Alternating minimal energy methods for linear systems in higher dimensions

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When high-dimensional problems are concerned, not much algorithms can break the curse of dimensionality, and solve them efficiently and reliably. Among those, tensor product algorithms, which implement the idea of separation of variables for multi-index arrays (tensors), seem to be the most general and also very promising. They originated in quantum physics and chemistry and descent broadly from the *density matrix renormalization group* (DMRG) [12] and *matrix product states* (MPS) [6] formalisms. The same tensor formats were recently re-discovered in the numerical linear algebra (NLA) community as the *tensor train* (TT) format [9, 8].

Algorithms developed in the quantum physics community are based on the optimisation in tensor formats, that is performed subsequently for all components of a tensor format (i.e. all *sites* or *modes*). The DMRG/MPS schemes are very efficient but very difficult to analyse, and at the moment only local convergence results for the simplest algorithm are available [10]. In the NLA community, a common approach is to use a classical iterative scheme (e.g. GMRES) and enforce the compression to a tensor format at every step [1]. The formal analysis is quite straightforward, but tensor ranks of the vectors which span the Krylov subspace grow rapidly with iterations, and the methods are struggling in practice.

The first attempt to merge classical iterative algorithms and DMRG/MPS methods was made in [13], where the second Krylov vector is used to expand the search space on the optimisation step. The idea proved to be useful, but the implementation was based on the fair amount of physical intuition, and the algorithm is not completely justified.

We have recently proposed the AMEn algorithm for linear systems [3, 4], that also injects the gradient direction in the optimisation step, but in a way that allows to prove the **global convergence** of the resulted scheme. The scheme can be easily applied for the computation of the ground state — the differences to the algorithm of S. White [13] are emphasized in [5]. The AMEn scheme is already acknowledged in the NLA community — for example it was recently applied for the computation of extreme eigenstates [7], using the block-TT format proposed in [2].

At the moment, AMEn algorithm was applied to solve the Fokker-Planck equation for the non-Newtonian polymeric flows [4], to the chemical master equation describing the mesoscopic model of gene regulative networks [4], to solve the Heisenberg model problem for a periodic spin chain [5], to simulate the NMR spectra of large molecules (such as ubiquitin) [11]. We aim to extend this framework and the analysis to other problems of NLA: eigenproblems, time-dependent problems, high-dimensional interpolation, and matrix functions; as well as to a wider list of high-dimensional problems.

This is a joint work with Sergey Dolgov at the Max-Planck Institute for Mathematics in the Sciences, Leipzig, and Ilya Kuprov at the University of Southampton, UK.

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