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Preconditioned Thick-Restart Lanczos Method with Subspace Optimization for Symmetric Eigenvalue Problems

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The Thick-Restart Lanczos method (TRLAN) is an effective method for large sparse symmetric eigenvalue problems. However, the effectiveness of Lanczos method heavily depends on the distribution of eigenvalues and can converge very slowly when the desired eigenvalues are not well separated from the rest of the spectrum. In addition, restarting causes further deterioration of convergence. Thick restarting can recover some of the convergence loss but the restarting method of subspace optimization (also known as +k or locally optimal restarting) is the one that can result in near optimal methods. However, locally optimal restarting has only been implemented with Generalized Davidson (GD) or LOPBCG methods which have expensive iteration costs.

In this work, we propose a new near-optimal eigenmethod, TRLAN+K, that combines the efficiency of the Lanczos algorithm and the power of the subspace optimization techniques. Specifically, an inner-outer scheme is employed. The inner loop applies the Lanczos recurrence while the outside loop augments the Krylov subspace with a certain number of vectors from the previous restart cycle. We then apply the Rayleigh-Ritz procedure in the new subspace. Numerical experiments show that the proposed method can achieve almost optimal convergence when considering the unrestarted Lanczos as benchmark. Specifically, our method can converge up to ten times faster than TRLAN when both methods are operated with relatively small subspace under limited memory. The advantage of the proposed method slowly diminishes as the size of subspace increases compared to TRLAN, and then both methods converge similarly to the unrestarted Lanczos.

The generated Davidson (GD) method and its variants are a class of effective eigenmethods that can also take advantage of a preconditioner. Among them, GD+K utilizes the locally optimal conjugate gradient restarting and has been shown to deliver near-optimal convergence under severely limited memory. Without a preconditioner, it is well known that the GD method is mathemati-

cally equivalent to the Lanczos method and with thick restarting it is equivalent to TRLAN. GD+K, however, has slightly better convergence than TRLAN+K since it expands the subspace by the residuals from Rayleigh-Ritz optimization at every step. On the other hand TRLAN+K has smaller costs for Raryleigh-Ritz and orthogonalization and thus it can be more efficient than GD+K when the matrix is sufficiently sparse. In addition, as the size of the subspace increases, the differences between convergence rates become smaller and the low cost of the Lanczos recurrence further benefits TRLAN+K.

In addition to the usual shift-invert mode,TRLAN+K can also be adapted to use a preconditioner. We use an inverse-free type preconditioned Krylov subspace scheme in the inner iteration. Although the inner iteration is similar to the EIGIFP method, TRLAN+K differs in several ways and most importantly in the techniques used in the outer iteration, specifically thick restarting and the subspace optimization. These techniques are the key to achieving a near-optimal eigenmethod.