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On expansion of search subspaces for large non-Hermitian eigenproblems

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ABSTRACT

How to expand a given subspace efficiently is an important task for large sparse eigenvalue problems. In this paper, we are interested in the following question: which vector from a given subspace, after multiplied by the matrix A, will give a better expanded search subspace. In (2008) [33], Ye investigated this problem and determined how to choose the optimal expansion vector theoretically. Unfortunately, the result is not computable since it involves some unknown information on the desired eigenvector. When A is symmetric, it was suggested that the Ritz vector may lead to a good candidate for subspace expansion. However, when A is non-Hermitian, the Ritz vector may not be a satisfactory choice. The contribution of this paper is twofold. First, we suggest to use the refined Ritz vector to expand the search subspace, and propose a residual expansion Arnoldi method for subspace expansion. Theoretical results justify the use of the refined Ritz vector. Second, we prove that the elements of the primitive refined Ritz vector have a decreasing pattern going to zero. We then show that the decreasing pattern exists in an arbitrary primitive approximate eigenvector, and derive an inexact residual expansion Arnoldi method for subspace expansion. Numerical examples show the effectiveness of our

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theoretical results and illustrate the numerical behavior of the new method for subspace expansion.

1. Introduction

Large sparse eigenvalue problem

$$A\mathbf{x} = \lambda\mathbf{x} \tag{1.1}$$

is fundamental in scientific and engineering computations [2,6,20,26–28], where $A \in \mathbb{C}^{n\times n}$ is a large sparse matrix, and $(\lambda, \mathbf{x})$ is an eigenpair of A with $\|\mathbf{x}\| = 1$. Projection methods are very popular for computing a few selected eigenvalues and the corresponding eigenvectors or invariant subspace of a large sparse matrix [2,20,28]. These methods are often implemented as iterative algorithms in which matrix–vector products are exploited to construct search subspaces. A key point to the success of a projection method is whether the search subspace constructed contains good approximation to the desired eigenvector [33]. Indeed, how to expand a given search subspace efficiently is a very interesting topic in large sparse eigenvalue computations. A number of numerical algorithms are available for this problem [1,14,17–19,24,33]. In this paper, we are interested in the problem of constructing a search subspace via gradual expansion from an existing one using matrix–vector products.

The Arnoldi method is a well-known Krylov subspace method that can be used to find a few eigenpairs of a large matrix [1,2,20,28]. Given a unit norm vector $\mathbf{v}_1$, if computations are performed in exact arithmetic, the Arnoldi process will generate successively an orthonormal basis for the Krylov subspace $\mathcal{K}_m(A, \mathbf{v}_1) = \text{span}\{\mathbf{v}_1, A\mathbf{v}_1, \ldots, A^{m-1}\mathbf{v}_1\}$. Let $V_m = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m]$ be an orthonormal basis for $\mathcal{K}_m(A, \mathbf{v}_1)$, then the Arnoldi method expands the search subspace V_k by $\mathbf{v}_{k+1}$ which is obtained from orthogonalizing $A\mathbf{v}_k$ against V_k. In this Krylov subspace, the restriction of A is represented by an $m \times m$ upper Hessenberg matrix H_m with the entries h_{ij}, $1 \le i, j \le m$. Furthermore, the following Arnoldi relation holds [2,20,28]

$$AV_m = V_m H_m + h_{m+1,m}\mathbf{v}_{m+1}\mathbf{e}_m^{\mathrm{T}} = V_{m+1}\widetilde{H}_m,$$

where $\mathbf{e}_m$ is the m-th coordinate vector of dimension m, and $\widetilde{H}_m$ is an $(m+1)\times m$ upper Hessenberg matrix. Let $(\widetilde{\lambda}, \mathbf{y})$ be an eigenpair of H_m, then one can use $(\widetilde{\lambda}, \widetilde{\mathbf{x}}) := (\widetilde{\lambda}, V_m\mathbf{y})$, called Ritz pair of A, as an approximation to the desired eigenpair $(\lambda, \mathbf{x})$ of A. For more details, refer to [2,20,28] and the references given therein.

However, if we start from a general subspace or from a slight deviation of a Krylov subspace, then the subspace expanded in this way depends on the vector that we select from the subspace [33]. In this situation, our problem reduces to the following: which