

Low-rank Riemannian optimization for high-dimensional eigenvalue problems

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Abstract: In this work we focus on a solution of symmetric eigenvalue problems with eigenvectors that admit a low-rank representation in the Tensor Train format. The straightforward extension of iterative methods, e.g. locally-optimal block preconditioned conjugate gradient method (LOBPCG), leads to the instability and/or to the rank growth. Alternatively one can solve an eigenvalue problem as an optimization procedure, which is time-consuming when a large number of eigenvectors is to be found. We present a new solver which is based on the Riemannian optimization approach and which is capable of computing hundreds of eigenstates in high dimensions. The solver is implemented using TensorFlow software library and hence allows for a natural GPU parallelization. We showcase our method by calculating up to 100 eigenvalues and eigenvectors of a realistic Hamiltonian.