Contribution ID: **29** Type: **Poster**

Lanczos with compression for symmetric eigenvalue problems

Monday, 20 January 2025 16:00 (2 hours)

This work focuses on computing a few smallest or largest eigenvalues and their corresponding eigenvectors of a large symmetric matrix A.

Krylov subspace methods are among the most effective approaches for solving large-scale symmetric eigenvalue problems. Given a starting vector $\mathbf{q}_1$, the M-th Krylov subspace is generated by repeatedly multiplying a general square matrix A with $\mathbf{q}_1$:

\$$\mathcal{K}_M(A, \mathbf{q}_1) := \mathrm{span}\{\mathbf{q}_1, A\mathbf{q}_1, \ldots, A^{M-1}\mathbf{q}_1\}$.

An orthonormal basis $Q\_\{M\}$ for the Krylov subspace \mathcal{K}\{M}(A,\mathbf{q}_1)isconstructedusingtheLancz
to extract eigenvalue and eigenvector approximations, known as Ritz values and Ritz vectors.

A significant challenge of Krylov subspace methods is the need to store $Q\_\{M\}$. For slow convergence (with respect to M), available memory may be exhausted before achieving satisfactory approximations. Popular algorithms for large-scale eigenvalue problems address this issue by combining the Lanczos process with restarting.

As an alternative to restarting, this work proposes a novel compression approach based on Rational Krylov subspaces associated with small matrices, limiting the Lanczos method's memory requirements. To provide intuition for our approach, suppose the spectrum of A is ordered such that:

$\lambda_1 \leq \cdots \leq \lambda_m < \tau < \lambda_{m+1} \leq \cdots \leq \lambda_n$,

where a shift \tau separates the smallest m\lln eigenvalues to be computed from the rest. Let \chi\\tau(x)denotethestepfunc

In practice, however, evaluating \chi\tau(A)\mathbf{q}\1exactlyiscomputationallyinfeasible.Instead, arationalappr
can be used to compress \mathcal{K}_{M}(A, \mathbf{q}_1). This approach parallels the developments in [2], which employs a rational approximation of a general function f to compress the Lanczos method for approximating f(A)\mathbf{b}\$.Tomakethiscompressionpracticalforeigenvalueproblems, severaladditio

We present a series of numerical experiments involving matrices from various applications. These experiments demonstrate that, in terms of matrix-vector products, our new method is consistently competitive with or superior to the Krylov–Schur method, often achieving significant improvements.

References

1. A. C., D. Kressner, N. Shao. Lanczos with compression for symmetric eigenvalue problems. In preparation.
2. A. C., I. Simunec. A low-memory Lanczos method with rational Krylov compression for matrix functions. arXiv, 2024.

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Session Classification: Poster Session