

Due giorni di Algebra Lineare Numerica

Roma, 18-19 febbraio, 2019

Programma

Orario	Lunedì 18	Martedì 19
9:10	Antonio Cicone	Michela Redivo-Zaglia
9:35	Patricia Diaz De Alba	Stefano Cipolla
10:00	Anna Concas	Dario Fasino
10:25	Domitilla Brandoni	Pasqua D'Ambra
10:50	Coffee Break	Coffee Break
11:20	Federica Pes	Gian Maria Negri Porzio
11:45	Lothar Reichel	Matteo Ronchetti
12:10	Ivan Gerace	Paola Ferrari
12:35	Valentina Giorgetti	Monica Dessoie
13:00	Pranzo	Pranzo
14:15	Pietro Dell'Acqua	Lucia Romani
14:40	Noè Caruso	Rafael Diaz-Fuentes
15:05	Bruno Carpentieri	Stefano Massei
15:30	Mariarosa Mazza	Alice Cortinovis
15:55	Coffee Break	Coffee Break offerto da ADALTA
16:25	Mattia Tani	Nicola Mastronardi
16:50	Fabio Durastante	Leonardo Robol
17:15	Ken Trotti	Davide Palitta
17:40	Carlo Janna	Antonio Fazzi
18:05	Matteo Frigo	Stefano Maset

Abstracts

Domitilla Brandoni (Università di Bologna), Valeria Simoncini (Università di Bologna)

Tensor techniques for image recognition

Automatic Face Recognition has become increasingly important in the past few years due to its several applications in daily life, such as in social media platforms and security services. Numerical linear algebra tools such as the SVD (*Singular Value Decomposition*) have been extensively used to allow machines to automatically process images in the recognition and classification contexts. On the other hand, several factors such as expression, view angle and illumination can significantly affect the image, making the processing more complex. To cope with these additional features, multilinear algebra tools, such as high-order tensors are being explored.

We analyze tensor calculus and tensor approximation via several different decompositions that have been recently proposed, which include HOSVD (*Higher-Order Singular Value Decomposition*) and Tensor-Train formats. A new algorithm is proposed to perform data recognition for the latter format.

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Bruno Carpentieri (Free University of Bolzano, Bolzano, 39100, Italy), Donglin Sun (University of Electronic Science and Technology of China, Chengdu, Sichuan 611731, PR China)

Spectrally preconditioned and initially deflated variants of the block GMRES method for the simultaneous solution of multiple right-hand sides linear systems

We consider the iterative solution of multiple right-hand sides linear systems of the form

$$AX = B, \tag{1}$$

where $A \in \mathbb{C}^{n \times n}$ is a large square nonsingular matrix of dimension n , either sparse or dense, $B = [b_1, b_2, \dots, b_p] \in \mathbb{C}^{n \times p}$ is a full rank matrix of the p right-hand side vectors b_i , $i = 1, 2, \dots, p$ given simultaneously, and $X \in \mathbb{C}^{n \times p}$ is the unknown solution matrix. Block Krylov subspace methods can solve the whole sequence (1) performing block matrix-vector operations that achieve high computational efficiency on modern cache-based computer architectures. However, the large memory requirements due to the block orthogonalization procedure and slow convergence especially in the presence of approximately linear dependent right-hand sides can limit their use for solving large-scale applications.

We present a spectrally preconditioned and initially deflated version of the restarted block Generalized Minimum Residual Method that attempts to overcome these computational problems by gathering spectral information during the block Arnoldi procedure to adapt an existing preconditioner, and by applying an initial deflation strategy to monitor the approximate linear dependence of the block of right-hand sides over the iterates [1]. We test our solver for the solution of multiple right-hand sides linear systems arising from the discretization of the Dirac equation in lattice quantum chromodynamics applications and of boundary integral equations in the analysis of electromagnetics scattering problems. To the best of our knowledge, our method is the first block Krylov solver that combines initial deflation with eigenspace recycling in the same block Krylov subspace formulation.

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Noe Caruso (SISSA), Alessandro Michelangeli (SISSA), Paolo Novati (Università degli Studi di Trieste)

On Krylov solutions to infinite-dimensional inverse linear problems

We discuss, in the context of inverse linear problems in Hilbert space, the notion of the associated infinite-dimensional Krylov subspace and we produce necessary and sufficient conditions for the Krylov-solvability of the considered inverse problem. The presentation is based on theoretical results together with a series of model examples.

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Antonio Cicone (Istituto Nazionale di Alta Matematica & University of L'Aquila & Gran Sasso Science Institute)

Nonstationary signals decomposition: an overview on the state of the art, current applications and possible future directions of research

The development of new algorithms for the decomposition and analysis of nonstationary signals is a new and promising field of research in Mathematics. Many field of research, like Economy, Finance, Engineering, Physics and Medicine, just to name a few, require the development of fast and reliable techniques able to handle these kind of signals. However many problems are still waiting to be tackled.

In this talk I will give an overview on the state of the art with particular emphasis on the connections with classical topics in Numerical Linear Algebra. Furthermore I will present some of the most promising and interesting applications. Finally I will provide a list of open problems and possible future directions of research.

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Stefano Cipolla (University of Padua, Dept. of Mathematics, Padua, Italy), Michela Redivo-Zaglia (University of Padua, Dept. of Mathematics, Padua, Italy) and Francesco Tudisco (University of Strathclyde, Dept. of Mathematics and Statistics, Glasgow, UK.)

Extrapolation Methods for Data Science

In a series of recent papers [1][2], *Anderson extrapolation methods* are increasingly attracting attention for their impressive performance when applied to optimization problems arising in Data Science. In this talk, after a short survey on some extrapolation techniques based on Shanks sequence transformations [3], we will show how the *Simplified Topological ϵ -Algorithm* (STEA) in the restarted form [4][5], is able to speed up the Multilinear PageRank computation [6] and gradient based optimization techniques (work in progress). 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 further theoretical investigation concerning closeness to the Shanks Kernel of the generated sequences.

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A. Concas (Department of Mathematics and Computer Science, University of Cagliari), R. Dessì (General Motors Global Propulsion Systems), C. Fenu (Department of Mathematics and Computer Science, University of Cagliari), G. Rodriguez (Department of Mathematics and Computer Science, University of Cagliari), M. Vanzi (Department of Electrical and Electronic Engineering, University of Cagliari).

Photometric Stereo under unknown lights position.

A classical problem in Computer Vision consists in reconstructing the 3D shape of an object, starting from a set of images. Photometric Stereo technique is used to extract shape and color information from an object which is observed from the same fixed point of view but under different lighting conditions.

We will describe an algorithm to approximate the framed object, treating, in particular, the case when the position of the light sources is unknown. Numerical experiments will be illustrated, showing that the lights position can be estimated directly from the data when at least 6 pictures of the observed object are available.

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Alice Cortinovia (EPF Lausanne), Daniel Kressner (EPF Lausanne), Stefano Massei (EPF Lausanne)

On maximum volume submatrices and cross approximation

Given a real matrix A , the volume of a submatrix $A(I, J)$ for two index sets $I, J \subseteq \{1, 2, \dots, n\}$ of cardinality k is the absolute value of its determinant. The problem of finding the $k \times k$ submatrix of maximum volume is connected to low-rank approximations of A of the form $A(:, J) \cdot A(I, J)^{-1} \cdot A(I, :)$ (cross approximation) [1]. We show that the submatrix of maximum volume is always attained by a principal submatrix if A is symmetric positive semidefinite or diagonally dominant. Then we analyze the approximation error returned by a greedy method, cross approximation with complete pivoting. Our result for general matrices includes a result by Harbrecht et al. [2] for symmetric positive definite matrices as a special case and yields new results for diagonally dominant matrices.

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Bootstrap AMG in spectral clustering

Graph Laplacian is a popular tool for analyzing graphs, in particular in graph partitioning and clustering. Given a notion of similarity, graph clustering refers to identifying different groups such that vertices in the same group are more similar compared to vertices across different groups. Data clustering can be reformulated in terms of a graph partitioning problem when the given set of data is represented as a graph, also known as similarity graph. In this context, eigenvectors of the graph Laplacian are often used to obtain a new geometric representation of the original data set which generally enhances cluster properties and improves cluster detection. In this work, we apply a bootstrap Algebraic MultiGrid (AMG) method which constructs a set of vectors associated with the graph Laplacian. These vectors, referred to as algebraically smooth ones, span a low-dimensional euclidean space, which we use to represent the data, enabling cluster detection both in synthetic and in realistic well-clustered graphs. We show that in the case of a good quality bootstrap AMG, the computed smooth vectors employed in the construction of the final AMG operator, which by construction is spectrally equivalent to the originally given graph Laplacian, accurately approximate the space in the lower portion of the spectrum of the preconditioned operator. Thus, our approach can be viewed as a spectral clustering technique associated with the generalized spectral problem, and hence it can be seen as an extension of the classical spectral clustering which employs a standard eigenvalue problem.

Pietro Dell'Acqua (Libera Università di Bolzano), Fabio Durastante (Università di Pisa)

New boundary conditions for fast and accurate deblurring models

In recent years, several efforts were made in order to introduce boundary conditions for deblurring problems that allow to get accurate reconstructions. This resulted in the birth of Reflective, Anti-Reflective and Mean boundary conditions, which are all based on the idea of guaranteeing the continuity of the signal/image outside the boundary. In [1] new boundary conditions, obtained by suitably combining Taylor series and finite difference approximations, have been proposed. In case of low levels of noise and blurs able to perform a suitable smoothing effect on the original image (e.g. Gaussian blur), such boundary conditions lead to a significant improvement of the restoration accuracy with respect to those available in the literature. This research line has been further investigated in [2], with the goal of presenting fast and accurate deblurring models, whose computational efficiency is mainly based on Fast Fourier Transform (FFT).

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Monica Dessoie (Department of Mathematics “Tullio Levi Civita”, University of Padova), Fabio Marcuzzi (Department of Mathematics “Tullio Levi Civita”, University of Padova)

Solving ABD systems on GPUs

In this talk we discuss numerical methods for solving Almost Block Diagonal (ABD) systems on a GPU. For a survey of serial and parallel algorithms for both Bordered Almost Block Diagonal (BABD) and ABD systems see [4] and [2]. We specialize these methods for the massive parallel computations made on a GPU. The most frequently occurring ABD matrix has the following structure

$$\begin{pmatrix} B_0 & & & & & \\ S_1 & T_1 & & & & \\ & S_2 & T_2 & & & \\ & & \ddots & \ddots & & \\ & & & S_N & T_N & \\ & & & & & B_{N+1} \end{pmatrix},$$

where $S_i, T_i, i = 1, \dots, N$ are square blocks all of the same size equal to the sum of the number of rows in B_0 and B_{N+1} . A BABD matrix differs from the ABD matrix in its last block row (or column) and has the following structure

$$\begin{pmatrix} S_1 & T_1 & & & & \\ & S_2 & T_2 & & & \\ & & \ddots & \ddots & & \\ & & & S_N & T_N & \\ B_0 & & & & & B_{N+1} \end{pmatrix},$$

however it is well known that every BABD system can be converted to ABD form at the cost of doubling the size of the matrix. In the literature, [3] showed that Gaussian elimination with no pivoting or row partial pivoting is potentially unstable on BABD matrices and can lead to overflow. On the other side, full pivoting is prohibitive for this type of matrices on a massively parallel architecture.

Most efficient algorithms for direct methods for solving BABD and ABD matrices are based on the *divide-and-conquer* approach. Between the 1980s and the 1990s, the special ABD structure has been exploited in a number of algorithms to minimize fill-in and computational cost without compromising stability, see [4]. Naive approaches consider ABD systems as banded block tridiagonal systems. Such approaches are considered undesirable for many reasons, not last the introduction of fill-in.

The scope of this work is to review the algorithms seen in [4] on massively parallel architectures such as GPUs. Direct sequential solvers for ABD systems rely on the classical Gaussian elimination scheme (with different kind of pivoting), which results in limited opportunity for parallelism when handling banded systems [1], Sec. 5.1. This limitation becomes more pronounced as the system’s band gets narrower. For this reason we focus on ad-hoc algorithms for direct parallel ABD solvers.

There are two candidates for ABD direct solvers on GPUs:

- “non overlapping divide-et-impera” proposed in [5] (and reviewed in [4]), not optimized on GPUs;
- “overlapping-tearing” proposed in [1] for banded systems, which need adaptations in the ABD case.

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Patricia Díaz de Alba (Department of Mathematics and Computer Science, University of Cagliari)

Linear and nonlinear models for EMI data inversion

This presentation is concerned with numerical methods for inverse problems in applied Geophysics. Its main purpose is to reconstruct the electrical conductivity and the magnetic permeability of the soil by Electromagnetic induction (EMI) techniques.

By taking measurements by a Ground Conductivity Meter (GCM), we can gain information about the depth profile of electrical conductivity. Nevertheless, the noninvasive determination of it, using only aboveground electromagnetic induction measurements, remains difficult since it involves inverse problems which typically lead to mathematical models that are not well-posed. This means especially that their solution is unstable under data perturbations. Numerical methods that can cope with this problem are the so-called regularization methods.

We report distinct algorithms and techniques to overpass these difficulties since mathematical problems having these undesirable properties pose severe numerical adversities. We also deal with linear and nonlinear models, that involve the solution of ill-conditioned problems for reconstructing the electrical conductivity and the magnetic permeability of the soil, and we propose for each of these models an inversion procedure to get a good approximation of the solution.

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Rafael Díaz Fuentes (University of Insubria), Lucia Romani (University of Bologna)

Interpolation of points and tangent directions by linear approximating subdivision schemes

Abstract.

Univariate subdivision schemes are iterative methods to generate smooth curves by means of repeated refinements of a given starting polygon \mathbf{P}^0 . For the subclass of approximating subdivision schemes, the limit curve \mathbf{c} is contained in the convex hull of \mathbf{P}^0 and, in case of linear refinement rules, the values of $\{\mathbf{c}(\frac{i}{2^k}), i \in \mathbb{Z}\}$ and $\{\mathbf{c}'(\frac{i}{2^k}), i \in \mathbb{Z}\}$ can be described in terms of linear operators for any arbitrary $k \in \mathbb{N}$. By exploiting these properties of linear approximating subdivision schemes, we derive a linear algebra algorithm for generating a family of subdivision curves that interpolate a sequence of data points under tangent directions constraints. When the cubic B-spline scheme is used and some specific tangent vectors are prescribed, our algorithm gives back the same output curve of the geometric iterative method proposed in [1].

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D. Bertaccini (Università di Roma "Tor Vergata", Dipartimento di Matematica & IAC-CNR Roma), F. Durastante (Università di Pisa, Dipartimento di Informatica)

Some fast algorithms for the large structured linear systems of FPDEs

Our recent efforts on the efficient numerical solution of the large linear systems of linear and semilinear fractional differential equations is briefly reviewed here. The main key tools used were

- structured preconditioners applied in tensor form;
- the short-memory principle;
- hybrid update of approximate inverse preconditioners on GPUs.

In particular, the following peculiar aspects below, strictly related to the above mentioned tools, have been observed in [1]-[4] and will be also quickly recalled in our presentation.

- The exponential growth of the number of elements (n^d) makes impossible using component-wise storage and operations. We found that the compression (representation) of such objects using the TT-tensor format gave promising preliminary results and, at the same time, we were able to take advantage of the inherent multiple structure present in the linear systems generated by finite volume discretization of some FDEs. Up to the best of our knowledge, the structure of the underlying matrices was not considered in TT-tensor-based solvers before.
- The short-memory principle ensures the decay of the entries of the inverse of the discretized operator. These inverses are approximated by a sequence of sparse matrices (sparse approximate inverses of AINV and by inversion-and-sparsification) that we use to build up preconditioners for Krylov methods. There is almost no loss of accuracy in the discretization of the differential model because the decay properties of the operators are used to approximate their inverses.

- Updating approximate inverses were used to cheaply treat problems with coefficients that vary over time, or to apply methods of integration with variable time step.
- The hybrid updates (structured mixed with nonstructured approximations) of approximate inverse preconditioners on GPUs, generated on CPUs or on GPUs (work in progress) and applied on GPUs, gave interesting and competitive performances. They were able to take the advantages of the above mentioned structured TT and short-memory tools. Moreover, it is interesting to observe the performances of different approaches for approximating the inverses of the underlying matrices.

Some conclusions and works in progress are also proposed.

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Dario Fasino (University of Udine)

So, what is the Random Walk Centrality?

Let H be the matrix containing the hitting times of the random walk on a connected undirected graph on n nodes. It is well known that the matrix $H + H^T$ is a multiple of the resistance matrix. On the other hand, the matrix $H - H^T$ has rank 2. In fact, the authors of [1] define numbers c_1, \dots, c_n such that

$$H_{ij} - H_{ji} = \frac{1}{c_j} - \frac{1}{c_i}$$

and name c_i the *random walk centrality* of node i , since it quantifies how central node i is regarding its potential to receive information randomly diffusing over the network. In practice, the value of c_i is quite good at recognizing node i as being a ‘core’ node or a ‘peripheral’ node in the network.

In [1], the c_i ’s are expressed in terms of infinite series. In this talk I propose new formulas to compute random walk centralities from the knowledge of the resistance matrix, or the pseudoinverse of the Laplacian matrix of the graph. Extensive numerical experiments show that c_i is positive and has a striking correlation with the so-called *random walk closeness centrality*, $C(i) = n / \sum_{j=1}^n (H_{ij} + H_{ji})$. While the former property is quite simple to prove, the reason for the latter is, at the time of writing this abstract, still unclear.

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A. Fazzi (Gran Sasso Science Institute), N. Guglielmi (Gran Sasso Science Institute), I. Markovsky (Vrije Universiteit Brussel)

Computing approximate common factors of matrix polynomials

Computation of (approximate) polynomials common factors is an important problem in several fields of science, like control theory, and it is an active research topic. While the problem has been widely studied for scalar polynomials, the scientific literature in the framework of matrix polynomials seems to be limited to the problem of exact greatest common divisors computation. We are going to generalize two algorithms from scalar to matrix polynomials: the subspace method [2], and an ODE-based algorithm [1].

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The eigenvalue distribution of special 2-by-2 block matrix-sequences with applications to the case of symmetrized Toeplitz structures

Given a Lebesgue integrable function f over $[-\pi, \pi]$, we consider the sequence of matrices $\{Y_n T_n[f]\}_n$, where $T_n[f]$ is the n -by- n Toeplitz matrix generated by f and Y_n is the anti-identity matrix. Because of the unitary character of Y_n , the singular values of $T_n[f]$ and $Y_n T_n[f]$ coincide. However, the eigenvalues are affected substantially by the action of the matrix Y_n . Under the assumption that the Fourier coefficients are real, we prove that $\{Y_n T_n[f]\}_n$ is distributed in the eigenvalue sense as

$$\phi_g(\theta) = \begin{cases} g(\theta), & \theta \in [0, 2\pi], \\ -g(-\theta), & \theta \in [-2\pi, 0), \end{cases}$$

with $g(\theta) = |f(\theta)|$. We also consider the preconditioning introduced by Pestana and Wathen in [1] and, by using the same arguments, prove that the preconditioned sequence is distributed in the eigenvalue sense as ϕ_1 , under the mild assumption that f is sparsely vanishing. We emphasize that the mathematical tools introduced in this setting have a general character and in fact can be potentially used in different contexts. A number of numerical experiments are provided and critically discussed.

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Matteo Frigo (University of Padova, Italy), Nicola Castelletto (Lawrence Livermore National Laboratory), Massimiliano Ferronato (University of Padova)

A Relaxed Physical Factorization Preconditioner for Mixed Finite Element Coupled Poromechanics

In this talk, we present a Relaxed Physical Factorization (RPF) preconditioner for the iterative solution of coupled poromechanics equations. The use of mixed finite element method along with implicit time discretization of Biot equations leads to a sequence of unsymmetric linear systems with a 3×3 block structure. This work focuses on the development and implementation of a new preconditioner inspired by the Relaxed Dimensional Factorization (RDF) preconditioner introduced by Benzi et al. [1], [2] for the saddle-point problems arising from Navier-Stokes equations. The preconditioner is obtained by using a proper physical splitting of the block system and setting a relaxation parameter α . An automatic procedure performs the optimal selection of α . With the aim to keep under control the possible ill-conditioning of the α -dependent inner blocks, two strategies are provided. In the former, a lower-bound condition for α is advanced. Later, a novel strategy, based on the projection of the block onto the non-null space of the rank-deficient term, is discussed. Numerical experiments in both theoretical benchmarks and real-world poromechanical applications are presented to verify the theoretical properties, performance, and robustness. The proposed approach appears to be a promising alternative to existing techniques for large-size and ill-conditioned problems.

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Antonio Boccuto (Università degli Studi di Perugia), Ivan Gerace (Università degli Studi di Perugia), Valentina Giorgetti (Università degli Studi di Perugia), Anna Tonazzini (I.S.T.I. C.N.R. Pisa)

An Edge-Preserving Regularization Model for the Demosaicing of Noisy Color Images

We propose edge-preserving regularization to solve the color image demosaicing problem in the realistic case of noisy data. We enforce both local smoothness of the intensity (low frequency components), and inter-channel local similarities of the object borders and textures (high frequency components). To describe local correlation, discontinuities of both the low frequency components and the high frequency components are accounted for in an implicit manner, i.e. through suitable functions of the proper derivatives. For the treatment of even the finest image details, derivatives of first, second and third order are considered. The solution of the demosaicing problem is defined as the minimizer of an energy function, accounting for all these constraints plus a data fidelity term. This non-convex energy is minimized via an iterative deterministic algorithm, applied to a family of approximating functions, each implicitly referring to edge elements marking meaningful discontinuities. Our method is general, in the sense that it does not refer to any specific color filter array. However, to permit a quantitative comparison with other published results, we tested it in the case of the Bayer CFA, and on both the Kodak 24-image dataset and the McMaster (IMAX) 18-image dataset. The performed comparisons with some among the most recent demosaicing algorithms show the good performance of our method, in both the noiseless and noisy case. We deal with a Blind Source Separation problem. As a particular case, we consider reconstruction of digital documents degraded by bleed-through and show-through effects. We propose a nonstationary locally linear data model and we propose a solutions based on the assumption of cross-correlated the ideal sources. In order to solve the ill-posed local linear problem we impose that the mixing matrix is nonnegative and stochastic, and the ideal sources are assumed to be nonnegative, and with a estimated level of overlapping (i.e. estimated cross-correlation). The sought solutions are related to a factorization of the data covariance matrix that allows the given constraints to be satisfied at best. Our experimental results confirm the goodness of the method.

Antonio Boccuto (Università degli Studi di Perugia), Ivan Gerace (Università degli Studi di Perugia), Valentina Giorgetti (Università degli Studi di Perugia)

A Blind Source Separation Technique for Document Restoration

We deal with a Blind Source Separation problem. As a particular case, we consider reconstruction of digital documents degraded by bleed-through and show-through effects. We propose a nonstationary locally linear data model and we propose a solutions based on the assumption of cross-correlated the ideal sources. In order to solve the ill-posed local linear problem we impose that the mixing matrix is nonnegative and stochastic, and the ideal sources are assumed to be nonnegative, and with a estimed level of overlapping (i.e. estimed cross-correlation). The sought solutions are related to a factorization of the data covariance matrix that allows the given constraints to be satisfied at best. Our experimental results confirm the goodness of the method.

Massimo Bernaschi (CNR), Mauro Carrozzo (CNR), Andrea Franceschini (Stanford University), Carlo Janna (Università di Padova)

Solving large size linear systems of equations on modern high-performance computers

One of the most time-consuming tasks in the procedures for the numerical study of PDEs is the solution to linear systems of equations. To that purpose, iterative solvers are viewed as a promising alternative to direct methods on high performance computers since, in theory, they are almost perfectly parallelizable. Their main drawback is the need of finding a suitable preconditioner to accelerate convergence. The Factorized Sparse Approximate Inverse (FSAI), mainly in its adaptive form, has proven to be an effective parallel preconditioner and an excellent AMG smoother for several problems. In the present communication, we report about novel ideas to compute, on Graphics Processing Units, both static and dynamic FSAI preconditioners [1]. We will also show that FSAI can be used as a powerful smoother in adaptive AMG [2] allowing for a fast solution of severely ill-conditioned real-world problems.

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Stefano Maset (Dipartimento di Matematica e Geoscienze, Università di Trieste)

Relative error analysis of matrix exponential approximations for numerical integration

We consider the relative error in the numerical solution of a linear ordinary differential equation

$$y'(t) = Ay(t), \quad t \geq 0,$$

where A is a normal matrix. The numerical solution is obtained by using at any step an approximation of the matrix exponential, e.g. a polynomial or a rational approximation. The error of the numerical solution with respect to the exact solution is due to the use of the approximation as well as to a possible perturbation in the initial value. We analyze the long-time behavior of the relative error as well as the numerical integration of the long-time solution in the stiffness situation. New and surprising results are obtained.

Daniel Kressner (EPF Lausanne), Patrick Kürschner (KU Leuven), Stefano Massei (EPF Lausanne)

Low-rank updates and divide-and-conquer methods for quadratic matrix equations

In this work, we consider two types of large-scale quadratic matrix equations: Continuous-time algebraic Riccati equations, which play a central role in optimal and robust control, and unilateral quadratic matrix equations, which arise from stochastic processes on 2D lattices and vibrating systems. We propose a simple and fast way to update the solution to such matrix equations under low-rank modifications of the coefficients. Based on this procedure, we develop a divide-and-conquer scheme for quadratic matrix equations with coefficients that feature a specific type of hierarchical low-rank structure, which includes banded matrices. This generalizes earlier work on linear matrix equations [1].

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Teresa Laudadio (IAC–CNR, Bari, Italy), Nicola Mastronardi (IAC–CNR, Bari, Italy), Paul Van Dooren (UCLouvain, Belgium)

On computing the Jordan structure of Totally Nonnegative Matrices with high relative accuracy

Given a bidiagonal decomposition of a totally nonnegative matrix $A \in \mathbb{R}^{n \times n}$, an algorithm for computing its Jordan structure was proposed in [4] with high relative accuracy in floating point arithmetic and $O(n^4)$ computational complexity.

In this talk we propose a modification of the latter algorithm with $O(n^3)$ computational complexity.

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Mariarosa Mazza (University of Insubria), Jennifer Pestana (Strathclyde University)

Spectral properties of flipped Toeplitz matrices and related preconditioning

In this work, we investigate the spectra of “flipped” Toeplitz sequences, i.e., the asymptotic spectral behaviour of $\{Y_n T_n(f)\}_n$, where $T_n(f) \in \mathbb{R}^{n \times n}$ is a real Toeplitz matrix generated by a function $f \in L^1([-\pi, \pi])$, and Y_n is the exchange matrix, with 1s on the main anti-diagonal. One reason for characterizing the spectra of these flipped matrices relates to the solution of linear systems with Toeplitz coefficient matrices. Since $Y_n T_n(f)$ is symmetric, the resulting linear system may be solved by the (preconditioned) MINRES method [5,4], with its descriptive convergence rate bounds based on eigenvalues (see, e.g., [2, Chapters 2 & 4]).

Using the block generalized locally Toeplitz machinery [1], we show that the eigenvalues of $Y_n T_n(f)$ are asymptotically described by a 2×2 matrix-valued function, whose eigenvalue functions are $\pm|f|$ [3]. It turns out that roughly half of the eigenvalues of $Y_n T_n(f)$ are well approximated by a uniform sampling of $|f|$ over $[-\pi, \pi]$, while the remaining are well approximated by a uniform sampling of $-|f|$ over the same interval. When f vanishes only on a set of measure zero, this motivates that the spectrum is virtually half positive and half negative. Some insights on the spectral distribution of related preconditioned sequences are provided as well. Finally, a wide number of numerical results illustrate our theoretical findings.

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Gian Maria Negri Porzio (The University of Manchester), Françoise Tisseur (The University of Manchester)

A contour integral approach for the solution of nonlinear eigenvalue problems

Abstract: Recently many researchers have been focusing on the nonlinear eigenvalue problem (NEP/NLEVP) for holomorphic and meromorphic functions [1]. I will shortly introduce this problem and then I will explain how to use contour integrals to solve it for medium-sized, dense matrices. This approach is really easy to parallelise and few hypotheses are needed to use it. Finally, I will describe developments and improvements we are currently working on [2].

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Davide Palitta (Max Planck Institute for Dynamics of Complex Technical Systems)

The projected Newton-Kleinman method for the algebraic Riccati equation

The numerical solution of the algebraic Riccati matrix equation

$$AX + XA^T - XBB^T X + C^T C = 0, \tag{2}$$

where $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, $C \in \mathbb{R}^{p \times n}$, $p + m \ll n$, is an interesting and still challenging task especially when the problem dimension is very large, say $n > 10^4$, as the dense solution X cannot be store and a memory-saving approximation has to be sought.

Due to its quadratic nature, the algebraic Riccati equation has more than one solution in general. However, under certain conditions on the coefficient matrices A , B and C , it can be shown that there exists a unique stabilizing solution X to (2) such that all the eigenvalues of the matrix $A - BB^T X$ have negative real part. One of the most classical iterative methods for the computation of such an X is the so-called Newton-Kleinman method [3] that, given a stabilizing initial guess X_0 , computes an approximation X_{k+1} to X by sequentially solving Lyapunov equations of the form

$$(A - X_k BB^T)X_{k+1} + X_{k+1}(A - X_k BB^T)^T + C^T C + X_k BB^T X_k = 0, \quad k \geq 0. \quad (3)$$

Since the problem dimension is very large, equations (3) must be iteratively solved, leading to the inexact Newton-Kleinman method which provides a low-rank approximation to X [1, 2].

Other very efficient methods have been developed in the last years. In particular, it has been shown how projection methods are very effective in the numerical treatment of (2) and they straightforwardly generalize the approach used for linear matrix equations like (3). See, e.g., [4, 5]. However, to the best of our knowledge, it is not guaranteed that the solution computed by projection methods is the stabilizing solution we look for.

In this talk we present a novel approach that combines the inexact Newton-Kleinman scheme with projection methods for Lyapunov equations. In particular, we show that all the iterates X_{k+1} in (3) belong to the same space so that only one approximation space has to be constructed. This leads to remarkable reductions in the computational efforts. Moreover, the well-established convergence properties of the inexact Newton-Kleinman method are preserved.

Several numerical results are reported to illustrate the potential of the discussed method.

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Federica Pes (Department of Mathematics and Computer Science, University of Cagliari), Giuseppe Rodriguez (Department of Mathematics and Computer Science, University of Cagliari)

Regularization methods for nonlinear ill-posed problems

Let us assume that $F(\mathbf{x})$ is a nonlinear Fréchet differentiable function, with value in \mathbb{R}^m for any $\mathbf{x} \in \mathbb{R}^n$. For a given $\mathbf{b} \in \mathbb{R}^m$ we want to solve the least squares problem $\min_{\mathbf{x}} \|F(\mathbf{x}) - \mathbf{b}\|^2$. To do this we apply the Gauss-Newton method. The nonlinear function $F(\mathbf{x})$ is considered ill-conditioned in a domain $\mathcal{D} \subset \mathbb{R}^n$ when the condition number $\kappa(J)$ of the Jacobian $J = J(\mathbf{x})$ of $F(\mathbf{x})$ is very large for any $\mathbf{x} \in \mathcal{D}$. Under this assumption, it is common to apply a regularization method to each step of the Gauss-Newton method. We compare this situation to applying the same regularization method to the initial nonlinear least squares problem.

C. Brezinski (University of Lille, France), M. Redivo-Zaglia (University of Padova, Italy), Y. Saad (University of Minnesota, USA)

Shanks' transformations, Anderson acceleration, and applications to systems of equations

We present a general framework for Shanks' transformations of sequences of elements in a vector space. It is shown that the Minimal Polynomial Extrapolation (MPE), the Modified Minimal Polynomial Extrapolation (MMPE), the Reduced Rank Extrapolation (RRE), the Vector Epsilon Algorithm (VEA), and the Topological Epsilon Algorithm (TEA), which are standard general techniques for accelerating arbitrary sequences, all fall into this framework. Their properties are studied.

Then, we discuss the application of these methods to the solution of systems of linear and nonlinear equations. Their connections with quasi-Newton and Broyden methods are studied.

We then consider Anderson Acceleration (AA) which is a method for solving systems of equations. In the linear case, it is known that AA and GMRES are 'essentially' equivalent in a certain sense while GMRES and RRE are mathematically equivalent. We discuss the connection between AA, the RRE, the MPE, and other methods in the nonlinear case. Finally, Anderson-type methods are presented.

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Lothar Reichel (Kent State University, Kent, OH)

Arnoldi decomposition, GMRES, and preconditioning for linear discrete ill-posed problems

GMRES is one of the most popular iterative methods for the solution of large linear systems of equations that arise from the discretization of linear well-posed problems, such as boundary value problems for elliptic partial differential equations. The method is also applied to the iterative solution of linear systems of equations that are obtained by discretizing linear ill-posed problems, such as many inverse problems. However, GMRES does not always perform well when applied to the latter kind of problems. This talk seeks to shed some light on reasons for the poor performance of GMRES in certain situations, and discusses some remedies based on specific kinds of preconditioning. The standard implementation of GMRES is based on the Arnoldi process, which also can be used to define a solution subspace for Tikhonov or TSVD regularization, giving rise to the Arnoldi-Tikhonov and Arnoldi-TSVD methods, respectively. The performance of the GMRES and the latter methods is discussed. This talk presents joint work with Marco Donatelli, Silvia Gazzola, Silvia Noschese, and Paolo Novati.

G. M. Del Corso (Università di Pisa), F. Poloni (Università di Pisa), L. Robol (Università di Pisa), R. Vandebriel (KU Leuven)

Distance from rank-structured matrices

Hermitian and unitary matrices are two representatives of the class of normal matrices whose full eigenvalue decomposition can be stably computed in quadratic computing complexity. Recently, fast and reliable eigensolvers dealing with low rank perturbations of unitary and Hermitian matrices were proposed [1,2,4]. These structured eigenvalue problems appear naturally when computing roots, via confederate linearizations, of polynomials expressed in, eg, the monomial or Chebyshev basis. Often, however, it is not known beforehand whether or not a matrix can be written as the sum of a Hermitian or unitary matrix plus a low rank perturbation.

We propose necessary and sufficient conditions characterizing the class of Hermitian or unitary plus low rank matrices. The number of singular values deviating from 1 determines the rank of a perturbation to bring a matrix to unitary form. A similar condition holds for Hermitian matrices; the eigenvalues of the skew-Hermitian part differing from 0 dictate the rank of the perturbation. We prove that these relations are linked via the Cayley transform.

Based on these conditions we are able to identify the closest Hermitian and unitary plus low rank matrix in Frobenius and spectral norm and a practical Lanczos iteration to detect the low rank perturbation is presented. Numerical tests prove that this straightforward algorithm is robust with respect to noise.

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Lucia Romani (Università di Bologna)

Even-symmetric interpolatory subdivision schemes: a constructive algebraic strategy

Subdivision schemes are iterative algorithms to generate curves or surfaces as the limit of a refinement process starting from a polyline or a polygonal mesh. Interpolatory subdivision schemes are characterized by the property of generating curves/surfaces that pass through all the vertices of the assigned polyline/polygonal mesh. In the last two decades many proposals of interpolatory subdivision schemes have appeared in the literature. All of them are obtained via odd-symmetric subdivision masks which generate at each iteration a polyline/polygonal mesh whose set of vertices contains all the ones from the previous iterations. The aim of this work is to propose a constructive approach, that uses classical numerical linear algebra methodologies, to show the existence of univariate interpolatory subdivision schemes that do not enjoy the latter properties. In particular, the new schemes are identified by an even-symmetric mask that does not contain the submask $\delta_0 = \{\delta_{j,0}\}_{j \in \mathbb{Z}}$. Thus, they offer an insight of interpolatory subdivision schemes that is lacking in existing literature.

Matteo Ronchetti (Università di Pisa)

IKA: Independent Kernel Approximator

A kernel is a function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ such that given $x_1, x_2, \dots, x_N \in \mathcal{X}$ the matrix $G_{ij} = K(x_i, x_j)$ (called Gramian matrix) is symmetric positive-semidefinite. In this work we concentrate on the situation where $\mathcal{X} = \mathbb{R}^d$ and $\{x_1, x_2, \dots, x_N\}$ are drawn from an unknown probability distribution with density $p(x)$. The density $p(x)$ defines an inner product between real-valued functions in \mathbb{R}^d , while the kernel K defines a self-adjoint linear operator:

$$\langle f, g \rangle \stackrel{\text{def}}{=} \int_{\mathbb{R}^d} f(x)g(x)p(x)dx \quad Kf(x) \stackrel{\text{def}}{=} \int_{\mathbb{R}^d} K(x, y)f(y)p(y)dy.$$

The kernel has real nonnegative eigenvalues and orthonormal eigenfunctions.

The problem of low rank kernel approximation consists of approximating a kernel $K : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ with a function $\psi : \mathbb{R}^d \rightarrow \mathbb{R}^m$ such that $K(x, y) \approx \langle \psi(x), \psi(y) \rangle$. This problem arises for example when using a kernel method on a machine learning problem where the dataset size renders operating on the full Gram matrix practically unfeasible, or when one is interested in using $\psi(x)$ as a feature map.

IKA is a new method for low rank kernel approximation that defines $\psi(x)$ as a linear combination of arbitrarily chosen functions $b_1(x), b_2(x), \dots, b_n(x)$. The method approximates the kernel using an approximation of its leading eigenfunctions. The problem of finding the leading eigenfunctions of K is reduced to an $n \times n$ generalized eigenvalue problem by projecting the eigenfunctions on the span of $\{b_1(x), b_2(x), \dots, b_n(x)\}$.

The ability of freely choosing the functions $b_i(x)$ is the key advantage of IKA, this feature allows to approximate a numerically expensive kernel with an inexpensive function and can be further exploited by future work.

Currently ongoing work includes a variant of the method that allows to efficiently approximate the kernel when the Gramian matrix is sparse and the use of IKA for approximating other self-adjoint operators.

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G. Loli (Università di Pavia), M. Montardini (Università di Pavia), G. Sangalli (Università di Pavia), M. Tani (IMATI-CNR, Pavia)

Space-time isogeometric preconditioners for parabolic problems

In this talk we discuss preconditioning strategies suited for a isogeometric discretization of the heat equation based on a Galerkin weak formulation. Exploiting the tensor product structure of the basis functions, we propose a preconditioner that is the sum of Kronecker products. We are able to apply it in a very fast way, thanks to a solver similar to the Fast Diagonalization method considered in [1]. The time required by the application grows almost as the number of degrees-of-freedom. Our preconditioner is robust with respect to the spline degree and the mesh-size.

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Marco Donatelli (University of Insubria), Mariarosa Mazza (University of Insubria), Ken Trotti (University of Insubria)

Anisotropic multigrid preconditioners for space-fractional diffusion equations

Fractional Diffusion Equations (FDEs) are a generalization of the classical Partial Differential Equations (PDEs) obtained replacing standard derivatives with fractional ones. Their recent success is notably due to the non-local behavior of fractional differential operators that translates in the appropriate modeling of anomalous diffusion phenomena appearing in several applicative fields, like plasma physics or imaging.

In this work, we focus on a two-dimensional space-FDE problem discretized by means of a second order finite difference scheme obtained as combination of the Crank-Nicolson scheme and the so-called weighted and shifted Grünwald formula [2]. Efficient multigrid strategies for the resulting Toeplitz-like linear systems have been already introduced in [1]. Therein, a symbol-based study of the coefficient matrices has been used to define a multigrid preconditioner built using either rediscrization or a two-dimensional scaled-Laplacian matrix which is particularly effective when the fractional orders are both close to 2.

Here we seek to investigate how multigrid approaches can be efficiently extended to the case where only one of the two fractional order is close to 2, while the other is close to 1. In other words, we consider space-FDE problems that involve an intrinsic anisotropy in the direction corresponding to the minimum fractional order. We design a multigrid preconditioner where the grid transfer operator is obtained with a semicoarsening technique and the smoothing is performed with relaxed Jacobi whose damping parameter is accurately estimated by using the symbol approach. Moreover, for large-sized problems a further improvement in the robustness of the multigrid method can be reached using a V-cycle with semicoarsening as smoother (see [3]). Similarly to the proposal in [1], the scaled-Laplacian matrix is used in the direction where the fractional derivative order is close to 2, while in the other direction a rediscrization is adopted. Several numerical results confirm that the resulting multigrid preconditioner is computationally effective and outperforms current state of the art techniques.

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