Numerical Linear Algebra (NLACIRM24)

CIRM Luminy (France), September 16 - 20, 2024

dedicated to Michela Redivo-Zaglia for her birthday and her retirement,
and to the 65th birthday of Hassane Sadok

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Numerical Linear Algebra (NLACIRM24)
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(The abstracts are listed alphabetically by speaker's underlined name)

List of presentations

Vector extrapolation techniques for regularization of ill-posed problems

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Abstract

When dealing with severely ill-conditioned linear systems arising from the discretization of first-kind integral equations, we can use a regularization method that usually produces a sequence of solutions depending on a parameter. Various extrapolation methods have been proposed for the choice of a suitable value of the regularization parameter; see, e.g, [1, 2]. In this talk, an extrapolation procedure for choosing the parameter in TSVD/TGSVD will be presented. It involves a sequence of extrapolated solutions that are less sensitive to a wrong choice of the parameter. Its effectiveness will be tested by numerical experiments and compared to other existing methods. A new implementation of Wynn's vector epsilon algorithm [3] has been developed exploiting a feature of the sequence generated by TSVD. In this talk theoretical considerations and numerical results will highlight the advantages of the new implementation and its application to regularization methods.

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Randomized coordinate-descent-type iteration methods

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Abstract

We review and compare several representative and effective randomized coordinate-descent-type methods, and their modifications and extensions, for solving the large, sparse, consistent or inconsistent systems of linear equations. We also anatomize, extract, and purify the asymptotic convergence theories of these iteration methods, and discuss, analyze, and summarize their advantages and disadvantages from the viewpoints of both theory and computations.

Sensitivity of eigenvalues for Hankel matrix pencils

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Abstract

We consider a matrix pencil $(A - \lambda B)$, $A, B \in \mathbb{C}^{m\times r}$ and we want to study the stability of eigenvalues and eigenvectors for different classes of pencils.

In the case where the pencil is regular (A and B square matrices, det$(A-\lambda B)$ not identically zero), with distinct eigenvalues $\lambda_1, \cdots, \lambda_r$ ans with right and left eigenvectors

$$(A - \lambda_j B)x_j = 0, \quad y_j(A - \lambda_j B) = 0,$$

if we denote a perturbed pencil $(\tilde{A} - \lambda\tilde{B})$ and measure the perturbation

$$\epsilon := \sqrt{||\tilde{A} - A||_2^2 + ||\tilde{B} - B||_2^2}$$

we give bounds on the chordal distance of the eigenvalues $\chi(\lambda_j, \tilde{\lambda}_j)$ and also relative errors of eigenvalues. We also study the case of a Hankel pencil $\lambda H^{(0)}_{m,n} - H^{(1)}_{m,n}$ with the entries

$$h_k = \sum_{j=1}^{r} \alpha_j \lambda_j^k, \quad k = 0, \cdots, m + n + 1, \quad \alpha_j \neq 0, \quad \lambda_j \text{ distinct.}$$

These pencils are important in the estimation of the parameters λ_j of exponential sums. We want to reconstruct the quantities λ_j from the Hankel matrices $\lambda\tilde{H} - \tilde{H}^{(1)}$ polluted by noise, specially in the case where r is small compared to n giving raise to singular pencils. Using some perturbation theory results, we give bounds on $|\lambda_j - \tilde{\lambda}_j|$ and corresponding eigenvectors.

Interpolation problems with spherical harmonics using various grids on the sphere*

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Abstract

Spherical harmonic (SH) expansions are commonly used for approximation problems on the sphere. However, when restricted to a particular spherical grid, compatibility problems between the grid and a particular subset of SH functions can appear. This is encoded in the associated VanDerMonde collocation matrix.
In this talk, we consider different SH subsets well adapted to different spherical grids of interest: the Cubed-Sphere, the Icosahedron grid and the Longitude-Latitude grid. The outcome is an algorithm based on an appropriate factorization of the VanDerMonde matrix in each case. The properties of these SH sets are analysed. Numerical results will be presented on a series of data interpolation problems as well as for quadrature on the sphere.

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An Alternating Direction Multiplier Method for the inversion of FDEM data*

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Abstract

We focus on the numerical solution of nonlinear inverse problems in applied geophysics. Our aim is to reconstruct the structure of the soil, i.e., either its electrical conductivity or the magnetic permeability distribution, by inverting Frequency Domain Electromagnetic (FDEM) data. This is a very challenging task since the problem is nonlinear and severely ill-conditioned. To solve the nonlinear inverse problem, we propose an Alternating Direction Multiplier Method (ADMM) algorithm, we prove its convergence, and propose an automated strategy to determine the parameters involved. Moreover, we present two heuristic variations of the ADMM that either improve the accuracy of the computed solutions or lower the computational cost. The effectiveness of the different proposed methods is illustrated through a few numerical examples. This work is based on [1].

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Landweber operator, its relaxations and extrapolations

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Abstract

Let A be a nonzero real matrix of type $m \times n$, $b \in \mathbb{R}^m$ and let $C \subseteq \mathbb{R}^n$ be a closed convex subset. We consider linear problems of type $Ax = b$ or $Ax \leq b$, where $x \in C$. Denoting $D = \mathrm{diag}(d)$, where $d \in \mathbb{R}^m$ is a vector with positive coordinates, the problems may be written equivalently as $\bar{A}x = \bar{b}$ or $\bar{A}x \leq \bar{b}$, where $x \in C$, respectively, where $\bar{A} = D^{\frac{1}{2}}A$ and $\bar{b} = D^{\frac{1}{2}}b$. There are many methods for solving these problems by fixed point iterations of type

$$x^{k+1} = P_C(Tx^k), \tag{1}$$

where $x^0 \in \mathbb{R}^n$ is arbitrary, $T : \mathbb{R}^n \to \mathbb{R}^n$ is an operator with $\mathrm{Fix}T$ being the solution set of the problem under consideration [1]-[5]. An important class of methods (1) for solving these problems are the projected Landweber methods, where T in (1) are the Landweber operators, i.e.

$$T(x) := x - \gamma A^T D(Ax - b) \tag{2}$$

or

$$T(x) := x - \gamma A^T D(Ax - b)_+, \tag{3}$$

respectively, where $\gamma \in (0, \frac{1}{\|A^T DA\|^2})$, $\|B\|$ denotes the spectral norm of a matrix B and $r_+ := \max(r, 0)$ denotes the nonnegative part or $r \in \mathbb{R}^m$. One can also take a relaxed version of the Landweber operator by replacing T in (2) and (3) by its relaxation $T_\lambda := \mathrm{Id} + \lambda(T - \mathrm{Id})$ with $\lambda \in (0, 2)$. We show that many iterative methods for solving the problems under consideration may be reduced to the projected Landweber method or to its scaled version. We give estimations of the parameters γ for particular methods. Moreover, we present some extrapolated versions of the projected Landweber methods for solving consistent systems of equations or inequalities, where the parameter γ in (2) and (3) may depend on $x \in \mathbb{R}^n$. We also compare the numerical behavior of particular methods.

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Convergence behavior of GMRES and MINRES for ("flopped") Toeplitz systems

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Abstract

Linear systems derived from discretisation of partial differential equations (PDEs) play a critical role across various applications such as climate change, personalised healthcare, and high-value manufacturing.While preconditioned Krylov subspace methods are frequently preferred for these systems,addressing preconditioners and solvers for nonsymmetric problems still lacks established theory, which is crucial for key industrially-relevant problems. The current objective of our research is to find out the reason why for Toeplitz systems, especially the preconditioined ones, GMRES for $Ax = b$ takes roughly half as many iterations as symmetrised MINRES for $YAx = Yb$, where Y is the reverse identity matrix. We will talk about why theories in current literature do not apply to our problems, how Hessenberg matrices derived from Arnoldi iterations may indicate the convergence behavior of GMRES/MINRES, why singular values or eigenvalues of A and/or YA may fail to predict their convergence behavior, etc.

A regularized Interior Point Method for sparse optimal transport on graphs

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Abstract

In this talk we present recent developments for the solution of Optimal Transport (OT) problems on graphs using Interior Point Methods (IPMs). In particular, we will show how to solve large scale OT problems on sparse graphs using a bespoke IPM algorithm able to suitably exploit a Proximal-Primal–Dual regularization in order to enforce scalability. Detailed theoretical results will be presented as well as extensive numerical results aiming at showcasing the efficiency and robustness of the proposed approach when compared to network simplex solvers. The presentation is based on [1].

References

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Some questions around my conjecture

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Abstract

In [1], I have proposed the conjecture

For all matrices A with complex entries and for all polynomials p

$$\|p(A)\| \leq 2 \max_{z \in W(A)} |p(z)|,$$

where $W(A)$ denotes the numerical range of A. This inequality has been shown for 2×2 matrices but is still open in the general case. At this time, the best result is the estimate (thanks to Cesar Palencia)

$$\|p(A)\| < (1+\sqrt{2}) \max_{z \in W(A)} |p(z)|.$$

I will speak about the difficulty to realize a numerical investigation of the conjecture even if we limit us to consider the 3×3 case.

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Linear algebra of data-driven ROMs in imaging applications

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Abstract

Data-driven reduced order models have recently emerged as an efficient tool for imaging applications in remote sensing and other noninvasive problems, such as radar imaging, seismic and electrical exploration, etc, where measurements are not available in the domain of interest, e.g., [1, 2, 3]. This approach fits measurements (components of MIMO transfer functions) using ladder network approximations, enabling the computation of the state solution in the inaccessible part of the model by embedding this approximation in the underlying partial differential equations (PDEs). This presentation will describe the linear algebraic foundations of this approach, including several classical and developing algorithms: the block-Lanczos algorithm, matrix-valued continued fraction, block-Cholesky decomposition of structured matrices, stabilization of reduced order models via data-driven Gramian truncation, and passive rational fitting of MIMO transfer functions. I will highlight some intriguing numerical matrix problems that arise in this context.

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Performance of the extended precision VRP processor on various Krylov subspace solvers

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Abstract

Numerical stability is a central aspect of high performance scientific computation, since the growing scale of modern problems has led researchers to complex numerical techniques which are vulnerable to round-off and quantization errors. This is particularly true for iterative Krylov subspace projective solvers, which are the workhorse the modern scientific applications. Here, higher precision, e.g. larger significand size, can mitigate these numerical instabilities and allow for simpler and more memory efficient computations.

The VRP Processor [1] is designed to accelerate extended precision arithmetics in hardware. It supports 1/ a fast arithmetic unit for up to 512 bits of mantissa and 2/ support in memory for unaligned floating-point (FP) arrays.

The objective of this study is to assess the performance impact of using the VRP with extended precision on common solver algorithms, e.g. conjugate gradient (CG), its preconditionned variant (PCG) and biconjugate gradient (BiCG).

We consider two metrics: 1/ convergence speed, which refers to the number of iterations necessary for reaching that objective and 2/ execution time, including memory access time, measured in clock cycles. Execution time depends from the actual implementation of both hardware and low-level software, and from the input matrix structure and values.

Our sample matrices principally come from the Florida sparse Matrix Collection [2]. We restrict ourselves to real matrices, which may be symmetric (for CG and PCG) or asymmetric (for BiCG). We compare execution time between different precisions (including standard double format) on the same VRP platform

Our results confirm the benefits of extended precision for Krylov subspace solvers. For the CG solver, extending precision around 128 mantissa bits appears optimal in terms of iteration count and mostly beneficial for cycle count. The benefit for the BiCG solver is even greater. When using precisions above 256 bits, BiCG convergence becomes predictable.

References

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Stochastic pth root approximation of a stochastic matrix: a Riemannian optimization approach*

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Abstract

The evolution of a discrete-time Markov chain, with a finite number n of states, is described in terms of an $n \times n$ matrix A, called *transition matrix*, whose (i, j)-th entry represents the probability to go from state i to state j in one unit of time. The matrix A is *stochastic*, i.e., belongs to the set

$$\mathbb{S}_n^0 = \{S \in \mathbb{R}^{n\times n} \,:\, S\mathbf{1} = \mathbf{1},\ S \geq 0\},$$

where $\mathbf{1} = (1, 1, \ldots, 1)^T \in \mathbb{R}^n$, and the symbol "$\geq$" represents the element-wise ordering. For the Perron-Frobenius theorem, any stochastic matrix A has a nonnegative Perron eigenvector $\boldsymbol{\pi}$ normalized so that $\boldsymbol{\pi}^T\mathbf{1} = 1$, and called steady state vector. In many applications, the entries of the matrix A are estimated through the analysis of historical series over long time intervals. The typical unit time at which transitions occur is generally smaller, compared with the characteristic time of the phenomenon to be analyzed. To know the transition probabilities in the typical time step of the phenomenon, it would therefore be necessary to investigate what happens in a fraction of a unit of time: for instance, which are the transition probabilities in a half-time unit? To this end, we might compute a matrix X such that $A = X^2$, or, in other terms, a *square root* of the transition matrix A. More generally, we can inquire about any number of intermediate steps p thus looking for a pth root X of A, $A = X^p$, $p \in \mathbb{N}$. Unfortunately, a *stochastic* pth root X does not exist in general [1], and several pathological cases can be readily produced. We propose two approaches, based on Riemannian optimization, for computing a stochastic approximation of the pth root of a stochastic matrix A [2]. In the first approach, the approximation is found in the Riemannian manifold of positive stochastic matrices [3]. In the second approach, we introduce the Riemannian manifold of positive stochastic matrices sharing with A the Perron eigenvector and we compute the approximation of the pth root of A in such a manifold. We will show examples from Markov chains used in applications and test examples to demonstrate the effectiveness of the proposed procedure.

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An Arnoldi-based approach to Sobolev polynomial and Sobolev rational least squares problems

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Abstract

In this research, we reformulate Sobolev polynomial and Sobolev rational least squares problems, which involve the derivate values up to an arbitrary order, based on orthogonal bases [1, 2]. Although the increase in the approximation degree allows us to fit the data better in attacking least squares problems, the ill-conditioning of the coefficient matrix fuels the dramatic decrease in the accuracy of the approximation at higher degrees. To overcome this drawback, we first show that the column space of the coefficient matrix is equivalent to a Krylov subspace generated by a Jordan-like matrix [3]. Then the connection between Sobolev orthogonal polynomials or Sobolev orthogonal rational functions and orthogonal bases for Krylov subspaces in order to exploit Krylov subspace methods like Arnoldi orthogonalization is established.

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Role extraction by random walks and matrix equations*

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Abstract

Nodes in a directed network can be grouped into equivalence classes according to the roles they play. The most prominent example of this is the Web's well-known bowtie structure: With few exceptions, websites can be divided into a large core group that forms a strongly connected subgraph, a group of nodes upstream of the core, and a group of nodes downstream of the core.

Generally, the roles are determined by defining appropriate measures of similarity between pairs of nodes. These are stored in a similarity matrix, which is often defined as the solution of a particular matrix equation or a low-rank approximation thereof, see e.g., [1, 2].

Here I propose a new node similarity measure to extract roles in a directed network. The idea exploits random walks that traverse the arcs both along their direction and in the opposite direction. The similarity matrix can be computed by a fixed-point iteration whose convergence allows a comprehensive analysis. Compared to other similarity measures, this one turns out to provide accurate results even on highly inhomogeneous networks.

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Efficient strategies for updating some resolvent-based centrality measures

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Abstract

Katz centrality is one of the most popular centrality index in networks analysis. Introduced in 1953 [1], it states that the importance of node i in a network is given by the i-th entry of the vector

$$\mathbf{k} := (I - \alpha A)^{-1}\mathbf{1} \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$ is the adjacency matrix of the network and $\alpha > 0$ is a damping parameter chosen such that the resolvent operator in (1) cannot be singular, i.e., $\alpha\rho(A) < 1$. In practice, the underlying indices for a given network is computed by solving the linear system

$$(I - \alpha A)\mathbf{k} = \mathbf{1}. \tag{2}$$

Although computing Katz centrality can be efficient even for large networks, recalculating the measure after sequentially removing a set of nodes or edges can be quite challenging. Indeed, multiple linear systems like (2) need to be solved in sequence, one after each elimination. For this reason, an interesting problem is to study how low-rank modifications of the adjacency matrix, such as the removal of a set of nodes or edges from the graph, affect the centralities of the remaining nodes, see, e.g., [2] and references therein.

In [3], we characterize how Katz centrality changes in networks when edges (resp., nodes) are removed from the graph, extending a previous result in [4]. Then, we derive bounds on the decay of the induced *total network communicability* [5]. Moreover, we introduce an efficient numerical strategy to update Katz centrality, significantly reducing the computational burden of recomputing it repeatedly from scratch.

This communication is based on [3] and [4].

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Analysis on aggregation and block smoothers in multigrid methods for block Toeplitz linear systems*

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Abstract

We present novel improvements in the context of symbol-based multigrid procedures for solving large block Toeplitz linear systems [4]. We study the application of aggregation-based grid transfer operators that transform the symbol of a block Toeplitz matrix from matrix-valued to scalar-valued at the coarser level [1]. The convergence analysis of the TGM reveals the connection between the features of the scalar-valued symbol at the coarser level and the properties of the original matrix-valued one [3]. This permits to prove the convergence of a V-cycle multigrid involving classical grid transfer operators for scalar Toeplitz systems at the coarser levels [2].

Moreover, we extend the class of suitable smoothers focusing on the efficiency of block strategies, particularly the relaxed block Jacobi method. General conditions on smoothing parameters are derived, with emphasis on practical applications where these parameters can be calculated with negligible computational cost.

We test the proposed strategies on linear systems stemming from discretization of differential problems. The numerical results show computational advantages compared to existing methods for block structured linear systems.

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What is new in domain decomposition?

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Abstract

Domain decomposition research intensified in the early nineties, and there is still substantial research activity in this field. There has been however an important shift in domain decomposition, and I will explain three new interesting research directions that are pursued very actively at the moment, and give newest results:

1. Iterative solvers for time harmonic wave propagation: time harmonic wave propagation problems are very hard to solve by iterative methods. All classical iterative methods, like Krylov methods, multigrid, and also domain decomposition methods, fail for the key model problem, the Helmholtz equation. There are new, highly promising domain decomposition methods for such problems, which I will present, and I will also state precisely under which conditions they can work well, and when they still fail.
2. Coarse space components: domain decomposition analysis has lacked behind multigrid in the precise understanding of the interaction between the domain decomposition smoother and coarse space solver, and all classical domain decomposition solvers need Krylov acceleration to be effective, while multigrid does not. I will present a new spectral analysis of the Schwarz iteration operator, which allows us to achive as an accurate understanding of two level Schwarz methods as the seminal Fourier analysis of multigrid methods.
3. Time parallelization: new computing architectures have too many computing cores to parallelize only in space for evolution problems. I will present time and space-time domain decomposition methods and explain which can be effective for parabolic and hyperbolic problems.

TRIPs-Py: Techniques for Regularization of Inverse Problems in Python

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Abstract

In this contribution we present TRIPs-Py, a new Python package of linear discrete inverse problems solvers and test problems. The solvers available in TRIPs-Py include direct regularization methods (such as truncated singular value decomposition and Tikhonov) and iterative regularization techniques (such as Krylov subspace methods and solvers for $\ell_p - \ell_1$ formulations, some of which have not been publicly available before, which enforce sparse or edge-preserving solutions and handle different noise types). Some of the test problems in TRIPs-Py arise from simulated image deblurring and computerized tomography, while other test problems model realistic problems in dynamic and hyperspectral computerized tomography. During this contribution we will give an overview of some of the state-of-the-art TRIPs-Py regularization methods, highlighting similarities and differences, and we will illustrate their use on some of the TRIPs-Py test problems.

Numerical solution of nonclassical boundary value problems by matrix function computations

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Abstract

In this poster we focus on the solution of a class of linear differential problems of the form

$$\frac{dv}{dt} = Av, \quad 0 < t < T,$$

set in a Banach space, with the nonlocal integral condition

$$\frac{1}{T}\int_0^T v(t)\, dt = f,$$

where the function f and the linear, closed, possibly unbounded operator A are given.

When A is a matrix, the solution of our differential problem can then be expressed as the action of a function of A on f, namely, $v(t) = \psi_t(A)f$. We first present some numerical methods based on the Fourier expansion of $\psi_t(z)$ for computing this action [1, 2]. Then, we place these methods in the classical framework of Krylov-Lanczos (polynomial-rational) techniques for accelerating Fourier series. This allows us to develop convergence results and to design suitable acceleration schemes [4].

For the more general case where the differential problem is set in a Banach space, we prove the existence and uniqueness of the solution $v(t)$ and characterize it via a family of mixed polynomial-rational expansions w.r.t. the operator A. Each expansion contains a purely polynomial term of arbitrary degree, which is related to the Bernoulli polynomials, followed by a series of rational terms. Each rational term is then computed as the solution of a boundary value problem [3].

The results presented in this poster are obtained jointly with P. Boito and Y. Eidelman [1, 2, 3] and L. Aceto [4].

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When is the resolvent like a rank one matrix?

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Abstract

Let A be a square matrix. The resolvent, $(A - zI)^{-1}$, $z \in \mathbb{C}$, plays an important role in many applications; for example, in studying functions of A, one often uses the Cauchy integral formula,

$$f(A) = -\frac{1}{2\pi i} \int_\Gamma (A - zI)^{-1} f(z)\, dz,$$

where Γ is the boundary of a region Ω that contains the spectrum of A and on which f is analytic.

If z is *very* close to a simple eigenvalue λ of A – much closer to λ than to any other eigenvalue of A – then $(A - zI)^{-1} \approx \frac{1}{\lambda - z} xy^*$, where x and y are right and left normalized eigenvectors of A corresponding to eigenvalue λ. It is sometimes observed, however, that $(A - zI)^{-1}$ is close to a rank one matrix even when z is not very close to an eigenvalue of A. In this case, one can write $(A - zI)^{-1} \approx \sigma_1(z) u_1(z) v_1(z)^*$, where $\sigma_1(z)$ is the largest singular value of $(A - zI)^{-1}$ and $u_1(z)$ and $v_1(z)$ are the corresponding left and right singular vectors.

We use singular value/vector perturbation theory to describe conditions under which $(A - zI)^{-1}$ can be well-approximated by rank one matrices for a wide range of z values. If λ is a simple *ill-conditioned* eigenvalue of A, if the smallest nonzero singular value of $A - \lambda I$ is *well-separated* from 0, and if a certain other condition involving the singular vectors of $A - \lambda I$ is satisfied, then it is shown that $(A - zI)^{-1}$ is close to a rank one matrix for a wide range of z values. An application of this result in comparing bounds on $\|f(A)\|$ is described [1].

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Right preconditioned GMRES for arbitrary singular systems

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Abstract

Brown and Walker [1] showed that GMRES determines a least squares solution of $A\boldsymbol{x} = \boldsymbol{b}$ where $A \in \mathbf{R}^{n\times n}$ without breakdown for arbitrary $\boldsymbol{b}, \boldsymbol{x}_0 \in \mathbf{R}^n$ if and only if A is range-symmetric, i.e. $\mathcal{R}(A^{\mathrm{T}}) = \mathcal{R}(A)$, where A may be singular and $\boldsymbol{b}$ may not be in the range space $\mathcal{R}(A)$ of A.

In this talk[2], we propose applying GMRES to $ACA^{\mathrm{T}}\boldsymbol{z} = \boldsymbol{b}$, where $C \in \mathbf{R}^{n\times n}$ is symmetric positive definite. This determines a least squares solution $\boldsymbol{x} = CA^{\mathrm{T}}\boldsymbol{z}$ of $A\boldsymbol{x} = \boldsymbol{b}$ without breakdown for arbitrary (singular) matrix $A \in \mathbf{R}^{n\times n}$ and $\boldsymbol{b} \in \mathbf{R}^n$.

To make the method numerically stable, we propose using the pseudoinverse (pinv of MATLAB) with an appropriate threshold parameter to suppress the influence of tiny singular values when solving the severely ill-conditioned Hessenberg systems which arise in the Arnoldi process of GMRES when solving inconsistent range-symmetric systems.

Numerical experiments show that the method taking C to be the identity matrix or $\{\mathrm{diag}(A^{\mathrm{T}}A)\}^{-1}$ give least squares solutions even when A is not range-symmetric, including the case when $\mathrm{index}(A) > 1$.

This is only a proof of concept, since pinv is too expensive. We are currently investigating more practical ways to implement the idea, as well as more efficient preconditioners for C.

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On the usage of Schur complements for post-processing techniques in electronic structure calculations

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Abstract

Molecular simulation and electronic structure calculation are fundamental tools used in chemistry, solid-state physics, molecular biology, materials science, nanosciences... Density functional theory (DFT) is one of the most widely used methods nowadays, as it offers a good compromise between efficiency and accuracy. It is a formidable problem that requires a whole hierarchy of choices, which lead to a number of approximations and associated errors: choice of model, choice of discretization basis, choice of solvers, truncation error, numerical error...

In this talk, I will present some recent works where known techniques in linear algebra (namely Schur complements) were successfully applied to solve numerical challenges in electronic structure calculations. First, I'll show how to enhance the numerical stability of response properties [1]. Such calculations require to solve successively many linear systems that are possibly badly conditioned, and using a Schur complement by decomposing the underlying Hilbert space into appropriate subspaces enables to achieve numerical stability, even for cases badly conditioned. If time allows, I'll explain how to use similar techniques to compute efficient *a posteriori* estimates in DFT [2, 3].

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Randomized low-rank approximation of parameter-dependent matrices

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Abstract

Randomized algorithms, like the randomized singular value decomposition (SVD) or the generalized Nyström method, have become standard approaches for computing a low-rank approximation of a matrix A when A is accessed through matrix-vector products. In a number of applications, A depends on a parameter t, like time, and it is of interest to obtain good low-rank approximation to $A(t)$ for many parameter values t. Examples include dynamical systems, spectral density estimation, and Gaussian process regression. In this talk, we discuss new randomized methods that aim at approximating $A(t)$ simultaneously for many values of t. Being direct extensions of the randomized SVD and the Nyström methods, our parameter-dependent methods share many of their practical and theoretical advantages. Both, theoretical results and numerical experiments show that these methods reliably return quasi-best low-rank approximations. This talk is based on joint work with Hysan Lam as well as Gianluca Ceruti, Haoze He, and Fabio Matti.

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A mixed-precision algorithm for the Sylvester matrix equation

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Abstract

In the usual one-precision environment the Bartels–Stewart algorithm [1] is the standard algorithm for solving small dense Sylvester matrix equations $AX + XB = C$. their algorithm consists of three steps, including the computation of the Schur decompositions, the substitution for solving the Sylvester equation with quasi-triangular coefficients, and the final recovering transformation.

In the new mixed-precision algorithm we propose, the computation of the Schur decompositions, which are the most expensive part of the algorithm, is performed in a low precision. Then the algorithm *refines* via a stationary iteration the approximate solution obtained by solving the quasi-triangular Sylvester equation with the low-precision quasi-triangular coefficient matrices; and this is in fact an iterative refinement scheme for the quasi-triangular Sylvester equation with the coefficient matrices in a perturbed form. Finally, in order to recover the solution from the Schur decompositions we need the unitary factors to be unitary to the working precision. In order to do so, we propose two efficient approaches to orthonormalize to the working precision the low-precision unitary factors, one based on orthonormalization and the other on inversion of the unitary factors.

We test the new mixed-precision methods on various problems from the literature containing both Sylvester and Lyapunov matrix equations. Numerical experiments show that the new methods are comparable with the classical Bartels–Stewart method in terms of accuracy, and they can be faster if the employed low-precision arithmetic is sufficiently cheaper than the working-precision arithmetic.

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Reorthogonalized Pythagorean variants of block classical Gram-Schmidt

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Abstract

Block classical Gram-Schmidt (BCGS) is commonly used for orthogonalizing a set of vectors X in distributed computing environments due to its favorable communication properties relative to other orthogonalization approaches, such as modified Gram-Schmidt or Householder. However, it is known that BCGS (as well as recently developed low-synchronization variants of BCGS) can suffer from a significant loss of orthogonality in finite-precision arithmetic, which can contribute to instability and inaccurate solutions in downstream applications such as s-step Krylov subspace methods. A common solution to improve the orthogonality among the vectors is reorthogonalization. Focusing on the "Pythagorean" variant of BCGS, introduced in [E. Carson, K. Lund, & M. Rozložník. *SIAM J. Matrix Anal. Appl.* 42(3), pp. 1365–1380, 2021], which guarantees an $O(\varepsilon)\kappa^2(X)$ bound on the loss of orthogonality as long as $O(\varepsilon)\kappa^2(X) < 1$, where ε denotes the unit roundoff, we introduce and analyze two reorthogonalized Pythagorean BCGS variants. These variants feature favorable communication properties, with asymptotically two synchronization points per block column, as well as an improved $O(\varepsilon)$ bound on the loss of orthogonality. Our bounds are derived in a general fashion to additionally allow for the analysis of mixed-precision variants. We verify our theoretical results with a panel of test matrices and experiments from a new version of the `BlockStab` toolbox.

Solving the parametric eigenvalue problem by Taylor series and Chebyshev expansion

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Abstract

We discuss two approaches to solving the parametric (or stochastic) eigenvalue problem. One of them uses a Taylor expansion and the other a Chebyshev expansion. The parametric eigenvalue problem assumes that the matrix A depends on a parameter μ, where μ might be a random variable. Consequently, the eigenvalues and eigenvectors are also functions of μ. We compute a Taylor approximation of these functions about μ_0 by iteratively computing the Taylor coefficients. The complexity of this approach is $O(n^3)$ for all eigenpairs, if the derivatives of $A(\mu)$ at μ_0 are given. The Chebyshev expansion works similarly. We first find an initial approximation iteratively which we then refine with Newton's method. This second method is more expensive but provides a good approximation over the whole interval of the expansion instead around a single point.

We present numerical experiments confirming the complexity and demonstrating that the approaches are capable of tracking eigenvalues at intersection points. Further experiments shed light on the limitations of the Taylor expansion approach with respect to the distance from the expansion point μ_0.

This work is joint work with Melina Freitag (University of Potsdam). There is a preprint available discussing significant parts of the research [1]. Other parts have been published in the proceedings paper [2].

The research has been partially funded by the Deutsche Forschungsgemeinschaft (DFG)—Project-ID 318763901—SFB1294.

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Spectral analysis of block preconditioners for double saddle-point linear systems*

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Abstract

Given positive integer dimensions $n \geq m \geq p$, consider the $(n+m+p) \times (n+m+p)$ double saddle point linear system of the form

$$\mathcal{A}w \equiv \begin{bmatrix} A & B^T & 0 \\ B & -D & C^T \\ 0 & C & E \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} f \\ g \\ h \end{bmatrix} \equiv b, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$ is a symmetric positive definite (SPD) matrix, $B \in \mathbb{R}^{m\times n}$ and $C \in \mathbb{R}^{p\times m}$ have full row rank, $D \in \mathbb{R}^{m\times m}$ and $E \in \mathbb{R}^{p\times p}$ are square positive semidefinite matrices. Moreover $f \in \mathbb{R}^n$, $g \in \mathbb{R}^m$ and $h \in \mathbb{R}^p$ are given vectors. Such linear systems arise in many scientific applications including constrained quadratic programming, magma-mantle dynamics, liquid crystal director modeling or in the coupled Stokes-Darcy problem, to name a few.

This work concerns the spectral analysis of an SPD block preconditioner for the iterative solution of (1). We consider the SPD preconditioner proposed in [1] in the framework of multiple saddle point linear systems, defined as $\mathcal{P} = \mathcal{P}_L \mathcal{P}_D^{-1} \mathcal{P}_L^\top$, where $\mathcal{P}_D$ and $\mathcal{P}_L$ are the well-known block diagonal and block triangular preconditioners, respectively.

We analyze the eigenvalue distribution of the preconditioned matrix $\mathcal{P}^{-1}\mathcal{A}$ and show that its eigenvalues are described in terms of the roots of a cubic polynomial with real coefficients. Through a constrained optimization procedure to bound the extremal roots of parameter-dependent polynomials, we derive tight eigenvalue bounds in the interesting practical case in which all the blocks of the preconditioner are applied inexactly.

If time permits, I will also present eigenvalue bounds for symmetric multiple saddle-point linear systems, preconditioned with block diagonal preconditioners. We have extended known results for 3×3 block systems and for 4×4 systems to an arbitrary number of blocks.

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On computing simultaneous Gaussian quadrature rules

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Abstract

The computation of simultaneous Gaussian quadrature rules associated to multiple orthogonal polynomials (MOP) [1, 3, 4] is considered in this talk. Suppose r weight functions $w^{(i)}(x) \geq 0$, with support $\Delta_i,\ i = 1, \ldots, r$, on the real line are given. The MOP $\{p_n(x)\}_{n=0}^{\infty}$ satisfy the following orthogonality conditions:

$$\int_{\Delta_i} p_n(x) x^k w^{(i)}(x) dx = 0, \quad 0 \leq k \leq n_{i-1},$$

with $n = \sum_{i=1}^{r} n_i$. We focus on the computation of the nodes x_j and weights $\omega_j^{(i)}$ of a simultaneous Gaussian quadrature rule

$$\sum_{j=1}^{n} f(x_j)\omega_j^{(i)} \approx \int_{\Delta_i} f(x) w^{(i)}(x) dx, \quad 1 \leq i \leq r.$$

They can be computed via the eigendecomposition of a banded lower Hessenberg matrix H_n, built on the coefficients of recurrence relations associated to the corresponding MOP. The Golub–Welsch algorithm [2] can be adapted to compute the eigendecomposition of H_n, but it suffers from tremendous instability due to the high non-normality characterizing the latter matrix [5, 3, 4]. Here, we propose a new balancing procedure that drastically reduces the condition of the Hessenberg eigenvalue problem, allowing to compute the simultaneous Gaussian quadrature rule,in floating point arithmetic, in a reliable way for different kinds of MOP, requiring $O(n^2)$ computational complexity and $O(n)$ memory.

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Exploring rational approximations of nonlocal operators for preconditioning

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Abstract

Let $\mathcal{L}$ be a self-adjoint positive operator acting in a Hilbert space $\mathcal{H}$, where the eigenfunctions of $\mathcal{L}$ form an orthonormal basis of $\mathcal{H}$. Then, for $\beta \in (0,1)$ and a given $g \in \mathcal{H}$, $\mathcal{L}^{-\beta}$ can be expressed through the spectral decomposition of $\mathcal{L}$. The numerical approximation of $\mathcal{L}^{-\beta}$ finds immediate application when solving equations involving a fractional super diffusion term like $(-\Delta)^{\frac{\alpha}{2}}$, $\alpha \in (1,2)$, where Δ denotes the standard Laplacian. This has driven significant interest in recent years toward efficient approximations of fractional powers.

Among the approaches recently introduced are methods based on quadrature rules for the integral representation of $\lambda^{-\frac{\alpha}{2}}$; see, e.g., [2, 3, 4]. Starting from the Dunford integral representation (see, e.g., [5]) with suitable changes of variables and quadrature rules, one typically finds rational approximations of the type $(m-1, m)$, where m is equal or closely related to the number of points of the quadrature formula.

Exploiting the Gauss-Jacobi quadrature approach given in [3], we define and investigate a preconditioner for a discretization of $\lambda^{-\frac{\alpha}{2}}$ that results in the sum of m inverses of shifted Laplacian matrices; see [1]. While comparable to the Laplacian for α close to 2, for α close to 1 and m reasonably small, the resulting preconditioner provides better results than the Laplacian itself, while maintaining the same computational complexity. Aiming to improve these results, we further explore the preconditioning feasibility of exponentially convergent quadrature rules, like those in [2, 4]. We discuss a method for choosing the involved parameters that keeps the number of inverses small and allows the exponential convergence to be reflected in the preconditioning numerical optimality.

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An edge centrality measure based on Kemeny's constant

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Abstract

In the context of random walks on graphs, Kemeny's constant is a measure of the non-connectivity of the graph [2, 3]. The higher the constant, the closer the graph is to be non-connected.

In [1] an edge centrality measure in graphs, based on the variation of Kemeny's constant under removal of an edge, has been introduced. Roughly speaking, according to this measure, an edge is important if its removal causes a large increase of Kemeny's constant. Some regularization and filtering techniques have been introduced in [1] to deal with cut-edges, whose removal would disconnect the graph.

This measure is effective in determining important connections in road networks. However, it still presents some weaknesses in evaluating the importance of peripheral roads.

Here, we present an improvement of this measure, based on the directional derivative of Kemeny's constant. We prove that the new measure continues to be non-negative, as the previous one. We provide an explicit expression of this measure, given in terms of the inverse of a modified Laplacian matrix of the graph, together with an effective algorithm for its computation.

For barbell graphs, an expression given in terms of the weights of the edge is provided that confirms its good behavior in assessing the importance of peripheral roads.

Numerical experiments performed on the road map of Tuscany confirm the nice features of this measure.

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Polynomial eigenvalue inclusion and exclusion sectors

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Abstract

We derive zero inclusion and exclusion sectors for scalar polynomials whose coefficients have sign restrictions. These sectors are determined only by the sign of the coefficients, which easily allows them to be applied to polynomial eigenvalue problems with positive and negative definite matrix coefficients. Such problems are often encountered in applications, one of which, in aerodynamics, provided the initial motivation for this work.

Although, strictly speaking, not related to linear algebra, the geometric approach used to obtain the aforementioned sectors can also be used to locate the zeros of complex valued harmonic polynomials, which have a fascinating connection to gravitational lensing. Such polynomials are not analytic, complicating their analysis, an illustration of which is, e.g., the fact that the number of their zeros is generally unknown a priori. We briefly describe an application to harmonic trinomials, which has been of recent interest, and for which surprisingly precise regions can be found for the location of their zeros.

A note on the Grcar matrix

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Abstract

The Grcar matrix is often used as a test matrix for algorithms designed for solving linear systems or eigenvalue problems. It is a banded Toeplitz upper Hessenberg matrix with sensitive eigenvalues.

In this note we provide closed form expressions for the factors of its LU factorization and for its inverse. More importantly, we also show how to obtain a parametric description of its asymptotic spectrum, which is the location of the eigenvalues in the complex plane when the order $n \to \infty$.

Enhancing multigrid solvers for IGA of linear and nonlinear problems using extrapolation methods

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Abstract

Multigrid methods (MG) are at the heart of the most powerful linear algebra solvers. They are powerful methods for solving large problems arising from the discretization of linear partial differential equations. In this study, geometric multigrid techniques for the isogeometric discretization of second-order elliptic problems are presented. The smoothing and approximation properties of the relaxation approach are investigated. These properties imply that two-grid and multigrid techniques will achieve uniform convergence. As the spline degree is increased, the application of the multigrid to the isogeometric situation leads to a large degradation of the convergence rates. Therefore, a specific combination of multigrid methods and preconditioning Krylov solvers is used to make the iteration numbers robust with respect to the spline degree [1, 2]. Our main focus revolves around using vector polynomial extrapolation methods [3] to enhance the convergence behavior of multigrid techniques. Numerical investigations for both linear and nonlinear problems demonstrate how well these extrapolation methods perform in accelerating the multigrid solver's convergence.

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H-LSLU: an inner product free Hybrid krylov subspace method for large scale inverse problems

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Abstract

In this presentation we describe two new Krylov subspace methods for solving rectangular large-scale linear inverse problems. The first approach is a modification of the Hessenberg iterative algorithm that is based off an LU factorization and is therefore referred to as the least squares LU (LSLU) method. The second approach incorporates Tikhonov regularization in an efficient manner; we call this the Hybrid LSLU (H-LSLU) method. Both methods are inner-product free, making them advantageous for high performance computing and mixed precision arithmetic. Theoretical results and extensive numerical results show that H-LSLU can be effective in solving large-scale inverse problems and has comparable performance with existing iterative projection methods.

Riemann-Oracle: An adaptable Riemannian solver for matrix nearness problems

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Abstract

In this talk, we propose a versatile approach to address a large family of matrix nearness problems. The method is based on splitting a matrix nearness problem into two nested optimization problems, of which the inner one can be solved either exactly or cheaply, while the outer one can be recast as an unconstrained optimization task over a smooth real Riemannian manifold. We also show that the objective function to be minimized on the Riemannian manifold can be discontinuous, thus requiring regularization techniques, and we give conditions for this to happen. Finally, we demonstrate the practical applicability of our method by implementing it for a number of matrix nearness problems that are relevant for applications, including nearest singular matrix with a given sparsity structure, nearest singular matrix polynomial, approximate GCD and nearest unstable matrix.

Filtering of mixed precision iterative refinement for linear inverse problems

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Abstract

Many problems in science and engineering give rise to linear systems of equations that are commonly referred to as large-scale linear discrete ill-posed problems. The matrices that define these problems are typically severely ill-conditioned and may be rank deficient. Because of this, the solution of linear discrete ill-posed problems may not exist or be extremely sensitive to perturbations caused by error in the available data. These difficulties can be reduced by applying regularization. We explore the connections between iterated Tikhonov regularization and iterative refinement on the Tikhonov problem in mixed precision using a filter factor analysis.

Row-aware randomized SVD with applications

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Abstract

We introduce a novel procedure for computing an SVD-type approximation of a tall matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$, $m \geq n$. Specifically, we propose a randomization-based algorithm that improves over the standard Randomized Singular Value Decomposition (RSVD) from [1]. Most significantly, our approach, the Row-aware RSVD (R-RSVD), explicitly constructs information from the row space of $\mathbf{A}$. This leads to better approximations to Range$(\mathbf{A})$ while maintaining the same computational cost. The efficacy of the R-RSVD is supported by both robust theoretical results and extensive numerical experiments. Furthermore, we present an alternative algorithm inspired by the R-RSVD, capable of achieving comparable accuracy despite utilizing only a subsample of the rows of $\mathbf{A}$, resulting in a significantly reduced computational cost. This method, that we name the Subsample Row-aware RSVD (Rsub-RSVD), is supported by a weaker error bound compared to the ones we derived for the R-RSVD, but still meaningful as it ensures that the error remains under control. Additionally, numerous experiments demonstrate that the Rsub-RSVD trend is akin to the one attained by the R-RSVD even for small subsampling parameters. Finally, we consider the application of our schemes in two very diverse settings which share the need for the computation of singular vectors as an intermediate step: the computation of CUR decompositions by the discrete empirical interpolation method (DEIM) and the construction of reduced-order models in the Loewner framework, a data-driven technique for model reduction of dynamical systems.

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A posteriori error estimates based on multilevel decompositions with large problems on the coarsest level

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Abstract

Multilevel methods represent a powerful approach in numerical solution of partial differential equations. The multilevel structure can also be used to construct estimates for total and algebraic errors of computed approximations. We consider residual-based error estimates based on properties of quasi-interpolation operators, stable-splittings, or frames and we focus on the settings where the system matrix on the coarsest level is still large and the associated terms in the estimates can only be approximated. We show that the way in which the error term associated with the coarsest level is approximated is substantial. In particular, it can significantly affect both the efficiency (accuracy) of the overall error estimates and their robustness with respect to the size of the coarsest problem. We propose a new approximation of the coarsest-level term based on using the conjugate gradient method with an appropriate stopping criterion. We prove that the resulting estimates are efficient and robust with respect to the size of the coarsest-level problem. Numerical experiments illustrate the theoretical findings.

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Efficient dynamic image reconstruction with motion estimation

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Abstract

Large-scale dynamic inverse problems are typically ill-posed and suffer from complexity of the model constraints and large dimensionality of the parameters. A common approach to overcome ill-posedness is through regularization that aims to add constraints on the desired parameters in both space and temporal dimensions. In this work, we propose an efficient method that incorporates a model for the temporal dimension by estimating the motion of the objects alongside solving the regularized problems. In particular, we consider the optical flow model as part of the regularization that simultaneously estimates the motion and provides an approximation for the desired image. To overcome high computational cost when processing massive scale problems, we combine our approach with a generalized Krylov subspace method that efficiently solves the problem on relatively small subspaces. The effectiveness of the prescribed approach is illustrated through numerical experiments arising in dynamic computerized tomography and image deblurring applications.

Tensor oriented truncated LSQR for tensor least squares problems

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Abstract

We are interested in the numerical solution of the tensor least squares problem

$$\min_{\mathcal{X}} \| \sum_{i=1}^{p} \mathcal{X} \times_1 A^{(i)} \times_2 B^{(i)} \times_3 C^{(i)} - \mathcal{D} \|_F,$$

where $\mathcal{D}$ is low rank. In our case low rank means that $\mathcal{D} = D_{\text{core}} \times_1 D_1 \times_2 D_2 \times_3 D_3$, with each D_i low rank and the core tensor having small dimensions. We will focus on the implementation for $p = 2, 3$, but it can be generalized to the multiterm setting, particularly useful for applications such as PDEs. The solution of the problem above has attracted significant interest in the recent literature, see, e.g., [1,2]. Along the same lines, we derive a truncated tensor-oriented LSQR. To this end, we generalize the work presented in [5] for the matrix least squares problem, where we have studied truncated matrix-oriented LSQR and compared it with the truncated matrix-oriented Conjugate Gradient (see [3,4]). We devise an implementation for the truncation step taking advantage of the structure of tensors, allowing us to work with low rank approximations. Natural applications and experiments arise from the numerical solutions of PDEs; we illustrate the performance of the new method with some examples in the 3D case, and compare truncated LSQR with already existing approaches based on the matricization of the problem.

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A fast numerical method for the operator solution of the generalized Rosen-Zener model

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Abstract

In quantum mechanics, the Rosen-Zener model represents a two-level quantum system. Its generalization to multiple degenerate sets of states leads to a non-autonomous linear system of ordinary differential equations (ODEs). We propose a new method for computing the solution operator of this system of ODEs. This new method is based on a recently introduced expression of the solution in terms of an infinite matrix equation, which can be efficiently approximated by truncation, fixed point iterations, and low-rank approximation. This expression is possible thanks to the so-called $\star$-product approach for linear ODEs. The numerical experiments show that the new method's computing time seems to scale linearly with the model's size.

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Convergence analysis and parameter choice for the iterated Arnoldi-Tikhonov method

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Abstract

The Arnoldi-Tikhonov method is a well-established regularization technique for solving large-scale ill-posed linear inverse problems. This method uses the Arnoldi decomposition to reduce computational complexity by projecting the discretized problem into a lower-dimensional Krylov subspace, in which it is solved. This talk explores the iterated Arnoldi-Tikhonov method and provides an analysis that addresses all approximation errors. Additionally, it introduces a novel strategy for choosing the regularization parameter.

Analysis of stochastic probing methods for estimating the trace of functions of sparse symmetric matrices

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Abstract

We consider the problem of estimating the trace of a matrix function $f(A)$. In certain situations, in particular if $f(A)$ cannot be well approximated by a low-rank matrix, combining probing methods based on graph colorings with stochastic trace estimation techniques can yield accurate approximations at moderate cost. So far, such methods have not been thoroughly analyzed, though, but were rather used as efficient heuristics by practitioners. In this manuscript, we perform a detailed analysis of stochastic probing methods and, in particular, expose conditions under which the expected approximation error in the stochastic probing method scales more favorably with the dimension of the matrix than the error in non-stochastic probing. Extending results from [1], we also characterize situations in which using just one stochastic vector is always—not only in expectation—better than the deterministic probing method. Several numerical experiments illustrate our theory and compare with existing methods.

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On the computation of the pseudoinverse of large and sparse regularization matrices

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Abstract

In [1] an algorithm for regularization problems in general form, based on projections on the null space of the regularization operator and its orthogonal complement, was introduced. This algorithm was further discussed in [2], where some properties and implementation details were highlighted. When this approach is applied to large scale general form problems by means of the LSQR method, it becomes necessary to solve, at each iteration step, a least-squares problem for the regularization matrix and one for its transpose. We will discuss this aspect of the computation, in the case of large and sparse regularization matrices, which is rather common in image reconstruction.

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Anderson acceleration. Convergence analysis and applications to equilibrium chemistry

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Abstract

In this paper, we study theoretically and numerically the Anderson acceleration method. First, we extend the convergence results of Anderson's method for a small depth to general nonlinear cases. More precisely, we prove that the Type-I and Type-II Anderson(1) are locally q-linearly convergent if the fixed point map is a contraction with a Lipschitz constant small enough. We then illustrate the effectiveness of the method by applying it to the resolution of chemical equilibria. This test case has been identified as a challenging one because of the high nonlinearity of the chemical system and stiffness of the transport phenomena. The Newton method (usually Newton-Raphson) has been adopted by quite all the equilibrium and reactive transport codes. But the often ill-conditioned Jacobian matrix and the choice of a bad initial data can lead to convergence problems, especially if solute transport produces sharp concentrations profiles. Here we propose to combine the Anderson acceleration method with a particular formulation of the equilibrium system called the method of positive continued fractions (usually used as preconditioning). As shown by the numerical simulations, this approach makes it possible to considerably improve the robustness of the resolution of chemical equilibria algorithms, especially since it is coupled with a strategy to monitor the depth of the Anderson acceleration method in order to control the condition number.

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The linear algebra of Large Language Models*

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Abstract

In an era where Artificial Intelligence (AI) is permeating virtuallly every single field of science and engineering, it is becoming critical to members of the numerical linear algebra community to understand and embrace AI, and to contribute to its advancement, and more broadly to the advancement of machine learning. What is fascinating and rather encouraging is that Numerical Linear Algebra (NLA) is at the core of machine learning and AI. In this talk we will give an overview of Deep Learning with an emphasis on Large Language Models (LLMs) and Transformers [3, 4]. The very first step of LLMs is to convert the problem into one that can he exploited by numerical methods, or to be more accurate, by optimization techniques. All AI methods rely almost entirely on essentially 4 ingredients: data, optimization methods, statistical intuition, and linear algebra. Thus, the first task is to map words or sentences into tokens which are then imbedded into Euclidean spaces. From there on, the models refer to vectors and matrices. We will show a few examples of important developments in ML, that were heavily based on linear algebra ideas. Among these, we will briefly discuss *LoRa* [1] a technique in which low-rank approximation was used to reduce computational cost in some models, leading to gains of a few orders of magnitude. Another contribution that used purely algebraic arguments and that had a major impact on LLMs is the article [2]. Here the main discovery is that the nonlinear "self-attention" in LLMs can be approximated linearly, resulting in huge savings in computations, as the computational complexity was decreased from $O(n^2)$ to $O(n)$.

The talk will be mostly a survey of known recent methods in AI with the primary goal of unraveling the mathematics of Transformers. A secondary goal is to initiate a discussion on the issue of how NLA specialitst can participate in AI research.

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Efficient SAA methods for hyperparameter estimation in Bayesian inverse problems

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Abstract

In Bayesian inverse problems, it is common to consider several hyperparameters that define the prior and the noise model that must be estimated from the data. In particular, we are interested in linear inverse problems with additive Gaussian noise and Gaussian priors defined using Matern covariance models. In this case, we estimate the hyperparameters using the maximum a posteriori (MAP) estimate of the marginalized posterior distribution. However, this is a computationally intensive task since it involves computing log determinants.

To address this challenge, we consider a stochastic average approximation (SAA) of the objective function and use the preconditioned Lanczos method to compute efficient function evaluation approximations. We can therefore compute the MAP estimate of the hyperparameters efficiently by building a preconditioner which can be updated cheaply for new values of the hyperparameters; and by leveraging numerical linear algebra tools to reuse information efficiently for computing approximations of the gradient evaluations.

We demonstrate the performance of our approach on inverse problems from tomography and atmospheric transport.

Shanks transformation for vector sequences, inner product free

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Abstract

Shanks transformation transforms a real sequence (s_n) into a real sequence (t_n) such that the convergence of (s_n) is accelerated via (t_n). Each term t_n appears as a solution of a linear system for which the size grows with n. Wynn's scalar Epsilon-algorithm is an appropriate way for computing t_n without explicitly solving the related linear system.

In the literature, generalisations of Shanks transformation to vector sequences (v_n) are derived with a strong connection to the scalar case, by using inner product $y^T v_n$ for some choosen vector y. This approach gives rise to topological Epsilon-algorithms for computing the transformed sequence.

In this talk, we introduce Shanks transformation for a vector sequences, inner product free. The construction of such transformation is achieved through the use of the powerful tools of Clifford algebra, which is a matrix algebra. Each term of the transformed sequence can be viewed as a solution of a generalized linear system with coefficients in Clifford algebra. We show also that the well-known vector Epsilon-algorithm introduced by P. Wynn allows us to compute the desired transformed sequence in an efficient way, without explicitly solving the generalized linear system.

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A low-memory Lanczos method with rational Krylov compression for matrix functions

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Abstract

We introduce a memory-efficient method for computing the action of a Hermitian matrix function on a vector. Our method consists of an outer rational Lanczos algorithm combined with an inner basis compression procedure based on rational Krylov subspaces that only involve small matrices. The cost of the compression procedure is negligible with respect to the cost of the outer Lanczos algorithm. This enables us to avoid storing the whole Krylov basis, leading to substantial reductions in memory requirements. This method is particularly effective when the outer rational Lanczos algorithm needs a significant number of iterations to converge and each iteration involves a low computational effort, a scenario that often occurs when polynomial Lanczos, as well as extended and shift-and-invert Lanczos are employed. Theoretical results prove that, for a wide variety of functions, the proposed algorithm differs from rational Lanczos by an error term that is usually negligible. The algorithm is compared with other low-memory Krylov methods from the literature on a variety of test problems, showing competitive performance.

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Symbol-based numerical solvers for fractional diffusion equations on convex domains

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Abstract

Fractional diffusion equations (FDEs) have rapidly gained attention and popularity in the last decades, mainly due to the fractional derivative order, a non-integer parameter that can be fine-tuned to a variety of situations and makes FDEs a strong and flexible model for anomalous diffusion. On the downside, analytical solutions are often difficult to acquire, unavailable or computationally inefficient. Hence, numerical methods need to be investigated.

Here we consider two-dimensional space-fractional diffusion equations defined on convex domains and introduce specialized tools for addressing the discretized problems. More in detail, the resulting linear systems fall in the Generalized Locally Toeplitz (GLT) class, a large algebra of matrix sequences equipped with several tools for performing an accurate spectral analysis of the coefficient matrices in an asymptotic sense, as the finesse parameters tend to zero and the precision of the discretization grows along with the size of the matrices. The acquired spectral information is then used to design numerical solvers, such as fast multigrid methods and preconditioners for the conjugate gradient or GMRES, and to assess their expected performance. Numerical experiments are presented and critically discussed.

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Convergence of preconditioned, weighted and deflated GMRES and a new deflation space

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Abstract

We present new convergence bounds for weighted, preconditioned, and deflated GMRES applied to non-Hermitian linear systems. These bounds are given for the case when the Hermitian part of the coefficient matrix is positive definite, the preconditioner is Hermitian positive definite, and the weight is equal to the preconditioner. The decrease in residual is bounded with respect to:

- the condition number of the preconditioned Hermitian part of the problem matrix,
- a certain measure of how non-Hermitian the problem is.

This indicates how to choose the preconditioner and the deflation space in order to accelerate convergence. One such choice of deflation space is proposed, and numerical experiments illustrate the effectiveness of such space.

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Analysis of randomized Householder-Cholesky QR factorization with multisketching

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Abstract

CholeskyQR2 and shifted CholeskyQR3 are two state-of-the-art algorithms for computing tall-and-skinny QR factorizations since they attain high performance on current computer architectures. However, to guarantee stability, for some applications, CholeskyQR2 faces a prohibitive restriction on the condition number of the underlying matrix to factorize. Shifted CholeskyQR3 is stable but has 50% more computational and communication costs than CholeskyQR2.

In this talk, a randomized QR algorithm called Randomized Householder-Cholesky (`rand_cholQR`) is analyzed. Using one or two random sketch matrices, it is proved that with high probability, its orthogonality error is bounded by a constant of the order of unit round-off for any numerically full-rank matrix, and hence it is as stable as shifted CholeskyQR3. An evluation of the performance of `rand_cholQR` on a NVIDIA A100 GPU demonstrates that for tall-and-skinny matrices, `rand_cholQR` with multiple sketch matrices is nearly as fast as, or in some cases faster than, CholeskyQR2. Hence, compared to CholeskyQR2, `rand_cholQR` is more stable with almost no extra computational or memory cost, and therefore a superior algorithm both in theory and practice.

On error norm estimation in CGLS and LSQR

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Abstract

One of the directions of our research is the problem of estimating the A-norm of the error in the conjugate gradient (CG) method for solving linear systems $Ax = b$ with a real symmetric positive definite matrix A. This quantity is one of the most relevant characteristics for measuring the quality of an approximation, and plays an important role in stopping criteria in many applications. For a summary and state of the art on error estimation in CG, see our book [1].

Let us recall a preferred way of estimating the A-norm of the error in CG; see [1, 2]. Denoting k the current CG iteration, we have developed a heuristic technique to obtain a sufficiently accurate estimate of the A-norm of the error at some of the previous iterations ℓ while keeping the delay $k - \ell$ as small as possible to avoid unnecessary iterations. This technique always provides a lower bound, but can also be used to construct a (not guaranteed) upper bound.

In this talk, we extend the above mentioned results to CG-like algorithms for solving least-squares problems; see [3]. In particular, we consider the CGLS and LSQR algorithms, which are mathematically equivalent to CG applied to a system of normal equations. We show how to estimate the unknown A^TA-norm of the error in CGLS and LSQR, and discuss the role of this quantity in stopping criteria for least-squares problems. The resulting estimate preserves its main properties: it can be evaluated cheaply, it is numerically reliable in finite-precision arithmetic, and it can be used in preconditioned algorithms. Numerical experiments confirm the robustness and satisfactory behavior of the estimates.

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Deflation strategies for nonlinear eigenvalue problems

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Abstract

Deflation for linear eigenvalue problems is a standard technique that consists of removing a known eigenvalue or changing it so that the other eigenvalues are easier to find. In this talk we discuss and compare different strategies to deflate eigenvalues of nonlinear eigenvalue problems. We will pay particular attention to the quadratic eigenvalue problem, describe a structural engineering application where deflation is needed, and introduce a deflation strategy based on a new class of transformations.

Rational functions in quantum computing

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Abstract

Polynomial Krylov subspaces form the basis for several powerful algorithms in classical computing. For certain problems, algorithms based on rational Krylov subspaces are more effective, e.g., approximation of certain matrix functions and computation of internal eigenvalues.

Quantum computing holds the promise that one day it can compute with matrices much larger than those that can be handled by classical computers. In recent years several effective quantum algorithms based on polynomials have been proposed, some of them inspired by Krylov subspace methods. However, rational functions as a building block for quantum algorithms remains underexplored. One major obstacle for the use of rational functions is the lack of an effective way to compute a resolvent, i.e., a single term in a partial fraction expansion, on a quantum computer. Procedures used on classical computers cannot be used directly, since some operations that are cheap on a classical computer can be expensive on a quantum computer, and vice versa.

We propose a procedure for computing a resolvent on quantum hardware that starts from the representation of the resolvent as an integral of a matrix exponential over an infinite interval. Our procedure employs a truncation of the integration interval and a quadrature rule in order to represent this integral in terms of objects that can be efficiently computed on a quantum computer. We compare several quadrature rules, analyze the quantum computational cost of this procedure and show that it outperforms the state of the art methods.

We also describe how our procedure can be used to construct a rational filter that can combined with existing quantum eigensolvers to improve convergence to internal eigenvalues significantly. Furthermore, we comment on the possibility of developing quantum analogues to classical rational function based algorithms and the corresponding challenges.

On convergence rate of the randomized multiplicative Schwarz method

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Abstract

The randomized coordinate descent (RCD) method and the randomized Kaczmarz (RK) method are two classical and widely-used randomized iteration methods for solving large-scale linear systems, they can be regarded as two special cases of the randomized multiplicative Schwarz (RMS) method. Motivated by the exact error analysis of the RCD method and the RK method, we conduct a closed-form formula for the solution error of the RMS method and further give a tighter upper bound for its convergence rate. On this basis, we unify the convergence results of the RCD method and the RK method, and generalize them to the more general extrapolated RCD method and extrapolated RK method. Numerical experiments confirm that the new estimate for the convergence rate of the RMS method is more accurate, and it can help us to find a more proper relaxation parameter.

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Quaternion tensor low rank approximation using quasi-norms

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Abstract

In this paper, we propose a new approach for low rank approximation of quaternion tensors [4, 1, 2]. The proposed method is based on the use of quasi-norms to approximate the tensor by a low rank tensor using the QT-product [3] that generalize the L-product to N-mode quaternions. We show that the proposed method is able to well approximate the tensor compared to the convexifying of the rank, i.e, the nuclear norm. We give theoretical results and numerical experiments to show the efficiency of the proposed method in the Inpainting and Denoising applications.

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Randomized projected successive iterations for symmetric and asymmetric linear complementarity problem

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Abstract

For solving large and sparse linear complementarity problems arsing from scientific computing and engineering applications, we propose a class of projected successive iteration methods with randomized or greedy selection of update indices in each iteration. The theoretical convergence analysis including the expected convergence rate are proposed when the system matrix are symmetric positive definite and nonsymmetric P-matrix, respectively. Numerical experiments on the linear complementarity problems arising from American option pricing and nonnegative matrix factorization show the efficiency of the proposed methods.

Block Gauss-Radau quadrature

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Abstract

In this talk we explore quadratures for $B^T\phi(A,s)B$ where A is a symmetric nonnegative-definite matrix in $\mathbb{R}^{n\times n}$, B is a tall matrix in $\mathbb{R}^{n\times p}$, and $\phi(\cdot,s)$ is a matrix function with parameter $s\in\mathbb{R}^+$ [1]. These formulations commonly arise in the computation of multiple-input multiple-output transfer functions for diffusion PDEs.

We propose an approximation scheme for $B^T\phi(A,s)B$ leveraging the block Lanczos algorithm [2] and its representation through Stieltjes matrix continued fractions. Using Stieltjes matrix continued fractions we show that the block-Lanczos algorithm converges monotonically for $\phi(\cdot,s) = B^T(A+sI)^{-1}B$ and we extend the notion of Gauss-Radau quadrature to the block case, (see for instance [3] for the non-block case). Together, the Gauss and Gauss-Radau quadrature facilitate the derivation of easily computable error bounds.

These Stieltjes matrix continued fractions can be defined via the recursion

$$\mathcal{C}_j(s) = \cfrac{1}{s\hat{\boldsymbol{\gamma}}_j + \cfrac{1}{\boldsymbol{\gamma}_j + \mathcal{C}_{j+1}(s)}}, \text{ with symmetric positive definite } \hat{\boldsymbol{\gamma}}_j, \boldsymbol{\gamma}_j \in \mathbb{R}^{p\times p},$$

where $\hat{\boldsymbol{\gamma}}_j$ and $\boldsymbol{\gamma}_j$ are directly related to the block-Lanczos coefficients. We show that the Gauss quadrature approximation to $B^T(A+sI)^{-1}B$ after m iterations of block-Lanczos corresponds to $\mathcal{C}_1(s)$ defined through the upper recursion terminated with $\mathcal{C}_{m+1}=0$, whereas the Gauss-Radau quadrature corresponds to a truncation with $\mathcal{C}_{m+1}=\infty$.

Finally, we present extrapolation schemes using averages of Gauss and Gauss-Radau quadrature and provide qualitative reasoning for such extrapolation, grounded in potential theory for Padé approximations. We show numerical examples for various $\phi(A,s)$ where A is a graph Laplacian or discretization of an operator with continuous spectrum, e.g., PDE operators in unbounded domains. We demonstrate that the derived error-bound is tight in important applications and that the extrapolation decreases the approximation error by one order of magnitude.

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