Luka Grubišić

RandLRAP Workshop 2024

Validating tensor reduced resolvent sampling algorithms and tensor structured DEIM

HRZZ IP2019-4-6268 Randomized low rank algorithms and applications to parameter dependent problems

HrZZ
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Contents

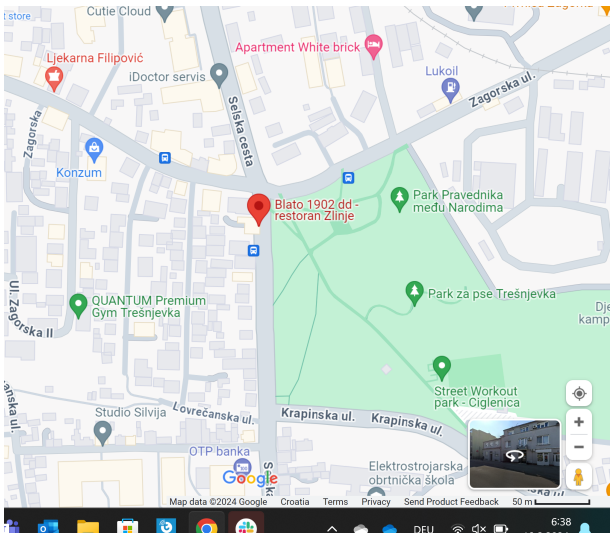
Programme

Monday 18.03.2024.

13:00-13:45	Daniel Kressner	105
14:00-15:00	Luka Grubišić	105
15:00	Lunch	001

Tuesday 19.03.2024.

12:15-13:00	Harri Hakula	105
13:00-13:30	Zvonimir Bujanović	105
13:30-14:00	Ivana Šain Glibić	105
14:00	Coffee break	108
15:45 - 16:15	Marko Hajba	108
16:15 - 16:45	Nela Bosner	108
19:30	Dinner `https://blato1902.hr/poslovnice/poslovnice-zagreb/`	



First session

Randomization for solving difficult linear algebra problems

Daniel Kressner
EPFL, Swizerland

Randomized algorithms are becoming increasingly popular in matrix computations. Recent software efforts, such as RandLAPACK, testify that randomization is on the brink of replacing existing deterministic techniques for several large-scale linear algebra tasks. The poster child of these developments, the randomized singular value decomposition is nowadays one of the state-the-of-art approaches for performing low-rank approximation. In this talk, we will discuss numerous further examples for the potential of randomization to facilitate the solution of notoriously difficult linear algebra tasks. This includes a simple numerical algorithm for jointly diagonalizing a family of nearly commuting matrices, the solution of challenging singular and nonlinear eigenvalue problems, as well as the low-rank approximation of matrix functions and matrix-valued functions. A common theme of all these developments is that randomization helps turn linear algebra results that only hold generically into robust and reliable numerical algorithms.

This talk is based on joint work with Alice Cortinovis, Stefan Güttel, Haoze, Hysan Lam, David Persson, Bor Plestenjak, Ivana Sain Glibic, Bart Vandereycken, and others.

Low rank methods for mesh adapted solutions of eigenvalue problems with Kronecker product structure - WP O4

Grubisic Luka
UNIZG-PMF-MO, Croatia

Solving stationary problems for operators with the Kronecker product structure (operators expressible as sums of Kronecker products) can be reduced to analyzing the solutions of operator Laypunov equations. We present a mesh adaptation algorithm for constructing piece-wise polynomial spaces of lowermost degree where we can achieve guaranteed approximation errors for the solutions of the spectral problem (eigenvalues and spectral projections). We further discus the use of randomised sampling techniques using Khatri-Rao products of random vectors to further economise the computational burden.

This is a joint work with Harri Hakula, Daniel Kressner, Zoran Bujanović and Haoze, Hysan Lam.

Second session

On Multiparamatric Eigenvalue Problems

Harri Hakula
Aalto University, Finland

Deterministic stochastic partial differential equations have received a lot of attention over the past twenty years. Both intrusive and non-intrusive methods have been proposed with emphasis on the non-intrusive ones due to natural desire to preserve existing investment in software. Random information is typically introduced via truncated Karhunen-Loeve expansions, where the coefficients are assumed to be i.i.d. with some known distributions.

The number of the coefficients is the dimension of the parameter space. The multiparametric PDE eigenvalue problems have their own characteristic features that have led much slower progress than in the static problems. First, all eigenmodes must be normalised over the whole parameter space. Second, the right quantity of interest is a subspace and not an individual eigenmode.

In this talk features of multiparametric eigenvalue problems are illustrated via numerical experiments covering multiple sources of uncertainty including material parameters and domains.

Randomized algorithms for large-scale eigenvalue problems

Zvonimir Bujanović
UNIZG-PMF-MO, Croatia

In this talk, we discuss two approaches to solving large-scale eigenvalue problems for matrices that have a special structure: they are short sums of Kronecker products. Such matrices occur, e.g., from the discretization of PDE eigenvalue problems on tensor product domains. Both approaches use randomized algorithms, but from very different perspectives.

First, we study a method based on contour integration of the matrix resolvent. Computing the eigenvalues of the matrix A that lie inside a contour $\Gamma \subseteq \mathbb{C}$ reduces to approximating the integral of the resolvent applied to a random matrix Ω by using a quadrature formula. In order to drastically increase the computational efficiency, it is advantageous to run the algorithm with Ω that is compatible with the underlying structure of the problem. Therefore, instead of using standard random Gaussian matrices, in this talk we discuss the use of random Khatri–Rao product

matrices: each column of Ω is generated as the Kronecker product of two Gaussian random vectors. We provide theoretical and numerical evidence that the use of such structured random matrices Ω instead of unstructured Gaussian random matrices leads to good estimates.

The second method we analyze is the LOBPCG method for computing extreme eigenvalues of a large symmetric positive definitive matrix. This method can also be implemented so that it exploits a random initial iteration with a Khatri–Rao product structure. We show that this is possible by keeping the subsequent iterations in a low-rank factored form, and by limiting the rank of the iterates via recompression. This does not hamper convergence, and leads to an efficient algorithm.

This is joint work with Luka Grubišić, Daniel Kressner, and Hysan Lam.

Singular quadratic eigenvalue problem: Linearization and weak condition numbers

Ivana Šain Glibić
UNIZG-PMF-MO, Croatia

In this talk we will study the numerical computation of singular quadratic eigenvalue problem associated with matrix polynomial $Q(\lambda) = \lambda^2 M + \lambda C + K$ such that $\det(Q(\lambda)) \equiv 0$. Since small matrix perturbation of singular problems can move eigenvalues anywhere in the complex plain these problems are known to be ill–conditioned. However, it was recognized by Wilkinson, and later proven by De Terán, Dopico and Moro that perturbation directions causing arbitrary large eigenvalue changes are rare.

More recently, in order to quantify the eigenvalue sensitivity, Lotz and Noferini introduced the so called δ–weak condition number.

Since linearization is logical first step for the solution of polynomial eigenvalue problems, we prove that one can always choose the linearization for this problem so that δ–weak condition number increases only marginally. We propose an algorithm for computing well–conditioned eigenvalues of singular quadratic eigenvalue problem by adding random perturbations to the coefficients. As a criterion for detecting and excluding spourious eigenvalues created from the singular part, we use eigenvalue condition number. We prove that this is, with high probability, a reliable criterion.

This is joint work with Daniel Kressner.

Tensorial Neural Networks for Eigenvalue Problems

Hajba Marko
Virovitica University of Applied Sciences, Croatia

We study eigenmode localization for a class of elliptic reaction-diffusion operators. As the prototype model problem we use a family of Schrödinger Hamiltonians parametrized by random potentials. Our computational model is posed in the truncated finite domain, and this is an approximation of the standard Schrödinger Hamiltonian. Our chosen task is to compute localized bounded states at the lower end of the spectrum. Tensorial neural networks (TNN) are used as surrogate models which represent dependence of the ground state or landscape function on the localizing potential, depending on a problem we are solving. Tensor neural networks contain large compress dense layers, reducing the number of parameters in a neural network through the use of truncated tensor factorizations. Further, we will also demonstrate the use of Variational Physics Informed Neural Network, together with the residual type error estimates, to obtain the ground state of the eigenvalue problem. Error estimators will be introduced to monitor the performance of the model. We present a host of numerical experiments to benchmark the accuracy and performance of the proposed algorithms.

Parallel Prony's method with multivariate matrix pencil approach

Bosner Nela
UNIZG-PMF-MO, Croatia

Prony's method is a standard tool for parameter identification in sparse exponential sums

$$f(k) = \sum_{j=1}^{T} c_j e^{-2\pi i \langle t_j, k \rangle}, \quad k \in \mathbb{Z}^d,$$

where the parameters are pairwise different $\{t_j\}_{j=1}^M \subset [0,1)^d$, and nonzero $\{c_j\}_{j=1}^M \subset \mathbb{C} \setminus \{0\}$. The focus of our investigation is on a Prony's method variant based on a multivariate matrix pencil method [M. Ehler et al.,2019]. The method constructs matrices $S_1, \ldots, S_d$ from the sampling values, and their simultaneous diagonalization yields the parameters $\{t_j\}_{j=1}^M$. The joint eigenbasis is obtained from the eigendecomposition of a single matrix that is random linear combination of $S_1, \ldots, S_d$. The parameters $\{c_j\}_{j=1}^M$ are computed as the solution of an linear least squares problem, where the matrix of the problem is determined from $\{t_j\}_{j=1}^M$. Since the method involves independent generation and manipulation of certain number of matrices, there is intrinsic capacity for parallelization of the whole computation process on several levels. On the first level, the tasks concerning generation of matrices is divided among GPU's block of threads and CPU, where heavier load is put on the GPU. On the second level, the individual threads are dealing with individual matrix elements. From the algorithmic point of view, the CPU is dedicated to the more

complex tasks of computing SVD, eigendecomposition, and solution of the least squares problem, while the GPU is performing matrix–matrix multiplications and summations. With careful choice of the algorithms solving the subtask, the load between CPU and GPU can be balanced. Besides the parallelization techniques, we are also concerned with some numerical issues, and we provide some numerical analysis results of the method.

Author Index