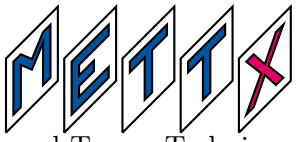

Matrix Equations and Tensor Techniques X
Aachen, September 13–15, 2023

Book of Abstracts

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Sketched and truncated Krylov subspace methods for matrix equations

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Sketching can be seen as a randomized dimensionality reduction technique able to preserve the main features of the original problem with probabilistic confidence. This kind of technique is emerging as one of the most promising tools to boost numerical computations and it is quite well-known by theoretical computer scientists. Nowadays, sketching is gaining popularity also in the numerical linear algebra community even though its use and understanding are still limited.

In this talk we will present cutting-edge results about the use of sketching in numerical linear algebra. In particular, we will focus on showing how sketching can be successfully combined with Krylov subspace methods. We will specialize our results to the solution of large-scale matrix equations but similar techniques can be applied to a variety of important algebraic problems, including the solution of linear systems, eigenvalue problems, and the numerical evaluation of matrix functions.

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A defect-correction algorithm for quadratic matrix equations, with applications to quasi-Toeplitz matrices

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We address the problem of solving a quadratic matrix equation $A_1X^2+A_0X+A_{-1}=0$, where the matrix coefficients A_i, $i=-1,0,1$, and the sought solution G, are infinite matrices endowed with the quasi-Toeplitz structure (QT matrices).

Since the Toeplitz part of the solution G can be easily computed, we introduce a method based on a defect correction formula, to exploit this information.

More specifically, assume that $\widetilde{G}$ is an approximation of the sought solution G. Then, by following the ideas of [2] and [3], we derive an equation for the defect $H=G-\widetilde{G}$ and express H in terms of an invariant subspace of a suitable pencil. This equation allows us to introduce a modification of the Structure-preserving Doubling Algorithm (SDA), that enables refining an initial approximation to the sought solution.

Numerical experiments confirm the effectiveness of the proposed method. More details can be found in [1].

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On the benefits of the LDL^T factorization for (large-scale) Riccati equations

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Our object of interest is the general continuous-time symmetric algebraic Riccati equation (ARE) of the form

$$A^\mathsf{T}XE + E^\mathsf{T}XA + C^\mathsf{T}QC - (E^\mathsf{T}XB + S)R^{-1}(B^\mathsf{T}XE + S^\mathsf{T}) = 0, \tag{1}$$

where $A, E \in \mathbb{R}^{n\times n}$, with E invertible, $B, S \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$, $Q \in \mathbb{R}^{p\times p}$ symmetric, and $R \in \mathbb{R}^{m\times m}$ symmetric and invertible.

Equation (1) shows up in various system-theoretic contexts, in which it is of particular interest to find—if it exists—the stabilizing symmetric solution $X \in \mathbb{R}^{n\times n}$ of (1) such that the matrix $A - BR^{-1}(B^\mathsf{T}XE + S^\mathsf{T})$ is Hurwitz. The most well-known application is the linear quadratic optimal control problem, where R is positive definite in addition. However, the formulation above also allows to cover equations relevant, for example, in model order reduction related to energy functions similar to balanced truncation. In particular, for model order reduction of passive systems via positive-real balanced truncation; see, e.g., [7]; Riccati equations with a positive sign in front of the quadratic term are needed. This can be covered by (1) choosing R^{-1} to be negative definite.

While for the RADI [1] algorithm and Krylov subspace projection methods [5, 6, 3] the benefit of using an LDL^T-type factorization of the solution X of (1) is evident from the procedures, in this contribution we are focusing on Newton-type approaches. For special formulations of (1), there exist Newton-type solvers in the literature [4, 2]. However, except for the standard LQR ARE; i.e., $S = 0$, Q symmetric positive semi-definite and R

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symmetric positive definite in (1); the Lyapunov equations solved in the Newton steps have indefinite right-hand sides. When aiming for low-rank factored solutions, the authors of [2] suggest splitting this into two Lyapunov equations with definite right-hand sides and compute the solution by superposition. This approach roughly doubles the costs of each Newton step. Moreover, this technique has been observed to be highly numerically unstable in the context of Rosenbrock solvers for differential Riccati equations, leading to the suggestion to use instead a factorization of the form $X = LDL^{\mathsf{T}}$, with D symmetric but potentially indefinite.

In this contribution, we follow up on this idea and formulate a general Newton method for (1) in terms of this type of factorization. This allows us to efficiently compute the solution of (1) in the case of large-scale sparse coefficient matrices.

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An extension of the low-rank Lyapunov ADI to non-zero initial values and its applications

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We derive the Alternating-Direction Implicit (ADI) method based on a commuting operator split following Schulze [6] and apply the results to the Lyapunov equation

$$AXE^T + EXA^T = -GSG^T \tag{1}$$

with low-rank constant term and approximate solution $X \approx LDL^T$. Previously, it has been mandatory to start the low-rank ADI with zero. The approach above generalizes the iteration scheme of Li and White [5] and the residual formulation of Benner, Kürschner, and Saak [2] to arbitrary initial values for the ADI method in a low-rank setting at the expense of an indefinite residual.

We demonstrate the benefit of arbitrary initial values using two other algorithms. First, we solve a differential Riccati equation with a first-order Rosenbrock method. Each time step requires the solution of an algebraic Lyapunov equation; see e.g., Lang, Mena, and Saak [4]. Due to the smoothness of the solution, the solution at the previous time step is a natural candidate to start the ADI with.

Second, we solve an algebraic Riccati equation with the Newton-ADI method; see e.g., Benner, Li, and Penzl [3]. Every Newton step requires the solution of a Lyapunov equation. Thus, the solution of the previous Newton step is a natural candidate to start the ADI with. We investigate whether such an ADI warm start makes the Newton-ADI method competitive to the RADI method of Benner et al. [1].

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Inexact Low-rank Sylvester ADI

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We consider large-scale Sylvester equations

$$AX + XB + fg^T = 0, \quad A \in \mathbb{R}^{n\times n}, \quad B \in \mathbb{R}^{m\times m}$$

with an inhomogeneity of low rank, $f \in \mathbb{R}^{n\times s},\ g \in \mathbb{R}^{m\times s},\ s \ll n, m$.
The low-rank ADI iteration [2], [3] iteratively computes a low-rank solution approximation $X \approx ZY^T$ with $Z \in \mathbb{R}^{n\times r},\ Y \in \mathbb{R}^{m\times r},\ r \ll n, m$. In every iteration step of this process one has to solve two shifted linear systems

$$(A + \beta_k I_n)v_k = s_{k-1} \quad (B + \alpha_k I_m)^T w_k = t_{k-1}, \quad k \geq 1$$

for $v_k,\ w_k$. We investigate the situation when those inner linear systems are solved inexactly by an iterative methods such as, e.g., preconditioned Krylov subspace methods. For this we first review this situation in the easier case of Lyapunov equations and the associated inexact Lyapunov low-rank ADI iteration investigated in [1] . Then we present estimates for the required accuracies regarding the inner linear systems which dictate when the employed inner Krylov subspace methods can be safely terminated. The goal is to save some computational effort without endangering the functionality of the low-rank Sylvester-ADI method. Ideally, the inexact ADI method mimics the convergence behavior of the more expensive exact ADI method. For the pair of linear systems in every step of the low-rank Sylvester-ADI iteration, there is also the interesting question if a low solution accuracy for one linear system can be compensated by a higher solution accuracy for the other linear system. If time permits, we will also show some possible applications to more general linear matrix equations.

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Projected exponential methods for stiff dynamical low-rank approximation problems

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The numerical integration of stiff equations is a challenging problem that needs to be approached by specialized numerical methods. Exponential integrators [2] form a popular class of such methods since they are provably robust to stiffness and have been successfully applied to a variety of problems. The dynamical low-rank approximation [3] is a recent technique for solving high-dimensional differential equations by means of low-rank approximations. However, the domain is lacking numerical methods for stiff equations since existing methods [1, 4, 5] are either not robust-to-stiffness or have unreasonably large hidden constants, see Figure 1.

In this talk, we focus on solving large-scale stiff matrix differential equations with a Sylvester-like structure,

$$\dot{X}(t) = AX(t) + X(t)B + G(t, X(t)), \quad X_0 = X(0),$$

that admit good low-rank approximations. We propose two new methods that have good convergence properties, small memory footprint and that are fast to compute. The theoretical analysis shows that the new methods have order one and two, respectively. We also propose a practical implementation based on Krylov techniques. The approximation error is analyzed, leading to a priori error bounds and, therefore, a mean for choosing the size of the Krylov space. Numerical experiments are performed on several examples, confirming the theory and showing good speedup in comparison to existing techniques.

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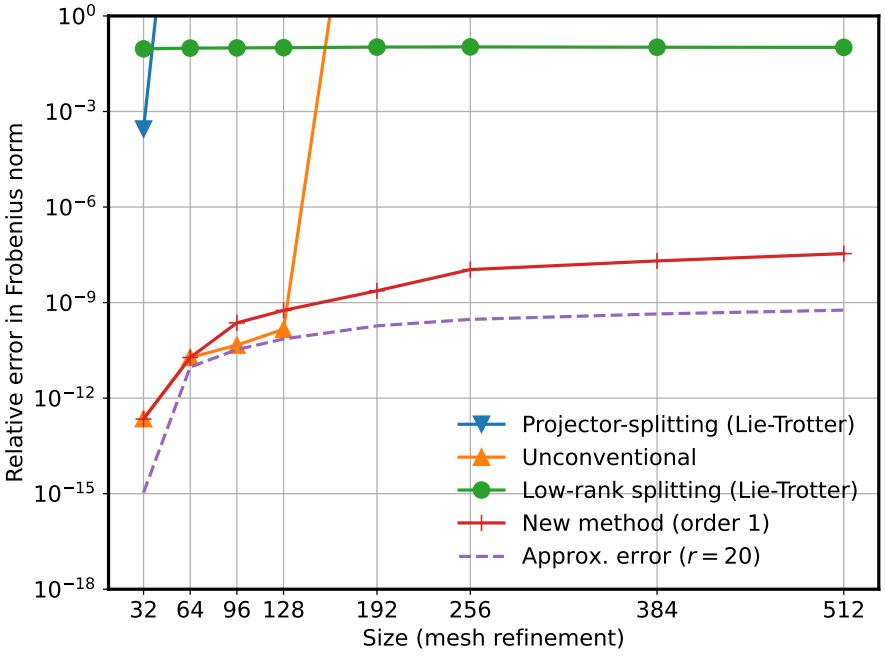

Figure 1: Relative error of existing techniques and the new method on a stiff problem (heat equation) under mesh refinements.

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Tensorized block rational Krylov methods for tensor Sylvester equations

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We introduce the definition of tensorized block rational Krylov subspaces and their relation with multivariate rational functions, extending the formulation of tensorized Krylov subspaces introduced in [2]. Moreover, we develop methods for the solution of tensor Sylvester equations with low multilinear or Tensor Train rank, based on projection onto a tensor block rational Krylov subspace. We provide a convergence analysis and some strategies for poles selection based on the techniques developed in [1].

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Low-Rank Tensor-Product approximations for Radiative Transfer in Slab Geometry

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Let us consider the even-parity formulation of the stationary Radiative Transfer Equation (RTE) in slab or plane-parallel geometry

$$-\partial_z\left(\frac{\mu^2}{\sigma_t}\partial_z u\right)+\sigma_t u=\sigma_s\int_0^1 u(\cdot,\mu')\,d\mu'+q\quad\text{in }\Omega:=(0,Z)\times(0,1),\tag{1}$$

for the specific intensity $u=u(z,\mu)$, complemented with Robin boundary conditions $u+\frac{\mu}{\sigma_t}\partial_n u=g$ on the inflow boundary $\partial\Omega_-:=\Gamma_0\cup\Gamma_Z$, where $\Gamma_z:=\{z\}\times(0,1)$. z and μ are a spatial and angular variables, respectively. The normal derivative $\partial_n u(z,\mu)$ reads $\partial_n u(0,\mu)=-\partial_z u(0,\mu)$ and $\partial_n u(Z,\mu)=\partial_z u(Z,\mu)$. In (1), the optical parameters σ_a, σ_s and σ_t model absorption, scattering and transport properties, respectively. We refer to [2] for a complete derivation and analysis of the even-parity formulation and its equivalence with the standard form of the RTE. Classical numerical schemes to solve the RTE approximate u by functions of the form $\sum_{j=0}^{J}\sum_{n=0}^{N}u_{j,n}\psi_j(z)H_n(\mu)$, but this representation is affected by the *curse of dimensionality*, which represents the exponential scaling of the computational complexity with the dimension of the problem. With this project, we aim to introduce a novel method to deal with the dimensionality issue for stationary radiative transfer, by developing a low-rank tensor product framework. Let us first introduce the matrix $\mathbf{U}=[u_{j,n}]_{j,n}\in\mathbb{R}^{(J+1)\times(N+1)}$. Employing a weak formulation of the even-parity equations as described in [2], allows to recast (1) as a linear system $\mathbb{A}\mathbf{U}=\mathbf{F}$, where the tensor $\mathbb{A}$ has the format $\mathbb{A}=\sum_{l=1}^{4}\mathbf{A}_l\otimes\mathbf{B}_l$, with matrices $\mathbf{A}_l\in\mathbb{R}^{(N+1)\times(N+1)}$ and $\mathbf{B}_l\in\mathbb{R}^{(J+1)\times(J+1)}$. Choosing suitable basis functions, such as the hat functions of standard finite elements in space (or multiwavelets for computational

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reasons) and the (shifted and scaled) Legendre polynomials in angle, the matrices $\mathbf{A}_l$ and $\mathbf{B}_l$ stemming from the angular and spatial part, respectively, are either sparse or low-rank. Let us call $\mathbb{A}_L$ and $\mathbf{F}_L$ the differential operator and the right-hand side in the aforementioned bases. Supposing now $\mathbf{U}$ in low-rank format $\mathbf{U} = \sum_{k=1}^{r} \mathbf{u}_k \otimes \mathbf{v}_k$, for vectors $\mathbf{u}_k \in \mathbb{R}^{J+1}$ and $\mathbf{v}_k \in \mathbb{R}^{N+1}$, $1 \leq k \leq r$, the storage requirement for $\mathbf{U}$ is $\mathcal{O}(r(J+N+2))$ and thus, if r is small, much smaller than the one for the standard representation. The compatibility between the differential operator structure and the low-rank format allows to never compute the Kronecker products, since the application of $\mathbb{A}_L$ to $\mathbf{U}$ writes as

$$\mathbb{A}_L \mathbf{U} = \sum_{k=1}^{r} \sum_{l=1}^{4} (\mathbf{B}_l \mathbf{u}_k) \otimes (\mathbf{A}_l \mathbf{v}_k).$$

Thus, the result $\mathbb{A}_L \mathbf{U}$ has again storage requirement $\mathcal{O}(r(J+N+2))$. However, in general, the rank has increased from r to $4r$. In order to prevent uncontrolled growth of the ranks in the iterative process, we will construct *(i)* a suitable preconditioner together with *(ii)* a rank truncation technique. Let $\mathbb{P}_L$ be a preconditioner for $\mathbb{A}_L$. We would like to solve the system using a preconditioned Richardson iteration defined on the matrix space, i.e. $\mathbf{U}_{k+1} = \mathbf{U}_k - \mathbb{P}_L^{-1}(\mathbb{A}_L \mathbf{U}_k - \mathbf{F}_L)$. In order to store and apply $\mathbb{P}_L^{-1}$ efficiently, we require for $\mathbb{P}_L^{-1}$ a similar format as for $\mathbb{A}$. For this reason, we replace $\mathbb{P}_L$ with a spectrally equivalent operator $\mathbb{P}_J$, obtained through a change of basis coded in a matrix $\mathbb{T}$, and acting on a transformed differential operator $\mathbb{A}_J = \mathbb{T}^{-T} \mathbb{A}_L \mathbb{T}^{-1}$. The new Kronecker-sum structure of $\mathbb{P}_J$ allows to use exponential sum approximations for the cheap application of its inverse powers to vectors. Since we cannot associate to $\mathbf{U}$ a Hilbert-Schmidt operator, established rank truncation methods, such as soft thresholding [1], applied to $\mathbf{U}$ do not have a proper meaning in the energy space. To overcome this issue, we denote by $\mathbb{P}$ the operator such that $\mathbb{P}^{-1/2}$ is the exponential sums approximation of $\mathbb{P}_J^{-1/2}$, and we introduce a new variable $\mathbf{W} = \mathbb{P}^{1/2} \mathbb{T} \mathbf{U}$. Since $\|\mathbf{U}\|_{\mathbb{P}_L} = \|\mathbf{W}\|_{\mathrm{F}}$, where $\|\cdot\|_{\mathrm{F}}$ denotes the Frobenius norm for matrices, rank truncation techniques that are based on the standard singular value decomposition of $\mathbf{W}$ can be employed and their error analysis implies error estimates in the energy norm for the original variable. Denoting $\mathcal{S}_{\delta_k}$, being $\delta_k > 0$ a sequence of thresholding parameters, any operator that is non-expansive with respect to $\|\cdot\|_{\mathrm{F}}$ (for us it will be a soft-thresholding operator), we define the next iterate by

$$\mathbf{W}_{k+1} = \mathcal{S}_{\delta_k}(\mathbf{W}_k - \omega(\mathbb{A}\mathbf{W}_k - \mathbf{F})),$$

where $\mathbb{A} = \mathbb{P}^{-1/2} \mathbb{A}_J \mathbb{P}^{-1/2}$, $\mathbf{F} = \mathbb{P}^{-1/2} \mathbb{T} \mathbf{F}_L$ and $\omega > 0$ is an acceleration parameter depending on the spectral properties of $\mathbb{A}$ and the exponential sums approximation of $\mathbb{P}_J^{-1/2}$. We can establish upper and lower bounds, depending on the contraction rate, for the distance between the true solution of the discretized equation and the fixed point of the thresholded iteration. Moreover, optimal ranks bounds are obtained knowing *a priori* the decay of the singular value of a manufactured exact solution. For all the other cases, when the decay of the singular values is unknown, we provide an algorithm which adjust the thresholding parameter *a posteriori*, based on the current iterate, retaining quasi-optimal ranks throughout the process.

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Compositional Tensor Trains (Deep TTs)

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Neural Network applications have shown a superior power of expressivity of compositional structures in function regression. Inspired by the notion of compositional sparsity as well as neural ODEs we want to find a class of functions that can be well approximated by a composition of functional tensor trains. For the computation of the underlying tensors, we can define an optimal control problem on the tensor train manifold.

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Gauss-Southwell type descent methods for low-rank matrix optimization

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We consider gradient-related methods for low-rank matrix optimization with a smooth strongly convex cost function. The methods operate on single factors and share aspects of both alternating and Riemannian optimization. We compare two possible choices for the search directions based on Gauss-Southwell type selection rules: one using the gradient of a factorized non-convex formulation, the other using the Riemannian gradient. Both methods provide convergence guarantees for the gradient that are analogous to the unconstrained case.

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Iteratively Reweighted Least Squares Recovery on Tensor Networks

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One fundamental approach to matrix recovery, being a predecessor to tensor recovery, traces back to the affine rank minimization problem. While there are various surrogate approaches within that setting, we emphasize here that the *asymptotic minimization* of the well-known, so called *log-det* objective functions always yields the desired, minimal rank matrices within the given, affine set; whereas such may or may not recover an a-priorly sought for ground truth. Concerning the commonly applied method of iteratively reweighted least squares (IRLS-0), one thus remains with two concerns. How problematic are local minima inherent to the log-det approach truly; and opposingly, how influential instead is the numerical realization. With higher dimensions in mind, based on the concept of matricization, affine sum-of-ranks minimization then generalizes the setting from matrices to tensors. While convergence properties are directly transferable, we demonstrate that in numerical experiments, the corresponding IRLS-0 method can be exhausted in order to observe the theoretical phase transition for generic tensor recoverability. In large-scale applications in turn, alternating, reweighted optimization on tensor tree networks allows to avoid exponential computational complexity, without substantial loss of approximation quality.

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Canonical Polyadic Decomposition and Sets of Polynomial Equations

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The task of solving systems of polynomial equations is important in engineering practice. In this talk, we present a novel strategy to find all (approximate) common roots of an overdetermined polynomial system corrupted by noise (e.g., caused by measurement error). In comparison to earlier approaches that reduce the problem to the generalized eigenvalue problem associated with a matrix pencil, we introduce a multi-pencil approach that translates the problem into the computation of a canonical polyadic decomposition (CPD) of a tensor (or a block term decomposition (BTD) in the case of coinciding roots) [2, 3]. The tensor is obtained from the null space of a so-called Macaulay matrix. For high polynomial degrees, the Macaulay matrix suffers from the curse of dimensionality. However, its algebraic structure can be exploited for efficiency [1]. The benefits of this approach, both from a conceptual and numerical standpoint, are analyzed. The technique is illustrated with an application involving the localization of two transmitters from the power received in arbitrary antenna configurations [4].

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Matrix Equations and Tensor Techniques X
Aachen, September 13–15, 2023

CP decomposition and low-rank approximation of antisymmetric tensors

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In this talk we are going to explore the antisymmetric tensors, their CP decomposition and the low-rank approximation algorithms. The idea of the CP decomposition is to write a tensor as a sum of its rank-one components. This decomposition is closely related to the tensor rank R, which is defined as the minimal number of rank-1 summands in the exact CP decomposition. Contrary to the matrix case, the rank of a tensor can exceed its dimension, and it can be different over $\mathbb{R}$ and over $\mathbb{C}$. It is known that the problem of finding the rank of a given tensor is NP-hard.

When computing the CP decomposition, the main question is the choice of the number of rank-one components. Assuming the antisymmetric structure of our tensors, we impose an additional constraint on the CP decomposition. This constraint assures that the resulting tensor is, indeed, antisymmetric, and it gives a bound on the minimal number of rank-one components. We focus on the tensors of order three. For a given non-zero antisymmetric tensor $\mathcal{A} \in \mathbb{R}^{n\times n\times n}$ our goal is to find its low-rank antisymmetric approximation which is represented via only three vectors.

For three vectors $x, y, z \in \mathbb{R}^n$ we define an $n \times n \times n$ antisymmetric tensor associated with these vectors as

$$\mathcal{A}_6(x, y, z) := \frac{1}{6}(x \circ y \circ z + y \circ z \circ x + z \circ x \circ y - x \circ z \circ y - y \circ x \circ z - z \circ y \circ x).$$

Then, we are looking for a tensor $\tilde{\mathcal{A}} = \mathcal{A}_6(x, y, z)$, i.e., vectors $x, y, z \in \mathbb{R}^n$, such that

$$\|\mathcal{A} - \tilde{\mathcal{A}}\|^2 \to \min .$$

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We propose an alternating least squares structure-preserving algorithm for solving this problem. The algorithm is based on solving a minimization problem in each tensor mode. Set

$$a = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \in \mathbb{R}^{3n}.$$

Then, similarly to what was done in [1], we define the objective function $f\colon \mathbb{R}^{3n} \to \mathbb{R}$,

$$f(a) = 6\|\mathcal{A} - \mathcal{A}_6(x, y, z)\|^2,$$

and consider three partial minimization problems:

$$\min_x f(a), \quad \min_y f(a), \quad \min_z f(a).$$

We compare our algorithm with a "naive" idea which uses a posteriori antisymmetrization.

Moreover, we study the tensors with partial antisymmetry, that is, antisymmetry in only two modes. Correspondingly to what we do for the tensors that are antisymmetric in all modes, we first determine a suitable format of the CP decomposition, which is going to be simpler for the partial antisymmetry. Based on this format, for a given non-zero tensor $\mathcal{C} \in \mathbb{R}^{n\times n\times m}$ antisymmetric in two modes, we are looking for its approximation $\tilde{\mathcal{C}}$ of the same structure such that $\tilde{\mathcal{C}}$ is represented by three vectors and $\operatorname{rank}(\tilde{\mathcal{C}}) = 2$.

We provide numerical examples for the comparison of the CP with a posteriori antisymmetrization and the antisymmetry preserving CP. Additionally, for the sake of completeness, we compare these algorithms with the CP-ALS algorithm that does not preserve antisymmetry. All algorithms are implemented and tested in Julia programming language

The talk is based on the preprint [2].

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Second-order algorithms for canonical polyadic decomposition with non-least-squares cost functions

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Signal processing and data analysis applications often rely on rank-1 terms to extract meaningful information from tensor data. By using the least-squares loss when computing this canonical polyadic decomposition, one implicitly assumes normally distributed errors, which might not be suitable for, e.g., count data. Therefore, we derive a generalized Gauss-Newton-type algorithm for non-least-squares loss functions and discuss how exploiting tensor structure and randomization lead to an efficient algorithm.

This work is based on [1] and [2]. Implementations of the algorithm and the experiments can be found at tensorlabplus.net.

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Alternating nonnegative factorization for low-rank tensor formats

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We discuss the problem of determining the nonnegative, high-dimensional solution $x^\star \in \mathbb{R}_{\geq 0}$ to a linear system $Ax = b$. The solution $x^\star$ can represent, for example, a probability distribution over a high-dimensional state space [1]. In order to deal with the high dimensionality, we approximate the solution $x^\star$ using low-rank tensor formats. Since the solution is nonnegative, we want the low-rank approximation to preserve this property by constraining each of its factors to be nonnegative. Common alternating strategies for nonnegative tensor factorization reduce the high-dimensional problem to a sequence of low-dimensional subproblems, but often suffer from slow convergence and persistence in local minima. In the setting without nonnegativity constraints, the factors of the low-rank representation are typically orthogonalized as an intermediate step between the alternating minimization steps. However, orthogonalization of the factors generally violates the nonnegativity constraints and therefore cannot be used for nonnegative tensor factorization.

Similar to [2] for nonnegative matrix factorization, we illustrate that nonnegative updates (unlike classical low-rank ones) are not representation invariant. Therefore, our goal is to increase the range of nonnegative factorization that can be discovered in the next minimization step. We propose a quasi-orthogonalization as an intermediate step. Numerical experiments suggest that this quasi-orthogonalization reduces the problematic issues of common alternating strategies for factorizing nonnegative tensors.

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Matrix Equations and Tensor Techniques X
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An algebraic algorithm for blind source separation and tensor decomposition

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The Blind Source Separation (BSS) problem is a classical signal processing problem. We want to retrieve the source signals from an observed mixture of signals. Mathematically this problem translate into the factorization of the $R \times N$ observed signal matrix $\mathbf{X}$ into

$$\mathbf{X} = \mathbf{M}\mathbf{S}^\top$$

where $\mathbf{M}$ is the mixing matrix and $\mathbf{S}$ is the source signal one. For some classes of BSS, e.g., sparsity [1], constant modulus [7], Vandermonde structure [6], or statistical independence of non-Gaussian signals [2], the problem has a unique solution, under mild conditions.

In [5], the authors study the uniqueness of the structured rank-1 factorization for the observed signal matrix $\mathbf{X}$ defined as

$$\mathbf{X} = \sum_{r=1}^{R} \mathbf{m}_r(\mathbf{z})\mathbf{s}_r(\mathbf{z})^T \qquad \text{for} \qquad \mathbf{z} \in \Omega \tag{1}$$

where the $\mathbf{m}_r(\mathbf{z})$ and $\mathbf{s}_r(\mathbf{z})$ are vector-value functions defined on Ω, a subset of the vector space $\mathbb{F}^N$. The fundamental contribution is checking-list criteria, which guarantee for a class of deterministic methods the generic uniqueness of the factorization in (1) up to trivial indeterminacy, as permutations or scaling.

These criteria, arising from the algebraic geometry framework, allow us to design an algorithm to retrieve the unique decomposition in various more specific cases, including

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the blind source separation problem if the source signals can be modeled as rational functions, and the canonical polyadic tensor decomposition. We assume that the matrix $\mathbf{X}$ has full row rank and that the columns of $\mathbf{S}$ belong to an algebraic variety $\mathcal{V}$, i.e.,

$$\mathcal{V} = \{\mathbf{z} \in \mathbb{F}^N : p_1(\mathbf{z}) = \cdots = p_K(\mathbf{z}) = 0\}$$

where $p_1, \ldots, p_K$ are polynomials. Thanks to the results of [3, 4], we prove that the rows of $\mathbf{M}^{-1}$ belong to the intersection of the vectorized symmetric tensor subspace and the kernel of a matrix $\mathbf{Q}$, obtained from the polynomials $p_1, \ldots, p_K$ defining the algebraic variety $\mathcal{V}$. Once the rows of $\mathbf{M}^{-1}$ are retrieved, we can easily obtain the wanted unique factorization.

As a consequence, a key step in the algebraic algorithm is computing the matrix $\mathbf{Q}$, which has large dimensions. However, the highly structured nature of $\mathbf{Q}$ allows an efficient computation on which we will particularly focus.

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Matrix Equations and Tensor Techniques X
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Oblique projection for scalable reduced-order modeling of nonlinear PDEs on low-rank matrix manifolds

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Dynamical low-rank approximation (DLRA) has successfully been used for approximating the solution to nonlinear partial differential equations (PDEs) on low-rank matrix manifolds. For many practical problems of interest, discretizing high-dimensional PDEs results in massive matrix differential equations (MDEs) that are too expensive to solve using conventional methods. While DLRA has the potential to significantly reduce this computational burden, it still suffers from the following challenges: (i) inefficient for general nonlinearities, (ii) intrusive implementation, (iii) ill-conditioned in the presence of small singular values, and (iv) error accumulation due to fixed rank. To this end, we present a scalable method for solving MDEs on low-rank matrix manifolds that is computationally efficient, minimally intrusive, robust in the presence of small singular values, rank-adaptive, and highly parallelizable. These favorable properties are achieved via oblique projections that require evaluating the MDE at a small number of rows and columns. The columns and rows are selected using the discrete empirical interpolation method (DEIM), which yields near-optimal matrix low-rank approximations. We show that the proposed algorithm is equivalent to a CUR matrix decomposition. Numerical results demonstrate the accuracy, efficiency, and robustness of the new method for a diverse set of problems [1].

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Alternating projections for low-rank approximation in the maximum norm

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When measured in a unitarily invariant norm, the distance from a matrix X to the set of low-rank matrices is determined by the singular values of X and is achieved at its truncated singular value decomposition. However, this theory does not cover other important norms such as the maximum norm $\|X\|_{\max} = \max_{i,j} |X(i,j)|$.

It was shown in [1] that for every $X \in \mathbb{R}^{m\times n}$ with $m \geq n$ and every $\varepsilon \in (0,1)$ there exists a matrix $Y \in \mathbb{R}^{m\times n}$ of rank at most $\lceil 72 \log(2n+1)/\varepsilon^2 \rceil$ such that $\|X - Y\|_{\max} \leq \varepsilon \|X\|_2$. In other words, every sufficiently large matrix with bounded spectral norm is close to a low-rank matrix in the maximum norm.

We propose to successively compute (quasi)optimal projections onto the set of fixed-rank matrices and the maximum-norm ball centered at X to obtain such low-rank approximations. In a series of numerical experiments with different classes of matrices we study how well the theoretical estimate of [1] describes the approximation errors achieved with the method of alternating projections.

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Matrix Equations and Tensor Techniques X
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Two relaxations of the best rank-1 tensor approximation problem using different norms

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Tensors as the extension of vectors and matrices, provide the natural tool for representing high-dimensional data. Similar to the matrix case, in order to extract the important patterns and discarding the redundant information, there is a need for dimensionality reduction techniques. Decomposing tensors and using the low-rank forms is one of these approaches. Using low-rank tensors is usual in applications like signal processing and optimal control. Of particular interest is the use of rank-1 CP approximation due to its simpler form and unlike the rank-r CP approximation ($r > 1$), it always exists [2].

In this work, first it is shown that the best rank-1 approximation of a real mth-order tensor is equal to solving m 2-norm optimization problems that each corresponds to a factor of the best rank-1 approximation. These problems are relaxed by using the Frobenius and L_1 norms instead of 2-norm. It is proved that the solution for the Frobenius relaxation of optimization problems is the leading eigenvector of a positive semi-definite matrix and the solution of the L_1 relaxation can be obtained efficiently by summing over all modes of the associated tensor but one. The numerical examples show that these relaxations can be faster than the alternating least squares (ALS) method and they are reasonably close to the solutions obtained by the ALS method.

For an m-th order tensor $\mathcal{A}$ in $\mathbb{R}^{n_1 \times n_2 \times \ldots \times n_m}$, the following problem is called the best (CP) rank-1 approximation,

$$\left\| \mathcal{A} - \mu \mathbf{a}^{(1)} \circ \mathbf{a}^{(2)} \circ \ldots \circ \mathbf{a}^{(m)} \right\|_F = \min_{c, \left\|\mathbf{x}^{(1)}\right\|_2 = \ldots = \left\|\mathbf{x}^{(m)}\right\|_2 = 1} \left\| \mathcal{A} - c \mathbf{x}^{(1)} \circ \mathbf{x}^{(2)} \circ \ldots \circ \mathbf{x}^{(m)} \right\|_F \tag{1}$$

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where μ and c are real scalars, $\mathbf{a}^{(i)}, \mathbf{x}^{(i)} \in \mathbb{R}^{n_i}, 1 \leq i \leq m$ are real vectors, $\circ$ denotes the vector outer product and $\mu\mathbf{a}^{(1)} \circ \mathbf{a}^{(2)} \circ \ldots \circ \mathbf{a}^{(m)}$ is called the best rank-1 approximation of $\mathcal{A}$.

It is known that the problem of finding a best (CP) rank-one approximation is NP-hard [1]. In this work, two relaxations for the best rank-one approximation of a real tensor are defined in order to create cost-effective methods. The purpose of a relaxation of an optimization problem is to approximate it by weakening the constraints or the objective function in order to have an easier-to-solve problem that approximates the optimal solution of original problem. The optimal solution of the relaxed maximization (minimization) problem is a lower bound (upper bound) for the optimal solution of the original problem.

Here, using relaxations leads to having simpler algorithms for calculating the best rank-1 approximation of a tensor. In addition, these new algorithms are of complexity class NC. Also, the output of one of relaxations (L_1) can be used to initialize alternating least squares (ALS) and create a faster and more accurate version of ALS than with random initialization.

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Matrix Equations and Tensor Techniques X
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A multilinear Nyström algorithm for low-rank approximation of tensors in Tucker format

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The Nyström method [**Nystrom1930**] offers an effective way to obtain low-rank approximation of SPD matrices, and has been recently extended and analyzed to nonsymmetric matrices [**Nakatsukasa2020**] (leading to the randomized, single-pass, streamable, cost-effective, and accurate alternative to the randomized SVD, and it facilitates the computation of several matrix low-rank factorizations.

In this presentation, we take these advancements a step further by introducing a higher-order variant of Nyström's methodology tailored to approximating low-rank tensors in the Tucker format: the multilinear Nyström technique. We show that, by introducing appropriate small modifications in the formulation of the higher-order method, strong stability properties can be obtained. This algorithm retains the key attributes of the generalized Nyström method, positioning it as a viable substitute for the randomized higher-order SVD algorithm [**Cichoki2014**] .

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Particle Number Conservation in Second Quantization and Block-Sparse Tensor Trains

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Low-rank tensor formats such as tensor trains [4], which in physics are known as matrix products states [5], are an important tool for representing wave functions in quantum physics. However, their direct application to approximations of fermionic wave functions in particle coordinates is problematic due to the antisymmetries under coordinate exchange that such wave functions need to satisfy, which cannot readily be treated using such hierarchical tensor formats [3].

An alternative is provided by a second-quantized representation, where the antisymmetric wave functions are parameterized in terms of *occupation numbers* with respect to a given set of single-particle basis functions, here called *orbitals*; for a brief overview, see, e.g., [1]. An additional difficulty that arises in this approach, however, is that the number of particles in the system is not a prior fixed and generally needs to be constrained to the desired value in some manner.

Constraining the particle number (or other quantum numbers) in matrix product states leads to a block-sparsity pattern in tensor components, as illustrated in 1. This is exploited in many tensor network codes, in particular in density matrix renormalization group algorithms. In this talk, based on the results in [2] we look at such block-sparsity properties from a more general point of view, with potential applications in other contexts.

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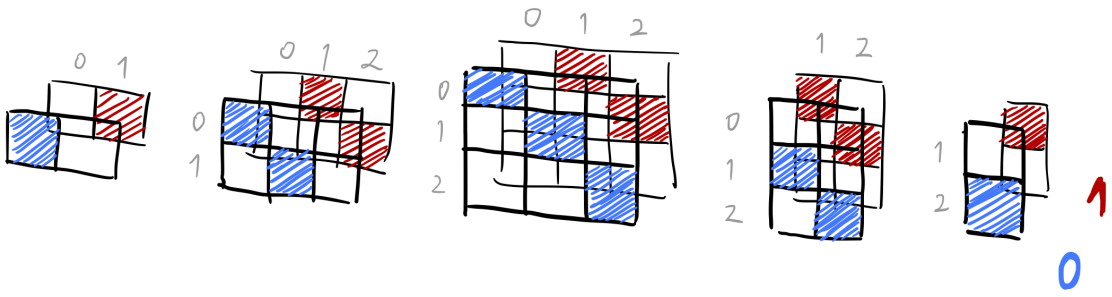

Figure 1: Blocks in a matrix product state with two particles encoding unoccupied (0, blue) and occupied (1, red) states for five orbitals.

We then consider the interaction of the block structure with matrix product operator representations of Hamiltonians in quantum chemistry. We obtain explicit representations of such Hamiltonians operating directly on the block structures, with improved rank bounds under sparsity assumptions on the Hamiltonian coefficients. Finally, we discuss their application in low-rank eigensolvers using full residual information.

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A Space-Time Adaptive Low-Rank Method for High-Dimensional Parabolic PDEs

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We present the construction and analysis of a space-time adaptive method for parabolic partial differential equations that combines sparse wavelet expansions in time with adaptive low-rank approximations in the spatial variables [2].

Similar to the existing adaptive low-rank method for elliptic problems [1], we use a perturbed Richardson iteration, where we apply two reduction operators to the iterates to keep the support as well as the arising ranks of the low-rank approximations near-optimal for a given error tolerance. This perturbed Richardson iteration is applied to a bi-infinite matrix-vector problem based on the space-time variational formulation [3] which is equivalent to the parabolic initial boundary value problem.

For the analysis of the method we propose a new approximation class for the temporal operator which is necessary due to the interaction between hierarchical tensor formats of different time indices. One of the main challenges is the fact that the parabolic operator is an isomorphism with respect to spaces not endowed with a cross norm. Therefore, as in [1], we use a method for preconditioning operators in low-rank format by exponential sum approximations.

The method is shown to converge and satisfy similar complexity bounds as the existing adaptive low-rank method for elliptic problems [1, 2], establishing its suitability for parabolic problems on high-dimensional spatial domains and does not suffer from the curse of dimensionality. The construction also yields computable rigorous a posteriori error bounds for the total error depending on the activated basis functions and ranks in the approximation.

The results are illustrated by numerical experiments for the heat equation in high dimensions, demonstrating the practical efficiency.

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Parameter-dependent multigrid method using low-rank tensor formats

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We consider a parameter-dependent linear system motivated by a diffusion problem. The combination of all finitely many parameters leads to an exponential scaling of the computational effort in the number of parameters, the so-called curse of dimensionality. To break this curse, we use low-rank tensor formats to represent this system. We introduce the parameter-dependent multigrid method to solve such a high-dimensional system within low-rank tensor formats.

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