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Accelerating large partial EVD/SVD calculations by filtered block Davidson methods.
(English) Zbl 1353.65029

Summary: Partial eigenvalue decomposition (PEVD) and partial singular value decomposition (PSVD) of large sparse matrices are of fundamental importance in a wide range of applications, including latent semantic indexing, spectral clustering, and kernel methods for machine learning. The more challenging problems are when a large number of eigenpairs or singular triplets need to be computed. We develop practical and efficient algorithms for these challenging problems. Our algorithms are based on a filter-accelerated block Davidson method. Two types of filters are utilized, one is Chebyshev polynomial filtering, the other is rational-function filtering by solving linear equations. The former utilizes the fastest growth of the Chebyshev polynomial among same degree polynomials; the latter employs the traditional idea of shift-invert, for which we address the important issue of automatic choice of shifts and propose a practical method for solving the shifted linear equations inside the block Davidson method. Our two filters can efficiently generate high-quality basis vectors to augment the projection subspace at each Davidson iteration step, which allows a restart scheme using an active projection subspace of small dimension. This makes our algorithms memory-economical, thus practical for large PEVD/PSVD calculations. We compare our algorithms with representative methods, including ARPACK, PROPACK, the randomized SVD method, and the limited memory SVD method. Extensive numerical tests on representative datasets demonstrate that, in general, our methods have similar or faster convergence speed in terms of CPU time, while requiring much lower memory comparing with other methods. The much lower memory requirement makes our methods more practical for large-scale PEVD/PSVD computations.

MSC:
65F15 Numerical computation of eigenvalues and eigenvectors of matrices
65F20 Numerical solutions to overdetermined systems, pseudoinverses
65F50 Computational methods for sparse matrices

Keywords:
polynomial filter; rational filter; kernel; graph; partial eigenvalue decomposition; partial singular value decomposition; algorithm; block Davidson method; Chebyshev polynomial; numerical test

Software:
CheFSI; LIBSVM; MNIST; JDQR; SNAP ; JDQZ; PROPACK; eigs; PRIMME; IRAM; SLEPc; softImpute; UCI-ml; ARPACK; lobpcg.m; JDCG

Full Text: DOI

References:


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