Tensor Computations in Linear and Multilinear Algebra

Lek-Heng Lim, Berkeley, CA, USA
Eugene Tyrtyshnikov, RAS Moscow, Russia

Matrix computations with huge-size multilevel matrices, e.g. of order of 2 to power 100, are not easy to make feasible even with structure and supercomputers. However, the former seems much more essential for problems on that scale. Most important structure on that scale is related with separation of variables and eventually with tensors. Thus, successful matrix computations are becoming tensor computations. The purpose of this minisymposium is to present the state of the art in representation and approximation of tensors in higher dimensions. The accent is made on recent findings, in particular on the use of matrix methods for generalized unfolding matrices associated with tensors.

Approximation of High-Order Tensors by Partial Sampling: New Results and Algorithms

C. Caiafa, LABSP-Brain Science Institute, RIKEN, Japan
ccaiafa@gmail.com
Thu 11:00, Room B

Recently [1,2,3], a new formula was provided that allows one to reconstruct a *rank*-$(R_1, R_2, ..., R_N)$ *Tucker tensor* $\underline{\mathbf{Y}} \in \mathbb{R}^{I_1 \times I_2 \dots \times I_N}$ from a subset of its entries which are determined by a selected subset of R_n indices in each mode $(n = 1, 2, ..., N)$. As a generalization of the column-row matrix decomposition (also known as **CUR** or "skeleton" decomposition), which approximates a matrix from a subset of its rows and columns, our result provides a new method for the approximation of a high dimensional $(N \geq 3)$ tensor by using only the information contained in a subset of its *n-mode fibers* $(n = 1, 2, .., N)$. The proposed algorithm can be applied to the case of arbitrary number of dimensions $(N \geq 3)$ and the indices are sequentially selected in an optimal way based on the previously selected ones. In this talk, we analyze and discuss the properties of this method in terms of the subspaces spanned by the *unfolding matrices* of the *subtensor* determined by the selected indices. We also discuss about its applications for signal processing where low dimensional signals are mapped to higher dimensional tensors and processed with tensor tools. Experimental results are shown to illustrate the properties and the potential of this method.

[1] C. Caiafa and A. Cichocki, Generalizing the Column-Row Matrix Decomposition to Multi-way Arrays, To appear.
[2] C. Caiafa and A. Cichocki, Reconstructing Matrices and Tensors from Few Vectors, Proc. NOLTA 2009, Oct. 18-21, 2009, Sapporo, Japan.
[3] C. Caiafa and A. Cichocki, Methods for Factorization and Approximation of Tensors by Partial Fiber Sampling, Cesar F. Caiafa and Andrzej Cichocki, Proc. CAMSAP 2009, Dec. 13-16, 2009, Aruba, Dutch Antilles.

Joint work with A. Cichocki (LABSP-Brain Science Institute, RIKEN)

Computing structured tensor decompositions in polynomial time

P. Comon, I3S, CNRS, Univ. of Nice Sophia-Antipolis
pcomon@unice.fr
Thu 11:25, Room B

Tensor decompositions permit to estimate in a deterministic way the parameters in a multi-linear model. Applications have been already pointed out in antenna array processing and digital communications [1], among others, and are extremely attractive provided some diversity at the receiver is available. In addition, they often involve structured factors. These deterministic techniques may be opposed to those based on cumulants, which require the decomposition of symmetric tensors [2]. More generally, the goal is to represent a function of three variables (or more) as a sum of functions whose variable separate.

As opposed to the widely used Alternating Least Squares algorithm, it is shown that non-iterative algorithms with polynomial complexity exist, when one or several factor matrices enjoy some structure, such as Toeplitz, Hankel, triangular, band, etc. Necessary conditions are first given, concerning dimensions, bandwidth, and rank [3]. Then sufficient conditions are provided, along with constructive algorithms, in the case of third order tensors. These algorithms require solving linear systems, and computing best rank-1 matrix approximations. Hence the overall complexity is polynomial if one admits that the latter rank-1 approximations also have a polynomial complexity.

[1] N. D. Sidiropoulos, G. B. Giannakis, and R. Bro, Blind Parafac receivers for DS-CDMA systems, IEEE Trans. on Sig. Proc., vol. 48, no. 3, pp. 810–823, Mar. 2000.
[2] P. Comon and G. Golub and L-H. Lim and B. Mourrain, Symmetric Tensors and Symmetric Tensor Rank, SIAM Journal on Matrix Analysis Appl., vol.30, no.3, Sept. 2008, pp.1254–1279.
[3] P. Comon and M. Sorensen and E. Tsigaridas, Decomposing tensors with structured matrix factors reduces to rank-1 approximations, Icassp, Dallas, March 14-19, 2010.

Joint work with M. Sorensen (I3S, University of Nice)

Optimization Problems in Contracted Tensor Networks

Mike Espig, Max-Planck-Institute for Mathematics in the Sciences, Germany
espig@mis.mpg.de
Fri 16:45, Room B

In this talk we discuss a calculus of variations in arbitrary tensor representations with a special focus on contracted tensor networks and apply it to functionals of practical interest. The survey provides all necessary ingredients for applying minimization methods in a general setting. The important cases of target functionals which are linear and quadratic with respect to the tensor product are discussed, and combinations of these functionals are presented in detail. As an example, we consider the representation rank compression in tensor networks. For the numerical treatment, we introduce efficient methods. Furthermore, we demonstrate the rate of convergence in numerical tests.

Joint work with Wolfgang Hackbusch (Max-Planck-Institute for Mathematics in the Sciences) and Reinhold Schneider (Technical University Berlin)

Most Tensor Problems are NP Hard

Christopher Hillar, Mathematical Sciences Research Institute, Berkeley

chillar@msri.org
Thu 11:50 Room B

The idea that one might extend numerical linear algebra, the collection of matrix computational methods that form the workhorse of scientific and engineering computing, to numerical multilinear algebra, an analogous collection of tools involving hypermatrices/tensors, appears very promising and has attracted a lot of attention recently. We examine here the computational tractability of some core problems in numerical multilinear algebra. We show that tensor analogues of several standard problems that are readily computable in the matrix (i.e. 2-tensor) case are NP hard. Our list here includes: determining the feasibility of a system of bilinear equations, determining an eigenvalue, a singular value, or the spectral norm of a 3-tensor, determining a best rank-1 approximation to a 3-tensor, determining the rank of a 3-tensor over the real or complex numbers. Hence making tensor computations feasible is likely to be a challenge.

Joint work with Lek-Heng Lim (University of Berkeley)

Numerical solution of the Hartree-Fock equation in the multilevel tensor structured format

V. Khoromskaia, Max-Planck-Institute for Mathematics in the Sciences, Leipzig, Germany
vekh@mis.mpg.de
Fri 17:10, Room B

We consider the numerical solution of the Hartree-Fock equation (nonlinear eigenvalue problem) by the novel tensor-structured methods based on tensor approximation of arising functions and operators represented on 3D $n \times n \times n$ Cartesian grid [1]. Tensor-structured techniques enable "agglomerated" computation of the three- and six- dimensional volume integrals [2], with complexity that scales linearly in the one-dimension grid size n. High accuracy is achieved due to the multigrid accelerated rank reduction algorithm for 3-rd order tensors which provides computation of the Hartree potential on large spacial grids, with $n \leq 10^4$, necessary to resolve multiple strong cusps in electron density [3]. The discrete nonlinear eigenvalue problem in 3D is solved iteratively by the multilevel tensor-truncated DIIS scheme on a sequence of refined grids with robust and fast convergence in a moderate number of iterations, uniformly in n, so that the overall computational cost also scales linearly in n. We present numerical illustrations for the all electron case of H_2O, and pseudopotential case of CH_4 and CH_3OH.

[1] B. N. Khoromskij, V. Khoromskaia, and H.-J. Flad. Numerical Solution of the Hartree-Fock Equation in the Multilevel Tensor-structured Format. Preprint MPI MiS 44/2009, Leipzig, July 2009, submitted.
[2] V. Khoromskaia. Computation of the Hartree-Fock Exchange in the Tensor-structured Format. Preprint MPI MiS 25/2009, Leipzig, June 2009.
[3] B. N. Khoromskij and V. Khoromskaia. Multigrid Tensor Approximation of Function Related Arrays. SIAM J. on Sci. Comp., **31**(4), 3002-3026 (2009).

Joint work with H.-J.Flad and B. Khoromskij

Prospects of Quantics-TT Approximation in Scientific Computing

Boris N. Khoromskij, Max-Planck-Institute for Mathematics in the Sciences, Leipzig, Germany
bokh@mis.mpg.de
Fri 11:00, Room B

We discuss the prospects of super-compressed tensor-structured quantics-TT data formats [1,3,5] in high dimensional numerical modeling. The respective multilinear algebra is based on the multi-folding or quantics representation of multidimensional data arrays [1,3]. Low rank tensor approximation via the TT-type dimension splitting scheme [2,4] leads to logarithmic complexity scaling in the volume size of a target N-d tensor. Numerical illustrations indicate that the quantics-TT tensor method has proved its value in application to various function related tensors arising in quantum chemistry and in the traditional FEM/BEM—the tool apparently works. In particular, this method can be applied in the framework of truncated iteration for solution the high dimensional elliptic/parabolic problems including stochastic PDEs.

[1] B.N. Khoromskij, *$O(d \log N)$-Quantics Approximation of N-d Tensors in High-Dimensional Numerical Modeling.* Preprint 55/2009, MPI MiS, Leipzig 2009, submitted.
[2] I.V. Oseledets, and E.E. Tyrtyshnikov, *Breaking the Curse of Dimensionality, or How to Use SVD in Many Dimensions.* SIAM J. Sci. Comput., 31, 5(2009), 37-44-3759.
[3] I.V. Oseledets, *Tensors Inside of Matrices Give Logarithmic Complexity.* SIAM J. Matrix Anal., 2009, accepted.
[4] I.V. Oseledets, and E.E. Tyrtyshnikov, *TT-Cross Approximation for Multidimensional arrays.* Linear Algebra Appl., 432 (2010), 70-88.
[5] B.N. Khoromskij, I.V. Oseledets, *Quantic-TT approximation of elliptic solution operators in higher dimensions.* Preprint MPI MiS 79/2009, Leipzig 2009, submitted.

Tensor train and QTT decompositions for high-dimensional tensors

I. Oseledets, Institute of Numerical Mathematics, Russ. Acad. Sci.
ivan.oseledets@gmail.com
Fri 11:25, Room B

In this talk we develop the basic idea of tensor-train decomposition, which can be considered as natural extention of singular value decomposition to high dimensions. It does not suffer from the curse of dimensionality, and can be computed with the reliability and SVD. Basic subroutines are simple to implement and are available online. QTT decomposition opens a new application area for tensor decompositions – approximation of tensors of "physically small" dimension. It includes compact representation of functions on sufficiently fine tensor grids with 2^D points in each direction, leading to d log n complexity. When the tensor is in structured format, it is interesting to perform some operations with it. Some operations are very intuitive in the tensor-train format, however some are not. An important operation is finding maximal and minimal elements. An algorithm usin maximal-volume submatrices will be presented for finding maximal in modulus element in the TT format.

Joint work with E. E. Tyrtyshnikov (INM RAS), B. N. Khoromskij (MIS MPG)

Krylov subspace methods for tensor computations

Berkant Savas, The University of Texas at Austin
berkant@cs.utexas.edu
Fri 11:50, Room B

In this talk we will present a few generalizations of matrix Krylov methods to tensors. The general objective is to obtain a rank-(p,q,r) approximation of a given $l \times m \times n$ tensor $\mathcal{A}$. The problem can be viewed as finding low dimensional signal subspaces associated to the different modes of $\mathcal{A}$.

Krylov methods, similar to the matrix case, are particularly well suited for problems involving large and sparse tensors or for tensors that allow efficient multilinear tensor-times-vector multiplications. We will consider several different types of tensor in evaluating the proposed methods: (1) tensors with specified low ranks; (2) low rank tensors with added noise; and (3) large and sparse tensors. For a few special cases we will prove that our methods captures the true signal subspaces associated to the tensor within certain number of steps in the algorithm. For more general cases we propose an approach, based on the Krylov-Schur method for computing matrix eigenvalues, to improve the subspaces obtained from the tensor-Krylov procedures. Test results confirm the usefulness of the proposed methods for the given objective. The technical report [1] covers part of the topics discussed in this talk.

[1] B. Savas and L. Eldén, Krylov subspace methods for tensor computations, Technical Report LITH-MAT-R-2009-02-SE, 2009, Dept. of Math., Linköping University.

Joint work with Lars Eldén (Linköping University)

New algorithms for Tucker approximation with applications to multiplication of tensor-structured matrices and vectors

D. V. Savostyanov, Institute of Numerical Mathematics RAS, Moscow
dmitry.savostyanov@gmail.com

Fri 12:15, Room B

New algorithms are proposed for Tucker approximation of tensors (multidimensional arrays) that are not given explicitly, but are defined by a tensor-by-vectors multiplication operation. As well as in matrix case, this framework applies to structured tensors, like sparse tensors, tensors with multilevel Toeplitz or Hankel structure and so on. We discuss the merits and drawbacks of minimal Krylov recursion [1] and suggest some possible optimisation for it. We also propose new approximation methods based on Wedderburn rank-reduction.

As an important application we consider approximate multiplication of d-dimensional matrices given as Tucker or canonical decomposition with the result being approximated in Tucker format with optimal values of ranks possible in the desired accuracy bound. Since mode sizes can be very large, the result should never appear as full array. Here we compare Krylov and Wedderburn approaches with previously studied independent factor filtering [3] and modified variable-rank Tucker-ALS procedure without a priori knowledge of ranks [2]. We also propose cheap initialization of Tucker-ALS using an intrinsic tensor structure of result. Numerical examples include structured evaluation of typical operators from Hartree-Fock/Kohn-Sham model, by means of Canonical-to-Tucker and Tucker-to-Tucker multiplication.

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[1] B. Savas, L. Eldén, Krylov subspace method for tensor computation. Preprint LITH-MAT-R-2009-02-SE, Dep. Math. Linköpings Univ., February 2009.
[2] I. V. Oseledets, D. V. Savostyanov, E. E. Tyrtyshnikov, Linear algebra for tensor problems. Computing. 2009. V. 85(3):169-188.
[3] D. V. Savostyanov, E. E. Tyrtyshnikov,Approximate multiplication of tensor matrices based on the individual filtering of factors. J. Comp. Math. Math. Phys. 2009. V. 49(10):1662-1677.
[4] I. V. Oseledets, D. V. Savostianov, E. E. Tyrtyshnikov, Tucker dimensionality reduction of three-dimensional arrays in linear time. SIAM J. Matrix Anal. Appl. 2008. V. 30(3):936–956.
[5] I. V. Oseledets, D. V. Savostianov, E. E. Tyrtyshnikov, Cross approximation in tensor electron density computations. J. Numer. Lin. Alg. Appl. 2009, doi: 10.1002/nla.682.

Joint work with S. A. Goreinov, I. V. Oseledets (Institute of Numerical Mathematics RAS, Moscow)

Generalized Cross Approximation for 3d-tensors

Jan Schneider, Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany
jschneid@mis.mpg.de

Fri 17:35, Room B

In this talk we present a generalized version of the Cross Approximation for 3d-tensors. The given tensor $a \in \mathbb{R}^{n\times n\times n}$ is represented as a matrix of vectors and 2d adaptive Cross Approximation is applied in a nested way to get the tensor decomposition. The explicit formulas are derived for the vectors in the decomposition. The computational complexity of the proposed algorithm is shown to be linear in n.

Joint work with K. K. Naraparaju (MPI for Mathematics, Leipzig, Germany)

The future of tensor computations, or how to escape from the curse of dimensionality

E. Tyrtyshnikov, Insitute of Numerical Mathematics, Russ. Acad. Sci.
tee@inm.ras.ru

Thu 12:15, Room B

Even "simple" cases in higher dimensions may require data elements as many as atoms in the universe. Structure in data in such cases is the key issue. However, existing tensor reprensentations of tensors (multilinear forms, multidimensional arrays) suffer from various drawbacks. We propose new tensor decompositions called TENSOR-TRAIN DECOMPOSITIONS and the corresponding numerical algorithms with then complexity linear in the number of axes. Applications include interpolation of multi-variate functions, computation of multi-dimensional integrals, solving PDEs, fast inversion of tensor structured matrices etc. The new algorithms appeared as recently as just in the beginning of 2009 and will certainly be leading to a new generation of numerical algorithms. For more details see http://pub.inm.ras.ru.

[1] I.Oseledets, E.Tyrtyshnikov, Recursive decomposition of multidimensional tensors, Doklady Mathematics, vol. 80, no. 1 (2009), pp. 460-462.
[2] N.Zamarashkin, I.Oseledets, E.Tyrtyshnikov, The tensor structure of the inverse of a banded Toeplitz matrix, Doklady Mathematics, vol. 80, no. 2 (2009), pp. 669-670.
[3] I. Oseledets, E. Tyrtyshnikov, Breaking the curse of dimensionality, or how to use SVD in many dimensions. SIAM J. Sci. Comput., vol 31, no. 5 (2009), pp. 3744-3759.
[4] I. Oseledets, E. Tyrtyshnikov, TT-cross approximation for multidimensional arrays, Linear Algebra Appl., 432 (2010), pp. 70-88.

Joint work with I. Oseledets (INM RAS)
