TT-FEAST: A High-Dimensional Eigenvalue Solver using Contour Integration and Tensor Train format

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Abstract

Eigenvalue problems in high-dimensional spaces are particularly challenging due to the curse of dimensionality, especially when computing eigenpairs within a given spectral interval. To address this complexity, we propose an extension of the FEAST algorithm, originally developed for Hermitian problems using contour integration, by integrating it with the Tensor Train (TT) decomposition. This approach enables efficient representations of both the operators and the eigenvectors in TT format, leading to significant savings in storage and computation requirements.

An adaptive approach is introduced to determine the dimension of the projection space by incorporating a rank-revealing Modified Gram-Schmidt process with pivoting, adapted for TT-vectors. A corresponding perturbation analysis provides an explicit bound on the attainable residual norm, which serves as a stopping criterion for the TT-FEAST algorithm. Furthermore, a continuation procedure is proposed to progressively refine convergence and rounding thresholds, allowing effective control over memory consumption throughout the computation.

The proposed method is applied to high-dimensional test cases, including the Laplacian operator and a vibrational Hamiltonian, demonstrating both efficiency and accuracy. For validation, we compare the results with analytical solutions in the case of the Laplacian, and with an existing TT-based method for computing low-lying eigenpairs of the vibrational Hamiltonian.

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