Ruipeng Li A Thick-Restart Lanczos algorithm with polynomial filtering for Hermitian eigenvalue problems

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Polynomial filtering can provide a highly effective means of computing all eigenvalues of a real symmetric (or complex Hermitian) matrix that are located in a given interval, anywhere in the spectrum. This work presents a technique for tackling this problem by combining a Thick-Restart version of the Lanczos algorithm with deflation ('locking') and a new type of polynomial filters. Thick restarting is employed to limit the cost of orthogonalization. The polynomial filter that maps eigenvalues within a given interval to eigenvalues with the largest magnitude of the transformed problem, is obtained from a least-squares approximation to an appropriately centered Dirac- δ distribution. The resulting algorithm can be utilized in a 'spectrum-slicing' approach whereby a very large number of eigenvalues and associated eigenvectors of the matrix are computed by extracting eigenpairs located in different sub-intervals independently from one another. Numerical experiments show that such a construction yields effective polynomial filters which along with a Thick-Restart Lanczos procedure enable desired eigenpairs to be computed efficiently.