University of Belgrade
Faculty of Mechanical Engineering

Numerical Methods for Large Scale Problems

Dedicated to Professor Lothar Reichel
(Kent State University, Ohio, USA)
on the occasion of his 70th Anniversary

A B S T R A C T   B O O K

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Plenary Talks

Richard Steven Varga (1928-2022)

Claude Brezinski

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Abstract

In this talk, I will evoke the life of Richard Varga and I will review his most important contributions to numerical analysis and approximation theory. I will also tell some personal reminiscences of Richard.

Finite-difference quadrature and inverse scattering

Jörn Zimmerling, Mikhail Zaslavsky, Rob Remis, Shari Moskow, Alexander Mamonov, Murthy Guddati, Vladimir Druskin[1], Liliana Borcea

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Abstract

One of classical tasks of the network synthesis is to construct ROMs realized via ladder networks matching rational approximations of a targeted filter transfer function. The inverse scattering can be also viewed in the network synthesis framework. The key is continuum interpretation of the synthesized network in terms of the underlying medium properties, aka embedding. We describe such an embedding via finite-difference quadrature rules (FDQR), that can be viewed as extension of the concept of the Gaussian quadrature to finite-difference schemes. One of application of this approach is the solution of earlier intractable large scale inverse scattering problems. We also discuss an important open question in the FDQR related to Lothar's earlier contributions, in particular, a possibility of finite-difference Gauss-Kronrod rules.

Orthogonality on the Semicircle and Applications: Old and New Results

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Abstract

One nonstandard type of orthogonality – orthogonality on the semicircle – was introduced and studied by Gautschi and Milovanović [2], and later generalized in [3] and [5]. Applications in numerical differentiation were given in [4] and [1]. Beside this background, starting from recent results given in [6], in this lecture we present new results on orthogonal Laurent polynomials on the semicircle, their properties, as well as some new applications in numerical integration and numerical differentiation.

Keywords: Complex orthogonal systems, Recurrence relations, Quadrature formula, Numerical differentiation, Zeros

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Variable selection in statistical modelling via a numerical linear algebra approach

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Abstract

Variable selection requires the minimization of $||X\beta - y||_2$ with respect to β, where $X \in R^{n\times p}$ is the design matrix, $\beta \in R^p$ is a vector of predictors and $y \in R^n$ is the response of the model. The identification of predictors is important for statistical modelling and numerical analysis can bring to statistics community advanced linear algebra techniques for handling this issue. In this work, for a given model $y = X\beta + \epsilon$, where $\epsilon \in R^n$ is the vector of random errors, we study the following problems:

(P1) *Regularization and condition estimation*
It is crucial to decide whether the given model needs regularization or not for the derivation of the vector β. The notion of the effective condition number is introduced, which provides a measure for the stability of β due to a perturbation in y.

(P2) *Fast GCV estimates for correlated matrices*
When regularization is applied and therefore the minimization of $\{||X\beta - y||_2 + \lambda||\beta||_2\}$ is needed, the specification of appropriate values of the tuning parameter λ is an important issue. When the design matrix has correlated columns, its eigenvalue structure leads to a fast estimate for the generalized cross validation (GCV) function which can provide a good value for the parameter λ.

(P3) *Numerical methods for high dimensional data*
When the design matrix has much more columns than rows we deal with high dimensional data. In such cases, it is needed the appropriate computation of β in a way preserving the sparsity and the stability of the solution.

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Model-based and Learning-based Methods for Hyperspectral Image Processing

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Abstract

In this talk, hyperspectral image processing based on model-based optimization methods, e.g., denoising, demosaicing, and destriping, etc are discussed and reported. Also learning-based models for hyperspectral image denoising are also studied.

Banded Toeplitz structured eigensensitivity

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Abstract

The sensitivity of the spectrum of a matrix under general or structured perturbations of the matrix entries has received attention in the literature, and both bounds and graphical tools such as the pseudospectrum or structured pseudospectrum have been developed. Also, characterizations of the algebraic variety of normal matrices and distance measures to this variety have received considerable attention. It is the purpose of my talk to carry out an investigation that focuses on analyzing the eigensensitivity of a banded Toeplitz matrix in relation to its distance to normality and to the structure of the perturbations to which it is subjected. Also, the distance of a banded Toeplitz matrix to the variety of similarly structured positive semidefinite matrices will be taken into account. In order to illustrate explicit expressions for the conditioning of eigenvalues and eigenvectors as well as algorithms for the construction of approximate structured pseudospectra, I will focus on the special case of the tridiagonal matrices, whose eigenvalues and eigenvectors are known in closed form.

(Joint work with Lothar Reichel)

Error bounds of quadrature formulae for analytic functions

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Abstract

In certain spaces of analytic functions the error term of a quadrature formula is a continuous linear functional. We give a survey of the methods used in order to compute or estimate the norm of the error functional, which leads to bounds for the error term. The results, some of which are fairly recent, cover, among others, interpolatory, Gauss and Gauss-Kronrod formulae.

Electrostatic models for zeros of orthogonal and multiple orthogonal polynomials. The legacy of Stieltjes.

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Abstract

In this talk, we review the legacy of T. J. Stieltjes (1856–1894) on the electrostatic interpretation of zeros of classical orthogonal polynomials and present an extension of this approach to the case of (type II) multiple (Hermite–Padé) orthogonal polynomials. We particulary focus on the well–known examples of Angelesco and Nikishin settings.

This is a joint work with A. Martínez Finkelshtein (Univ. Baylor, TX, USA, and Univ. Almería, Spain) and J. Sánchez Lara (Univ. Granada, Spain).

Gauss-like quadrature through manipulations with Jacobi matrices

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Abstract

We discuss a construction of several types of Gauss and *rational* Gauss quadrature rules through manipulations with Jacobi or Jacobi-like matrices. We pay particular attention to the rational anti-Gauss, simplified Gauss and Gauss-Radau rules. The interest in these rules stems from the need to approximate the matrix functionals of the form $v^T f(A)v$ arising in many applications, where v is a vector, A is a large symmetric positive matrix, and f is a function defined on the spectrum of A. Although a distribution function in the functional $v^T f(A)v$ is not explicitly known, we can compute the corresponding Jacobi or Jacobi-like matrix (and therefore the Gauss or rational Gauss quadrature for the mentioned functional) by several steps of Lanczos or rational Lanczos method with input v and A. By modifying such a matrix we can compute some other quadrature that enables us to estimate the error in the Gauss or rational Gauss quadrature.

This is a joint work with Lothar Reichel and Jihan Alahmadi.

Keywords: Gauss quadrature, Jacobi matrices, rational Gauss quadrature

Regularized Recycling and Subspace Augmentation Methods: Theory and Applications in Adaptive Optics

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Abstract

Subspace recycling techniques have been used quite successfully for the acceleration of iterative methods for solving large-scale linear systems. These methods often work by augmenting a solution subspace generated iteratively by a known algorithm with a fixed subspace of vectors which are "useful' for solving the problem. Often, this has the effect of inducing a projected version of the original linear system to which the known iterative method is then applied, and this projection can act as a deflation preconditioner, accelerating convergence. In this talk we consider subspace augmentation-type iterative schemes applied to linear ill-posed problems in a continuous Hilbert space setting, based on a recently developed framework describing these methods. We show that under suitable assumptions, a recycling method satisfies the formal definition of a regularization, as long as the underlying scheme is itself a regularization. We then develop an augmented subspace version of the gradient descent method and Tikhonov regularization and demonstrate their effectiveness, both on an academic Gaussian blur model and on problems arising from the adaptive optics community for the resolution of large sky images by ground-based extremely large telescopes. Specifically, we consider wavefront reconstruction from Pyramid sensor data and the atmospheric tomography problem.

Finding the optimal regularization parameter: old and new methods

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Abstract

Discrete ill-posed inverse problems arise in various areas of science and engineering. The presence of noise in the data often makes it difficult to compute an accurate approximate solution. To reduce the sensitivity of the computed solution to the noise, one replaces the original problem by a nearby well-posed minimization problem, whose solution is less sensitive to the noise in the data than the solution of the original problem. This replacement is known as regularization. In this talk we consider the situation when the minimization problem consists of a fidelity term, that is defined in terms of a p-norm, and a regularization term, that is defined in terms of a $\mathrm{q}-$norm,$0 < \mathrm{p}, \mathrm{q} \leq 2$. The relative importance of the fidelity and regularization terms is determined by a regularization parameter. We will present and compare esperimentally the well known $\mathrm{L}-$curve, Generalized Cross Validation, Discrepancy approaches with a new one which is based on the so-called residual whiteness principle. We also discuss methods for the solution of the minimization problem and automatic selection of the regularization parameter. The first method is based on the majorization-minimization in generalized Krylov subspaces of increasing dimension while the second one is an iterative framework based on the alternating direction method of multipliers.

Construction of a sequence of orthogonal rational functions

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Abstract

Orthogonal polynomials are an important tool to approximate functions. Orthogonal rational functions provide a powerful alternative if the function of interest is not well approximated by polynomials.

Polynomials orthogonal with respect to certain discrete inner products can be constructed by applying the Lanczos or Arnoldi iteration to appropriately chosen diagonal matrix and vector. This can be viewed as a matrix version of the Stieltjes procedure. The generated nested orthonormal basis can be interpreted as a sequence of orthogonal polynomials. The corresponding Hessenberg matrix, containing the recurrence coefficients, also represents the sequence of orthogonal polynomials.

Alternatively, this Hessenberg matrix can be generated by an updating procedure. The goal of this procedure is to enforce Hessenberg structure onto a matrix which shares its eigenvalues with the given diagonal matrix and the first entries of its eigenvectors must correspond to the elements of the given vector. Plane rotations are used to introduce the elements of the given vector one by one and to enforce Hessenberg structure. The updating procedure is stable thanks to the use of unitary similarity transformations. In this talk rational generalizations of the Lanczos and Arnoldi iterations are discussed. These iterations generate nested orthonormal bases which can be interpreted as a sequence of orthogonal rational functions with prescribed poles. A matrix pencil of Hessenberg structure underlies these iterations.

We show that this Hessenberg pencil can also be used to represent the orthogonal rational function sequence and we propose an updating procedure for this case. The proposed procedure applies unitary similarity transformations and its numerical stability is illustrated.

SESSION M1

Regularization of ill-posed inverse problems

Inverse problems arise in most scientific fields. These problems are usually ill-posed and can be of very large dimension. Developing fast and accurate methods for their solution is of fundamental importance. Moreover, since most methods require the estimation of one or more regularization parameters, the development of automatic strategies for the selection of these parameters is of considerable importance, especially for real-world applications. This minisymposium presents new approaches to the solution of inverse problem and to the automatic estimation of regularization parameters.

Organizers:

- Alessandro Buccini
- Marco Donatelli

Krylov subspace based Fista-type methods for ill-posed problems

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Abstract

A group of iterative shrinkage-thresholding algorithms (ISTA) have been proposed for solving regularized linear inverse problems that arise in many applications in science and engineering. This group of methods, which can also be viewed as an extension of classical gradient algorithm, are simple and applicable to large-scale ill-posed problems. One of the difficulties that arise when applying those methods is the slow rate of convergence. Faster versions of ISTA such as fast iterative shrinkage-thresholding algorithms (FISTA), two-step ISTA (TWIST) and monotonic version of TWIST (MTWIST), are proposed to overcome this issue. While there are made improvements in terms of convergence, the computational cost of each iteration remains a concern, particularly for large scale problems. In this paper we propose a novel approach to speed up the convergence of the ISTA type methods, and decrease the computational cost by the aid of Krylov subspace methods. For applications such as image reconstruction, where the pixel values are nonnegative, one may impose nonnegativity constraint so that the reconstructed solution lies on the nonnegative orthant but such approach is known to cause slower convergence. We find a simply post nonnegative projection, i.e., setting all negative values of a solution to 0, improves the quality of the of the reconstructed solution. While working with regularization methods, the quality depends on the regularization parameter that balances the data fitting term and the regularization term. We propose a method that automatically selects the regularization parameter without significantly increasing the computational cost. This is especially useful for large-scale problems. Several numerical examples are presented to illustrate the efficiency of the proposed methods.

Keywords: Projected FISTA, Krylov subspace, nonnegativity constraint, regularization parameter choice rules, image reconstruction

Identifying a conductive sphere by time-domain electromagnetic data via Prony-like methods

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Abstract

We consider a homogeneous sphere with radius r_s, magnetic permeability μ_s, and electrical conductivity σ_s, immersed in a uniform time-varying electromagnetic field. The impulsive response of the system can be modeled by an exponential sum of the type

$$\varphi(t) = \sum_{n=1}^{\infty} c_n e^{-d_n t},$$

whose coefficients and exponents depend on the parameters r_s, μ_s, and σ_s. Prony-like methods allow one to identify the physical parameters of the sphere, starting from time-domain electromagnetic data. In this talk, we discuss several numerical implementations of such methods and illustrate the effectiveness of the approaches through numerical experiments.

Keywords: Electromagnetic induction, time domain electromagnetic (TDEM) method, exponential sums, Prony-like methods

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Fractional Tikhonov regularization revisited

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Abstract

It is well known and observed again and again that classical Tikhonov regularization for ill-posed inverse problems leads to rather smooth reconstructions, often smoother than one would like. In an attempt to remedy this, fractional Tikhonov regularization was introduced. In fact, two methods with the name were suggested. The method of [1] aims at solving the normal equation

$$((A^*A)^{(\alpha+1)/2} + \mu I)x = (A^*A)^{(\alpha-1)/2}A^*b^\delta,$$

where the parameter $0 < \alpha < 1$ is used to reduce the smoothing compared to standard Tikhonov regularization which corresponds to $\alpha = 1$. The second method, proposed in [2], aim at solving the linear system

$$(A^*A + \mu I)^\alpha x = (A^*A)^{\alpha-1}A^*b^\delta$$

where α plays the same role and $\alpha = 1$ yields standard Tikhonov regularization. Both methods were compared in [3], and several papers transferred the concept of fractional regularization to approaches other than Tikhonov regularization.

A main point that, to the best of the authors knowledge, has not been answered anywhere up to now is the choice of the fractional parameter α. In this talk, we give an answer to that based on a new way of interpreting regularization introduced in [4]. We also discuss why, from the point of regularization theory, fractional regularization proposes no significant benefit over classical Tikhonov regularization and even fractional regularization with $\alpha > 1$, i.e., amplified smoothing of the solutions. A main ingredient to this is understanding the role of the optimal choice of the regularization parameter μ, which leads to all methods yielding, up to constants, the same upper and lower bound on the reconstruction error.

Keywords: Tikhonov regularization, inverse problem, fractional regularization

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A preconditioned Arnoldi-Tikhonov method for the solution of linear discrete ill-posed 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. These problems arise for instance, from the discretization of Fredholm integral equations of the first kind. 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 Tikhonov regularization. We describe a novel "approximate Tikhonov regularization method" based on constructing a low-rank approximation to the matrix in the linear discrete ill-posed problem by carrying out a few steps of the Arnoldi process. The iterative method so defined is transpose-free. Our work is inspired by Donatelli and Hanke whose approximate Tikhonov regularization method seeks to approximate a severely ill-conditioned block-Toeplitz matrix with Toeplitz-blocks by a block-circulant matrix with circulant-blocks. Computed examples illustrate the performance of our proposed iterative regularization method.

Regularized solution in a RKHS of an overdetermined system of first kind integral equations

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Abstract

Overdetermined systems of first kind integral equations arise in many applications. It is well-known that Fredholm integral equations of the first kind are often ill-posed problems. When the right-hand side is discretized, e.g., when it consists of experimental measurements, the difficulties related to ill-posedness are enforced, as the problem admits infinitely many solutions. We propose a numerical method to compute the minimal-norm solution of a system of the form

$$\begin{cases} \displaystyle\int_a^b k_\ell(x_{\ell,i},t)\, f(t)\, dt = g_\ell(x_{\ell,i}), \qquad \ell = 1,\dots,m, \quad i = 1,\dots,n_\ell, \\ f(a) = f_0, \ f(b) = f_1, \end{cases}$$

in the presence of boundary constraints. The algorithm stems from the Riesz representation theorem and operates in a reproducing kernel Hilbert space (RKHS). Since the resulting linear system is strongly ill-conditioned, we construct a regularization method based on a truncated expansion of the minimal-norm solution in terms of the singular functions of the integral operator defining the problem. Numerical experiments, both artificial and deriving from an application in applied geophysics, are presented to show that the new method is extremely effective when the sought solution is smooth, but produces significant information even for non-smooth solutions. This is a joint work with Patricia Díaz de Alba, Luisa Fermo, and Giuseppe Rodriguez [1], [2].

Keywords: Fredholm integral equations, Riesz representation theorem, Reproducing kernel Hilbert space, Linear inverse problems, Regularization, FDEM induction

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2. Díaz de Alba, P., Fermo, L., Pes, F., Rodriguez, G.: Regularized minimal-norm solution of an overdetermined system of first kind integral equations, Numer. Algorithms (2022) https://doi.org/10.1007/s11075-022-01282-2.

SESSION M2

Approximation methods and applications

The session focuses on new developments and recent advances in the areas of approximation and interpolation of functions, and related methods to approximate integral transforms and solutions of functional equations.

Organizers:

- Maria Carmela De Bonis
- Donatella Occorsio

On some weighted quadrature rules on equispaced nodes through constrained mock-Chebyshev interpolation

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Abstract

We get accurate quadrature formulas from equispaced nodes with high degree of exactness, by using Gaussian-Christoffel formulas and a mixed interpolation-regression process, in combination. More in detail, we substitute the exact values $f(\xi_k)$ with the values at Christoffel abscissas ξ_k of the constrained mock-Chebyshev least-squares interpolant $\hat{P}_{r,n}[f]$ of a suitable degree r [1, 2]. We develop an adaptive algorithm for determining the optimal degree r of the constrained mock-Chebyshev least-squares interpolation to get quadrature formulas as much accurate as possible. The algorithm generalizes to the bivariate case by means of the constrained mock-Chebyshev least-squares tensor product interpolation [2].

Keywords: Quadrature formulas, degree of exactness, equispaced points

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Optimal selection of shape parameters in radial kernels

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Abstract

The problem of selecting an optimal shape parameter in radial kernels has been a relevant problem for many years. The predictive capacity of radial basis functions (RBFs) methods greatly depends on this parameter both in the PDE approximation using RBF collocation methods and in the interpolation setting (see [3, 4]). This is also important for Machine Learning applications by kernel methods. In this talk some recent results will be discussed for interpolation and integration [1, 2]. Several experiments and some open problems will be presented.

Keywords: radial basis functions, meshfree approximation, radial kernel methods, approximation algorithms

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Averaged Nyström interpolants for the solution Fredholm integral equations of the second kind

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Abstract

In this talk we explore the application of weighted averaged Gauss quadrature rules, recently proposed in [2] (see also [3]), to the numerical solution of Fredholm integral equations of the second kind,

$$f(y) + \int_{\mathcal{D}} k(x,y) f(x) d\mu(x) = g(y), \quad y \in \mathcal{D}, \tag{1}$$

where the kernel k and right-hand side function g are given, the function f is to be determined, and $d\mu(x)$ is a nonnegative measure supported on a bounded or unbounded domain $\mathcal{D} \subset \mathbb{R}$.

In particular, we focus on the estimate of the error in the Nyström interpolants.

Several iterative methods are also presented and numerical tests showing the performance of the proposed approaches are discussed.

Keywords: Fredholm integral equations of the second kind, Gauss quadrature rule, Averaged quadrature rule, Nyström method.

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A Nyström method for 2D linear Fredholm integral equations on curvilinear polygons

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Abstract

The talk deals with the numerical approximation of 2D Fredholm linear integral equations of the type

$$f(x,y) - \mu \int_S k(x,y,s,t) f(s,t) ds dt = g(x,y), \qquad (x,y) \in S,$$

where S is a general bi-dimensional domain whose boundary is a piecewise smooth Jordan curve (curvilinear polygon), g and k are known functions defined on S and S^2, respectively, μ is a fixed real parameter and f is the unknown in S.

For 2D Fredholm integral equations very few methods were proposed. The most considered case is that of rectangular domains (see for istance [1] and the references therein).If a global approximation strategy is chosen, the most simple and powerful approach seems to be Nyström methods based on cubature rules obtained as the tensor product of two univariate rules.

On the contrary no global approach was proposed for the case of curvilinear domains that cannot be transformed in a square. On the other hand even if the transformation is possible, the smoothness of the known functions could be not preserved and this can produce a severe loss in the rate of convergence of the method.

Here we propose a numerical method of Nyström type based on cubature formulas introduced in [2]. This choice allows to consider general curvilinear domains, to use a global approximation approach and avoids the loss of convergence due to transformations.

Keywords: Fredholm integral equations, Nyström method, Curvilinear polygons

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A Nyström method for Volterra integral equations based on equally spaced nodes

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Abstract

In this talk, we present a Nyström-type method based on equally spaced points of $[0,1]$, for Volterra integral equation of the type

$$f(s) + \mu \int_0^s k(t,s) f(t)(t-s)^\alpha t^\beta dt = g(s), \quad s \in (0,1),$$

where f is the unknown function, k and g are given functions, $\mu \in \mathbb{R}$, and $\alpha, \beta \geq 0$.

The use of equidistant points is crucial in many engineering and mathematical physics problems which are modeled by Volterra equations, and k and g are available only in a discrete set of equispaced nodes. In all these cases, the classical methods based on piecewise polynomial approximation offer a lower degree of approximation, while the efficient procedures based on the zeros of orthogonal polynomials cannot be used.

Here, we present a Nyström method based on a quadrature formula obtained by means of the sequence $\{B_{m,\ell}(f)\}_m$ of the so called Generalized Bernstein polynomials, where $B_{m,\ell}(f)$ is the ℓ iterated boolean sum of the classical Bernstein polynomial $B_m(f)$, i.e.

$$B_{m,\ell}(f) = f - (f - B_m(f))^\ell, \qquad \ell \in \mathbb{N}, \quad B_{m,1}(f) = B_m(f).$$

$B_{m,\ell}(f)$ requires the samples of f at equally spaced nodes as well as the "original" Bernstein polynomials $B_m(f)$. However, differently from $B_m(f)$, the rate of convergence of $B_{m,\ell}(f)$ improves as the smoothness of the function increases. Indeed, by approximating $f \in C^{2\ell}([0,1])$ by $\{B_{m,\ell}(f)\}_{m,\ell}$, it is $\|f - B_{m,\ell}(f)\|_\infty \sim \mathcal{O}(m^{-\ell})$.

Stability and convergence of the Nyström method are proved in Hölder–Zygmund type spaces and some numerical tests are shown to confirm the theoretical estimates.

Keywords: Nyström Methods, Volterra Integral Equations, Bernstein Polynomials

Marcinkiewicz–Zygmund type inequalities with exponential weights

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Abstract

As is well known, Marcinkiewicz–Zygmund type inequalities are widely used in the study of the convergence of various approximation processes [6, 4, 1].

The classical inequalities were proved for trigonometric polynomials in 1937, whereas the algebraic case is more difficult and the first results were obtained by R. Askey in 1973 [2, 5]. In fact, the direct inequality

$$\left(\sum_{k=1}^{m} \Delta x_k \left|P_{lm}\left(x_k\right) u(x_k)\right|^p\right)^{1/p} \leq \mathcal{C}\left(\int_{-1}^{1} \left|P_{lm}(x)u(x)\right|^p \mathrm{d}x\right)^{1/p}, \quad 1 \leq p < \infty\,,$$

holds for any polynomial P_{lm} of degree lm (l fixed integer) with $\mathcal{C}$ depending only on p, $\Delta x_k = x_{k+1} - x_k$, x_k arbitrary arcsin distributed nodes and u a doubling weight [3], but the converse inequality requires more restrictive assumptions.

In this talk we discuss the case of non-doubling weights, namely exponential weights on bounded or unbounded intervals of the real line.

Keywords: Marcinkiewicz–Zygmund inequalities, orthogonal polynomials, exponential weights.

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A numerical method for hypersingular integrals of highly oscillatory functions on $[0, +\infty)$.

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Abstract

We consider the approximation of the following integrals

$$H_p^{\omega,\gamma}(f,t) = \int_0^{+\infty} \frac{f(x)e^{i\omega x}}{(x-t)^{p+1}} u_\gamma(x)\, dx, \tag{1}$$

where $t > 0, p \geq 0$ is an integer, $i^2 = -1$, $\omega \gg 1$, $u_\gamma(x) = x^\gamma e^{-\frac{x}{2}}, \gamma \geq 0$, is a generalized Laguerre weight and the integral is understood in the Cauchy principal value sense if $p = 0$ and in the finite part Hadamard sense if $p > 0$.

Integrals $H_p^{\omega,\gamma}(f,t)$ are of great interest in many scientific areas, such image analysis, optics, electrodynamics and electromagnetism. In particular, they frequently appear in boundary element methods and their efficiency often depends upon the accuracy of the numerical evaluation of (1).

To our knowledge a wide literature is available on the approximation of singular and hypersigular integrals for non oscillatory function. The same is true for integrals of non singular highly oscillatory functions. Moreover, most of the papers present in literature about integrals having both singularity and oscillation are devoted to the case of bounded intervals, and very few references deal with $H_p^{\omega,\gamma}(f,t)$ with $p = 0$.

In order to evaluate (1) we propose a product quadrature rule based on the approximation of function f by a truncated Lagrange polynomial using the Laguerre zeros and the additional point $4m$. Stability and convergence are proved in suitable weighted Sobolev type spaces. Comparison with the results obtained using the methods introduced in [1, 2] are also given. Finally we present an application of the proposed quadrature rule for the construction of a Nyström type method for the numerical solution of the following integral equations

$$f(t) + \int_0^{+\infty} \frac{f(x)e^{i\omega x}}{(x-t)^{p+1}} u_\gamma(x)\, dx = g(t), \quad t > 0,$$

where g is a given function and f is the unknown.

Keywords: Product rule, Hadamard integrals, Cauchy integrals, Nyström methods

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Finite difference approximation of a initial-boundary value problem with Dirac delta function and time-dependent coefficients

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Abstract

One interesting class of parabolic problems model processes in heat-conduction media with concentrated capacity in which the heat capacity coefficient contains a Dirac delta function. In this paper we study the convergence of a finite difference scheme that approximates the initial-boundary problem for the heat equation with concentrated capacity and time-dependent coefficients. We assume that the generalized solution of the problem belongs to the Sobolev space $W_2^{s,\,s/2}$, $5/2 < s \leq 3$. Order convergence rate estimate in the discrete $W_2^{1,1/2}$ norm is obtained. The result is based on some nonstandard a priori estimates involving fractional order discrete Sobolev norms.

Keywords: Partial differential equations, Delta function, Sobolev space, Convergence

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De la Vallée Poussin Interpolation method for image resizing

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Abstract

The aim of this talk is to show how de la Vallée Poussin type interpolation based on Chebyshev zeros of first kind, can be applied to resize an arbitrary color digital image. In fact, using such kind of approximation, we get an image scaling method running for any desired scaling factor or size, in both downscaling and upscaling. The peculiarities and the performance of such method will be discussed.

Keywords: Image resizing, Lagrange interpolation, de la Vallée Poussin filtered interpolation, Chebyshev zeros

SESSION M3

Methods for Large-Scale and High-Dimensional Data Analysis

Large-scale computational problems arise from mathematical formulations of applications in science and engineering including medical and astronomical imaging. This minisymposium describes several novel techniques for handling this kind of problems. The solution of discrete ill-posed problems, dynamic problems, as well as quadrature are considered.

Organizers:

- Mirjeta Pasha
- Lothar Reichel

New Block Generalized Averaged Gauss Quadrature Rules

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Abstract

Golub and Meurant presented the way of using the symmetric block Lanczos algorithm for calculating the block Gauss quadrature rules for approximating of matrix functions $w^T f(A)u$, where A is a large square matrix, u and v are block-vectors and f is a function. We describe a new block quadrature rules . These rules can be calculated using the symmetric or nonsymmetric block Lanczos algorithms for calculating error estimates for computed quantities, and shows how to achieve more accuracy than standard block Gauss rules for the same computational effort. Our methods are based on block generalizations of the generalized averaged Gauss quadrature rules that were recently proposed by Spalevic. The new representation suggested by Spalevic is a new averaged Gauss quadrature rule that has higher degree of exactness and the same number of nodes as the averaged rule proposed by Laurie. Numerical experiments reported in this paper show the latter averaged rule to yield higher accuracy than Laurie's averaged rule for smooth integrals and, therefore, also can be used to estimate the error in Gauss rules and to approximate integrals. In addition, We describe how to use a symmetric or nonsymmetric adjacency matrix for a network to evaluate functions as applications.

Keywords: Gauss quadrature, Block quadrature rules, Averaged Gauss rule, Generalized averaged Gauss rule

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A Kaczmarz approach to Galactic Archaeology

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Abstract

We consider the problem of reconstructing a galaxy's stellar population distribution function from spectroscopy measurements. These quantities can be connected via the single-stellar population spectrum, resulting in a very large scale integral equation with a system structure. To solve this problem, we propose a projected Nesterov-Kaczmarz reconstruction (PNKR) method, which efficiently leverages the system structure and incorporates physical prior information such as smoothness and non-negativity constraints.

Keywords: Astrophysics, Galactic Archaeology, Inverse and Ill-Posed Problems, Kaczmarz Method, Nesterov Acceleration, Large Scale Problems

Hybrid Projection Methods for Solution Decomposition in Large-scale Bayesian Inverse Problems

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Abstract

In this work, we develop hybrid projection methods for computing solutions to large-scale inverse problems, where the solution represents a sum of different stochastic components. Such scenarios arise in many imaging applications (e.g., anomaly detection in atmospheric emissions tomography) where the reconstructed solution can be represented as a combination of two or more components and each component contains different smoothness or stochastic properties. In an inversion or inverse modeling framework, these assumptions correspond to different regularization terms for each solution in the sum. Although various prior assumptions can be included in our framework, we focus on the scenario where the solution is a sum of a sparse solution and a smooth solution. For computing solution estimates, we develop hybrid projection methods for solution decomposition that are based on a combined flexible and generalized Golub-Kahan processes. This approach integrates techniques from the generalized Golub-Kahan bidiagonalization and the flexible Krylov methods. The benefits of the proposed methods are that the decomposition of the solution can be done iteratively, and the regularization terms and regularization parameters are adaptively chosen at each iteration. Numerical examples from image processing demonstrate the potential for these methods to be used for anomaly detection.

Keywords: inverse problems, hybrid methods, generalized Golub-Kahan, flexible methods, Tikhonov regularization, Bayesian inverse problems

On Deterministic and Statistical Methods for Large-scale Dynamic Inverse Problems

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Abstract

Inverse problems are ubiquitous in many fields of science such as engineering, biology, medical imaging, atmospheric science, and geophysics. Three emerging challenges on obtaining relevant solutions to large-scale and data-intensive inverse problems are ill-posedness of the problem, large dimensionality of the parameters, and the complexity of the model constraints. In this talk we discuss efficient methods for computing solutions to dynamic inverse problems, where both the quantities of interest and the forward operator may change at different time instances. We consider large-scale ill-posed problems that are made more challenging by their dynamic nature and, possibly, by the limited amount of available data per measurement step. In the first part of the talk, to remedy these difficulties, we apply efficient regularization methods that enforce simultaneous regularization in space and time (such as edge enhancement at each time instant and proximity at consecutive time instants) and achieve this with low computational cost and enhanced accuracy [1]. In the remainder of the talk, we focus on designing spatial-temporal Bayesian models for estimating the parameters of linear and nonlinear dynamical inverse problems [2]. Numerical examples from a wide range of applications, such as tomographic reconstruction, image deblurring, and chaotic dynamical systems are used to illustrate the effectiveness of the described approaches.

Keywords: dynamic inverse problems, Bayesian, large-scale, regularization, computerized tomography, dynamical systems

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Ill-posed problems for third order tensors: *tensorize or matricize?*

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Abstract

In this talk, we describe solution methods for linear discrete ill-posed problems defined by third-order tensors and the t-product formalism introduced by Kilmer et al., (2013). We discuss extensions of the standard Arnoldi iteration for matrices to third-order tensors, namely, the t-Arnoldi, global t-Arnoldi, and generalized global t-Arnoldi processes, for which the latter two processes involve flattening. Several algorithms based on these extensions are presented. Solution methods considered are based on computing a few steps of the extended Arnoldi process. Each of the t-Arnoldi-type processes is applied to reduce a large-scale Tikhonov regularization problem for third-order tensors to a problem of small size. Regularization by truncated iterations is considered. This gives rise to extensions of the standard GMRES method, referred to as the tGMRES-type methods. The data is represented by a laterally oriented matrix or a third-order tensor, and the regularization operator is a third-order tensor. The discrepancy principle is used to determine the regularization parameter and the number of steps of the t-Arnoldi-type process. Numerical examples discuss applications to (color) image and video restorations. We compare results for several solution methods and illustrate the potential superiority of solution methods that tensorize over solution methods that matricize linear discrete ill-posed problems for third-order tensors.

Keywords: discrepancy principle, linear discrete ill-posed problem, tensor Arnoldi process, t-product, tensor Tikhonov regularization

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SESSION M4

Recent developments in projection methods with applications

Many existing iterative methods for linear and nonlinear systems of equations exploit, in a way or another, the idea of projecting the original problem into smaller subspaces where a solution can be "easily" computed. Projection Methods have been hugely developed in the last 30 years and represent one of the main computational paradigm in modern scientific computing. The main objective of this session is to bring together researchers with different expertise to discuss and overview novel computational approaches, related to Projection Methods, which target a range of modern large scale applications.

Organizers:

- Michela Redivo Zaglia
- Hassane Sadok
- Stefano Cippola

An enhancement of the convergence of IDR method

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Abstract

IDR is a short-recurrence method for large non-symmetric systems of linear equations introduced by Sonneveld [2]. This method generates residuals that are forced to be in a sequence of nested subspaces. For this reason, it is necessary to calculate some vectors of all this subspaces to obtain the next residual. In this talk, we study the convergence of this method and propose an enhancement of its convergence and a slight improvement of its stability using orthogonal projectors constructed using all vectors already computed. Numerical experiments are provided to illustrate the performance of the derived algorithm compared with the known GMRES method [1].

Keywords: Linear equations, iterative methods, IDR(s) method, Krylov subspace

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Towards a matrix-free parallelization of the scalable deflation method for the 3D heterogeneous high-frequency Helmholtz equation

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Abstract

The Helmholtz equation arises in many applications such as seismic imaging, sonar, antennas, and medical imaging. It is one of the hardest problems to solve both in terms of accuracy and convergence due to scalability issues of the numerical solvers. Motivated by the observation that for large wavenumbers, the eigenvalues of the preconditioned system with the well-known Complex Shifted Laplacian Preconditioner (CSLP) shift towards zero, deflation techniques were incorporated to accelerate the convergence of preconditioned Krylov subspace methods [1]. Deflation aims at projecting the small eigenvalues to zeros. But the near-zero eigenvalues will reappear for larger wavenumber. In [2, 3], the adapted deflation preconditioning (ADP) methods, using higher-order deflation vectors, combined with CSLP can lead to scalable convergence. Targeting modern large-scale applications, parallelization of the scalable deflation techniques is in progress. As CSLP is the cornerstone, we start with a matrix-free parallel variant of the CSLP preconditioned Krylov subspace methods for the 3D heterogeneous Helmholtz equation. The CSLP is approximately inverted using one parallel multigrid cycle. The matrix-vector multiplications and preconditioning operators are all implemented in a matrix-free way. Numerical experiments of 3D model problems show that the matrix-free parallel solution method has improved parallel performance and weak scalability.

Keywords: Helmholtz equation, Parallel computing, Deflation, Multigrid, Preconditioner, Scalable, Matrix-free

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Complex moment-based method with nonlinear transformation for computing partial singular triplets

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Abstract

Given a rectangular matrix $A \in \mathbb{R}^{m \times n}$ $(m \geq n)$, let

$$A = U\Sigma V^{\mathrm{T}} = \sum_{i=1}^{n} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^{\mathrm{T}}$$

be a singular value decomposition of A, where σ_i are singular values and $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$ are the corresponding left and right singular vectors, respectively, and $U = [\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_n]$, $V = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_n]$ and $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$. To compute partial singular triplets specifically corresponding to the larger part of singular values, there are several projection-type methods such as Golub-Kahan-Lanczos method, Jacobi-Davidson type method and randomized SVD algorithm.

This study considers computing partial singular triplets corresponding to the singular values in some interval,

$$(\sigma_i, \boldsymbol{u}_i, \boldsymbol{v}_i), \quad \sigma_i \in \Omega := [a, b], \tag{1}$$

where $0 \leq a < b$. One of the simplest ideas to compute (1) is to apply some eigensolver for solving the corresponding symmetric eigenvalue problems of $A^{\mathrm{T}}A$ or AA^{T}. However, this simple strategy does not work well in some situation due to the numerical instability.

Based on the concept of the complex moment-based eigensolvers [1, 2], in this study, we propose a novel complex moment-based method to compute partial singular triplets (1). Based on the concept of the complex moment-based parallel eigensolvers, now, we have the following theorem.

Theorem 1. *Let $L, M \in \mathbb{N}_+$ be the input parameters and $V_{\mathrm{in}} \in \mathbb{R}^{n \times L}$ be an input matrix. We define $S \in \mathbb{R}^{n \times LM}$ and $S_k \in \mathbb{R}^{n \times L}$ as follows:*

$$S := [S_0, S_1, \ldots, S_{M-1}], \quad S_k := \frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} z^k (zI - A^{\mathrm{T}}A)^{-1} V_{\mathrm{in}} \mathrm{d}z, \tag{2}$$

where Γ is a positively oriented Jordan curve around $[a^2, b^2]$. Then, the subspaces $\mathcal{R}(AS)$ and $\mathcal{R}(S)$ are equivalent to subspaces with respect to the left and right singular vectors corresponding to the singular values in a given interval $\Omega = [a, b]$, i.e.,

$$\mathcal{R}(AS) = \mathrm{span}\{\boldsymbol{u}_i | \sigma_i \in \Omega = [a, b]\}, \quad \textit{and} \quad \mathcal{R}(S) = \mathrm{span}\{\boldsymbol{v}_i | \sigma_i \in \Omega = [a, b]\},$$

if and only if $\mathrm{rank}(S) = t$, *where t is the number of target singular values.*

This theorem denotes that the singular triplets corresponding to $\sigma_i \in [a, b]$ (1) can be obtained by some projection method with $\mathcal{R}(AS)$ and/or $\mathcal{R}(S)$ constructed by contour integral (2). In practice, the contour integral (2) is approximated by a numerical integration rule such as the N-point trapezoidal

rule, as follows:

$$\widehat{S} := [\widehat{S}_0, \widehat{S}_1, \ldots, \widehat{S}_{M-1}], \quad \widehat{S}_k := \sum_{j=1}^{N} \omega_j z_j^k (z_j I - A^{\mathrm{T}} A)^{-1} V_{\mathrm{in}},$$

where $(z_j, \omega_j), j = 1, 2, \ldots, N$, are the quadrature points and the corresponding weights, respectively. Then, the approximate singular triplets are computed by a projection method.

From the analysis of error bounds, we also show that the accuracy of the proposed method can be improved by a nonlinear transformation. Details of the proposed method and numerical results will be reported in the presentation.

The present study is supported in part by JSPS KAKENHI (Nos. 19KK0255 and 21H03451).

Keywords: Partial singular triplets, Complex moment-based method, nonlinear transformation

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The LSQR method for solving tensor least squares problem

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Abstract

In this paper, we are interested in finding an approximate solution $\hat{\mathcal{X}}$ of the tensor least squares minimization problem
$\min_{\mathcal{X}} \left\| \mathcal{X} \times_1 A^{(1)} \times_2 A^{(2)} \times_3 \cdots \times_N A^{(N)} - \mathcal{G} \right\|$ where $\mathcal{G} \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N}$ and $A^{(i)} \in \mathbb{R}^{J_i \times I_i}$ $(i = 1, \ldots, N)$ are known, and $\mathcal{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is the unknown tensor to be approximated. Our approach is based on two steps. Firstly, we apply the CP or HOSVD decomposition to the right-hand side tensor $\mathcal{G}$. Secondly, we perform the well-known Golub-Kahan bidiagonalization to each coefficient matrix $A^{(i)}(i = 1, \ldots, N)$ to obtain a reduced tensor least squares minimization problem. This type of equations may appear in color image and video restorations as we described below. Some numerical tests are performed to show the effectiveness of our proposed method.

Keywords: HOSVD, CP decomposition, color image restoration, video restoration, LSQR

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Regularized solution of large scale underdetermined nonlinear least-squares problems

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Abstract

We will describe a regularized Newton-type method for the computation of the minimal-norm solution to underdetermined nonlinear least-squares problems, recently proposed in [1, 2]. The iterative algorithm is obtained by adding a correction vector to the Gauss–Newton iteration, and depends on two relaxation parameters which are automatically estimated. We will discuss a modified algorithm for the solution of medium and large scale problems, which projects each linearized step in a suitable Krylov space. Numerical experiments concerning imaging science will be presented to illustrate the performance of the method.

Keywords: Nonlinear least-squares problem, Minimal-norm solution, Gauss–Newton method

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Regularization by inexact Krylov methods with applications to blind deblurring

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Abstract

In this talk I will present a new class of algorithms for separable nonlinear inverse problems based on inexact Krylov methods. In particular, I will focus in semi-blind deblurring applications. In this setting, inexactness stems from the uncertainty in the parameters defining the blur, which are computed throughout the iterations. After giving a brief overview of the theoretical properties of these methods, as well as strategies to monitor the amount of inexactness that can be tolerated, the performance of the algorithms will be shown through numerical examples. This is a joint work with Silvia Gazzola (University of Bath).

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Stein-based preconditioners for weak-constraint 4D-var

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Abstract

Algorithms for data assimilation try to predict the most likely state of a dynamical system by combining information from observations and prior models. One of the most successful data assimilation frameworks is the linearized weak-constraint four-dimensional variational assimilation problem (4D-Var), that can be ultimately interpreted as a minimization problem. The linear algebraic problem can be solved by means of a Krylov method, like MINRES or GMRES, that needs to be preconditioned to ensure fast convergence in terms of the number of iterations.

The saddle point formulation of weak-constraint 4D-Var offers the possibility of exploiting modern computer architectures and algorithms due to its underlying block structure. Developing good preconditioners which retain the highly-structured nature of the saddle point system has been an area of recent research interest, especially for applications to numerical weather prediction [3, 1]. In this talk I will present a new preconditioning approach which exploits inherent Kronecker structure within a matrix GMRES implementation [1, 2]. In addition to achieving better computational performance, the latter machinery allows us to derive tighter bounds for the eigenvalue distribution of the preconditioned saddle point linear system. A panel of diverse numerical results displays the effectiveness of the proposed methodology compared to current state-of-the-art approaches.

Keywords: Stein equations, data assimilation, preconditioners

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Discretization of the $\star$-Lanczos procedure

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Abstract

The time ordered exponential $U(t)$ is the solution to the ODE

$$\frac{d}{dt}U(t) = A(t)U(t), \quad U(s) = I, \quad t \geq s,$$

where $A(t)$ is a time dependent matrix and s is the starting time. The bilinear form $w^H U(t)v$, with vectors v and w can be approximated by the $\star$-Lanczos procedure. This is a new symbolic algorithm which generalizes the nonHermitian Lanczos iteration to work on bivariate functions. It projects $A(t)\Theta(t-s)$, with Θ the Heaviside step function, onto a Krylov-type subspace which is constructed from bivariate functions using a convolution-like product, the $\star$-product.

We aim to develop a numerical algorithm discretizing the $\star$-Lanczos procedure. This discretized procedure uses a discretization of the $\star$-product and of the related $\star$-inverse.

In this talk we will discuss suitable discretizations and their properties. We mainly focus on an approximation with Legendre polynomials. Such an approximation allows us to transform the $\star$-product between two bivariate functions into the usual matrix-matrix product and the $\star$-inverse into the matrix inverse. The matrices contain the coefficients of the bivariate functions expanded in the Legendre basis. Because of the nature of the problem, the functions of interest are the product of a smooth function and the heaviside step function, i.e., discontinuous, but piecewise smooth. This leads to the Gibbs phenomenon in the discretized functions and corrupts the reconstruction of a function from its coefficients. We show that most of the Legendre coefficients can be computed up to machine precision and they satisfy a decay property, i.e., the coefficient matrices are numerically banded matrices. The properties of these banded Legendre coefficient matrices, and the product of two such matrices, are fundamental to an effective discretization of the $\star$-product and $\star$-inverse and to overcome the Gibbs phenomenon.

Accuracy and early termination of Krylov solvers in interior point methods

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Abstract

When an iterative method is applied to solve the linear equation system in Interior Point Methods (IPMs), the attention is usually placed on accelerating their convergence by designing appropriate preconditioners, but the linear solver is applied as a black box solver with a standard termination criterion which asks for a sufficient reduction of the residual in the linear system. Such an approach often leads to an unnecessary "oversolving" of linear equations. In this talk, it is shown how an IPM can preserve the polynomial worst-case complexity when relying on an inner termination criterion that is not based on the residual of the linear system. Moreover, a practical criterion is derived from a deep understanding of IPM needs. The new technique has been adapted to the Conjugate Gradient (CG) and to the Minimum Residual method (MINRES) applied in the IPM context. The new criterion has been tested on a set of quadratic optimization problems including compressed sensing, image processing and instances with partial differential equation constraints, and it has been compared to standard residual tests with variable tolerance. Evidence gathered from these computational experiments shows that the new technique delivers significant improvements in terms of inner (linear) iterations and those translate into significant savings of the IPM solution time.

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SESSION M5

Large scale techniques in Numerical Linear Algebra

Recently we are facing a serious growth in data from all sorts of applications that needs to be processed. In this session experts in numerical linear algebra will present their research to deal with these immense datasets. Advances in the field will be presented linked to fast and stable linear algebra methods, structure exploiting linear algebra, iterative methods, tensors, dimensionality reduction, fast algorithms, and image processing.

Organizers:

- Giuseppe Rodriguez
- Raf Vandebril

Fast Alternating Direction Multipliers Method by Generalized Krylov Subspaces

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Abstract

The Alternating Direction Multipliers Method (ADMM) is a very popular and powerful algorithm for the solution of many optimization problems. In the recent years it has been widely used for the solution of ill-posed inverse problems. However, one of its drawback is the possibly high computational cost, since at each iteration, it requires the solution of a large-scale least squares problem.

In this talk we propose a computationally attractive implementation of ADMM, with particular attention to ill-posed inverse problems. We significantly decrease the computational cost by projecting the original large scale problem into a low-dimensional subspace by means of Generalized Krylov Subspaces (GKS). The dimension of the projection space is not an additional parameter of the method as it increases with the iterations. The construction of GKS allows for very fast computations, regardless of the increasing size of the problem. Several computed examples show the good performances of the proposed method.

Keywords: ADMM, Ill-posed inverse problems, Generalized Krylov subspaces

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Proximal stabilized Interior Point Methods for large scale quadratic programming and *low-frequency-updates* preconditioning techniques

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Abstract

Computational evidence suggests that the Primal-Dual Regularization for Interior Point Methods (IPMs) is a successful technique able to stabilize and to speed-up the linear algebra used in IPM implementations [1].

On the other hand, many issues remain open when IPMs are used in their primal-dual regularized form and, in particular, to the best of our knowledge, the known convergence theory requires strong assumptions on the uniform boundedness of the Newton directions [2].

Recently, the study of the interaction of primal-dual regularized IPMs with the Augmented Lagrangian Method and the Proximal Point Algorithm has permitted to prove the convergence when the regularization parameter is driven to zero at a suitable speed [3].

In this talk, we will show that it is possible to naturally frame the primal-dual regularized IPMs in the context of the Proximal Point Algorithm [4]. Among the benefits of the proposed approach, we will show how convergence can be guaranteed without any supplementary assumptions and how the rate of convergence can be explicitly estimated in relation to (fixed) regularization parameters. Moreover, we will show how regularization could be exploited in order to devise suitable preconditioners of the Newton system which are required to be re-computed just a fraction of the total IPM iterations.

Keywords: Interior point methods, Proximal point methods, Regularized primal-dual methods, Convex quadratic programming

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Sampling methods for large adjacency matrices

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Abstract

The adjacency matrix of a graph is a construction that plays an important role in network analysis. Important global properties of a network, and of stochastic processes that take place on the network, can determined by properties of the adjacency matrix, like the magnitude of its Perron eigenvalue. Also, matrix functions evaluated on the adjacency matrix can provide important information about global communicability, as well as the centrality of nodes and edges.

In applications, the networks of interest can be very large. If that is the case, the adjacency matrix is large as well, and computations involving it can become onerous. Furthermore, it can be difficult or impractical to collect the data to form the full adjacency matrix. In these cases, the strategies used to collect a subset of the network data become crucial, as well as the methods for computing approximate eigenvalues, eigenvectors, and/or matrix functions of the adjacency matrix from a partial submatrix.

In this talk we describe some sampling strategies and computational approaches to perform computations with partially known adjacency matrices. We show some simulations, and discuss an application involving the spread, detection, and control of infectious diseases.

Keywords: Matrix functions, network sampling

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Graph Laplacian in $\ell^2 - \ell^q$ regularization for image reconstruction

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Abstract

The use of the Laplacian of a properly constructed graph for denoising images has attracted a lot of attention in the last years. Recently, a way to use this instrument for image deblurring has been proposed in [1].

In this talk, we consider the $\ell^2 - \ell^q$ regolarization method, $0 < q < 2$, for image reconstruction with application in computer tomography and image deblurring [2]. Using the majorization-minimization method, we reduce to the minimization of a quadratic functional, whose solution is approximated in a subspace of fairly small dimension. Thanks to the projection into properly constructed subspaces of small dimension, the proposed algorithm can be used for solving large scale problems. Moreover, the projected problem can be also used for estimating the regularization parameter by the generalized cross validation or the discrepancy principle. Some numerical results compare our proposal with total variation and sparse wavelets reconstructions.

Keywords: Graph Laplacian, image deblurring, regularization

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Primal and dual descent regularization algorithms for imaging

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Abstract

Let us consider the functional equation $Ax = y$ characterized by an ill-posed linear operator $A : X \longrightarrow Y$ between two Banach spaces X and Y. In this talk, we study on-step iterative gradient methods to minimize the residual functional $\Phi(x) = \frac{1}{p}\|Ax - y\|_Y^p$, with $p > 1$. It is well-known that gradient methods can be considered as implicit regularization algorithm if combined with an early-stopping criterion to prevent over-fitting of the noise.

We prove that gradient methods in Banach spaces can be fully explained and understood in the context of proximal operator theory, with appropriate norm (for primal schemes) or Bregman (for dual schemes) distances as proximity measure, which shows a deep connection between iterative regularisation and convex optimisation. In particular, we consider the following proximal iterative method

$$x_{k+1} = \arg\min_{x\in X}\Big\{B_r^X(x, x_k) + \alpha_k\langle\partial\Phi(x_k), x\rangle\Big\}$$

where $\alpha_k > 0$ is a proper step length, and B_r^X is the Bregman distance with respect to the functional $\frac{1}{r}\|\cdot\|_X^r$ with $r > 1$, that is

$$B_r^X(x, x_k) = \frac{1}{r}\|x\|_X^r - \Big(\frac{1}{r}\|x_k\|_X^r + \langle\partial\big(\frac{1}{r}\|x_k\|_X^r\big), x - x_k\rangle\Big)\,,$$

where ∂ denotes the (sub-)differential operator.

Hence, we study the special setting where X and Y are both two variable exponent Lebesgue spaces $L^{q(\cdot)}$, that is, Lebesgue spaces where the exponent is not a constant value but rather a function of the position of the domain. We first review the key concept of duality map, providing an explicit formulation, then we apply the iterative scheme to deblurring imaging problems. By using an heuristic adaptive strategy to select the point-wise variable exponent function $q(\cdot)$, numerical tests will show the advantages of considering variable exponent Lebesgue spaces w.r.t. both the standard L^2 Hilbert and the constant exponent Lebesgue space Banach L^q spaces, in terms of both reconstruction quality and convergence speed.

Keywords: iterative regularization, proximal operators, variable exponent Lebesgue spaces

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The seriation problem in the presence of a double Fiedler value

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Abstract

Seriation is a problem consisting of seeking the best enumeration order of a set of units whose interrelationship is described by a bipartite graph, that is, a graph whose nodes are partitioned in two sets and arcs only connect nodes in different groups. An algorithm for spectral seriation based on the use of the Fiedler vector of the Laplacian matrix associated to the problem was developed by Atkins et al. [1], under the assumption that the Fiedler value is simple. The algorithm has been analyzed and improved in [2].

In this talk, we analyze the case in which the Fiedler value of the Laplacian is not simple, discuss its effect on the set of the admissible solutions, and study possible approaches to actually perform the computation. Examples and numerical experiments illustrate the effectiveness of the proposed methods.

Keywords: seriation problem, Fiedler vector, bipartite graph

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A nonlinear singular value decomposition

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Abstract

While linear functions are widely used and well-understood, for nonlinear (multivariate vector) functions it is unclear how to

– define their complexity,
– reduce the complexity and
– increase their interpretability.

To solve these problems, we propose a decomposition of nonlinear functions, which can be viewed as a generalization of the singular value decomposition. In this decomposition, univariate nonlinear mappings replace the simpler scaling performed by the singular values. For example, the simplest such nonlinear functions would be pure powers, but more generally, we can use non-homogeneous polynomials. We discuss the computation of the decomposition, which is based on tensor techniques. We also mention an application in nonlinear system identification.

Keywords: singular value decomposition, nonlinear functions, tensors

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SESSION M6

Recent advances in numerical integration by Gaussian rules

Gaussian formulas occupy a special place in numerical integration. They were introduced in 1814 by the famous German mathematician Carl Friedrich Gauss. They have been intensively developing in various directions. Practical error estimation in these effective formulas is an issue to which special attention is paid, especially in the last 60 years since the introduction of Gauss-Kronrod formulas. It turns out that in many cases the latter formulas cannot be effectively constructed and applied. That was the reason for looking for their alternatives. This mini-symposium is dedicated to recent progress in this area.

Organizers:

- Miodrag Spalević
- Marija Stanić

Some properties of orthogonal polynomials with respect to the Abel weight

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Abstract

While a lot is known about the classical orthogonal polynomials, their counterparts with respect to non-classical weights are not as well explored. Nevertheless, sometimes such weights come handy as well. For example, the famous Abel-Plana summation formula offers a convenient method of summing an infinite series, reducing the sum to an integral with the Abel weight function on the real line,

$$w(x) = \frac{x}{e^{\pi x} - e^{-\pi x}}.$$

Orthogonal polynomials with respect to this weight [1, 3] naturally arise when we have to numerically evaluate this integral using the Gauss quadrature rule [2]. These polynomials turn out to possess various symmetry properties. Here we investigate some properties of these polynomials and give some relations between these and some related polynomials.

Keywords: Orthogonal polynomials, Abel weight function, Non-classical weight function

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Error term in Gauss quadrature with Legendre weight function for analytic functions

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Abstract

We studied the error bound of Gauss-Legendre quadrature for analytic functions. It is well known when f is an analytic function then remainder term can be represented as contour integral with a complex kernel:

$$R_n(f) = I(f;\omega) - \sum_{i=1}^{n} \omega_i f(\xi_i) = \frac{1}{2\pi i} \oint_{\Gamma} K_n(z;\omega) f(z)\, dz,$$

where

$$I(f;\omega) = \int_{-1}^{1} \omega(t)\, f(t)\, dt, \quad \omega_i = \int_{-1}^{1} \omega(t)\, l_i(t)\, dt.$$

Then the error bound is reduced to find the maximum of the kernel function. $K_n(z) = K_n(z;\omega)$ can be expressed in the form

$$K_n(z;\omega) = \frac{\varrho_n(z;\omega)}{\Omega_n(z)}, \quad \varrho_n(z;\omega) = \int_{-1}^{1} \omega(t)\, \frac{\Omega_n(t)}{z-t}\, dt, \quad z \in C \setminus [-1,1].$$

We derived explicit expression of the kernel function $K_n(z;\omega)$ and analysed behaviour of this expression in order to determine points where maximum is attained.

Keywords: Gaussian quadratures, Legendre polynomials, Error bound

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Optimal sets of quadrature rules for trigonometric polynomials

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Abstract

In this article we consider the optimal sets of quadrature rules in Borges' sense [On a class of Gauss-like quadrature rules, Numer. Math. 67, (1994) 271-288] for trigonometric polynomials. Also, we consider situations where some nodes are fixed and prescribed in advance. We analyse different cases depending on whether we have an even or odd number of total nodes.

Keywords: Quadrature rules, Trigonometric polynomials, Preassigned nodes

Optimal averaged Padé approximants

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Abstract

Padé-type approximants are rational functions of fixed degrees that approximate a given formal power series. It is well-known that the most accurate such approximants are related to the Gauss quadrature. Boutry [1] constructs a Padé-type approximant that corresponds to the anti-Gaussian quadrature and consequently to the averaged Gaussian quadrature. An alternative to this quadrature is the optimal averaged Gaussian quadrature [7], with a higher degree of precision. Here we give a construction of a Padé-type approximant that corresponds to the optimal averaged Gaussian quadrature and describe some of its properties.

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The error bounds of Gauss quadrature formula for the modified weight functions of Chebyshev type

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Abstract

We consider the Gauss quadrature formulae corresponding to some modifications of anyone of the four Chebyshev weights, considered by Gautschi and Li. As it is well known, in the case of analytic integrands, the error of these quadrature formulas can be represented as a contour integral with a complex kernel. We study the kernel, as it is often considered, on elliptic contours with foci at the points ∓ 1 and such that the sum of semi-axes is $\rho > 1$, of the mentioned quadrature formulas, and derive some error bounds for them. In addition, we obtain, for the first time as far as we know, a result about the behavior of the modulus of the corresponding kernels on those ellipses in some cases. Numerical examples checking the accuracy of such error bounds are included.

Anti-Gaussian quadrature rules for the optimal set of quadrature rules in Borges' sense

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Abstract

Anti-Gaussian quadrature rules, introduced by Laurie in [1], have the property that their error is equal in magnitude but of the opposite sign to the corresponding Gaussian quadrature rules. Guided by that idea, we define and analyse anti-Gaussian quadrature rules for the optimal set of quadrature rules in Borges' sense (see [2]), with respect to the set of r different weight functions. Also, we introduce the set of averaged quadrature rules and give some numerical examples.

Keywords: Anti-Gaussian quadratures, Optimal set of quadrature rules in Borges' sense, Weight function

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Gauss-type quadrature rules with respect to the external zeros of the integrand

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Abstract

In the present paper, we propose a Gauss-type quadrature rule into which the external zeros of the integrand (the zeros of the integrand outside the integration interval) are incorporated. This new formula with n nodes, denoted by $\mathcal{G}_n$, proves to be exact for certain polynomials of degrees greater than $2n-1$ (while the Gauss quadrature formula with the same number of nodes is exact for all polynomials of degrees less than or equal to $2n-1$). It turns out that $\mathcal{G}_n$ has several good properties: all its nodes belong to the interior of the integration interval, all its weights are positive, it converges, and it is applicable both when the external zeros of the integrand are known exactly and when they are known approximately. In order to economically estimate the error of $\mathcal{G}_n$, we construct its extensions that inherit the n nodes of $\mathcal{G}_n$, and that are analogous to the Gauss-Kronrod, averaged Gauss and generalized averaged Gauss quadrature rules. Further, we show that $\mathcal{G}_n$ with respect to the pairwise distinct external zeros of the integrand represents a special case of the (slightly modified) Gauss quadrature formula with preassigned nodes. The accuracy of $\mathcal{G}_n$ and its extensions is confirmed by numerical experiments.

Keywords: Gauss quadrature formula, External zeros of the integrand, Modified weight function, Quadrature error, Convergence of a quadrature formula

Talks outside of mini-symposia

Machine Learning Approach for Sentiment Polarity Detection in Different Languages

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Abstract

Sentiment Polarity Detection (SPD) is a challenging task that combines Natural Language Processing (NLP) and text mining techniques to automatically classify text documents into "positive" and "negative" categories regarding sentiment orientation. The proposed technique is based on the byte-level n-gram frequency statistics method for text representation, and Support Vector Machine (SVM) - Machine Learning (ML) algorithm for categorization process. It does not require any morphological analysis of texts, any preprocessing steps, or any prior information about document content or language. We avoid the necessity for use of taggers, parsers, feature selection, or other language-dependent and non-trivial NLP tools. Proposed approach fully relies on the power of ML algorithm based on strong mathematical foundations. For driving experiments we used seven publicly available movie review benchmarks in English, Spanish, Arabic, French, Turkish, Czech languages and Serbian. Despite their simplicity and broad applicability, experimental results confirm that the presented technique is comparable with the best ranked previously published techniques, when applied to movie reviews datasets.

Keywords: sentiment polarity detection, movie reviews, n-grams, SVM

Methodology for the solution of high-dimensional statistical problems

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Abstract

High-dimensional problems often appear in several studies, such as in medical studies in which the number of samples is less than the number of characteristics. In this case the corresponding design matrix is said to be high-dimensional. The solution of these problems is not unique and it is of great interest the way that a solution can be found. A usual choice is to keep the corresponding solution with the minimum norm. There are cases in which this solution is not a good one and regularization techniques have to be considered. A major issue is the classification of specific cases for which regularization is required or not. An analytical comparison among existing methods for estimating the coefficients of the model which corresponds to design matrices with correlated covariates is presented.

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One Modification of the Chebyshev Measure of the Second Kind and Corresponding Orthogonal Polynomials

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Abstract

The first results to the problem of modification of positive measure with finite support and construction of corresponding orthogonal polynomials were proposed by Christoffel and later by Uvarov (see [2] and [10]). The constructive theory of orthogonal polynomials on the real line was developed in the papers of Gautschi ([6], [7]). Investigations of polynomials orthogonal to non-standard measures and weights have great importance in numerous branches of science and it has been especially important in the development of modified Gaussian quadratures with maximal algebraic degree of exactness ([8]).

Starting from recent results given for example in [4], [3] and [1], in this paper we present our new results on polynomials $\{p_k^{n,s}(x)\}$ orthogonal to one modification of the Chebyshev measure of the second kind given by

$$d\sigma^{n,s}(x) = |\widehat{U}_n(x)|^{2s}(1-x^2)^{1/2+s}dx,\ n \in N,\ s > -1/2,$$

where $\widehat{U}_n(x)$ is $n-$th degree monic Chebyshev polynomial of the second kind. Here we determined the coefficients of the three-term recurrence for observed polynomials $\{p_k^{n,s}(x)\}$ in closed analytic form and derived a differential equality, as well as the differential equation of second order for $\{p_k^{2,s}(x)\}$.

In order to verify all complex formulas we have employed and implemented some symbolic computations in Mathematica, with the intensive use of software package OrthogonalPolynomials ([5], [9]).

Keywords: Orthogonal polynomials, Chebyshev measure, Chebyshev polynomials, recurrence relation

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