Computational aspects in large scale matrix function approximations

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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.

Tentative table of contents
– To be completed.

Tentative bibliography
– To be completed.

Error Bounds and Estimates for Matrix Functions

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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.

Model reduction of large scale dynamical systems

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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

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– A. C. Antoulas. Approximation of Large-Scale Dynamical Systems. Siam Publications, Philadelphia (2005).
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Theory and Computation of Matrix Functions with Applications to Network Analysis and Quantum Chemistry

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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.

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– M. Benzi and N. Razouk, "Decay bounds and $O(n)$ algorithms for approximating functions of sparse matrices", ETNA, 28 (2007), pp. 16–39.
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