Numerical approximation of multi-dimensional PDEs in quantized tensor spaces

Boris N. Khoromskij

Max-Planck-Institute for Mathematics in the Sciences,
Inselstr. 22-26, D-04103 Leipzig, Germany; *bokh*@mis.mpg.de

Modern methods of tensor-product approximation by separation of variables allow an efficient low-parametric calculus of functions and operators in higher dimensions. Most common separable representations combine the Tucker, canonical, tensor train (TT) and the more general MPS-type decompositions. The idea of data quantization makes it possible to represent (approximate) the multivariate functions, operators and dynamical systems in the quantized tensor spaces (QTT format) with the log-volume complexity scaling with respect to the grid size [2]. This opens the way to the profound numerical simulation of high-dimensional PDEs getting rid of the "curse of dimensionality" and rigorous restrictions on the grid size. However, the approach may be limited by the "curse of ranks" characterizing the essential entanglement in the system of interest.

We focus on the approximation and complexity results in the quantized tensor formats (Q-canonical, Q-Tucker, QTT) applied to the solution of d-dimensional elliptic and parabolic equations [1] - [5]. Numerical tests indicate the logarithmic computational complexity of the QTT tensor approximation for some parametric elliptic PDEs and in many-particle dynamics.

http://personal-homepages.mis.mpg.de/bokh

References

[1] I.V. Gavrilyuk, and B.N. Khoromskij. Quantized-TT-Cayley transform to compute dynamics and spectrum of high-dimensional Hamiltonians. Comp. Meth. in Applied Math., v.11 (2011), No. 3, 273-290.

[2] B.N. Khoromskij. $O(d \log N)$-*Quantics Approximation of* N-d *Tensors in High-Dimensional Numerical Modeling.* J. Constr. Approx. v. 34(2), 257-289 (2011).

[3] B.N. Khoromskij, *Tensors-structured Numerical Methods in Scientific Computing: Survey on Recent Advances.* Chemometrics and Intellingent Laboratory Systems, 110 (2012), 1-19.

[4] B.N. Khoromskij, and Ch. Schwab. *Tensor-Structured Galerkin Approximation of Parametric and Stochastic Elliptic PDEs.* SIAM J. Sci. Comp., **33**(1), 2011, 1-25.

[5] B.N. Khoromskij, and I. Oseledets. *DMRG+QTT approach to the computation of ground state for the molecular Schrödinger operator.* Preprint 68/2010, MPI MiS, Leipzig 2010 (Numer. Math., submitted).