PROGRAM

Time	**Wednesday 15th May**
9h – 9h 30	Welcome of participants
9h 30– 10h 30	Valeria Simoncini (University of Bologna, Italy) Computational aspects in large scale matrix functions approximations Lesson 1
10h30 – 11h00	Coffee break
11h 00– 12h 30	Valeria Simoncini Lesson 2
13h 00 - 14h 30	Lunch (Restaurant Universitaire Charles Barrois)
14h 30 – 16h 00	Valeria Simoncini Lesson 3
16h 00 - 16h 30	Coffee break
16h 30 - 18h 00	Lothar Reichel (University of Kent, USA) Error bounds and estimates for matrix functions Lesson 1

Time	**Thursday16th May**
9h 30– 10h 30	Lothar Reichel Lesson 2
10h30 – 11h00	Coffee break
11h 00– 12h 30	Lothar Reichel Lesson 3
13h 00 - 14h 30	Lunch (Restaurant Universitaire Charles Barrois)
14h 30 – 16h 00	Paul Van Dooren (Université Catholique de Louvain) Model reduction of large scale dynamical systems Lesson 1
16h 00 - 16h 30	Coffee break
16h 30 - 18h 00	Paul Van Dooren Lesson 2
20h 00	Conference Dinner

Time	**Friday 17th May**
9h 30– 10h 30	Paul Van Dooren Lesson 3
10h30 – 11h30	Coffee break and POSTER session
11h 30– 12h 30	Michele Benzi (University of Emory, USA) Theory and computation of matrix functions with applications to network analysis and quantuum chemistry Lesson 1
13h 00 - 14h 30	Lunch (Restaurant Universitaire Charles Barrois)
14h 30 – 16h 00	Michele Benzi Lesson 2
16h 00 - 16h 30	Coffee break
16h 30 - 18h 00	Michele Benzi Lesson 3

Lectures

Theory and Computation of Matrix Functions with Applications to Network Analysis and Quantum Chemistry

Michele Benzi
Emory University, Georgia, USA

The purpose of these lectures is to introduce the audience to some mathematical and computational aspects of matrix functions relevant for applications in two major areas: network analysis and quantum chemistry. While these two applications appear to be rather far removed from each other, there are interesting points of contact and even overlap between the two. Indeed, not only many of the matrix functions that are found to be fundamental in these two areas are essentially the same, but also similar techniques, in particular from classical approximation theory, are used to study and to numerically evaluate these matrix functions.

In the lectures we will emphasize issues related to sparsity, decay, and the use of computational methods based on Chebyshev polynomials, the Lanczos algorithm, and matrix moments.

The only prerequisites are a basic knowledge of linear algebra and numerical analysis. The necessary background material on graphs, networks, approximation theory and the applications will be provided during the lectures or by means of printed material distributed in advance of the course.

Tentative table of contents

- Introduction to the analysis of complex networks using matrix functions.
- Functions of symmetric adjacency matrices and graph Laplacians.
- The case of directed networks.
- Lanczos-based approaches to estimating matrix functions relevant to network analysis.
- Matrix functions in quantum chemistry.

- Decay results for functions of sparse matrices, with applications.

Tentative bibliography

- M. Benzi, P. Boito and N. Razouk, "Decay properties of spectral prjectors with applications to electronic structure", SIAM Review, 55(1) (2013), pp. 1–62.
- M. Benzi, E. Estrada and C. Klymko, "Ranking hubs and authorities using matrix functions", Linear Algebra and its Applications, published online, December 2013. DOI:10.1016/j.laa.2012.10.022
- M. Benzi and G. H. Golub, "Bounds for the entries of matrix functions with applications to preconditioning", BIT, 39 (1999), pp. 417–438.
- M. Benzi and N. Razouk, "Decay bounds and $O(n)$ algorithms for approximating functions of sparse matrices", ETNA, 28 (2007), pp. 16–39.
- E. Estrada, "The Structure of Complex Networks: Theory and Applications", Oxford University Press, Oxford, UK, 2012.
- E. Estrada, N. Hatano, and M. Benzi, "The physics of communicability in complex networks", Physics Reports, 514 (2012), pp. 89–119.
- E. Estrada and D. J. Higham, "Network properties revealed by matrix functions", SIAM Review, 52 (2010), pp. 696–714.
- N. J. Higham, "Functions of Matrices: Theory and Computations", SIAM, Philadelphia, PA, 2008.
- G. H. Golub and G. Meurant, "Matrices, Moments and Quadrature with Applications", Princeton University Press, Princeton, NJ, 2010.

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Model reduction of large scale dynamical systems

Paul Van Dooren
Département d'ingénierie mathématique
Université catholique de Louvain, Belgium

Model reduction aims at replacing a system of differential or difference equations of high complexity by one of much lower complexity. In so doing, one tries to preserve certain critical properties of the system (e.g. stability) and approximate well important features (e.g. the system response). During the last two decades, a lot of progress has been made in the theory of this approximation problem. The first part of the course will review the foundations of this theory and will present the key results of frequency and time domain approximations (Grammian based balanced truncation and Hankel norm approximation). More recently, the need has arisen to apply these methods to problems of very high complexity; in such cases the resulting computational complexity becomes prohibitively high and different approaches to the problem have to be developed. In the second part of the course we will present techniques that can be applied to large scale systems provided the models are sparse or structured (Padé like approximations and Krylov based methods). Basic knowledge of systems theory (state-space models) and some background in linear algebra and numerical linear algebra is recommended.

Tentative table of contents

- Introduction to Approximation of State-Space Models
- Gramians of State-Space Models and Balanced Realizations
- Balanced Truncation and Hankel Norm Approximations
- Approximation by Moment Matching and Rational Interpolation
- Padé Approximations and the Lanzcos Algorithm
- Multi Point Padé Approximations
- Krylov Space Methods

- Extensions to Time Varying Systems

Tentative bibliography

- A. C. Antoulas. Approximation of Large-Scale Dynamical Systems. Siam Publications, Philadelphia (2005).
- J. Ball, I. Gohberg and L. Rodman. Interpolation of Rational Matrix Functions, Birkhauser Verlag (1990).
- A. Bunse-Gerstner, D. Kubalinska, G. Vossen, and D. Wilczek. H2-norm optimal model reduction for large-scale discrete dynamical MIMO systems. Internal Report Bremen University, 2007.
- K. Gallivan, A. Vandendorpe, and P. Van Dooren. Sylvester equations and projection-based model reduction. J. Comp. Appl. Math., 162:213-229, 2004.
- K. Gallivan, A. Vandendorpe, and P. Van Dooren. Model reduction of MIMO systems via tangential interpolation. SIAM J. Matrix Anal. Appl., 26(2):328-349, 2004.
- S. Gugercin. Projection methods for model reduction of large-scale linear dynamical systems. PhD Thesis, ECE Dept., Rice Univ., December 2002.
- S. Gugercin, A. Antoulas and C. Beattie. H2 model reduction for large-scale linear dynamical systems. SIAM J. Matrix Anal. Appl., 30:609-638, 2008.
- L. Meier and D. Luenberger. Approximation of linear constant systems. IEEE Trans. Aut. Contr., 12:585-588, 1967.
- P. Van Dooren, K. Gallivan and P.-A. Absil. H2-optimal model reduction of MIMO systems. Appl. Math. Lett., 21(12):1267-1273, 2008.

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Error Bounds and Estimates for Matrix Functions

Lothar Reichel
Kent State University, Ohio, USA

Let A be a square matrix and f a function that is analytic in a set Ω in the complex plane that contains the spectrum of A. For many such functions, the value $f(A)$ is typically typically computed by first approximating f by a polynomial or rational function, and then evaluating the latter. These lectures will discuss approaches to bound or estimate the error in the computed approximations. We will first review error bounds for polynomial and rational approximation of analytic functions on regions in the complex plane and then discuss how these bounds shed light on convergence of the error for best polynomials and rational approximants as their degree or order is increased. K-spectral sets are introduced and their application to the determination of error bounds is explored. We define the Faber transform and show how it allows us to map approximation problems on simply connected sets in the complex plane to approximation problems on the unit disk. This transform also can be helpful for computing near-best polynomial and rational approximants. Finally, we describe the application of the Cauchy transform to the computation of matrix functions. In particular, we discuss the evaluation of the Cauchy transform with the aid of quadrature rules.

In some application, one is interested in evaluating expressions of the form $V^T f(A)W$, where the matrices V and W have many more rows than columns. We will discuss how estimates of upper and lower bounds for each entry can be determined with the aid of Gauss and anti-Gauss quadrature rules.

Tentative table of contents

- Polynomial and rational approximation in the complex plane by interpolation: Error bounds, conformal mapping.
- The Faber transform, standard and rational Krylov methods, error bounds.

- Application of the Cauchy integral to the evaluation of matrix functions. Gauss and anti-Gauss quadrature rules for determining error bounds or estimates of bounds.

Tentative bibliography

- To be completed.

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Computational aspects in large scale matrix function approximations

Valeria Simoncini
Universitá di Bologna, Italy

This series of lectures will focus on some main computational issues one has to face when numerically approximating the action of a matrix function to a vector, as it occurs in many large scale application problems.

We will first survey two of the main streams of action: rational function approximation, including contour integrals, and projection-type methods. We will emphasize the pros and cons of these two venues, and point to their similarities and connections.

We will then discuss the effective application of these strategies to some well established frameworks stemming from the numerical solution of evolutionary PDE problems.

If time allows, we will show how matrix function approximation strategies have motivated the numerical solution of other, apparently unrelated, mathematical problems.

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Posters

Superlinear convergence of the rational Arnoldi method for the approximation of matrix functions

Bernd Beckermann
Université de Lille (France)

A superlinear convergence bound for rational Arnoldi approximations to functions of matrices is derived. This bound generalizes the well-known superlinear convergence bound for the CG method to more general functions with finite singularities and to rational Krylov spaces. A constrained equilibrium problem from potential theory is used to characterize a max-min quotient of a nodal rational function underlying the rational Arnoldi approximation, where an additional external field is required for taking into account the poles of the rational Krylov space. The resulting convergence bound is illustrated at several numerical examples, in particular, the convergence of the extended Krylov method for the matrix square root.

Joint work with Stefan Gttel (Manchester).

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Fast computation of centrality indices for complex networks

Caterina Fenu
University of Cagliari (Italy)
Kent State University, Ohio (USA)

In complex networks theory, matrix functions can be used to extract global information from a graph G, when applied to its adjacency matrix. We will introduce a new computational method to rank the nodes of an undirected unweighted network according to the values of these functions. The procedure uses a low-rank approximation of the adjacency matrix, in order to obtain a list of nodes candidates to being the most important, their ranking is then refined by using an algorithm based on Gauss quadrature. The method is compared to other approaches to perform the computation, both on a set of test problems, and on real networks coming from applications, e.g. in software engineering, bibliometry and social network. This is a joint work with D. Martin, L. Reichel, G.Rodriguez.

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A residual based error estimate for the Leja interpolation

Peter Kandolf
University of Innsbruck , Austria

Exponential integrators require a reliable implementation of the action of the matrix exponential and related φ functions. For possibly large matrices an approximation up to a certain tolerance needs to be obtained in an efficient way. In this work we consider the Leja method for performing this task. Our focus lies on an a posteriori error estimate of the method. We introduce the notion of a residual based error estimate where the residual is obtained from differential equations defining the φ functions. The properties of this new error estimate are investigated and compared to the existing a posteriori estimate. Further, a numerical investigation is performed based on test examples from spatial discretizations of time dependent partial differential equations in two and three space dimensions. The experiments show that this new approach is robust for various types of matrices and applications.

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A moment-matching Arnoldi method for phi-functions

Antti Koskela
University of Innsbruck , Austria

We consider a new Krylov subspace algorithm for computing expressions of the form $\sum_{k=0}^{p} h^k \varphi_k(hA) w_k$, where $A \in \mathbb{C}^{n\times n}$, $w_k \in \mathbb{C}^n$, and φ_k are matrix functions related to the exponential function. Computational problems of this form appear when applying exponential integrators to large dimensional ODEs in semilinear form $u'(t) = Au(t) + g(u(t))$. Using Cauchy's integral formula we give a representation for the error of the approximation and derive a priori error bounds which describe well the convergence behaviour of the algorithm. In addition an efficient a posteriori estimate is derived. Numerical experiments in MATLAB illustrating the convergence behaviour are given.

This is a joint work with Alexander Ostermann.

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Approximation of the transfer function and of quadratic forms

Zdeněk Strakoš
Charles University of Prague

Model reduction in linear dynamical systems can be formulated (in a simplified form) as an approximation of the transfer function $T(\lambda) = c^*(\lambda I - A)^{-1}b$ using the reduced order matrices and vectors A_n, I_n, c_n, and b_n. Approximation of the quadratic form $c^*A^{-1}b$ can seemingly be interpreted as using the previous approach with taking $\lambda = 0$. This, however, does not lead to efficient numerical algorithms for the second problem. In the contribution we give a short overview of the existing approaches with emphasizing their computational efficiency and numerical stability properties.

This is a joint work with Petr Tichý.

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Sparse matrix reordering via the eigenvectors of Laplacian

Omer Tari
Middle East Technical University

We present a new sparse matrix reordering scheme which uses the eigenvectors of the Laplacian of a given sparse matrix. Using this reordering, we show that one can obtain a sparsity structure similar to saddle point problems. We show the effectiveness of our scheme by applying it on sparse matrices from the University of Florida Sparse Matrix Collection.

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