient computations with arbitrary tensors [2]. Basically, a tensor train (TT) decomposition of a d -dimensional tensor \mathbf{A} with size $n_1 \times n_2 \times \dots \times n_d$ is a sequence G_1, \dots, G_d of 3-tensors (the *carriages*); the size of G_i is $r_{i-1} \times n_i \times r_i$ with $r_0 = r_d = 1$ (that is, G_1 and G_d are ordinary matrices) and

$$\mathbf{A}(i_1, i_2, \dots, i_d) = \sum_{\alpha_1, \dots, \alpha_{d-1}} G_1(i_1, \alpha_1) G_2(\alpha_1, i_2, \alpha_2) \cdots G_d(\alpha_{d-1}, i_d).$$

The index α_i runs from 1 to r_i , for $i = 1, \dots, d-1$, and the numbers r_1, \dots, r_{d-1} are the *TT-ranks* of \mathbf{A} . We will use the notation $\mathbf{A} = \text{TT}(G_1, \dots, G_d)$.

We present a backward error analysis of two algorithms found in [3] which perform computations with tensors in TT-format. The first one produces an exact or approximate TT-decomposition G_1, \dots, G_d of a tensor \mathbf{A} given in functional form, depending on a tolerance ε . If $\varepsilon = 0$ then the output of the algorithm is an exact TT-decomposition, that is, $\mathbf{A} = \text{TT}(G_1, \dots, G_d)$. If $\varepsilon > 0$ then $\text{TT}(G_1, \dots, G_d)$ is an $\mathcal{O}(\varepsilon)$ -approximation of \mathbf{A} which can realize significant savings in memory space. The computational core of the algorithm is a suitable (approximate) matrix factorization that, in the original paper, relies on SVD computations. We prove that analogous performances and backward stability can be obtained by means of QR factorizations.

The second algorithm computes the *contraction* (multilinear form) of a tensor in TT-format and vectors v_1, \dots, v_d ,

$$a = \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} \sum_{\alpha_1, \dots, \alpha_{d-1}} G_1(i_1, \alpha_1) G_2(\alpha_1, i_2, \alpha_2) \cdots G_d(\alpha_{d-1}, i_d) v_1(i_1) \cdots v_d(i_d).$$

By means of known error bounds for inner products in floating point arithmetic [1], we prove backward stability of the proposed algorithm under very general hypotheses on the evaluation order of the innermost summations. More precisely, if $\mathbf{A} = \text{TT}(G_1, \dots, G_d)$ and no underflows or overflows are encountered then the output \hat{a} computed by the algorithm in floating point arithmetic is the exact contraction of $\hat{\mathbf{A}} = \text{TT}(G_1 + \Delta G_1, \dots, G_d + \Delta G_d)$ and v_1, \dots, v_d where $|\Delta G_i| \leq (n_i + r_{i-1})u|G_i| + \mathcal{O}(u^2)$ and u is the machine precision.

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An ODE based method for computing the Approximate Greatest Common Divisor of polynomials

9 Feb
12:35

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Computing the greatest common divisor of a set of polynomials is a problem which plays an important role in different fields, such as linear system, control and network theory. In practice, the polynomials are obtained through measurements and computations, so that their coefficients are inexact. This poses the problem of computing an approximate common factor. We propose an improvement and a generalization of the method recently proposed in [1], which restates the problem as a (structured) distance to singularity of the Sylvester matrix. We generalize the algorithm in order to work with more than 2 polynomials and to compute an Approximate GCD of degree $k \geq 1$; moreover we show that the algorithm becomes faster by replacing the eigenvalues by the singular values.

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A numerical method for bisingular Cauchy integral equations

8 Feb
12:20

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This talk deals with the numerical solution of bisingular Cauchy integral equations of the first kind, defined on the square $S = [-1, 1] \times [-1, 1]$, having the following form

$$(D + K)f = g$$

where f is the bivariate unknown function, g is a given right-hand side, D is the dominant operator

$$Df(t, s) = \frac{1}{\pi^2} \oint_S \frac{f(x, y)}{(x-t)(y-s)} \sqrt{\frac{1-x}{1+x}} \sqrt{\frac{1-y}{1+y}} dx dy,$$

and K is the perturbation operator

$$Kf(t, s) = \int_S k(x, y, t, s) f(x, y) \sqrt{\frac{1-x}{1+x}} \sqrt{\frac{1-y}{1+y}} dx dy$$

with k a given kernel function.

For its solution we propose a numerical method based on a polynomial approximation of the unknown function f . We examine the stability of the proposed method, discuss the convergence, and analyze the conditioning of the linear system we solve. Moreover, we illustrate numerical tests showing the efficiency of the approach.

Iterative Construction of Non-Symmetric Factored Sparse Approximate Inverse Preconditioners

9 Feb
15:45

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Factored sparse approximate inverses (FSAI) play a key-role in the efficient algebraic preconditioning of sparse linear systems of equations. For SPD problems remarkable results are obtained by building the FSAI non-zero pattern iteratively during its computation [1]. Unfortunately, an equivalent algorithm still is missing in the non-symmetric case. In the present contribution we explore the possibility of iteratively computing FSAI for non-symmetric matrices by using an incomplete Krylov subspace bi-orthogonalization procedure. Another adaptive technique relies on the idea of directly minimizing the two norm of the off-diagonal row(/column) of the preconditioned matrix. Finally, as reference algorithm, a factorized sparse approximate inverse on static pattern is considered.

The main idea behind these approaches is to build two real sparse triangular factors (W is lower triangular and Z is upper triangular) such that:

$$WAZ = D \tag{2}$$

where $A \in \mathbb{R}^{n \times n}$ is the original non-symmetric matrix and D is the preconditioned matrix. Factors W and Z should be sparse, cheap to compute and effective, i.e. D tends to be diagonal.

The three mentioned algorithms are intrinsically parallel as they compute the approximate inverse row(/column)-wisely, with each row independently computed from the others. In this preliminary work, we show the effectiveness of the bi-orthogonalization based preconditioner for Krylov subspace iterative methods, like BiCGstab and GMRES. We compare this approach also with the norm minimization technique and with the computation relying on a static pattern.

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Exact Formulae and Matrix-less eigensolvers for Block Banded Toeplitz-like matrices

8 Feb
18:15

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Bogoya, Böttcher, Grudsky, and Maximenko have recently obtained the precise asymptotic expansion for the eigenvalues of a sequence of Toeplitz matrices $\{T_n(f)\}_n$, under suitable assumptions on the associated generating function f [2]. An evident restriction is that f has to be polynomial, monotone and scalar-valued.

In this talk we focus on the case of f being a $s \times s$ matrix-valued trigonometric polynomial, $s \geq 1$, and $\{T_n(f)\}_n$ a sequence of block Toeplitz matrix generated by f , with size $N(n, s) = sn$, where the case $s = 1$ corresponds to that already treated in the literature [6].

Following the proposal in the scalar-valued case, we devise an extrapolation algorithm [1, 4, 5, 6] (see also [3]) for computing the eigenvalues in the present setting regarding banded symmetric block Toeplitz matrices, with a high level of accuracy and with a low computational cost. We use the asymptotic expansion to study the spectral properties of special block Toeplitz structures and we show exact formulae for the eigenvalues of the stiffness matrices coming from the Q_p Lagrangian FEM approximation of a second order elliptic differential problem [7]. Numerical results are presented and critically discussed.

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Fast Computation of Toeplitz Eigenvalues through Asymptotic Expansions and Extrapolation

8 Feb
17:25

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Extrapolation is known to be one of the most successful ways for accelerating the convergence of numerical methods [2]. In the words of Birkhoff and Rota, “its usefulness for practical computations can hardly be overestimated”. In the presence of an asymptotic expansion for the quantity to be approximated, a “canonical” extrapolation method arises; think, for example, to Romberg’s integration method, which arises from the Euler–Maclaurin expansion associated with the trapezoidal formula.

In this presentation, we discuss a recently conjectured asymptotic expansion for the eigenvalues of banded symmetric Toeplitz matrices [5]. We also describe the related extrapolation method, which allows the fast computation of the spectrum of such matrices [4, 5]. Further applications of this method include the fast computation of the eigenvalues of both preconditioned banded symmetric Toeplitz matrices [1, 4] and PDE discretization matrices [3].

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A Schur algorithm for rational matrix equations

8 Feb
09:25

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Let r be a rational function. We consider the matrix equation $r(X) = A$, where A and X are a given and an unknown square complex matrix, respectively, and $r(X)$ should be understood in the sense of functions of matrices [1].

After a brief classification of the solutions, we describe an algorithm, based on a recursion on the Schur normal form of A , to compute all the *well-posed* solutions of the aforementioned equation. The algorithm is constructed in a fashion similar to existing algorithms for specific problems, such as the ones for the equation $X^p = A$ [2], and behaves in a similar, stable way. Moreover, in the case of real data, it is able to compute the real solutions using only real arithmetic.

As an application, we propose a new algorithm for computing the matrix logarithm, built on the inverse scaling and squaring method [3], but relying on a different rational approximation.

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A novel AMG approach based on adaptive smoothing and prolongation for ill-conditioned linear systems

9 Feb
10:25

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The numerical simulation of modern engineering problems can easily incorporate millions or even billions degrees of freedom. In several applications, these simulations require the solution to sparse linear systems of equations, and algebraic multigrid (AMG) methods are often standard choices as iterative solvers or preconditioners [1]. This happens due to their high convergence speed guaranteed even in large size problems, which is a consequence of the AMG ability of reducing particular error components across their multilevel hierarchy. Despite carrying the name “algebraic”, most of these methods still rely on additional information other than the global assembled sparse matrix, as for instance the knowledge of the operator near kernel. This fact somewhat limits their applicability as black-box solvers. In this work, we introduce a novel AMG approach featuring the adaptive Factored Sparse Approximate Inverse (aFSAI) [2] method as a flexible smoother as well as three new approaches to adaptively compute the prolongation operator. We assess the performance of the proposed AMG through the solution of a set of model problems along with real-world engineering test cases. Moreover, comparisons are made with the aFSAI and BoomerAMG preconditioners, showing that our new method proves to be superior to the first strategy and comparable to the second one, if not better as in the elasticity problems.

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Conditioning and relative error propagation in linear autonomous ordinary differential equations

9 Feb
12:10

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In this talk, we study the relative error propagation in the solution of linear autonomous ordinary differential equations with respect to perturbations in the initial value. We also consider equations with a constant forcing term and a nonzero equilibrium. The study is carried out for equations defined by normal matrices.

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In this work we study how the solutions of certain linear matrix equations behave when the original coefficients are modified with low-rank perturbations. More precisely, given the solution X_0 of the Sylvester equation $AX_0 + X_0B = C$, and 3 low-rank matrices $\delta A, \delta B$ and δC , we are interested in characterizing the update δX that verifies

$$(A + \delta A)(X_0 + \delta X) + (X_0 + \delta X)(B + \delta B) = C + \delta C.$$

Under reasonable assumptions, δX turns out to have a low numerical rank and allows to be efficiently approximated by means of Krylov subspace techniques. We show how to exploit this property to design divide and conquer methods for solving large-scale Sylvester equations whose coefficients are represented in the HODLR and HSS formats. This comprises the case of banded and quasiseparable coefficients.

Numerical methods for Lyapunov matrix equations with banded symmetric data

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We are interested in the numerical solution of the large-scale Lyapunov equation

$$A\mathbf{X} + \mathbf{X}A^T = C,$$

where $A, C \in \mathbb{R}^{n \times n}$ are both large and banded matrices. We suppose that A is symmetric and positive definite and C is symmetric. While the case of low-rank C has been successfully addressed in the literature, the more general banded setting has not received much attention, in spite of its possible occurrence in applications. In this talk we aim to fill this gap.

It has been recently shown that if A is well conditioned, the entries of the solution matrix \mathbf{X} decay in absolute value as their indexes move away from the sparsity pattern of C . This property can be used in a memory-saving matrix-oriented Conjugate Gradient method to obtain a banded approximate solution.

For A not well conditioned, the entries of \mathbf{X} do not sufficiently decay to derive a good banded approximation. Nonetheless, we show that it is possible to split \mathbf{X} as $\mathbf{X} = \mathbf{Z}_b + \mathbf{Z}_r$, where \mathbf{Z}_b is banded and \mathbf{Z}_r is numerically low rank. We thus propose a novel strategy that efficiently approximates both \mathbf{Z}_b and \mathbf{Z}_r with acceptable memory requirements.

Numerical experiments are reported to illustrate the potential of the discussed methods.

Numerical linear algebra techniques for efficient RBFs interpolation and collocation

9 Feb
11:20

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Scattered data interpolation using Radial Basis Functions (RBFs) involves solving ill-conditioned Symmetric Positive Definite (SPD) linear systems; refer e.g. to [6] for further details. We will discuss the properties (conditioning, density) of the interpolation matrices for both global and compactly supported kernels, depending on the value of the shape parameter for both classical global interpolation and local methods based on Partition of Unity (PU). The severe ill-conditioning of the interpolation matrices causes theoretically SPD matrices to be not numerically SPD. We will discuss the benefits provided by Tikhonov regularization techniques to guarantee the stability of the solution, as well as preconditioned iterative methods for the solution by collocation of elliptic boundary value problems [2].

Also efficient numerical linear algebra tools are needed in the computation of rational RBF interpolants [4, 5]. Rational RBF interpolation reveals particularly suitable for approximating functions that display oscillations or steep gradients. The study described in [3] reveals that the method is robust enough to accurately fit data coming from applications, such as Earth's topography. Moreover, when compactly supported RBFs are used, it enables us to increase the sparsity of the kernel matrices and at the same time to maintain a good accuracy. Furthermore, since a global interpolation method cannot handle truly large sets of points, an efficient implementation via the PU method is carried out. The resulting scheme requires the solution of a set of generalized eigenvalue problems, one for each local subdomain. We will describe an efficient algorithm for solving these local eigenvalue problems by means of the combination of the power method and the Deflation-Accelerated Conjugate Gradient (DACG) method [1]. We will present results showing that with this efficient implementation the proposed method outperforms the classical and rescaled PU schemes.

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In [2], the authors obtain a backward stable algorithm for computing the eigenvalues of a matrix polynomial $P(z) = z^d + A_{d-1}z^{d-1} + \dots + A_1z + A_0 \in \mathbb{C}[z]^{k \times k}$ using a fast eigensolver on the classical Frobenius (column-based) companion matrix. The two main properties that make it possible are:

1. this companion matrix can be factored into the product of k analogous companion matrices of *scalar* polynomials ($k = 1$);
2. this companion matrix is a small-rank modification of an orthogonal matrix.

We show that both these results hold also for a larger class of companion matrices introduced by Fiedler [1, 3]. The matrices in this class can be obtained as products of elementary matrices of the form

$$\begin{bmatrix} 0 & I_k \\ I_k & A \end{bmatrix}, \quad A \in \mathbb{C}^{k \times k}, \quad (3)$$

suitably padded with identities.

To obtain the first result, the main ingredient is extending the flow graph notation for Fiedler matrices introduced in [4] with the novel idea of ‘breaking up’ a block elementary Fiedler matrix (3) into the product of several scalar ones (i.e., with the same structure but $k = 1$). The decompositions arising from this factorization are easy to visualize graphically.

The second result also stems from factoring Fiedler pencils and rearranging the various terms, and leads to a more general result that on when a matrix is orthogonal-plus-low-rank.

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Lanczos algorithm, Gauss quadrature, and minimal partial realization

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Gauss quadrature can be naturally generalized to approximate quasi-definite linear functionals [1], where the interconnections with formal orthogonal polynomials, Padé approximants, complex Jacobi matrices and Lanczos algorithm are analogous to those in the positive definite case. The existence of the n -weight complex Gauss quadrature corresponds to performing successfully the first n steps of the non-Hermitian Lanczos algorithm. Some further results on the relation between the *non-definite* case, the look-ahead Lanczos algorithm and the minimal partial realization will be shown.

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A Krylov-based trust region scheme for model updating

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We consider the problem of optimizing finite element models arising from structural analysis of buildings using some free parameters describing the mechanical characteristics of the underlying materials. This problem — usually known in engineering as *model updating* — arises when trying to match the theoretical characteristic frequencies predicted by the finite element model with the ones recovered using accelerometers combined with a system identification approach. In particular, one desires to optimize the eigenvalues at the lowest end of the spectrum of a symmetric definite pencil $K(\mathbf{x}) - \lambda M(\mathbf{x})$, depending on a vector of ℓ parameters \mathbf{x} . A relevant application is understanding the characteristic of unknown materials, whose properties cannot be analyzed directly because of lack of samples [3].

We describe the numerical challenges in tackling large scale problems (with typically more than 10^5 degrees of freedom for 3D models) — where repeated computation of the eigenvalues for many values of \mathbf{x} is often too expensive. For this reason, we rely on a trust region optimizer to efficiently perform the optimization task. To this end, we need a local model of the objective function that approximates it cheaply. The model can be obtained by a slightly modified inverse Lanczos projection, based on the one used to approximate the smallest eigenvalues. The idea is to re-use the projection space at one point also in a small neighborhood (similarly to Krylov recycling methods [2]), and update the projection computing a first order local approximation of $K(\mathbf{x})^{-1}$, and of the inner product induced by $M(\mathbf{x})$. This approximation can be interpreted as an instance of parametric model order reduction [1].

We show that this choice provides a first-order accurate local model, and that this can be used to prove the convergence of the scheme. In particular, the obtained method allows to optimize the frequency response of the buildings to match the one experimentally recovered at the cost of very few evaluations of the objective function. Several practical examples are shown, that further confirm the applicability and efficiency of the method.

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Matrix-free iterative solvers for isogeometric analysis

9 Feb
10:25

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Isogeometric analysis (IGA) is a method to numerically solve partial differential equations (PDEs). It is based on the idea of using B-splines (and their generalizations) both for the parametrization of the domain, as it is typically done by computer aided design software, and for the representation of the unknown solution. One interesting feature of IGA is the possibility of using high-degree high-regularity splines (the so-called k -refinement) as they deliver higher accuracy per degree-of-freedom in comparison to C^0 finite elements [1].

The computational cost of a solver for a linear PDE problem is the sum of the cost of the formation of the system matrix and the cost of the solution of the linear system. Unfortunately, it is known if these two steps are performed using the approaches that are standard in the context of C^0 finite elements, their computational cost increases dramatically with the spline degree. This makes the k -refinement unfeasible for practical problem, where quadratic or cubic splines are typically preferred.

Several improvements have been achieved recently. In [2], the authors discuss a preconditioner for scalar elliptic problems, based on an old idea, which is robust with respect to both the mesh size h and the spline degree p . Moreover, in [3] a novel method is developed that allows the formation of the stiffness matrix with almost optimal complexity. In the recent work [4], these two approaches are combined with a third ingredient: a matrix-free implementation.

In this talk we discuss the overall strategy, which is very beneficial in terms of both memory and computational cost. In particular, we show that memory required is practically independent of p and that the cost depends on p only mildly. The numerical experiments show that, with the new implementation, the k -refinement becomes appealing from a computational point of view. Indeed, increasing the degree and continuity leads to orders of magnitude higher computational efficiency.

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8 Feb
15:40

Multi-dimensional nonlinear Perron-Frobenius theorem and its application to network centrality

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The nonlinear Perron-Frobenius theory (see [1] e.g.) addresses existence, uniqueness and maximality of positive eigenpairs for order-preserving homogeneous functions. This is an important and relatively recent generalization of the famous results for nonnegative matrices. In this talk I present a further generalization of this theory to “multi-dimensional” order-preserving and homogeneous maps, which we briefly call multi-homogeneous maps [2]. The results presented are then used to discuss a new eigenvector-based centrality measure for nodes and layers of a multi-layer network [3].

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8 Feb
9:00

Recent Developments of Low Rank Approximation of Matrices

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In this talk we survey recent essential developments [2, 3] of the ideas of low-rank matrix approximation proposed in [1]. The practical importance of the very approach consists in its paradigm of using only small part of matrix entries that allows one to construct a sufficiently accurate approximation in a fast way for “big data” matrices that cannot be placed in any available computer memory and are accessed implicitly through calls to a procedure producing any individual entry in demand. During the two recent decades the approach has become a powerful numerical instrument in a tremendous variety of applications. However, its theoretical grounds still invite the researchers to provide them a better look. We discuss the notable new findings and as well some perspectives and open questions.

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Preconditioning for non-symmetric Toeplitz matrices with application to time-dependent PDEs

9 Feb
08:45

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Gil Strang proposed the use of circulant matrices (and the FFT) for preconditioning symmetric Toeplitz (constant-diagonal) matrix systems in 1986 and there is now a well-developed theory which guarantees rapid convergence of the conjugate gradient method for such preconditioned positive definite symmetric systems developed by Raymond Chan, Michael Ng, Fabio Di Benedetto, Stefano Serra Capizzano and Eugene Tyrtshnikov amongst others.

In this talk we describe our recent approach which provides a preconditioned MINRES method with the same guarantees for real nonsymmetric Toeplitz systems regardless of the non-normality. We demonstrate the utility of these ideas in the context of time-dependent PDEs.

Computation of matrix functions with fully automatic Schur-Parlett and Rational Krylov methods

8 Feb
10:40

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We present MatFun, a Julia package for computing dense and sparse matrix functions fully automatically (no user input required, other than the code to compute the function f and the matrix A themselves). This is achieved by combining specifically chosen algorithms and some peculiar feature of Julia. For dense matrices, the Schur-Parlett algorithm [1] has been implemented, leveraging Julia's automatic differentiation capabilities. The algorithm has also been improved from a performance standpoint, making the Parlett recurrence cache-oblivious and enabling the whole procedure to work mostly in real arithmetic, for real inputs. For sparse matrices, we implemented a Rational Krylov method [2], alongside the AAA Rational Approximation [3]. Given a function's samples, AAA is often able to accurately identify its poles, which can then be used by the Rational Krylov method itself for the approximation of $f(A)b$. The accuracy and performance of the algorithms are evaluated, in comparison with already existing specialized methods.

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