Solving high-dimensional PDEs by tensor product approximation

Reinhold Schneider
TU Berlin , Germany
schneidr@math.tu-berlin.de

Hierarchical Tucker tensor format introduced by Hackbusch et al. including Tensor Trains (TT) (Tyrtyshnikov) have been introduced in 2009. These representations offer stable and robust approximation of high order tensors and multi-variate functions by a low order cost . For many high dimensional problems, including many body quantum mechanics, uncertainty quantification etc., this approach has great potential to circumvent from the *curse of dimensionality.* In case $\mathcal{V} = \bigotimes_{i=1}^{d} \mathcal{V}_i$ the complexity remains proportional to d and polynomial in some multilinear ranks. The approximation properties w.r.t. to these ranks are depending on bilinear approximation rates and corresponding trace class norms. Despite fundamental problems in multilinear approximation, under certain conditions optimal convergence rates could be shown. The present formats are equivalent to tree tensor networks states and matrix product states (MPS) introduced for the treatment of quantum spin systems. For numerical computations, we cast the PDEs into optimization problems constraint by restricting to set of d tensors of bounded multilinear ranks $\mathbf{r}$. The underlying admissible set is no longer convex, but it is an algebraic variety. We consider optimization on Riemannian manifold and corresponding gradient schemes. Numerical examples include electronic Schrödinger equations, uncertainty quantification and molecular dynamics.

Joint work with A. Uschmajew (U Bonn).