Student Krylov Day 2015

SIAM Student Chapter Delft

February 2, 2015

Preface

Krylov subspace methods have been applied successfully to solve various problems in Numerical Linear Algebra. The Netherlands have been a pioneer country in the development of Krylov methods over the past years. Methods like the Conjugate Gradient Squared (CGS), Bi-Conjugate Gradient Stabilized (BiCG-STAB), Nested GMRES (GMRESR), and the Induced Dimension Reduction method (IDR) are examples of Krylov methods developed at Dutch universities. In this context, we are proud to welcome Peter Sonneveld as invited speaker to our workshop. We are organizing the Student Krylov Day 2015 at TU Delft in the framework of the SIAM Student Chapter Delft.

Sponsors:

Program

The Student Krylov Day takes place on February 2nd, 2015 at Technische Universiteit Delft, Faculteit Elektrotechniek, Wiskunde en Informatica. We meet at **Snijderszaal LB 01.010.** Mekelweg 4, 2628 CD Delft, The Netherlands.

10:00 - 10:10		Welcoming
10:10 - 10:50	P. Sonneveld	IDR-CGS-BiCGSTAB-IDR(s) - a case of serendipity -
11:00 - 11:20	Manuel	Krylov methods for shifted linear systems
11:20 - 11:40	Xian-Ming	Recent progresses in Krylov subspace methods for solving complex symmetric linear systems
11:40 - 12:00	Ian	Krylov and Matrix Balancing for fast Field of Value Type Inclusion Regions
		Chairman: Reinaldo
12:00 - 13:30		Lunch at TU Delft Sports Center
13:30 - 13:50	Heiko	Preconditioning of Large-Scale Saddle Point Systems for Coupled Flow Problems
13:50 - 14:10	Jörn	A Krylov Subspace Approach to Modeling of Wave Propagation in Open Domains
14:10 - 14:30	Jing	A conjugate gradient based method for frictional contact problems
		Chairman: Tomáš
15:00 - 15:20	Tomáš	On the numerical behaviour of the CG method
15:20 - 15:40	Patrick	Krylov subspace methods for matrix equations which include matrix functions
15:40 - 16:00	Ana	On Low-rank Updates of Matrix Functions
		Chairman: Heiko
16:30 - 16:50	Reinaldo	Induced Dimension Reduction method to solve the Quadratic Eigenvalue Problem
16:50 - 17:10	Mario	Rational Least Squares Fitting using Krylov Spaces
17:10 - 17:30	Sarah	Probabilistic bounds for the matrix condition number with extended Lanczos bidiagonalization
		Chairman: Manuel
17:30 - 18:30		Snacks & drinks at TU Delft

In the evening we will go to San Marco (Brabantse Turfmarkt 23, 2611 CL Delft). This is a nice restaurant close to the main train station. Everybody is welcome to join!

IDR-CGS-BiCGSTAB-IDR(s)
- a case of serendipity -

Peter Sonneveld [1]

In about 1976, I was preparing a renovation of the elementary course on numerical analysis in Delft University. In relation to the problem of solving a single nonlinear equation iteratively, I wondered whether the so-called 'secant method' could be generalized to systems of N nonlinear equations with N unknowns.
Before starting to read everything on a subject, I always try to think about it unbiased, and so I started with (probably) re-inventing the wheel. Had I seen the book by Ortega and Rheinboldt at that time, CGS, BiCGSTAB and IDR(s) probably wouldn't exist today. After a week of rather primitive numerical experiments, I decided that generalisations of the secant method to N dimensions were far too complicated for an elementary course. However, the experiments showed a surprising phenomenon, that appeared to be useful in the machinery of solving large sparse nonsymmetric *linear* systems.
The first application of this 'new wheel' was called IDR (Induced Dimension Reduction). Afterwards, CGS (Conjugate Gradients Squared) was developed as an 'improvement' of IDR, and also for other reasons. From then, starting with BiCGStab in cooperation with Henk van der Vorst, a lot of other methods of this kind were developed by many others. This went on until about 10 years ago.
In this short presentation I'll give a reconstruction of the strange history of these so-called 'Lanczos-type product methods'. It will be explained why this 'sleeping theory' woke up just after my retirement in 2006, resulting in a brand new family of methods: IDR(s). Since history is a continuing story, also some recently discovered interesting features of the IDR(s) methods are already part of it. Some will be mentioned in the lecture.

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Krylov methods for shifted linear systems

Manuel Baumann

PhD student at TU Delft

In my research, we focus on Krylov methods for so-called *shifted linear systems* of the form

$$(A - \omega_k I)\mathbf{x}_k = \mathbf{b}, \tag{1}$$

where $\{\omega_k\}_{k=1}^{K} \in \mathbb{C}$ is a sequence of distinct *shifts*. During the last 20 years, almost every Krylov method has been adapted to solve (1) efficiently for many shifts. In my presentation, I will show you how multi-shift Krylov methods work and, afterwards, point to some more recent research questions like:

- Can we allow multiple right-hand sides?
- Which preconditioners preserve the shifted structure?
- Can we apply restarting and nested algorithms?
- Can we benefit from deflation?
- Where do shifted systems arise in practice?

One of the above questions has been answered in [1].

References

[1] M. Baumann and M.B. van Gijzen, *Nested Krylov methods for shifted linear systems*, Technical Report 14-01, Delft University of Technology, The Netherlands, 2014. Available for download at http://manuelbaumann.de/phd.html.

Recent progresses in Krylov subspace methods for solving complex symmetric linear systems

Xian-Ming Gu

PhD student at Rijksuniversiteit Groningen and University of Electronic Science and Technology of China

Complex symmetric linear systems (CSLSs) with the following form

$$A\boldsymbol{x} = \boldsymbol{b}, \quad A \neq A^H, \text{ but } A = A^T \in \mathbb{C}^{n\times n}, \quad \boldsymbol{b} \in \mathbb{C}^n$$

arise in many important applications such as numerical computations in quantum chemistry, eddy current problems, modeling the waveguide discontinuities and electromagnetic simulations. Hence, there is a strong need for the fast solutions of complex symmetric linear systems. During the past few years, a variety of specified Krylov subspace methods (KSMs) for solving such systems are proposed and used, such as COCG, COCR, QMR-SYM and BiCGCR methods.

In this talk, I will mainly revisit and focus on SCBiCG, which is also known as one of methods for solving such linear system. SCBiCG can be derived by substituting a matrix polynomial, which is expressed by the complex conjugate coefficient matrix and initial residual vector, to the initial shadow residual of the BiCG algorithm. Moreover, we clarify that SCBiCG can be transformed to some methods which have been previously proposed. Besides, in our talk we will prove that the preconditioned BiCGCR is mathematically equivalent to preconditioned COCR in detail, and then give an overview of the recent progress in other KSMs with suitable preconditioning techniques for solving CSLSs. Finally, numerical experiments involving many electromagnetic model problems are employed to investigate the convergence behaviors of these solvers, and then some remarks on future research of this topic will be also summarized.

This is joint work with Ting-Zhu Huang, Liang Li, Tomohiro Sogabe, Markus Clemens, Bruno Carpentieri, Hou-Biao Li.

Krylov and Matrix Balancing for fast Field of Value Type Inclusion Regions

Ian Zwaan*

PhD student at TU/e

The field of values may be an excellent tool for generating a spectral inclusion region: it is easy to approximate numerically, and for many matrices this region fits relatively tightly around the eigenvalues. However, for some matrices the field of values may be a poor eigenvalue inclusion region: the numerical radius may be much larger than the spectral radius. We show that balancing the matrix may be helpful for generating a quality inclusion region based on the field of values. and introduce a new Krylov based balancing method. We believe that both the (sparse) balancing and the new "Krylov and balance" technique, combined with a projected field of values, render spectral inclusion regions that may be hard to beat in both quality and efficiency.

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*Joint work with Michiel E. Hochstenbach

Preconditioning of Large-Scale Saddle Point Systems for Coupled Flow Problems

Heiko Weichelt

PhD student at Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg, Germany

In order to explore boundary feedback stabilization of coupled flow problems, we consider the Navier-Stokes equations that describe instationary, incompressible flows coupled with a diffusion convection equation. Using a standard finite element discretization, we get a differential-algebraic system of differential index two. We show how to reduce this index with a projection method to get a generalized state space system, where a linear quadratic control approach can be applied.

This leads to large-scale saddle point systems which have to be solved in a threefold nested iteration. For obtaining a fast iterative solution of those non-symmetric systems, we derive efficient preconditioners based on the approaches due to Wathen et al. [Elamn/Silvester/Wathen 2005, Stoll/Wathen 2011]. Finally, we show recent numerical results regarding the arising nested iteration.

A Krylov Subspace Approach to Modeling of Wave Propagation in Open Domains

Jörn Zimmerling

PhD student at TU Delft

Simulating electromagnetic or acoustic wave propagation in complex open structures is extremely important in many areas of science and engineering. In a wide range of applications, ranging from photonics and plasmonics to seismic exploration, efficient wave field solvers are required in various design and optimization frameworks.

In this talk, a Krylov subspace projection methodology is presented to efficiently solve wave propagation problems on unbounded domains. To model the extension of the computational domain to infinity, an optimal, frequency independent complex scaling method is introduced, that allows us to simulate wave propagation on unbounded domains provided we compute the propagating waves via a stability-corrected wave function.

In our Krylov subspace framework, this wave function is approximated by polynomial or rational functions, which are obtained via Krylov subspace projection on Polynomial, Extended and Rational Krylov subspaces. In this talk we compare the convergence within these three Krylov subspaces. Further we show how symmetry relations in the finite difference approximation of wave equations can be used to efficiently construct Polynomial and Extended Krylov subspaces.

Numerical examples illustrate the performance of the method and show that our Krylov resonance expansions significantly outperform conventional solution methods.

A conjugate gradient based method for frictional contact problems

J. Zhao, E.A.H. Vollebregt and C.W. Oosterlee

Delft Universiry of Technology

In the simulation of railway vehicles dynamics, the interaction between vehicles' wheels and rails attracts a lot of interest, involving the solution of frictional contact problems. Frictional stress arises between two contacting bodies when they are brought into relative motion. The question is to find out which parts of the surfaces are sticking together versus where local relative sliding occurs, and further to find the distribution of frictional stress. Fast solvers are demanded for such problems.

In this talk, I would like to present a conjugate gradient based method, called TangCG, which is incorporated in an active set strategy. One significant difference with the conventional solvers lies in the change of unknowns in the slip area, where the magnitude of tractions reaches the traction bound. Instead of using tractions there, we solve for angles, since they uniquely determine the tractions. This yields a transformation of the governing equations. A linearization technique is employed for some necessary approximation. Moreover, the fast Fourier transform (FFT) is adopted to accelerate the matrix-vector products encountered in the algorithm. Numerical tests confirm the efficiency and robustness of our method.

On the numerical behaviour of the CG method

Tomáš Gergelits

PhD student at Faculty of Mathematics and Physics, Charles University in Prague

The method of conjugate gradients (CG) is computationally based on short recurrences. Assuming exact arithmetic, they ensure global orthogonality of the residual vectors which span the associated Krylov subspace. Due to rounding errors in practical computations, however, the use of short recurrences leads to the loss of the global orthogonality and even linear independence of the computed residual vectors. Consequently, the computed Krylov subspaces are typically not of full dimensionality which causes a significant delay of convergence in finite precision CG computations.

As a result, the practical CG behaviour significantly differs, in general, from the behaviour of CG in exact arithmetic. Through the example of composite polynomial convergence bounds based on Chebyshev polynomials we show that any consideration concerning the CG rate of convergence relevant to practical computations may not assume exact arithmetic and must include the analysis of effects of rounding errors.

Furthermore, we address the question of the difference between Krylov subspaces generated by the CG method in finite precision arithmetic and their exact arithmetic counterparts. Apart from the loss of dimensionality, we observe that the computed Krylov subspaces remain very close to their exact arithmetic counterparts. This sort of inertia of finite precision CG computations represents a remarkable phenomenon which deserves further investigation.

Krylov subspace methods for matrix equations which include matrix functions

Patrick Kürschner

PhD student Max Planck Institute for Dynamics of Complex Technical Systems, Germany

We consider the numerical solution of large-scale Lyapunov equations of the form

$$AX + XA^T + f(A)BB^T + BB^T f(A) = 0, \quad A \in \mathbb{R}^{n\times n},\ B \in \mathbb{R}^{n\times m},$$

where f is an analytic function of A. Such matrix equations arise in certain model order reduction methods. Our focus are projection type approaches which employ rational or extended Krylov subspaces. For dealing with the above problem we propose efficient methods that deal with both the Lyapunov equation and the matrix function $f(A)$ at the same time.

On Low-rank Updates of Matrix Functions

Ana Šušnjara

PhD student at EPF Lausanne

The efficient and reliable update computation of large-scale matrix functions subject to low-rank perturbations is of interest in several applications, such as the analysis of networks. For addressing this problem, Beckermann and Kressner have proposed the use of tensor polynomial and rational Krylov subspace methods. Starting from the exactness property of (rational) Krylov subspaces, convergence bounds for the tensor Krylov subspace method have been derived. In this talk, we discuss how these bounds provide important insight into the choice of poles for setting up the rational Krlyov subspaces. In particular, we discuss $\exp(A)$ and $\mathrm{sign}(A)$. The matrix sign function immediately yields the corresponding spectral projector and we discuss how tensorized Krylov subspace methods can be used in the solution of eigenvalue problems. For the case of the matrix exponential, the error expansion in terms of $\varphi-$ functions as well as the resulting corrected scheme proposed by Saad are extended to the tensor Krylov subspace method. While the corrected scheme itself may not offer advantages, it has been observed useful in deriving stopping criteria.

Induced Dimension Reduction method to solve the Quadratic Eigenvalue Problem

Reinaldo Astudillo*

PhD student at TU Delft, The Netherlands

The Induced Dimension Reduction method (IDR(s)) was originally proposed for solving systems of linear equations, and recently adapted to solve the standard eigenvalue problem. In this talk, I am going to present an extension of IDR(s) to solve the Quadratic Eigenvalue Problem (QEP)

$$(\lambda^2 M + \lambda D + K)\mathbf{x} = \mathbf{0},$$

where M, D, and K are given matrices of order n. Using the short-recurrences formulas of IDR, we obtain a Hessenberg decomposition to approximate eigenvalues and eigenvectors of the linearized QEP. Also, exploiting the structure of the Krylov subspace vectors, we reduced the memory consumption of the proposed algorithm in almost a half. Numerical results generated by IDR for QEP are competitive with respect to another specialized algorithm like Second Order Arnoldi.

*Joint work with M. B. van Gijzen

Rational Least Squares Fitting using Krylov Spaces

Mario Berljafa* Stefan Güttel*

For given matrices $\{A, F\} \subset \mathbb{C}^{N \times N}$ and a vector $\mathbf{v} \in \mathbb{C}^N$, we consider the problem of finding a rational function $R_m^{\min}$ of type (m, m) such that

$$\|F\mathbf{v} - R_m(A)\mathbf{v}\|_2^2 \to \min,$$

and propose an iterative algorithm [1, 2] for its solution. At each iteration the algorithm constructs a rational Krylov space $\mathcal{Q}_{m+1}(A, \mathbf{v})$ and manipulates an associated Arnoldi decomposition to find better approximations to the poles of $R_m^{\min}$. In the special case when $A = \operatorname{diag}(\lambda_j)$ and $F = \operatorname{diag}(\psi_j)$ are diagonal we have a weighted rational least squares fitting problem $\sum_{j=1}^{N} |v_j|^2 \cdot |\psi_j - R_m(\lambda_j)|^2 \to \min$, and compare our method to the popular *vector fitting* [3].

References

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Probabilistic bounds for the matrix condition number with extended Lanczos bidiagonalization

Sarah W. Gaaf*

PhD student at Eindhoven University of Technology

Reliable estimates for the condition number of a large (sparse) matrix A are important in many applications. To get an approximation for the condition number $\kappa(A)$, an approximation for the smallest singular value is needed. Krylov subspaces are usually unsuitable for finding a good approximation to the smallest singular value. Therefore, we study extended Krylov subspaces which turn out to be ideal for the simultaneous approximation of both the smallest and largest singular value of a matrix. First, we develop a new extended Lanczos bidiagonalization method. With this method we obtain a lower bound for the condition number. Moreover, the method also yields probabilistic upper bounds for $\kappa(A)$. The user can select the probability with which the upper bound holds, as well as the ratio of the probabilistic upper bound and the lower bound.

*Joint work with Michiel E. Hochstenbach

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We will tweet about the workshop using the account `@SSC_Delft` and hashtag `#KD15`.

http://sscdelft.github.io/