Numerical Methods and Scientific Computing (NMSC21)

CIRM Luminy, November 8 - 12, 2021

dedicated to Claude Brezinski for his 80th birthday and to Numerical Algorithms for its 30th birthday

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Numerical Methods and Scientific Computing (NMSC21)
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(The abstracts are listed alphabetically by speaker's underlined name)

List of presentations

Best rational approximants of Markov functions

Joanna Bisch[1], Bernhard Beckermann[1]

[1] *Laboratoire Painlevé UMR 8524, Université de Lille, France*
email: bisch_j_2a@outlook.fr, Bernhard.Beckermann@univ-lille.fr

Abstract

The study of the error of rational approximants of Markov functions

$$f^{[\mu]}(z) = \int \frac{d\mu(x)}{z-x}, \quad \text{supp}(\mu) \subset [a,b],$$

on some $\mathbb{E} \subset \mathbb{R} \setminus [\alpha, \beta]$ has a long history, with a well-established link to orthogonal polynomials. For example, Zolotarev more than 100 years ago described best rational approximants and their error for the particular Markov function

$$f^{[\nu]}(z) = \frac{\sqrt{|a|}}{\sqrt{(z-a)(z-b)}} = \int \frac{d\nu(x)}{z-x}, \quad \frac{d\nu}{dx}(x) = \frac{\sqrt{|a|}}{\pi\sqrt{(x-a)(b-x)}},$$

for closed intervals $\mathbb{E}$. The aim of this talkis to show that

$$\min_{r \in \mathcal{R}_{m-1,m}} \|1 - r/f^{[\mu]}\|_{L^\infty(\mathbb{E})} \le 3 \min_{r \in \mathcal{R}_{m-1,m}} \|1 - r/f^{[\nu]}\|_{L^\infty(\mathbb{E})},$$

that is, up to some modest factor, the particular Markov function $f^{[\nu]}$ gives the worst relative error among all Markov functions $f^{[\mu]}$. In our proof we show similar inequalities for rational interpolants and Padé approximants.

References

[1] Bernhard Beckermann, Joanna Bisch, Robert Luce, Computing Markov functions of Toeplitz matrices, arXiv:2106.05098 (2021).

Extrapolation quadrature from equispaced samples of functions with jumps

Jean-Paul Berrut[1], Manfred R. Trummer[2]

[1] *Université de Fribourg, Suisse*
email: jean-paul.berrut@unifr.ch
[2] *Simon Fraser University, Vancouver, Canada*
email: trummer@sfu.ca

Abstract

Based on the Euler–Maclaurin formula, the Romberg quadrature method extrapolates trapezoidal values to improve their accuracy when computing the integral of smooth functions from equispaced samples. It has been known at least since an article of Lyness in 1971 that the Euler–Maclaurin formula may be extended to accomodate functions with jumps. In the present work, we develop an extrapolation method, based on this extended formula, for the quadrature of such discontinuous functions. We illustrate the method with numerical examples, using one as well as several sample vectors.

Some NLAA aspects on nonlocal dynamics of complex networks through a time-dependent Laplacian

Daniele Bertaccini[1], Fabio Durastante[2]

[1] *Universià di Roma Tor Vergata and*
Consiglio Nazionale delle Ricerche, Istituto per le Applicazioni del Calcolo "M. Picone", Roma, Italy
email: bertaccini@mat.uniroma2.it

[2] *Università di Pisa, Pisa, Italy*
email: fabio.durastante@unipi.it

Abstract

Road networks, coupled biological and chemical systems, neural networks, social interacting species, the Internet and the World Wide Web, are only a few examples of systems composed of a large number of highly interconnected dynamical units. The first approach to capture the global properties of such systems is to model them as graphs whose nodes represent the units, and whose links stand for the interactions between them. A popular approach is to explore the underlying network structure by means of random walks and other processes with diffusive nature defined on these graphs.

In our talk we investigate some aspects of the behavior of certain nonlocal dynamical processes evolving on the networks whose Jacobian matrix is based on a fractional version of a nonsymmetric Laplacian. In the considered models, a random walker on the network is not constrained to hop only from one node to adjacent nodes, but is allowed to perform long distance jumps.

In particular, we focus on some numerical linear algebra aspects of the underlying nonlocal dynamics on directed and undirected networks. An extension with order variable with time is considered with some comments on existence, uniqueness, and uniform asymptotic stability of the solutions. Some examples giving a sample of the behavior of the above dynamics are also included.

References

[1] M. Benzi, D. Bertaccini, F. Durastante, I. Simunec, *Nonlocal network dynamics via fractional graph Laplacians*, Journal of Complex Networks, **8** (2020), no. 3, 1–27.

[2] D. Bertaccini, F. Durastante, *Nonlocal diffusion of variable order on graphs*, (2021), submitted.

Computing the eigenvalues of quasi-Toeplitz matrices

Dario A. Bini[1], Bruno Iannazzo[2], Beatrice Meini[1], Jie Meng[1], Leonardo Robol[1]

[1] *Università di Pisa*
email: dario.bini@unipi.it, beatrice.meini@unipi.it, jie.meng@dm.unipi.it, leonardo.robol@unipi.it
[2] *Università degli Studi di Perugia*
email: bruno.iannazzo@unipg.it

Abstract

A quasi-Toeplitz matrix (in short QT-matrix) is a semi-infinite matrix of the form $A = T(a)+E$ where $T(a) = (a_{j-i})_{i,j\in\mathbb{Z}^+}$, $a = (a_i)_{i\in\mathbb{Z}} \in \ell^1$, is a Toeplitz matrix, and $E = (e_{i,j})_{i,j\in\mathbb{Z}^+}$ represents a compact operator in ℓ^2. QT matrices are encountered in certain applications, in particular in the analysis of queuing models associated with random walks in the quarter plane, and in other stochastic processes from the applications [1], [2], [4], [6].

We investigate the problem of numerically computing the eigenpairs (λ, v) such that $Av = \lambda v$, $v = (v_j)_{j\in\mathbb{Z}^+}$, and $\sum_{j=1}^{\infty} |v_j|^2 = 1$. We provide locally convergent algorithms for computing these eigenpairs in the case where A is finitely representable, i.e., $a_k = 0$ for $k < -m$ and for $k > n$, where m, n are given positive integers and E has a finite number of nonzero entries.

Relying on the theoretical properties in [5], we show that the problem is reduced to a finite generalized nonlinear eigenvalue problem of the kind $L(\lambda)w = \lambda R(\lambda)w$, that can be equivalently formulated as $\det WV(\lambda) = 0$, where W is a constant matrix and V, L, R depend on λ. The matrix V can be given either in terms of a Vandermonde matrix or in terms of a Frobenius companion matrix. The algorithms rely on fixed point iterations or on Newton's method applied to the above determinantal equation. Numerical experiments are presented. Some interesting theoretical and algorithmic issues remain open. The algorithms provide an integration tool of the CQT-Toolbox [3] for performing computations with QT matrices.

References

[1] D. A. Bini, S. Massei, and B. Meini. Semi-infinite quasi-Toeplitz matrices with applications to QBD stochastic processes. *Math. Comp.*, **87** (2018), 2811–2830.

[2] D. A. Bini, S. Massei, B. Meini, and L. Robol. A computational framework for two-dimensional random walks with restarts. *SIAM J. Sci. Comput.*, **42** (2020), A2108–A2133.

[3] D. A. Bini, S. Massei, and L. Robol. Quasi-Toeplitz matrix arithmetic: a MATLAB toolbox. *Numerical Algorithms*, **81** (2019), 741–769.

[4] D. A. Bini, B. Meini, and J. Meng. Solving quadratic matrix equations arising in random walks in the quarter plane. *SIAM J. Matrix Anal. Appl.*, **41** (2020), 691–714.

[5] A. Böttcher and S. M. Grudsky. *Spectral properties of banded Toeplitz matrices*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2005.

[6] T. Ozawa. Asymptotic properties of the occupation measure in a multidimensional skip-free Markov-modulated random walk. *Queueing Syst.*, **97** (2021), 125–161.

Solving Kepler's equation via nonlinear sequence transformations

Riccardo Borghi[1]

[1] *Dipartimento di Ingegneria. Università "Roma Tre", Italy*
email: Riccardo.Borghi@uniroma3.it

Abstract

Likely, there are a very few equations in the world (if any) which can boast such a large number of solving strategies as much as the celebrated *Kepler equation* (KE henceforth),

$$\boxed{M \,=\, \psi \,-\, \epsilon \,\sin\, \psi}$$

The task is to solve KE for ψ, given $M \,\in\, [0, \pi]$ and $\epsilon \,\in\, [0, 1]$. Despite its apparent simplicity, solving KE has gained over three centuries a pivotal role in the science of computation. As it was pointed out in the classical textbook by Colwell [1],

> *Any new technique for the treatment of trascendental equations should be applied to this illustrious case; any new insight, however slight, lets its conceiver join an eminent list of contributors.*

In the present work we intend to give a further contribution to the subject, by focusing our attention on a semi-analytic approach to solve KE based on the following Fourier series expansion:

$$\boxed{\psi \,=\, M \,+\, \sum_{n=1}^{\infty} \frac{2\, J_n(n\,\epsilon)}{n} \,\sin\, nM}$$

where $J_n(\cdot)$ denotes the nth-order Bessel function of the first kind. Although the above series converges for any $\epsilon \,\in\, [0, 1)$, it turns out that such a convergence is extremely slow, especially when $\epsilon \,\to\, 1$. This, together with the fact that a considerable number of Bessel function evaluations has to be implemented, unavoidably brought the Fourier series to be abandoned as far as practical applications of KE are concerned. Nevertheless, such a series expansion presents features that still make it a subject of considerable interest, both in math and in theoretical physics. It was the first example of a class of Bessel function based expansions called *Kapteyn series* (KS henceforth) [2]. One of the scope of the present work is to provide numerical evidences supporting the conjecture that the KS representation of the KE solution is related to the so-called *Stieltjes* series, which are mathematical object playing a pivotal role in theoretical physics. To this end, the well known Debye representation of Bessel functions will be used together with a special type of nonlinear sequence transformation, namely the Weniger transformation [3]. Moreover, some basic features of the the so-called *Debye polynomials* will be explored on a purely numerical ground. Finally, it will be shown how an efficient decoding of the KS series representation of the KE equation can be achieved again by using the Weniger transformation.

References

[1] P. Colwell, *Solving Kepler's Equation Over Three Centuries* Willmann-Bell, Richmond, 1993.

[2] W. Kapteyn, Ann. Sci. de l'Ecole Norm. Sup. Ser. **3,** 91-122 (1893).

[3] E. J. Weniger, Comput. Phys. Rep. **10,** 189 - 371 (1989).

Peter Wynn and Co.

Claude Brezinski[1], Michela Redivo-Zaglia[2], F. Alexander Norman[3]

[1] University of Lille, Laboratory Paul Painlevé, France
email: claude.brezinski@univ-lille.fr
[2] University of Padua, Dept. of Mathematics "Tullio Levi-Civita", Italy
email: michela.redivozaglia@unipd.it
[3] University of Texas at San Antonio, Dept. of Mathematics, USA
email: sandy.norman@utsa.edu

Abstract

In this talk, we tell how, at the occasion of the writing of a paper on the genesis and the development of Aitken's Δ^2 process, Shanks' transformation and the ε-algorithm [1], we learned the death of Peter Wynn in 2017. A special issue of *Numerical Algorithms* was the dedicated to him.

As soon as we learnt the death of Wynn, we began to write an analysis of his published works. But, for introducing them, we had to give an overview of the topics he covered. We also realized that the works of his predecessors should be described, and those of the followers also. Thus, our paper's project rapidly evolved into a book [2], which also contains the testimonies of several researchers in the domain.

Some time after, we received a message from Sandy Norman, from the University of Texas at San Antonio, USA, informing us that, from time to time, Peter Wynn was visiting some friends of him there and left mathematical documents at their home. He asked us if we were interested in them and he proposed to gather and scan them and send them to us. Of course we accepted and we analyzed these unpublished handwritten documents in an open access paper [3].

Finally, Andrea Rosolen, a student of the University of Padua, for his BSC thesis supervised by M. Redivo-Zaglia, constructed a web site dedicated to P. Wynn, and where all the documents we found in San Antonio could be downloaded. Thus, they are not lost and people in the scientific community that want to work on them could do so [4].

This is the story we tell in this talk, together with some biographical notes on Peter Wynn.

References

[1] C. Brezinski, M. Redivo-Zaglia, *The genesis and early developments of Aitken's process, Shanks' transformation, the ε–algorithm, and related fixed point methods*, Numer. Algorithms, **80** (2019), 11–133. https://link.springer.com/journal/11075/volumes-and-issues/80-1

[2] C. Brezinski, M. Redivo-Zaglia, *Extrapolation and Rational Approximation. The Works of the Main Contributors*, Springer Nature, Cham, Switzerland, 2020. https://www.springer.com/gp/book/9783030584177

[3] C. Brezinski, F.A. Norman, M. Redivo-Zaglia, *The Legacy of Peter Wynn*, Mathematics, **9** 11 (2021), 1240. https://www.mdpi.com/2227-7390/9/11/1240/xml

[4] Peter Wynn Legacy site, https://mathresearch.utsa.edu/Legacy/Peter-Wynn/

A variational non-linear constrained model for the inversion of FDEM data

Alessandro Buccini[1], Patricia Diaz de Alba[2]

[1]*Department of Mathematics and Computer Science, University of Cagliari, Italy*
email: alessandro.buccini@unica.it

[2]*School of Mathematics, Gran Sasso Science Institute, Italy*
email: patricia.diazdealba@gssi.it

Abstract

Reconstructing the structure of the soil using non invasive techniques is a very relevant problem in many scientific fields, like geophysics and archaeology. This can be done, for instance, with the aid of Frequency Domain Electromagnetic (FDEM) induction devices. Inverting FDEM data is a very challenging inverse problem, as the problem is extremely ill-posed, i.e., sensible to the presence of noise in the measured data, and non-linear. Regularization methods aim at reducing this sensitivity. In this talk we describe a regularization method to invert FDEM data. We propose to determine the electrical conductivity of the ground by solving a variational problem. The minimized functional is made up by the sum of two terms, the data fitting term ensures that the recovered solution fits the measured data, while the regularization term enforces sparsity on the Laplacian of the solution. The trade-off between the two terms is determined by the regularization parameter. This is achieved by minimizing an $\ell_2 - \ell_q$ functional with $0 < q \leq 2$. Since the functional we wish to minimize is nonconvex, we show that the variational problem admits a solution. Moreover, we prove that, if the regularization parameter is tuned accordingly to the amount of noise present in the data, this model induces a regularization method. Some selected numerical examples show the good performances of our proposal.

Quasi-paraorthogonal polynomials, their zeros and quadrature

Adhemar Bultheel[1], Ruyman Cruz-Barroso[2], Carlos Díaz Mendoza[2]

[1]*Dept. Computer Sci., KULeuven, Belgium*
email: adhemar.bultheel@kuleuven.be
[2]*Dept. Math. Analysis, U. La Laguna, Tenerife, Spain*
email: rcruzb@ull.es, cjdiaz@ull.es

Abstract

Real polynomials have zeros that are either real or appear in complex conjugate pairs, i.e., they are symmetric with respect to the real line $\mathbb{R}$. Complex polynomials whose zeros have similar properties with respect to the unit circle $\mathbb{T}$, i.e., their zeros are either on the circle or are symmetric with respect to it, are invariant polynomials. Invariant polynomials of degree n satisfy by definition $P_n(z) = \tau P_n^*(z)$ for some invariance parameter $\tau \in \mathbb{T}$ and where $P_n^*(z) = z^n\overline{P_n(1/\overline{z})}$.

In view of this spectral property, it should be clear that the natural counterpart of orthogonal polynomials on $\mathbb{R}$ are not the orthogonal, but the paraorthogonal polynomials on $\mathbb{T}$. These paraorthogonal polynomials are orthogonal to $\operatorname{span}\{z, z^2, \ldots, z^{n-1}, z^n - \hat{\tau}\}$ for some $\hat{\tau} \in \mathbb{T}$, and their zeros are important for the construction of (positive) quadrature formulas with maximal domain of validity.

By removing some of the orthogonality conditions for the polynomials, we gain extra free parameters, which can be used to place some of the zeros at preselected locations. This resulted in a number of papers on quasi-orthogonal polynomials on $\mathbb{R}$. In this talk we shall consider the analogue concept on $\mathbb{T}$ which are the quasi-paraorthogonal polynomials. We analyze the possibilities of preselecting some of the zeros, in order to build positive quadrature formulas with prefixed nodes and maximal domain of validity. We illustrate with a numerical example how the zeros behave as a function of an invariance parameter τ, when they are all simple and on $\mathbb{T}$, and when they are allowed as nodes in positive quadrature formulas.

References

[1] R. Cruz-Barroso, C. Díaz Mendoza, and F. Perdomo Pío, *Szegő-type quadrature formulas*, J. Math. Anal. Appl. **455** (2017) , no. 1, 592–605.

[2] A. Bultheel, R. Cruz-Barroso, C. Díaz Mendoza, *Zeros of quasi-paraorthogonal polynomials and positive quadrature*, (2021), Submitted.

[3] C. Jagels and L. Reichel, *Szegő-Lobatto quadrature rules*, J. Comp. Appl. Math. **200**(2007), no. 1, 116–126.

[4] F. Peherstorfer, *Positive trigonometric quadrature formulas and quadrature on the unit circle*, Math. Comp. **80** (2011) , no. 275, 1685-1701.

Training large scale SVMs using structured kernel approximations and ADMM

Stefano Cipolla[1], Jacek Gondzio[2]

[1] The University of Edinburgh, School of Mathematics, U.K.
email: scipolla@ed.ac.uk, j.gondzio@ed.ac.uk

Abstract

Despite their simplicity, non-linear Support Vector Machines (SVMs), are still recognised by practitioners of Machine Learning and Data Science as the preferred choice for classification tasks in certain situations.

On the other hand, the computational complexity of solving non-linear SVMs is prohibitive on large-scale datasets: the use of the Kernel Trick requires the storage of a value for the kernelized distance between any two pairs of points leading to a storage complexity of $O(d^2)$ where d is the dimension of the training set.

In this talk we will demonstrate how to efficiently merge a Hierarchically Semi-Separable [2] approximation of the kernel matrix with the Alternating Direction Method of Multipliers (ADMM) [1] for the solution of the underlying convex optimization problem. The proposed merger delivers a computational framework able to out-perform the state of the art training algorithms for large scale SVMs [3].

References

[1] S. Boyd, N. Parikh, and E. Chu. *Distributed optimization and statistical learning via the alternating direction method of multipliers*, Foundations and Trends in Machine Learning **3** (2010), no. 1 1–122.

[2] G. Chávez, Y. Liu, P. Ghysels, X.S. Li, E. Rebrova. *Scalable and Memory-Efficient Kernel Ridge Regression*. In 2020 IEEE International Parallel and Distributed Processing Symposium (IPDPS), IEEE, 2020, 956–965.

[3] S. Cipolla, J. Gondzio. *Training very large scale nonlinear SVMs using Alternating Direction Method of Multipliers coupled with the Hierarchically Semi-Separable kernel approximations*, arXiv:2108.04167.

Multidimensional exponential analysis: feasible at last

Annie Cuyt[1], Ferre Knaepkens[1], Wen-shin Lee[2]

[1] *Universiteit Antwerpen, Belgium*
email: annie.cuyt@uantwerpen.be, ferre.knaepkens@uantwerpen.be
[2] *University of Stirling, Scotland (U.K.)*
email: wen-shin.lee@stir.ac.uk

Abstract

The problem of d-dimensional exponential analysis consists in retrieving the linear parameters $\alpha_j \in \mathbb{C}$ and the nonlinear parameters $\phi_j \in \mathbb{C}^d$ in the exponential model

$$f(x) = \sum_{j=1}^{n} \alpha_j \exp\left(\langle \phi_j, x \rangle\right), \qquad x = (x_1, \ldots, x_d), \qquad \phi_j = (\phi_{j1}, \ldots, \phi_{jd}) \tag{1}$$

from as few function samples as possible. Until recently, algorithms to solve the problem required a number of samples of the order $O(n^d)$ or $O(2^d n)$ or at most $(d+1)n^2 \log^{2d-2} n$, all growing exponentially with the dimension of the problem statement. As a consequence, most of the methods were not employed in practice in higher dimensional problem statements where $d \geq 3$.

We propose to use a reliable implementation based on [1] which requires only $O((d+1)n)$ regularly gathered samples. Thus the new technique does not suffer the well-known curse of dimensionality. The computation cost of the new method is further reduced as we solve several smaller systems instead of one large system dealing with all measurements at the same time.

In addition, when the technique is combined with convergence theorems from approximation theory on the one hand and sparse interpolation results from computer algebra on the other hand, one is able to:

- filter unstructured noise in the data out of the structured exponential model (1) via a connection to Padé approximation theory,
- automatically deduce and validate the sparsity n of expression (1), which is usually regarded to be a hard problem,
- separate exponential components that are contained in a cluster of similar components, using a connection with sparse interpolation,
- and as a result of all of the above, tighten the numerical estimates for the parameters ϕ_j and α_j in case of a low signal-to-noise ratio.

We illustrate its use on several two-, three- and higher-dimensional applications and compare with existing techniques and optimisation methods.

References

[1] Annie Cuyt and Wen-shin Lee. Multivariate exponential analysis from the minimal number of samples. *Adv. Comput. Math.*, 44:987–1002, 2018. (Published online November 16, 2017).

Numerical solution of second-kind integral equations by means of anti-Gauss quadrature rules

Patricia Díaz de Alba[1], Luisa Fermo[2], Giuseppe Rodriguez[2]

[1]*Gran Sasso Science Institute, L'Aquila, Italy*
email: patricia.diazdealba@gssi.it
[2]*Department of Mathematics and Computer Science, University of Cagliari, Italy*
email: fermo@unica.it, rodriguez@unica.it

Abstract

The aim of this talk is concerned with a global approximation of the following Fredholm integral equation of the second-kind

$$f(y) - \int_{-1}^{1} k(x,y) f(x) w(x) dx = g(y), \quad y \in [-1,\, 1],$$

where f is the unknown function, k and g are two given functions and $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$ is a Jacobi weight with parameters $\alpha, \beta > -1$.

A numerical method based on the Nyström interpolants corresponding to Gauss and anti-Gauss quadrature formulae is developed [1, 2] providing upper and lower bounds for the solution of the equation under suitable assumptions, which are easily verified for a particular weight function.

The convergence and stability of the proposed method is discussed in proper weighted spaces. Moreover, an error estimate is available, and the accuracy of the solution is improved by approximating it by an averaged Nyström interpolant.

Numerical tests will show the accuracy of the approach.

References

[1] D.P. Laurie, *Anti-Gaussian quadrature formulas*, Mathematics of Computation, **65** (1996), 739–747.

[2] P. Díaz de Alba, L. Fermo, and G. Rodriguez, *Solution of second-kind Fredholm integral equations by means of Gauss and anti-Gauss quadrature rules*, **146(4)** (2020), 699–728.

Linear algebra in interior point methods for sparse approximation problems

Valentina De Simone[1], Daniela di Serafino[2], Jacek Gondzio[3], Spyridon Pougkakiotis[3], Marco Viola[1]

[1] *University of Campania "L. Vanvitelli", Italy*
email: valentina.desimone@unicampania.it, marco.viola@unicampania.it
[2] *University of Naples Federico II, Italy*
email: daniela.diserafino@unina.it
[3] *University of Edinburgh, U.K.*
email: J.Gondzio@ed.ac.uk, S.Pougkakiotis@sms.ed.ac.uk

Abstract

We focus on optimization problems with sparse solutions. Although first-order methods are widely applied to these problems, we believe that interior point methods equipped with suitable linear algebra can provide significant advantages, especially when the problems are large and not so-well conditioned. To this aim, we develop variants of an interior point-proximal method of multipliers by specializing its linear algebra phase, and show their effectiveness on applications of wide interest in science and engineering (see [1] and the references therein).

References

[1] V. De Simone, D. di Serafino, J. Gondzio, S. Pougkakiotis, M. Viola, *Sparse Approximations with Interior Point Methods*, Technical Report ERGO 21-001, School of Mathematics, University of Edinburgh, 2021, also available from Optimization Online and arXiv.

Multigrid methods for anisotropic space-fractional diffusion equations

Mariarosa Mazza[1], Marco Donatelli[1], Rolf Krause[2], Ken Lorenzo Trotti[1]

[1] *Università degli Studi dell'Insubria, Dept. of Science and High Technology, Como, Italy*
email: mariarosa.mazza@uninsubria.it, marco.donatelli@uninsubria.it kl.trotti@uninsubria.it
[2] *Università della Svizzera Italiana, Lugano-Viganello, Switzerland*
email: rolf.krause@usi.ch

Abstract

We are interested in a finite difference discretization of a two-dimensional time-dependent space-fractional diffusion equation (FDE) and in the solution of the related linear systems. Our focus is both on the case where the fractional orders are close to each other (isotropic case), and the one where they are not (anisotropic case). Driven by the fact that the discretization matrices have a block-Toeplitz-Toeplitz-blocks-like structure, and by the well-known negative results on multilevel circulant preconditioning, we opt for a multigrid approach. In this framework, the spectral properties of the matrices and the isotropic/anisotropic nature of the problem guide the selection of both projector and smoother.

In the isotropic case, based on the spectral analysis of the coefficient matrices, we define a multigrid method with classical linear interpolation as grid transfer operator and damped-Jacobi as smoother. In the anisotropic case, inspired by certain multigrid strategies for integer order anisotropic diffusion equations given in literature, we replace the classical linear interpolation with a semi-coarsening technique. Moreover, we estimate the Jacobi relaxation parameter by using an automatic spectral-based procedure. A further improvement in the robustness of the proposed method with respect to the anisotropy of the problem is attained employing the resulting V-cycle with semi-coarsening as smoother inside an outer full-coarsening.

References

[1] M. Donatelli, R. Krause, M. Mazza, K. Trotti, *Multigrid preconditioners for anisotropic space-fractional diffusion equations*, Advances in Computational Mathematics **46** (2020), no. 3.

Zeros of Jacobi polynomials

Kathy Driver[1]

[1] *University of Cape Town, South Africa*
email: kathy.driver@uct.ac.za

Abstract

Suppose $\{P_n^{(\alpha,\beta)}(x)\}_{n=0}^{\infty}$ is a sequence of Jacobi polynomials, $\alpha, \beta > -1$. It is known that the zeros of $P_n^{(\alpha,\beta)}(x)$ and $P_n^{(\alpha-t,\beta+s)}(x)$ are interlacing for $\alpha - t > -1, \beta > -1, 0 \leq t, s \leq 2$. We discuss the simplest cases of a question raised by Alan Sokal at OPSFA 2019 whether the zeros of $P_n^{(\alpha,\beta)}(x)$ and $P_{n+k}^{(\alpha+t,\beta+s)}(x)$ are interlacing when $s, t > 0$ and $k, n \in \mathbb{N}$. We prove that the zeros of $P_n^{(\alpha,\beta)}(x)$ and $P_{n+1}^{(\alpha,\beta+1)}(x)$, $\alpha > -1, \beta > 0, n \in \mathbb{N}$ are partially, but in general not fully, interlacing, depending on the values of α, β and n. We also consider interlacing of the zeros of $P_n^{(\alpha,\beta)}(x)$ and $P_{n+1}^{(\alpha+1,\beta+1)}(x)$, $\alpha, \beta > -1$ and provide examples confirming that our results cannot be strengthened in general. This is joint work with Jorge Arvesú Carballo and Lance Littlejohn.

Solving Richards equation: theoretical challenges and parallel implementation*

Daniele Bertaccini[1], Pasqua D'Ambra[2], Fabio Durastante[3], Salvatore Filippone[1]

[1] *Università di Roma "Tor Vergata", Dipartimento di Matematica, Italy*
email: bertaccini@mat.uniroma2.it, salvatore.filippone@uniroma2.it

[2] *Consiglio Nazionale delle Ricerche, Istituto per le Applicazioni del Calcolo "M. Picone", Italy*
email: pasqua.dambra@cnr.it

[3] *Università di Pisa, Dipartimento di Matematica, Italy*
email: fabio.durastante@unipi.it

Abstract

Groundwater flow in the unsaturated zone is a highly nonlinear problem. We describe it by Richards equation in the "mixed form", for which we consider a cell-centered finite-difference approximation [1]. The nonlinearities of the model lead to changes in soil conductivity over several orders of magnitude and long time integrations are often required in simulations. Thus, any discretization for space variables produces a stiff system of differential equations. To face it, we employ a fully implicit discretization. This require solving a nonlinear system by a quasi-Newton algorithm at each time step. In turn, it requires solving a sequence of linear systems with Jacobian matrices $\{J_k\}_k$.

We will show some results on the asymptotic distribution of the eigenvalues of each J_k that will connect the physical and numerical properties of the model. This analysis enables the possibility of constructing efficient preconditioners based on some recent developments on a package of AMG preconditioners aimed to improve the efficiency, scalability, and robustness of Krylov accelerators in solving extreme-scale problems on parallel hybrid architectures. Specifically, we will discuss the use of functionalities introduced by the AMG4PSBLAS [2] package as part of the PSCToolkit† (Parallel Sparse Computation Toolkit) that includes some parallel AMG methods designed to provide scalable and easy-to-use preconditioners in the context of the PSBLAS (Parallel Sparse Basic Linear Algebra Subprograms) computational framework, which implements distributed Krylov-type linear solvers. For the latter aspect, we will focus on the flexibility and efficiency of the proposed AMG methods and the related software framework on supercomputers.

References

[1] D. Bertaccini, P. D'Ambra, F. Durastante, S. Filippone, *Hybrid Preconditioning Richards Equation for Variably Saturated Flow*, **In preparation** (2021).

[2] P. D'Ambra, F. Durastante, S. Filippone *AMG Preconditioners for Linear Solvers towards Extreme Scale*, SIAM J. Sci. Comput. **In Press** (2021), S679–S703.

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†PSCToolkit website https://psctoolkit.github.io/.

Forward-backward regularization methods by modular-proximal operators

Marta Lazzaretti[1], Claudio Estatico[1], Luca Calatroni[2]

[1] *Department of Mathematics, University of Genova, Italy*
email: lazzaretti@dima.unige.it, estatico@dima.unige.it

[2] *CNRS, UCA, Inria, Lab. I3S, France*
email: calatroni@i3s.unice.fr

Abstract

We consider a variational approach to the solution of inverse problems by minimization of Tikhonov-like functionals of the form $\arg\min_{x\in X} f(x,y) + \lambda g(x)$, where $f : X \times Y \longrightarrow \mathbb{R}$ represents a smooth convex fidelity term between the data $y \in Y$ and the solution $x \in X$, $g : X \longrightarrow \mathbb{R}$ is a (possibly non-smooth) convex penalty term, and $\lambda > 0$ is the regularization parameter. In inverse problems modeled by a linear functional equation $Ax = y$, very basic examples include norm fidelity terms $f(x,y) = \|Ax - y\|_Y^p$ and L^1 regularization $g(x) = \|x\|_1$.

In Hilbert space setting, the Forward-Backward (FB) splitting algorithm for the minimization of $f(x,y) + \lambda g(x)$ enables to exploit the differentiability of the smooth function f in the anti-gradient minimization "forward step" $x_k \mapsto x_k - \tau_k \nabla_x f(x_k, y)$ for a proper step-size $\tau_k > 0$, and then to minimize with respect the (non smooth) function g by the "backward step" $x_{k+1} = \text{prox}_{\tau_k \lambda g}(x_k - \tau_k \nabla f(x_k, y))$, defined in terms of the proximal operator $\text{prox}_{\gamma g}(u) = \arg\min_{x\in X} \frac{1}{2}\|x - u\|_X^2 + \gamma g(x)$.

In this work, we study the generalization of FB algorithms to a Banach space X. This generalization is not straightforward. Indeed, since the gradient is an element of the dual space X^*, the forward step cannot be performed directly on x_k and requires the application of the so called duality maps, which link primal and dual spaces, allowing to perform the gradient step in the dual space X^* [1]. Moreover, duality maps are non-linear, leading to a different definition of the backward step in terms of Bregman distance and a more difficult convergence analysis.

We then introduce a FB algorithm suited for Variable exponent Lebesgue spaces [2], which are (non-Hilbertian) Banach spaces where the exponent used in the definition of the norm is not constant, but rather is a function $p(\cdot) > 1$ of the domain. In this case, the role of the norm in the proximal operator is replaced by the so called modular $m(x,u) = \sum_i p_i^{-1}|x_i - u_i|^{p_i}$, which allows effective computation of the backward step by virtue of separability. The proposed FB algorithm based on such a modular-proximity will be outlined and its convergence properties discussed. We mention that variable exponents Lebesgue spaces are endowed with space variant geometrical properties which are useful in adaptive regularization techniques [3].

References

[1] K. Bredies, *A forward—backward splitting algorithm for the minimization of non-smooth convex functionals in Banach space*, Inverse Problems **25** (2008), no. 1, 015005.

[2] L. Diening, P. Harjulehto, P. Hästö, M. Ruzicka, *Lebesgue and Sobolev Spaces with Variable Exponents*, Lecture Notes in Mathematics, vol. 2017, Springer, 2011.

[3] T. Schuster, B. Kaltenbacher, B. Hofmann and K. Kazimierski, *Regularization Methods in Banach Spaces*, Radon Series on Computational and Applied Mathematics, vol. 10, De Gruyter, 2012.

Cubature schemes on the real semi-axis

Dusan Lj. Djukić[1], Luisa Fermo[2], Rada M. Mutavdžić Djukić[1]

[1] University of Belgrade, Department of Mathematics, Faculty of Mechanical Engineering, Serbia
email: ddjukic@mas.bg.ac.rs, rmutavdzic@mas.bg.ac.rs

[2] University of Cagliari, Department of Mathematics and Computer Science, Italy
email: fermo@unica.it

Abstract

This talk deals with the numerical tretament of the following integral

$$I(f) = \int_0^\infty \int_0^\infty f(x,y)\, w(x,y)\, dx\, dy$$

where f is a known function defined on the domain $[0,\infty)\times[0,\infty)$ and $w(x,y) = x^\alpha\, y^\beta e^{-(x+y)}$, $\alpha, \beta > -1$.

Suitable truncated averaged rules based on Gauss-Laguerre formulae [1, 2, 3] will be introduced, and investigated in terms of stability and convergence. Numerical tests will be presented, in order to show the performance of the introduced cubature schemes.

References

[1] D. Lj. Djukić, L. Reichel, M. M. Spalević, *Truncated generalized averaged Gauss quadrature rules*, Journal of Computational and Applied Mathematics, **308** (2016), 408–418.

[2] D. P. Laurie. *Anti-Gaussian quadrature formulas*, Mathematics of Computation **65** (1996), 739–747.

[3] G. Mastroianni and G. Monegato. *Truncated quadrature rules over* $(0,\infty)$ *and Nyström-type methods*, SIAM Journal on Numerical Analysis **41** (2003), 1870–1892.

A multilevel approach to stochastic estimation of the trace*

Andreas Frommer[1], Mostafa Khalil Nasr[1], Gustavo Ramirez-Hidalgo[1]

[1]*Department of Mathematics, University of Wuppertal, Wuppertal, Germany*
email: frommer@uni-wuppertal.de, m.nasr@stimulate-ejd.eu, g.ramirez@stimulate-ejd.eu

Abstract

The trace of a matrix function $f(A)$, most notably of the matrix inverse, can be estimated stochastically using samples $x^* f(A)x$ if the components of the random vectors x obey an appropriate probability distribution. However such a Monte-Carlo sampling suffers from the fact that the accuracy depends quadratically of the samples to use, thus making higher precision estimation very costly. In this paper we suggest and investigate a multilevel Monte-Carlo approach which uses a multigrid hierarchy to stochastically estimate the trace. This results in a substantial reduction of the variance, so that higher precision can be obtained at much less effort. We illustrate this for the trace of the inverse using three different classes of matrices, the discrete 2d Laplace operator, the 2d gauge Laplace operator and the Schwinger model of electrodynamics as a quantum field theory.

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Iterative methods for linear systems

Martin J. Gander[1]

[1] University of Geneva, Switzerland
email: martin.gander@unige.ch

Abstract

Iterative methods for linear systems were invented for the same reasons as they are used today, namely to reduce computational cost. Gauss states in a letter to his friend Gerling in 1823: "you will in the future hardly eliminate directly, at least not when you have more than two unknowns".

Richardson's paper from 1910 was then very influential, and is a model of a modern numerical analysis paper: modeling, discretization, approximate solution of the discrete problem, and a real application. Richardson's method is much more sophisticated that how it is usually presented today, and his dream became reality in the PhD thesis of Gene Golub.

The work of Stiefel, Hestenes and Lanczos in the early 1950 sparked the success story of Krylov methods, and these methods can also be understood in the context of extrapolation, pioneered by Brezinski and Sidi, based on seminal work by Wynn.

This brings us to the modern iterative methods for solving partial differential equations, which come in two main classes: domain decomposition methods and multigrid methods. Domain decomposition methods go back to the alternating Schwarz method invented by Herman Amandus Schwarz in 1869 to close a gap in the proof of Riemann's famous Mapping Theorem. Multigrid goes back to the seminal work by Fedorenko in 1961, with main contributions by Brandt and Hackbusch in the Seventies.

I will show in my presentation how these methods function on the same model problem of the temperature distribution in a simple room. All these methods are today used as preconditioners for Krylov methods, which leads to the most powerful iterative solvers currently known for linear systems.

References

[1] L. F. Richardson, *The approximate arithmetical solution by finite differences of physical problems involving differential equations, with an application to the stresses in a masonry dam*, Philosophical Transactions of the Royal Society of London. Series A, **210** (1911), 307–357.

[2] E. Stiefel, *Über einige Methoden der Relaxationsrechnung, Edouard Stiefel*, Z. Angew. Math. Phys. **3** (1952), 1–33.

[3] H. A. Schwarz, *Über einen Grenzübergang durch alternierendes Verfahren*, Vierteljahrsschrift der Naturforschenden Gesellschaft in Zürich **15** (1870), 272—286.

[4] G. Ciaramella and M. J. Gander, *Iterative Methods and Preconditioners for Systems of Linear Equations*, to appear in SIAM (2021).

[5] M. J. Gander, P. Henry and G. Wanner, *A History of Iterative Methods*, in preparation (2021).

Regularization by inexact Krylov methods

Silvia Gazzola[1], Malena Sabaté Landman[2]

[1] *Department of Mathematical Sciences, University of Bath, U.K.*
email: S.Gazzola@bath.ac.uk

[2] *Department of Applied Mathematics and Theoretical Physics, University of Cambridge, U.K.*
email: ms2845@damtp.cam.ac.uk

Abstract

This talk will present theoretical and algorithmic aspects of regularization methods based on inexact Krylov methods for the solution of large-scale discrete inverse problems. Specifically, we will introduce two new inexact Krylov methods that can be efficiently applied to unregularized or Tikhonov-regularized least squares problems, and we present their theoretical properties, including links with their exact counterparts and strategies to monitor the amount of inexactness. We then describe how the new methods can be applied to solve separable nonlinear inverse problems arising in blind deblurring, where both the sharp image and the parameters defining the blur are unknown. We show that the new inexact solvers (which can naturally handle varying inexact blurring parameters while solving the linear deblurring subproblems within a variable projection method) allow for a much reduced number of total iterations and substantial computational savings with respect to their exact counterparts. This talk is based on the work described in [1].

References

[1] S. Gazzola and M. Sabaté Landman, *Regularization by inexact Krylov methods with applications to blind deblurring*, to appear in SIAM J. Matrix Anal. Appl., 2021. See also arXiv:2105.07378.

Padé approximation and Wavelet filters on logarithmic economic time series

Concepción González-Concepción[1]

[1] *University of La Laguna, Spain*
email: cogonzal@ull.edu.es

Abstract

The wavelet theory has been useful to study time economic data (see, among others, the handbook of Addison [1]), due to the possibility of working in the dual time-frequency domain and allowing to establish certain causal properties between variables. Due to its good properties, the Fourier transform is frequently used which acts as a wavelet filter.
Following the proposal in Haddad [2], in this presentation we explore the alternative use of the Laplace transform and the Padé approximation to build the transfer function of the wavelet filter, which may be more appropriate for logarithmic economic time series.

References

[1] P.S. Addison, *The illustrated wavelet transform handbook: introductory theory and applications in science, engineering, medicine and finance*, CRC press, 2017.

[2] S. A. Haddad, S. Bagga, & W. A. Serdijn, *Log-domain wavelet bases*, IEEE Transactions on Circuits and Systems I: Regular Papers **52** (2005), no. 10, 2023–2032.

Recent trends in adaptive regularisation under inexact evaluations for nonconvex optimisation and machine learning applications

Stefania Bellavia[1], Gianmarco Gurioli[2], Benedetta Morini[1], Philippe L. Toint[3]

[1] *Università degli Studi di Firenze, Italy*
email: stefania.bellavia@unifi.it, benedetta.morini@unifi.it
[2] *SISSA, Italy*
email: gianmarco.gurioli@unifi.it
[3] *University of Namur, Belgium*
email: philippe.toint@unamur.be

Abstract

Within the context of nonconvex unconstrained and inexpensively-constrained optimisation, a class of adaptive regularisation methods under inexact function and derivatives evaluations is presented.
At variance with the basic ARC framework, the underlying algorithm is not limited to refer to the cubic model, allowing for the use of potentially higher degrees to search for arbitrary order optimality points. At each iteration, it features an adaptive mechanism for determining the inexactness which is needed to compute objective function values and derivatives, in order to preserve the complexity results of its counterpart with exact evaluations.
Sharp global evaluation complexity bounds, assuming that the right accuracy level in function and derivatives estimates is deterministically achievable, are derived and hold for any model degree and any order of optimality, thereby generalising known results for first and second-order versions of the method. High probability and stochastic complexity bounds are also shown.
For lower orders, preliminary numerical tests are finally reported.

GMRES methods for tomographic reconstruction with an unmatched back projector*

Per Christian Hansen[1], Ken Hayami[2], Keiichi Morikuni[3]

[1]*Department of Applied Mathematics and Computer Science, Technical University of Denmark*
email: pcha@dtu.dk

[2]*Professor Emeritus, National Institute of Informatics, Japan*
email: hayami@nii.ac.jp

[3]*Faculty of Engineering, Information and Systems, University of Tsukuba, Japan*
email: morikuni@cs.tsukuba.ac.jp

Abstract

We consider iterative reconstruction methods for X-ray computed tomography that are based on a discretization $A\,x \approx b$. This approach does not assume any specific scanning geometry, and it produces good reconstructions in the case of limited-data and/or limited-angle problems [2].

The matrix A represents the *forward projector* while the transpose A^T represents the so-called *back projector* which maps the data back onto the solution domain. In large-scale CT problems, A is too large to store, and we must use functions that compute the multiplications with A and A^T in a matrix-free fashion. Optimal use of GPUs calls for the use of different discretization methods for the forward projector and the back projector [4]. Hence, the matrix $B \in \mathbb{R}^{n\times m}$ which represents the back projector is typically different from the transpose A^T of the forward projector, and we say that B is an *unmatched back projector*.

The consequence is that iterative solvers based on multiplications with A and B solve the *unmatched normal equations* [1] in one of the forms $B\,A\,x = B\,b$ or $A\,B\,y = b$, $x = B\,y$. It is natural to use the well-known GMRES algorithm to solve these systems, and our work is based on the preconditioned AB-GMRES and BA-GMRES methods for solving least squares problems [3] with B as a right and left preconditioner, respectively.

We study the performance and the regularizing effects of the AB- and BA-GMRES methods when applied to CT reconstruction problems, and we show how these methods depend on the difference between B and A^T. Specifically we show that AB-GMRES and BA-GMRES are equivalent to LSQR and LSMR, respectively, when $B = A^T$. We also show how to terminate the iterations before the noise starts to dominate the iteration vectors. Our numerical experiments demonstrate that AB- and BA-GMRES can be used successfully to solve algebraic formulations of large-scale CT reconstruction problems with an unmatched back projector.

References

[1] T. Elfving and P. C. Hansen, *Unmatched projector/backprojector pairs: perturbation and convergence analysis*, SIAM J. Sci. Comput., 40 (2018), A573–A591.

[2] P. C. Hansen, J. S. Jørgensen and W. R. B. Lionheart, *Computed Tomogrpahy: Algorithms, Insight and Just Enough Theory*, SIAM, PA, 2021.

[3] K. Hayami, J.-F. Yin and T. Ito, *GMRES methods for least squares problems*, SIAM J. Matrix Anal. Appl., 31 (2010), 2400–2430.

[4] W. J. Palenstijn, K. J. Batenburg and J. Sijbers, *Performance improvements for iterative electron tomography reconstruction using graphics processing units*, J. Struct. Biol., 176 (2011), 250–253.

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Normal equations can be more stable than equations.

Ken Hayami[1], Zeyu Liao[2], Keiichi Morikuni[3], Jun-Feng Yin[4]

[1] *Professor Emeritus, National Institute of Informatics, Japan*
email: hayami@nii.ac.jp
[2] *The Graduate University for Advanced Studies (SOKENDAI), Japan*
email: zeyu@nii.ac.jp
[3] *University of Tsukuba, Japan*
email: morikuni@cs.tsukuba.ac.jp
[4] *Tongji University, China*
email: yinjf@tongji.edu.cn

Abstract

A common belief in solving systems of linear equations is that explicitly forming the normal equations deteriorates the conditioning. Namely, let $A \in \mathbf{R}^{n\times n}$, and $\kappa_2(A)$ be the 2-norm condition number of A. Then, in exact arithmetic, $\kappa_2(A^{\mathrm{T}}A) = \kappa_2(A)^2$.

In this talk, we show that if A is extremely ill-conditioned, that is, $\kappa_2(A) = \dfrac{1}{o(n\sqrt{\epsilon})}$, then, generically, $\kappa_2(\mathrm{fl}(A^{\mathrm{T}}A)) = \dfrac{1}{O(n^2\epsilon)}$. Here, ϵ is the machine epsilon, $\mathrm{fl}(\cdot)$ denotes floating point computation. $O(\cdot)$ and $o(\cdot)$ are Landau's symbols,

Then, numerical experiments suggest that by Cholesky decomposition $\mathrm{fl}(A^{\mathrm{T}}A) = \mathrm{fl}(LL^{\mathrm{T}})$, we have $\kappa_2(\mathrm{fl}(L)) = \dfrac{1}{O(n\sqrt{\epsilon})}$, even when $\kappa_2(A) = \dfrac{1}{o(n\sqrt{\epsilon})}$.

This fact can be used, for instance, to stabilize the convergence of GMRES for extremely ill-conditioned linear systems. Namely, in the GMRES iteration, when the upper triangular matrix R becomes severely ill-conditioned, i.e. when $\kappa_2(R) = \dfrac{1}{o(n\sqrt{\epsilon})}$, instead of solving $R\boldsymbol{y} = \boldsymbol{t}$ by back substitution, we solve $R^{\mathrm{T}}R\boldsymbol{y} = R^{\mathrm{T}}\boldsymbol{t}$ using Cholesky decomposition: $R^{\mathrm{T}}R = LL^{\mathrm{T}}$, which stabilizes the convergence of GMRES [1]. In the talk, we will present numerical experiment results which demonstrate the validity of this approach.

References

[1] Z. Liao, K. Hayami, K. Morikuni, J.-F. Yin, *A Stabilized GMRES Method for Solving Underdetermined Least Squares Problems*, https://arxiv.org/abs/2007.10853, arXiv, arXiv:2007.10853, March, 2020.

Tensors Krylov-based subspace methods for image and video processing

Khalide Jbilou[1]

[1] *Université du Littoral Côte d'Opale, Calais Cedex, France*
email: Khalide.Jbilou@univ-littoral.fr

Abstract

In this poster, we propose some tensor Krylov-based subspace methods such as tensor GMRES or tensor Golub-Kahan methods for color image and video processing. The proposed methods are obtained using the tensor-tensor T-product which is derived by using the Fast Fourier Transform (or the Discrete Cosine Transform for the c-product). We give a small presentation of the proposed methods and present some numerical examples. We also show how to use the tensor Golub-Kahan algorithm in Tensor Principal Component Analysis (T-PCA) for classification and face recognition when using color objects.

References

[1] M. El Guide, A. El Ichi, K. Jbilou and R. Sadaka, On tensor GMRES and Golub-Kahan methods via the T-product for color image processing, The Electronic Journal of Linear Algebra 37(2021), 524-543.

[2] M. El Guide, A. El Ichi, and K. Jbilou, Discrete cosine transform LSQR methods for multidimensional ill-posed problems J. Mathematical Modeling, (2021), in press.

[3] F. P. A. Beik, A. El Ichi , K. Jbilou and R. Sadaka, Tensor extrapolation methods with applications, Numerical Algorithms, Numerical Algorithms 87 (2021) 1421–1444.

[4] M.E. Kimler and C.D. Martin, Factorization strategies for third-order tensors, Linear Algebra with Applications, 435(2011), 641—658.

[5] M. E. Kilmer, K. Braman, N. Hao and R. C. Hoover, Third-order tensors as operators on matrices: a theoretical and computational framework with applications in imaging, SIAM Journal of Matrix Analysis and Applications, 34(2013), 148–172.

[6] L. Reichel and O. Ugwu, The tensor Golub-Kahan-Tikhonov method applied to the solution of ill-posed problems with a t-product structure, Numerical Linear Algebra with Applications, in press.

Divide and conquer methods for functions of matrices with banded or hierarchical low-rank structure *

Alice Cortinovis[1], Daniel Kressner[1], Stefano Massei[2]

[1] *Institute of Mathematics, École Polytechnique Fédérale de Lausanne, Switzerland*
email: alice.cortinovis@epfl.ch, daniel.kressner@epfl.ch
[2] *CASA, TU Eindhoven, Netherlands*
email: s.massei@tue.nl

Abstract

This talk is concerned with approximating matrix functions for banded matrices, hierarchically semiseparable matrices, and related structures. We develop a new divide-and-conquer method based on (rational) Krylov subspace methods for performing low-rank updates of matrix functions. Our convergence analysis of the newly proposed method proceeds by establishing relations to best polynomial and rational approximation. When only the trace or the diagonal of the matrix function is of interest, we demonstrate – in practice and in theory – that convergence can be faster. For the special case of a banded matrix, we show that the divide-and-conquer method reduces to a much simpler algorithm, which proceeds by computing matrix functions of small submatrices. Numerical experiments confirm the effectiveness of the newly developed algorithms for computing large-scale matrix functions from a wide variety of applications.

References

[1] A. Cortinovis, D. Kressner, S. Massei, *Divide and conquer methods for functions of matrices with banded or hierarchical low-rank structure*, arXiv:2107.04337, 2021. .

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Smith normal form and rational approximation

George Labahn[1]

[1] *Cheriton School of Computer Science, University of Waterloo, Canada*
email: glabahn@uwaterloo.ca

Abstract

The Smith normal form of an $n \times n$ matrix $A$of integers or polynomials is a diagonal matrix $S = diag(s_1, s_2, \ldots, s_n)$ satisfying $s_1|s_2|..|s_n$ with $UAV = S$, where U and V are unimodular matrices (i.e. det U = det $V = \pm 1$ (integers) or a constant (polynomials)). The U and V matrices represent the row and column operations need to convert A into S.

In this talk we will discuss efficient algorithms for the computation of S, U and V. The tools used are closely related to algebraic tools used for fast algorithms for rational approximation problems such as Padé and Hermite-Padé approximation.

A boundary-layer preconditioner for singularly perturbed convection diffusion

Scott P. MacLachlan[1], Niall Madden[2], Thái Anh Nhan[3]

[1]*Memorial University of Newfoundland, Canada*
email: smaclachlan@mun.ca

[2]*National University of Ireland, Galway, Ireland*
email: Niall.Madden@NUIGalway.ie

[3]*Holy Names University, USA*
email: nhan@hnu.edu

Abstract

Motivated by a wide range of real-world problems whose solutions exhibit boundary and interior layers, the numerical analysis of discretizations of singularly perturbed differential equations is an established sub-discipline within the study of the numerical approximation of solutions to differential equations. Consequently, much is known about how to accurately and stably discretize such equations on *a priori* adapted meshes, in order to properly resolve the layer structure present in their continuum solutions. However, despite being a key step in the numerical simulation process, much less is known about the efficient and accurate solution of the linear systems of equations corresponding to these discretizations.

In this talk, we discuss problems associated with the application of direct solvers to these discretizations. We then propose a preconditioning strategy that is tuned to the matrix structure induced by using layer-adapted meshes for convection-diffusion equations, proving a strong condition-number bound on the preconditioned system in one spatial dimension, and a weaker bound in two spatial dimensions. Numerical results confirm the efficiency of the resulting preconditioners in one and two dimensions, with time-to-solution of less than one second for representative problems on 1024×1024 meshes and up to $40\times$ speedup over standard sparse direct solvers.

Rational spectral transformations, orthogonal polynomials and matrix factorization

Francisco Marcellán Español[1]

[1] Departamento de Matemáticas, Universidad Carlos III de Madrid, Spain
email: pacomarc@ing.uc3m.es

Abstract

Let $\mathbf{u}$ be a quasi-definite linear functional defined on the linear space of polynomials $\mathbb{P}$. For such a functional we can define a sequence of monic orthogonal polynomials (SMOP in short) $(P_n)_{n\geq 0}$, which satisfies a three term recurrence relation. Shifting one unity the recurrence coefficient indices we get the sequence of associated polynomials of the first kind $(P_n^{(1)})_{\geq 0}$ which are orthogonal with respect to a linear functional denoted by $\mathbf{u}^{(1)}$.

In the literature two special spectral transformations of the functional $\mathbf{u}$ are studied: the canonical Christoffel transformation $\widetilde{\mathbf{u}} = (x-c)\mathbf{u}$ and the canonical Geronimus transformation $\widehat{\mathbf{u}} = (x-c)^{-1}\mathbf{u} + M\delta_c$, where c is a fixed complex number, M is a free parameter and δ_c is the linear functional defined on $\mathbb{P}$ as $< \delta_c, p(x) >= p(c)$. They constitute a generating system of the so called linear spectral transformation set analyzed in [ZH97]. For the Christoffel transformation with **SMOP** $(\widetilde{P}_n)_{n\geq 0}$, we are interested in analyzing the relation between the linear functionals $\mathbf{u}^{(1)}$ and $\widetilde{\mathbf{u}}^{(1)}$. There, the super index denotes the linear functionals associated with the orthogonal polynomial sequences of the first kind $(P_n^{(1)})_{n\geq 0}$ and $(\widetilde{P}_n^{(1)})_{n\geq 0}$, respectively. This problem is also studied for Geronimus transformations. Here we give close relations between their corresponding monic Jacobi matrices by using the LU and UL factorizations. For more information, see [1].

Joint work with Juan Carlos Garcia Ardila (Universidad Politécnica de Madrid, España) and Paul H. Villamil-Hernández (Universidad Carlos III de Madrid, España).

References

[1] J. C. García Ardila, F. Marcellán, P. H. Villamil-Hernández, *Associated orthogonal polynomials of the first kind and Darboux transformations*, arXiv:2103.0232, [math.CA] **23** March 2021

[2] A. Zhedanov, *Rational spectral transformations and orthogonal polynomials*, J. Comput. Appl. Math. **85** (1997), 67-86.

On computing Gaussian quadrature rules with high relative accuracy

Teresa Laudadio[1], Nicola Mastronardi[1], Paul Van Dooren[2]

[1] *Istituto per le Applicazioni del Calcolo "M. Picone", Consiglio Nazionale delle Ricerche, sede di Bari, Italy*
email: teresa.laudadio@cnr.it, nicola.mastronardi@cnr.it

[2] *Department of Mathematical Engineering, Catholic University of Louvain, Louvain-la-Neuve, Belgium*
email: paul.vandooren@uclouvain.be

Abstract

The Golub–Welsch algorithm [1] is the classical way to compute the knots x_i and the weights $w_i,\ i = 1, \ldots, n$, of the Gaussian quadrature rule

$$\sum_{i=1}^{n} f(x_i) w_i$$

approximating the integral $\int_{-a}^{a} f(x)\omega(x)dx$, with f a continuous function and ω a positive weight.

The knots x_i, zeros of the orthogonal polynomial $p_n(x)$ associated to the weight ω, are also the eigenvalues of a tridiagonal matrix of order n, called *Jacobi* matrix, whose nonzero entries are the coefficients of the three–term recurrence relation of the sequence of the orthogonal polynomials $p_j(x), j = 0, 1, \ldots, n-1$, associated to ω.

Computed $x_i,\ i = 1, \ldots, n$, the corresponding weight w_i can be obtained from the first component of the eigenvector associated to x_i [1].

If ω is a symmetric weight, x_i and $w_i,\ i = 1, \ldots, n$, can be computed by solving a tridiagonal eigenvalue problem of size $\lfloor n/2 \rfloor$ [2].

Exploiting the method proposed in [2], we derive an efficient algorithm to compute the knots of Gaussian quadrature rules corresponding to symmetric weights ω with high relative accuracy.

Moreover, for a nonsymmetric weight $\hat{\omega}$, computed a knot $\hat{x}_i$, we consider different ways to compute the corresponding weight $\hat{w}_i$.

Among them, we consider [3]

$$\hat{w}_i = \frac{1}{\sum_{k=0}^{n-1} \hat{p}_k^2(\hat{x}_i)},$$

where $\hat{p}_k(x),\ k = 0, \ldots, n-1$, are the first n orthonormal polynomials associated to $\hat{\omega}$.

In particular, we analyze the stability of the forward and backward three–term recurrence relations generating $\hat{p}_k(x),\ k = 0, \ldots, n-1$, and develop a method for computing them with high relative accuracy.

References

[1] G.H. Golub, J.H. Welsch, *Calculation of Gauss quadrature rules*, Math. Comput. **23** (1969), 221–230.

[2] G. Meurant, A. Sommariva, *Fast variants of the Golub and Welsch algorithm for symmetric weight functions in matlab*, Numerical Algorithms, **67** (2014), 491–506.

[3] G. Szegö, *Orthogonal Polynomials*, fourth ed., American Mathematical Society, Providence, 1975.

Palindromic linearization and numerical solution of nonsymmetric algebraic T–Riccati equations

Peter Benner[1], Bruno Iannazzo[2], Beatrice Meini[3], Davide Palitta[4]

[1]*Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*
email: benner@mpi-magdeburg.mpg.de

[2]*Università degli Studi di Perugia, Italy*
email: bruno.iannazzo@unipg.it

[3]*Università di Pisa, Italy*
email: beatrice.meini@unipi.it

[4]*Università di Bologna, Italy*
email: davide.palitta@unibo.it

Abstract

We consider the Nonsymmetric algebraic T-Riccati equation (T-NARE)

$$DX + X^T A - X^T BX + C = 0, \tag{1}$$

where X is the unknown matrix and $A, B, C, D \in \mathbb{R}^{n\times n}$ are the coefficients, while the superscript T denotes transposition. Equation (1) has been considered in [1], with applications to solving large-scale Dynamic Stochastic General Equilibrium models.

We introduce a palindromic linearization for the T-NARE (1). More specifically, by using the coefficients of the matrix equation, we construct a T-palindromic pencil $\varphi(z) = M + zM^T$ of size $(2n) \times (2n)$, that linearizes the equation: we show that, if $\varphi(z)$ is regular and if X is a solution to (1), then the columns of $\begin{bmatrix} I \\ X \end{bmatrix}$ span a deflating subspace of $\varphi(z)$; also a kind of converse result holds under suitable assumptions. This linearization, besides being interesting *per se*, opens the way to find solutions of a T-NARE by relying on algorithms that compute bases of deflating subspaces of a matrix pencil, such as the QZ algorithm and the Doubling Algorithm [2, 3]. Moreover, the palindromic structure of $\varphi(z)$ can be exploited by a structured QZ algorithm [4]. We show the effectiveness of these algorithms, in terms of accuracy and execution time, with comparisons with the Newton method proposed in [1].

References

[1] P. Benner and D. Palitta. On the solution of the nonsymmetric T-Riccati equation. *Electron. Trans. Numer. Anal.*, 54:68–88, 2021.

[2] D. A. Bini, B. Iannazzo, and B. Meini. *Numerical Solution of Algebraic Riccati Equations*. Society for Industrial and Applied Mathematics, 2011.

[3] T.-M. Huang, R.-C. Li, and W.-W. Lin. *Structure-preserving doubling algorithms for nonlinear matrix equations*, volume 14 of *Fundamentals of Algorithms*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2018.

[4] D. S. Mackey, N. Mackey, C. Mehl, and V. Mehrmann. Numerical methods for palindromic eigenvalue problems: computing the anti-triangular Schur form. *Numer. Linear Algebra Appl.*, 16(1):63–86, 2009.

Generalizations of scalar polynomial properties to matrix polynomials

Aaron Melman[1]

[1]*Department of Applied Mathematics, Santa Clara University, Santa Clara, USA*
email: amelman@scu.edu

Abstract

The development of fast and reliable methods to compute the zeros of a polynomial, may, at first sight, appear to have diminished the need for zero approximations, localization results, and other properties. However, these properties become significantly more valuable if they can be generalized to matrix polynomials, as polynomial eigenvalues are much harder to compute than polynomial zeros. Clearly, not all properties can be so generalized, but many can.

We survey several recent results that were generalized from scalar to matrix polynomials, ranging from relatively basic ones, such as the well-known zero localizations by Cauchy and Pellet (and their less well-known improvements), to more refined ones such as properties related to the angular distribution of zeros.

Although many generalizations to matrix polynomials are traditionally expressed in terms of the norms of the coefficient matrices, we also make use of the numerical radius of the coefficients, which has led to remarkably good results.

Finally, we show how generalizations obtained for matrix polynomials can – somewhat paradoxically – be turned around to improve and even derive new results for scalar polynomials.

Detection and correction of silent errors in the Conjugate Gradient algorithm

Gérard Meurant[1]

[1] Paris, France
email: gerard.meurant@gmail.com

Abstract

There are more and more computing elements in modern supercomputers. This increases the probability of computer errors. Errors that do not stop the computation are called *soft errors* or *silent errors*. Of course, they could have a negative impact on the output of the code. So, it is of interest to be able to detect these silent errors and to correct them.

In this talk we are concerned with the detection and correction of silent errors in the conjugate gradient (CG) algorithm to solve linear systems $Ax = b$ with a symmetric positive definite matrix A. Silent errors in CG may affect or even prevent the convergence of the algorithm. We propose a new way to detect silent errors using a scalar relation that must be satisfied by CG variables,

$$\alpha_{k-1}^2 \frac{(Ap_{k-1}, Ap_{k-1})}{(r_{k-1}, r_{k-1})} = 1 + \beta_k, \tag{1}$$

where r_j's are the residual vectors, p_j's the descent directions and

$$\alpha_{k-1} = \frac{(r_{k-1}, r_{k-1})}{(p_{k-1}, Ap_{k-1})}, \quad \beta_k = \frac{(r_k, r_k)}{(r_{k-1}, r_{k-1})}$$

are the coefficients computed in CG.

We study how relation (1) is modified in finite precision arithmetic and define a criterion to detect when this relation is not satisfied.

Checking relation (1) involves computing an additional dot product, but, as it was shown some time ago in [1] and more recently in [2], relation (1) can be used to introduce more parallelism in the algorithm.

Assuming that the input data (A, b) is not corrupted, we model silent errors by bit flips in the output of some CG steps. When an error is detected in some iteration k, we could restore the CG data from iteration $k - 2$ to be able to continue the computation safely.

Numerical experiments will show the efficiency of this approach.

References

[1] G. Meurant, *Multitasking the conjugate gradient method on the CRAY X-MP/48* Parallel Comput. **5** (1987), 267–280.

[2] T. Chen and E. Carson, *Predict-and-recompute conjugate gradient variants* SIAM J. Sci. Comput. **42** (2020), A3084–A3108.

Randomized FEAST algorithm for generalized Hermitian eigenvalue problems with probabilistic error analysis

Nikita Kapur[1], Agnieszka Międlar[2], Arvind K. Saibaba[3], Eric de Sturler[4]

[1] *University of Iowa, USA*
email: nikita-kapur@uiowa.edu
[2] *University of Kansas, USA*
email: amiedlar@ku.edu
[3] *North Carolina State University, USA*
email: asaibab@ncsu.edu
[4] *Virginia Tech, USA*
email: sturler@vt.edu

Abstract

Randomized NLA methods have recently gained popularity because of their easy implementation, computational efficiency, and numerical robustness. We propose a randomized version of a well-established FEAST eigenvalue algorithm that enables computing the eigenvalues of the Hermitian matrix pencil $(\mathbf{A}, \mathbf{B})$ located in the given real interval $\mathcal{I} \subset [\lambda_{min}, \lambda_{max}]$. In this talk, we will present deterministic as well as probabilistic error analysis of the accuracy of approximate eigenpair and subspaces obtained using the randomized FEAST algorithm. First, we derive bounds for the canonical angles between the exact and the approximate eigenspaces corresponding to the eigenvalues contained in the interval $\mathcal{I}$. Then, we present bounds for the accuracy of the eigenvalues and the corresponding eigenvectors. This part of the analysis is independent of the particular distribution of an initial subspace, therefore we denote it as deterministic. In the case of the starting guess being a Gaussian random matrix, we provide more informative, probabilistic error bounds. Finally, we will illustrate numerically the effectiveness of all the proposed error bounds.

Eigensolvers using complex moments for operators

Akira Imakura[1], Keiichi Morikuni[1], Akitoshi Takayasu[1]

[1] *University of Tsukuba, Japan*
email: imakura@cs.tukuba.ac.jp, morikuni@cs.tukuba.ac.jp, takitoshi@risk.tsukuba.ac.jp

Abstract

The proposed solvers compute discrete eigenvalues in a simply connected region in the complex plane and the corresponding eigenfunctions of linear operators with boundary conditions. The operator eigenvalue problems widely appear in science and engineering, such as stability analysis in infinite-dimensional dynamical systems.

Inspired by recent studies of operator analogs [1, 2], this study extends eigensolvers for large-scale matrix eigenvalue problems to operators. Complex moment eigensolvers for matrix eigenvalue problems, including a class of projection methods [3, 4, 5], have been developed, attracting advantages in their highly hierarchical parallelizability. Our extension carries out those features in parallel by nature. The operator analogs of FEAST avoid discretizing operators, and the proposed methods likewise. Unlike the operator analogs of FEAST, the proposed methods reduce the computational costs by using high-order complex moments.

These eigensolvers construct complex moment matrices by a contour integral of a resolvent and extract the target eigenpairs. A complex moment matrix consisting of a resolvent filters out undesired eigencomponents and extracts the desired ones in a pseudorandom quasimatrix whose columns are supposed to have eigencomponents corresponding to the eigenvalues of interest. FEAST and its operator analogs use the zeroth-order complex moments, while the proposed methods use high-order complex moments to reduce computational costs. Numerical experiments show that the proposed methods are more efficient and accurate than previous methods.

References

[1] A. Austin, *Eigenvalues of Differential Operators by Contour Integral Projection*, `http://www.chebfun.org/examples/ode-eig/ContourProjEig.html` (2009).

[2] A. Horning, A. Townsend, *FEAST for differential eigenvalue problems*, SIAM J. Numer. Anal. **58** (2020), no. 2, 1239–1262.

[3] S. Goedecker, *Low complexity algorithms for electronic structure calculations*, J. Comput. Phys. **118** (1995), no. 2, 261–268.

[4] T. Sakurai, H. Sugiura, *A projection method for generalized eigenvalue problems using numerical integration*, J. Comput. Appl. Math. **159** (2003), no. 1, 119–128.

[5] E. Polizzi, *Density-matrix-based algorithm for solving eigenvalue problems*, Phys. Rev. B **79** (2009), no. 11, 115112.

Numerical algorithms for solving nonlinear systems via spectral residual methods

Enrico Meli[1], Benedetta Morini[1], Margherita Porcelli[2], Cristina Sgattoni[3]

[1] *Università di Firenze, Italy*
email: enrico.meli@unifi.it, benedetta.morini@unifi.it

[2] *Università di Bologna, Italy*
email: margherita.porcelli@unibo.it

[3] *Istituto per le Applicazioni del Calcolo "Mauro Picone", Italy*
email: cristina.sgattoni@fi.iac.cnr.it

Abstract

Spectral residual methods are derivative-free and low-cost per iteration procedures for solving systems of nonlinear equations [1]. They are generally coupled with a nonmonotone linesearch strategy and compare well with Newton-based methods in the solution of both large nonlinear systems and sequences of nonlinear systems. The residual vector is used as the search direction and the steplength is inspired by the Barzilai Borwein method [2]. Analogously to spectral gradient methods for minimization, choosing the steplength has a crucial impact on the performance of the procedure. In this talk we address, both theoretically and experimentally, the steplength selection and provide results on a real application such as the wheel-rail contact in railway systems. The talk is based on the work [3].

References

[1] W. La Cruz, J. M. Martinez, M. Raydan, M. *Spectral residual method without gradient information for solving large-scale nonlinear systems of equations*, Math. Comput. **75** (2006), 1429–1448.

[2] J. Barzilai, J. Borwein, 1988 *Two point step gradient methods*, IMA J. Numer. Anal. **8** (1988), 141–148.

[3] E. Meli, B. Morini, M. Porcelli, C. Sgattoni, *Solving nonlinear systems of equations via spectral residual methods: stepsize selection and applications*, arXiv:2005.05851v1

On the low-rank approximations in the Chebyshev norm*

Stanislav Morozov[1], Nikolai Zamarashkin[1], Eugene Tyrtyshnikov[1]

[1]*Marchuk Institute of Numerical Mathematics of the Russian Academy of Sciences, Russia*
email: stanis-morozov@yandex.ru

Abstract

Low-rank matrices and tensors are ubiquitous in science. To date, most of the methods have been developed to build effective low-rank approximations in the spectral or Frobenius norm. The quality of such approximations depends on the decrease rate of the singular values of the matrix. However, recent results show that low-rank approximations of matrices in other norms can be effective even without decreasing singular values. One fundamental result was proved in [1]:

Theorem. Let $X \in \mathbb{R}^{m\times n}$ with $m \geq n$ and $0 < \varepsilon < 1$. Then, with

$$r = \lceil 72 \log(2n+1)/\varepsilon^2 \rceil \tag{1}$$

we have

$$\inf_{\text{rank}Y \leq r} \|X - Y\|_C \leq \varepsilon \|X\|_2, \text{ where } \|X\|_C = \max_{i,j} |X_{ij}| \tag{2}$$

This paper is devoted to algorithms for constructing low-rank approximations of matrices in the Chebyshev norm. The problem of low-rank approximations in the Chebyshev norm formulates as follows

$$\mu = \inf_{U\in\mathbb{R}^{m\times r}, V\in\mathbb{R}^{n\times r}} \left\|A - UV^T\right\|_C, \tag{3}$$

As far as we know, the only work that addresses this problem is [2]. To begin with, we study the necessary and sufficient conditions for the optimality of the solution of problem

$$\mu = \inf_{U\in\mathbb{R}^{m\times r}} \left\|A - UV^T\right\|_C, \tag{4}$$

for a known matrix V and come to a method for constructing an exact solution to this problem. Then we repeatedly alternate between problems for matrices U and V, obtaining convergence to some solution. As the result, we obtain an algorithm that allows us to build low-rank approximations of matrices without decreasing singular values in the Chebyshev norm. The accuracy of the approximation of the method turns out to be significantly higher than (1), and the operating time grows polynomial with the matrix size.

References

[1] M. Udell, A. Townsend, *Why are big data matrices approximately low rank?*, SIAM Journal on Mathematics of Data Science, (2019)

[2] V. A. Daugavet, *The uniform approximation of a function of two variables that is given in tabular form by a product of functions of one variable*, U.S.S.R. Comput. Math. Math. Phys., (1971, in Russian)

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Numerical methods for CT reconstruction with unknown geometry parameters

James Nagy[1]

[1] *Department of Mathematics, Emory University, USA*
email: jnagy@emory.edu

Abstract

Computed tomography (CT) techniques are well known for their ability to produce high quality images needed for medical diagnostic purposes. Unfortunately standard CT machines are extremely large, heavy, require careful and regular calibration, and are expensive, which can limit their availability in point-of-care situations. An alternative approach is to use portable machines, but parameters related to the geometry of these devices (e.g., distance between source and detector, orientation of source to detector) cannot always be precisely calibrated, and these parameters may change slightly when the machine is adjusted during the image acquisition process. In this work we describe the nonlinear inverse problem that models this situation, and discuss algorithms that can jointly estimate the geometry parameters and compute a reconstructed image.

Numerical methods for fractional diffusion equations

Michael Ng[1]

[1] *The University of Hong Kong*
email: mng@maths.hku.hk

Abstract

In this talk, we discuss some preconditioning methods for fractional diffusion equations. Also preconditioning for time fractional diffusion inverse source problems is studied. Numerical examples are reported to demonstrate these preconditioning techniques. Also some deep learning methods are discussed in the talk.

On the convergence of Krylov methods with low-rank truncations

Davide Palitta[1], Patrick Kürschner[2]

[1]*Alma Mater Studiorum, Università di Bologna, Italy*
email: davide.palitta@unibo.it
[2]*Leipzig University of Applied Sciences, Germany*
email: patrick.kuerschner@htwk-leipzig.de

Abstract

Low-rank Krylov methods are one of the few options for solving general linear matrix equations, especially for large problem dimensions. An important step of these procedures consists in truncating the rank of the basis vectors, represented in terms of matrices, to maintain a feasible storage demand of the overall solution process. In principle, such truncations can severely impact on the converge of the adopted Krylov routine. In this talk we show how to perform the low-rank truncations in order to maintain the convergence of the selected Krylov procedure. In particular, our analysis points out that not only the thresholds employed for the truncations are important, but further care has to be adopted to guarantee the orthogonality of the computed basis. In particular, an auxiliary, exact Gram-Schmidt procedure in a low dimensional subspace may be adopted to retrieve the orthogonality of the computed basis – when lost – while preserving the memory-saving features of the latter. This additional orthogonalization step leads to a modified formulation of the inner problems. Nevertheless, this is still feasible in terms of computational efforts. We illustrate some numerical experiments which validate our theoretical findings.

References

[1] D. Palitta and P. Kürschner, *On the convergence of Krylov methods with low-rank truncations*, Numerical Algorithms (2021)

Regularized minimal-norm solution of a system of first kind integral equations

Patricia Díaz de Alba[1], Luisa Fermo[2], Federica Pes[2], Giuseppe Rodriguez[2]

[1]*School of Mathematics, Gran Sasso Scientific Institute, Italy*
email: patricia.diazdealba@gssi.it

[2]*Department of Mathematics and Computer Science, University of Cagliari, Italy*
email: fermo@unica.it, federica.pes@unica.it, rodriguez@unica.it

Abstract

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 only known at a finite set of points, e.g., when it consists of experimental measurements, the difficulties related to ill-posedness are enforced, as the problem has 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 problem is solved in a reproducing kernel Hilbert space (RKHS), by using the Riesz Representation Theorem. Indeed, the minimal-norm solution is written as a linear combination of the Riesz representers. 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. Numerical experiments are presented to illustrate the excellent performance of the method. This is a joint work with Patricia Díaz de Alba, Luisa Fermo, and Giuseppe Rodriguez [1, 2].

References

[1] P. Díaz de Alba, L. Fermo, F. Pes, and G. Rodriguez. *Minimal-norm RKHS solution of an integral model in geo-electromagnetism*. Accepted on the proceedings of the IEEE International Conference on Computational Science and its Applications (2021).

[2] P. Díaz de Alba, L. Fermo, F. Pes, and G. Rodriguez. *Minimal-norm solution of an overdetermined system of first kind integral equations: algorithms and applications*. Submitted (2021).

On symmetric orthogonal polynomials

Cleonice F. Bracciali[1], Miguel A. Piñar[2]

[1] *Departamento de Matemática, IBILCE, UNESP - Universidade Estadual Paulista, São José do Rio Preto, Brazil*
email: cleonice.bracciali@unesp.br

[2] *Departamento de Matemática Aplicada, Universidad de Granada, Granada, Spain*
email: mpinar@ugr.es

Abstract

We study families of multivariate orthogonal polynomials with respect to the symmetric weight function in d variables

$$B_\gamma(\mathtt{x}) = \prod_{i=1}^{d} w(x_i) \prod_{i<j} |x_i - x_j|^{2\gamma+1}, \quad \mathtt{x} \in (a,b)^d,$$

for $\gamma > -1$, where $w(t)$ is an univariate weight function in $t \in (a,b)$ and $\mathtt{x} = (x_1, x_2, \ldots, x_d)$ with $x_i \in (a,b)$. Using the change of variables $\mathtt{x} = (x_1, x_2, \ldots, x_d) \mapsto \mathtt{u} = (u_1, u_2, \ldots, u_d)$ where, u_r are the r**-th elementary symmetric functions** we study multivariate orthogonal polynomials in the variable $\mathtt{u}$ associated with the weight function $W_\gamma(\mathtt{u})$ defined by means of $W_\gamma(\mathtt{u}) = B_\gamma(\mathtt{x})$. For the new weight function, the domain is described in terms of the discriminant of the polynomial having x_i, $i = 1, 2, \ldots, d$, as its zeros and in terms of the associated Sturm sequence. Obviously, generalized classical orthogonal polynomials as defined by Lassalle [2, 3, 4] and Macdonald [5] are included in our study. Choosing the univariate weight function as the Hermite, Laguerre and Jacobi weight functions, we obtain the representation in terms of the variables u_r for the partial differential operators having the respective Hermite, Laguerre and Jacobi generalized multivariate orthogonal polynomials as the corresponding eigenfunctions. The case $d = 2$ coincides with the polynomials studied by Koornwinder in [1]. Finally, we present explicitly the partial differential operators for Hermite, Laguerre and Jacobi generalized polynomials in the cases $d = 2$ and $d = 3$.

References

[1] T. H. Koornwinder, *Orthogonal polynomials in two variables which are eigenfunctions of two algebraically independent partial differential operators I*, Indag. Math., **3**6 (1974), 48–58.

[2] M. Lassalle, *Polynômes de Jacobi généralisés*, C. R. Acad. Sci. Paris Sér. I Math. **312** (1991), 425–428.

[3] M. Lassalle, *Polynômes de Laguerre généralisés*, C. R. Acad. Sci. Paris Sér. I Math. **312** (1991), 725–728.

[4] M. Lassalle, *Polynômes de Hermite généralisés*, C. R. Acad. Sci. Paris Sér. I Math. **312** (1991), 579–582.

[5] I. G. Macdonald, *Hypergeometric Functions I*, arXiv:1309.4568 [math.CA]

From ESPRIT to ESPIRA: estimation of signal parameters by iterative rational approximation

Nadiia Derevianko[1], Gerlind Plonka[1], Markus Petz[1]

[1] University of Göttingen, Germany
email: n.derevianko@math.uni-goettingen.de, plonka@math.uni-goettingen.de, m.petz@math.uni-goettingen.de

Abstract

We introduce a new method for **E**stimation of **S**ignal **P**arameters based on **I**terative **R**ational **A**pproximation (ESPIRA) for sparse exponential sums. Our algorithm uses the AAA algorithm for rational approximation [2] of the discrete Fourier transform of the given equidistant signal values. We show that ESPIRA can be interpreted as a matrix pencil method applied to Loewner matrices. These Loewner matrices are closely connected with the Hankel matrices which are usually employed for recovery of sparse exponential sums. Due to the construction of the Loewner matrices via an adaptive selection of index sets, the matrix pencil method is stabilized. ESPIRA achieves similar recovery results for exact data as ESPRIT and the matrix pencil method in [3] but with less computational effort. Moreover, ESPIRA strongly outperforms ESPRIT and the matrix pencil method for noisy data and for signal approximation by short exponential sums.

References

[1] N. Derevianko, G. Plonka, and M. Petz, *From ESPRIT to ESPIRA: estimation of signal parameters by iterative rational approximation*, preprint, 2021, arXiv:2106.15140.

[2] Y. Nakatsukasa, O. Sete, and L.N. Trefethen, *The AAA algorithm for rational approximation*, SIAM J. Sci. Comput., **40** (2018), no. 2, A1494–A1522.

[3] D. Potts and M. Tasche, *Parameter estimation for nonincreasing exponential sums by Prony-like methods*, Linear Algebra Appl. **439** (2013), no. 4, 1024–1039.

Gauss quadrature, linear functionals, and Lanczos algorithm

Stefano Pozza[1], Miroslav Pranić[2], Zdeněk Strakoš[1]

[1] *Charles University, Czech Republic*
email: pozza@karlin.mff.cuni.cz, strakos@karlin.mff.cuni.cz

[2] *University of Banja Luka, Bosnia-Erzegovina*
email: miroslav.pranic@pmf.unibl.org

Abstract

The Gauss quadrature can be generalized to approximate quasi-definite linear functionals where the interconnections with (formal) orthogonal polynomials, (complex) Jacobi matrices, and Lanczos algorithm are analogous to those in the positive definite case. In particular, the existence of the n-weight (complex) Gauss quadrature corresponds to successfully performing the first n steps of the Lanczos algorithm. For general linear functionals, the series of (formal) orthogonal polynomials may not be complete. Nevertheless, the Gauss quadrature generalization is still possible and can be connected with the (look-ahead) Lanczos algorithm.

Approximation of Stieltjes matrix functions via rational Gauss-type quadrature rules

Jihan Alahmadi[1], Miroslav Pranić[2], Lothar Reichel[1]

[1] *Department of Mathematical Sciences, Kent State University, USA*
email: jalahma1@kent.edu, reichel@math.kent.edu

[2] *University of Banja Luka, Bosnia-Erzegovina*
email: miroslav.pranic@pmf.unibl.org

Abstract

This talk is concerned with the inexpensive approximation of expressions of the form $I(f) = v^T f(A)v$, when A is a large symmetric positive definite matrix, v is a vector, and $f(t)$ is a Stieltjes function. We are interested in the situation when A is too large to make the evaluation of $f(A)$ practical. Approximations of $I(f)$ are computed with the aid of rational Gauss quadrature rules. Error bounds or estimates of bounds are determined with rational Gauss-Radau or rational anti-Gauss rules.

Subspace iteration and variants, revisited

Yousef Saad[1]

[1] University of Minnesota, Twin Cities, USA
email: saad@umn.edu

Abstract

Computing invariant subspaces is at the core of many applications, from machine learning to signal processing, and control theory, to name just a few examples. Often one wishes to compute the subspace associated with eigenvalues located at one end of the spectrum, i.e., either the largest or the smallest eigenvalues. In addition, it is quite common that the data at hand undergoes frequent changes and one is required to keep updating or tracking the target invariant subspace. The talk will present standard tools for computing invariant subspaces, with a focus on methods that do not require solving linear systems. One of the best known techniques for computing invariant subspaces is the subspace iteration algorithm [2]. While this algorithm tends to be slower than a Krylov subspace approach such as the Lanczos algorithm, it has many attributes that make it the method of choice in many applications. One of these attributes is its tolerance of changes in the matrix. An alternative framework that will be emphasized is that of Grassmann manifolds [1]. We will derive gradient-type methods and show the many connections that exist between different viewpoints adopted by practitioners, e.g., the TraceMin algorithm [3]. The talk will end with a few illustrative examples.

References

[1] A. EDELMAN, T. A. ARIAS, AND S. T. SMITH, *The geometry of algorithms with orthogonality constraints*, SIAM J. Matrix Anal. Appl., 20 (1999), pp. 303–353.

[2] Y. SAAD, *Numerical Methods for Large Eigenvalue Problems- Classics in Appl. Math.*, SIAM, Philadelpha, PA, 2011.

[3] A. H. SAMEH AND J. A. WISNIEWSKI, *A trace minimization algorithm for the generalized eigenvalue problem*, SIAM Journal on Numerical Analysis, 19 (1982), pp. 1243–1259.

Characterization and convergence improvement of some Krylov subspace methods for solving linear systems

F. Bouyghf[1,3], A. Messaoudi[2,1], Hassane Sadok[3]

[1] *Laboratoire de Mathématiques, Informatique et Applications, Sécurité de l'Information, Département de Mathématiques, Faculté des sciences, Université Mohammed V, Rabat, Maroc*
email: fatima.bouyghf@etu.univ-littoral.fr

[2] *Ecole Normale Supérieure Takaddoum, Département d'Informatique, Rabat, Maroc*
email: abderrahim.messaoudi@gmail.com

[3] *Laboratoire de Mathématiques Pures et Appliquées, Université du Littoral Côte d'Opale, Calais, France*
email: hassane.sadok@univ-littoral.fr

Abstract

We consider some Krylov subspace methods for solving a linear system $Ax = b$, which converge in m iterations for a certain initial estimate x_0 and the corresponding residual $r_0 = b - A\,x_0$, being m the degree of the minimal polynomial M_m of A for r_0.

The Krylov methods considered are products methods and the kth residual polynomial is $Q_k P_k$, where P_k is a polynomial of degree k such that $P_m = M_m$ and Q_k is a polynomial of fixed or variable degree.

We first show how to compute recursively the sequence of polynomials P_k and provide some particular case. Then, we study some choices of polynomials Q_k involving local convergence, smoothing, and fixed memory and cost for each iteration. Numerical experiments are provided to illustrate the performance of the algorithms developed.

On the kernel of the vector Epsilon-algorithm

Claude Brezinski[1], Michela Redivo-Zaglia[2], Ahmed Salam[3]

[1] *Université de Lille, CNRS, UMR 8524 - Laboratoire Paul Painlevé, France*
email: Claude.Brezinski@univ-lille.fr
[2] *Università degli Studi di Padova, Dipartimento di Matematica "Tullio Levi-Civita", Padova, Italy*
email: Michela.RedivoZaglia@unipd.it
[3] *Université du Littoral, LMPA, Calais, France*
email: ahmed.salam@univ-littoral.fr

Abstract

The vector Epsilon-algorithm introduced by P. Wynn is a powerful method for accelarating the convergence of vector sequences. The algorithm is an extension of the scalar Epsilon algorithm, obtained by replacing the inverse of a real number in the scalar case, by the psoeudo-inverse of a vector in the vector case. The kernel of the vector Epsilon is the set of sequences transformed by the algorithm to stationnary sequences (the constant is a limit or anti-limit of the sequence). It is well-known that the kernel contains sequences satisfying some difference equations. In this paper, we show that this condition is only sufficient and that the kernel contains other kind of sequnces. We show also how the use of Clifford algebra, can be very helpful for understanding and deriving new results of the algorithm. In particular, we give necessary and sufficient condition for caracterizing the kernel. Examples for illustrations as well as geometrical interpretations are given.

References

[1] C. Brezinski, A. Salam, *Matrix and vector sequence transformations revisited*, Proc. Edinburgh Math. Soc., **38** (1995) 495-510.

[2] A. Salam, *An algebraic approach to the vector ε-algorithm*, Numer. Algorithms, **11** (1996) 327-337.

[3] P. Wynn, *Acceleration techniques for iterated vector and matrix problems*, Math. Comp., **16** (1962) 301–322.

Gaussian quadrature according to Gauss

J.M. Sanz-Serna[1]

[1] *Universidad Carlos III de Madrid, Spain*
email: jmsanzserna@gmail.com

Abstract

It is standard to present Gaussian quadrature in connection with orthogonal polynomials. However Gauss himself arrived at his quadrature rules by following a very different path. The talk will be a guided tour through Gauss's original memoir, a fascinating mathematical work that uses, in a masterly way, rational approximation, continued fractions, integral transforms, and many other resources. As any numerical analyst would do today, Gauss wraps up by presenting an experiment that shows the superiority of his approach when compared with other available techniques.

New numerical quadrature formulas of spectral accuracy for Hadamard finite parts of periodic divergent integrals

Avram Sidi[1]

[1] *Computer Science Department, Technion–Israel Institute of Technology, Haifa, Israel*
email: asidi@cs.technion.ac.il

Abstract

We consider the efficient numerical computation of Hadamard Finite Part (HFP) integrals

$$I[f] = \text{⨍}_a^b f(x)\,dx, \quad f(x) = \frac{g(x)}{(x-t)^m}, \quad g \in C^\infty[a,b], \quad m = 1,2,\ldots, \quad a < t < b,$$

$$f(x)\ \ T\text{-periodic}, \quad f \in C^\infty(\mathbb{R}_t), \quad \mathbb{R}_t = \mathbb{R} \setminus \{t + kT\}_{k=-\infty}^{\infty}, \quad T = b - a.$$

Such integrals, arise naturally in different scientific and engineering disciplines, such as fracture mechanics, elasticity, electromagnetic scattering, acoustics, to name some. Starting with a most recent generalization of the Euler–Maclaurin expansion [1], we determine the asymptotic expansion of the trapezoidal sum $h\sum_{j=1}^{n-1} f(t+jh)$, $h = T/n$, and use this and a "backward" extrapolation procedure to develop new numerical quadrature formulas we denote $\widehat{T}_{m,n}^{(s)}[f]$. For example, with $m = 3$, we have

$$\widehat{T}_{3,n}^{(0)}[f] = h\sum_{j=1}^{n-1} f(t+jh) - \tfrac{\pi^2}{3}\, g'(t)\, h^{-1} + \tfrac{1}{6}\, g'''(t)\, h$$
$$\widehat{T}_{3,n}^{(1)}[f] = h\sum_{j=1}^{n} f(t+jh-h/2) - \pi^2\, g'(t)\, h^{-1},$$
$$\widehat{T}_{3,n}^{(2)}[f] = 2h\sum_{j=1}^{n} f(t+jh-h/2) - \tfrac{h}{2}\sum_{j=1}^{2n} f(t+jh/2-h/4).$$

The important features of our formulas are as follows: (i) Unlike existing formulas that deal separately with each m (limited mostly to $m = 1, 2$), our formulas cover *all* values of m simultaneously. (ii) They are obtained by adding simple, yet sophisticated, "correction" terms to $h\sum_{j=1}^{n-1} f(t+jh)$. Thus, they are compact. (Most quadrature formulas in the literature have complex structures.) (iii) Unlike most quadrature formulas in the literature that achieve limited and low accuracy (like $O(n^{-\nu})$ for some small $\nu > 0$), our formulas achieve *spectral* accuracy, that is, for all m and s, we have $\widehat{T}_{m,n}^{(s)}[f] - I[f] = o(n^{-\mu})$ as $n \to \infty$ $\forall \mu > 0$.
We present numerical examples that confirm our theoretical results pertaining to the rates of convergence of the quadrature formulas developed. For details, see [2].

References

[1] A. Sidi, *Euler-Maclaurin expansions for integrals with arbitrary algebraic endpoint singularities*, Math. Comp. **81** (2012), no. 280, 2159–2173.

[2] A. Sidi, *Unified compact numerical quadrature formulas for Hadamard finite parts of singular integrals of periodic functions*, Calcolo **58** (2021), no. 2, article number 22.

Numerical approximation of the spectrum of self-adjoint operators and operator preconditioning

Tomáš Gergelits[1], Bjørn Fredrik Nielsen[2], Zdeněk Strakoš[1]

[1] *Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic*
email: gergelits@karlin.mff.cuni.cz, strakos@karlin.mff.cuni.cz

[2] *Faculty of Science and Technology, Norwegian University of Life Sciences, Norway*
email: bjorn.f.nielsen@nmbu.no

Abstract

We consider operator preconditioning $\mathcal{B}^{-1}\mathcal{A}$, which is employed in the numerical solution of boundary value problems. Here, the self-adjoint operators $\mathcal{A}, \mathcal{B} : H_0^1(\Omega) \to H^{-1}(\Omega)$ are the standard integral/functional representations of the partial differential operators $-\nabla \cdot (k(x)\nabla u)$ and $-\nabla \cdot (g(x)\nabla u)$, respectively, and the scalar coefficient functions $k(x)$ and $g(x)$ are assumed to be continuous throughout the closure of the solution domain. The function $g(x)$ is also assumed to be uniformly positive. When the discretized problem, with the preconditioned operator $\mathcal{B}_n^{-1}\mathcal{A}_n$, is solved with Krylov subspace methods, the convergence behavior depends on the distribution of the eigenvalues. Therefore it is crucial to understand how the eigenvalues of $\mathcal{B}_n^{-1}\mathcal{A}_n$ are related to the spectrum of $\mathcal{B}^{-1}\mathcal{A}$. Following the path started in the two recent papers published in SIAM J. Numer. Anal. [57 (2019), pp. 1369-1394 and 58 (2020), pp. 2193-2211], the first part of the talk addresses the open question concerning the distribution of the eigenvalues of $\mathcal{B}_n^{-1}\mathcal{A}_n$ formulated at the end of the second paper.

The second part generalizes some of the results to bounded and self-adjoint operators $\mathcal{A}, \mathcal{B} : V \to V^{\#}$, where $V^{\#}$ denotes the dual of V. More specifically, provided that $\mathcal{B}$ is coercive and that the standard Galerkin discretization approximation properties hold, we prove that the whole spectrum of $\mathcal{B}^{-1}\mathcal{A} : V \to V$ is approximated to an arbitrary accuracy by the eigenvalues of its finite dimensional discretization $\mathcal{B}_n^{-1}\mathcal{A}_n$.

The presented spectral approximation problem includes the continuous part of the spectrum and it differs from the eigenvalue problem studied in the classical PDE literature which addresses compact (solution) operators.

Optimal block size for block GMRES on GPUS

EriK G. Boman[1], Andrew J. Higgins[2], Daniel B. Szyld[2]

[1] *Sandia National Laboratories, Albuquerque, NM, USA*
email: egboman@sandia.gov
[2] *Temple University, Philadelphia, PA, USA*
email: andrew.higgins@temple.edu, szyld@temple.edu

Abstract

We report on our experiments with Block GMRES (BGMRES) on GPUs. We show that there are many cases in which BGMRES is slower than GMRES on CPUs, but faster on GPUs. Furthermore, when varying the number s of right hand sides, it is clear that there is an optimal such number, that is, one for which the advantage of BGMRES over GMRES is maximal. We develop a computational model, using CPU and GPU specific parameters such as latency, and communication time per word. The computational model shows qualitatively where this optimal value of s is, and helps exlpain this phenomena.

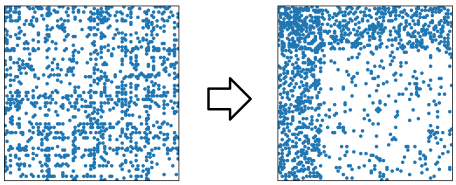
Optimal L-shaped matrix reordering via nonlinear matrix eigenvectors

Francesco Tudisco[1], Desmond J. Higham[2]

[1]School of Mathematics, Gran Sasso Science Institute, 67100 L'Aquila, Italy
email: francesco.tudisco@gssi.it
[2]School of Mathematics, University of Edinburgh, EH89YL Edinburgh, UK
email: d.j.higham@ed.ac.uk

Abstract

We are interested in finding a permutation of the entries of a given square matrix A, so that the maximum number of its nonzero entries are moved to one of the corners in a L-shaped fashion, as in the example figure below.



If we interpret the nonzero entries of the matrix as the edges of a graph, this problem boils down to the so-called core–periphery structure, consisting of two sets: the core, a set of nodes that is highly connected across the whole graph, and the periphery, a set of nodes that is well connected only to the nodes that are in the core.

Matrix reordering problems have applications in sparse factorizations and preconditioning, while revealing core–periphery structures in networks has applications in economic, social and communication networks.

This optimal reordering problem is a hard combinatorial optimization problem. In this work, we relax the combinatorial constraint and propose a method based on the continuous problem:

$$\max f(x) := \sum_{ij} |A_{ij}| \max\{x_i, x_j\} \qquad \text{s.t.} \qquad \|x\| = 1 \tag{1}$$

A solution of (1) would then be a vector that assigns a core score which indicates how "likely" it is that a node is in the core. While the quality measure f is still highly nonconvex and thus hardly treatable, we show that the global maximum of f coincides with the nonlinear Perron eigenvector of a suitably defined parameter dependent matrix $M(x)$, i.e. the positive solution to the nonlinear eigenvector problem $M(x)x = \lambda x$. Using recent advances in nonlinear Perron–Frobenius theory, we show that (1) has a unique solution and we propose a nonlinear power-method type scheme that allows us to solve (1) with global convergence guarantees and effectively scales to very large and sparse matrices. We present several numerical experiments showing that the new method largely outperforms baseline techniques.

References

[1] F. Tudisco, D. J. Higham *A nonlinear spectral method for core-periphery detection in networks*, SIAM J. Mathematics of Data Science **1** (2019), 269–292.

Construction of a sequence of orthogonal rational functions*

Niel Van Buggenhout[1], Marc Van Barel[1], Raf Vandebril[1]

[1]KU Leuven, Belgium
email: {niel.vanbuggenhout,marc.vanbarel,raf.vandebril}@kuleuven.be

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.

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The Weeks method for computing the forward Laplace transform in the complex plane

J.A.C. Weideman[1], Bengt Fornberg[2]

[1] *Stellenbosch University, South Africa*
email: weideman@sun.ac.za
[2] *University of Colorado at Boulder, USA*
email: Bengt.Fornberg@colorado.edu

Abstract

Numerical methods based on the Laplace transform are ubiquitous in scientific computing. Algorithms in the literature have focused predominantly on the computation of the inverse transform, the assumption presumably being that if the forward transform is needed then one can find it by analytical methods or table look-up. When these methods fail, the forward transform has to be computed numerically, a challenging task if the transform is needed in the left half of the complex plane. This need arises because many efficient inversion algorithms sample the transform at certain locations in the left half-plane. A method based on the well-known Weeks method [1] for the inverse transform is modified here for the computation of the forward transform. The method is compared with earlier methods based on sums of exponentials. A few applications are presented, including the solution of a fractional differential equation.

References

[1] W.T. Weeks, *Numerical inversion of the Laplace transform using Laguerre functions*, J. Assoc. Comput. Mach. **13** (1966), 419–429.