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DEFLATION BY RESTRICTION FOR THE INVERSE-FREE PRECONDITIONED KRYLOV SUBSPACE METHOD

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Abstract. A deflation by restriction scheme is developed for the inverse-free preconditioned Krylov subspace method for computing a few extreme eigenvalues of the definite symmetric generalized eigenvalue problem $Ax = \lambda Bx$. The convergence theory for the inverse-free preconditioned Krylov subspace method is generalized to include this deflation scheme and numerical examples are presented to demonstrate the convergence properties of the algorithm with the deflation scheme.

1. **Introduction.** The definite symmetric generalized eigenvalue problem for (A, B) is to find $\lambda \in \mathbb{R}$ and $x \in \mathbb{R}^n$ with $x \neq 0$ such that

$$Ax = \lambda Bx \tag{1}$$

where A, B are $n \times n$ symmetric matrices and B is positive definite. The eigenvalue problem (1), also referred to as a pencil eigenvalue problem (A, B), arises in many scientific and engineering applications, such as structural dynamics, quantum mechanics, and machine learning. The matrices involved in these applications are usually large and sparse and only a few of the eigenvalues are desired.

Iterative methods such as the Lanczos algorithm and the Arnoldi algorithm are some of the most efficient numerical methods developed in the past few decades for computing a few eigenvalues of a large scale eigenvalue problem, see [1, 11, 19]. Their speed of convergence depends on the spectral distribution of (1) and they may suffer from slow convergence when the desired eigenvalues are not well separated. Preconditioning techniques may be used to accelerate the convergence of these iterative methods. One of the most effective techniques is the shift-and-invert transformation. However, for truly large problems, it may be too expensive or even infeasible to employ the shift-and-invert method as it requires the LU factorization of a shifted matrix. To avoid the fill-in of zero entries of a sparse matrix caused by

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the LU factorization, one can consider incomplete factorizations that are used as preconditioners for solving linear systems. Several methods have been proposed that can effectively accelerate convergence of an eigenvalue algorithm without using the (complete) LU factorization of the shift-and-invert. The Jacobi-Davidson method [20, 4], the JDCG algorithm [16], the locally preconditioned conjugate gradient method (LOBPCG) [6, 7], and the inverse-free preconditioned Krylov subspace method [5, 14] are some of such methods, among many others (see [2, 3, 6, 7, 12, 13, 15, 21, 24] for example).

The inverse-free precondioned Krylov subspace method of [5] is a Krylov subspace projection method that computes the smallest (or the largest) eigenvalues of (1). The method is based on an inner-outer iteration that does not require the inversion of B or any shifted matrix $A - \lambda B$. Given an approximate eigenvector x_k and its Rayleigh quotient ρ_k, it approximates the smallest eigenvalue iteratively through the Rayleigh-Ritz projection on the Krylov subspace

$$\mathcal{K}_m(H_k, x_k) := \text{span}\{x_k, H_k x_k, H_k^2 x_k, \ldots, H_k^m x_k\} \tag{2}$$

where $H_k := A - \rho_k B$. It is proved in [5] that this method converges at least linearly with a rate determined by the spectral separation of the smallest eigenvalue of H_k. This convergence theory leads to a preconditioning scheme that accelerates the convergence through some equivalent congruent transformation based on incomplete factorizations. This procedure, however, computes one eigenvalue (the smallest) only. To compute additional eigenvalues, a deflation technique needs to be used. Note that a block version developed in [18] can compute several eigenvalues simultaneously, but it is efficient largely for severely clustered eigenvalues.

Deflation processes are standard methods used by iterative eigenvalue algorithms to compute additional eigenvalues after some eigenvalues have converged. Two widely used deflation techniques are the Wielandt deflation (or known as deflation by subtraction) where the matrix is modified with a low rank perturbation to move converged eigenvalue to a different part of spectrum, and deflation by restriction where approximate eigenvectors and relevant subspaces are projected to the orthogonal complement of the converged eigenvectors, see [17, 19, 23]. Both of these deflation schemes can be used in the standard Lanczos and Arnoldi algorithms. There are variations of these schemes that are suitable for some particular methods. For example, the implicitly restarted Arnoldi algorithm [9, 10, 11] employs an elaborate deflation scheme (locking and purging) that is similar to deflation by restriction. The Jacobi-Davidson method [20, 22] incorporates a partial Schur decomposition deflation.

For the inverse-free preconditioned Krylov subspace method [5, 14], a natural deflation scheme is the Wielandt deflation where the method is implicitly applied to a low rank modified problem. Specifically, assume that ℓ eigenpairs (λ_i, v_i)(for $1 \le i \le \ell$) of (A, B) have been found and let $V_\ell = [v_1, ..., v_l]$ with $V_\ell^T B V_\ell = I$ and $\Lambda_\ell = \text{diag}(\lambda_1, ..., \lambda_\ell)$. If $\lambda_{\ell+1} \le ... \le \lambda_n$ are the remaining eigenvalues, then $\lambda_{\ell+1}$ is the smallest eigenvalue of

$$(A_\ell, B) := (A + (BV_\ell)\Sigma(BV_\ell)^T, B) \tag{3}$$

where $\Sigma = \text{diag}\{\alpha - \lambda_i\}(1 \le i \le \ell)$ with α any value chosen to be greater than $\lambda_{\ell+1}$. Therefore $\lambda_{\ell+1}$ can be computed by applying the inverse-free preconditioned Krylov subspace algorithm to (A_ℓ, B) and all the known convergence theory is directly applicable. This deflation method is implemented in the MATLAB program `eigifp` of [14].

In some applications, the deflation (3) alters the structure of the problem which may cause some difficulties in its implementations. Consider computing a few smallest singular values of a matric C. In [8], the inverse-free Krylov subspace method is implicitly applied to $A = C^TC$ to compute the singular values of C. To carry out the Rayleigh-Ritz projection, it is proposed to apply the projection directly to C rather than to $A = C^TC$; namely, we compute the smallest singular values of $Y_m^TCZ_m$, rather than the smallest eigenvalues of $Z_m^TC^TCZ_m$, where Z_m and Y_m are orthogonal bases of the subspaces $\mathcal{K}_m$ and $C\mathcal{K}_m$ respectively. In this way, the singular values of C are approximated by the singular values of the projection matrix. Avoiding squaring of the singular values allows tiny singular values to be computed more accurately (see [8]). However, the deflation (3) changes the problem to the one for $C^TC + V_\ell\Sigma V_\ell^T$, for which the Ritz values can not be formulated as the singular values of some projection matrix. In this setting, therefore, it is more desirable to work with the original problem without the low rank modification.

The deflation by restriction is a method that ensures convergence to the desired eigenpairs through projecting all approximate eigenvectors (or subspaces of candidate eigenvectors) to the B-orthogonal complement of $\mathcal{V}_\ell := \text{span}\{v_1, \cdots, v_\ell\}$. This certainly ensures the resulting approximate eigenvectors are the ones desired, but the process alters the underlying algorithm which may change its convergence properties. For the inverse-free Krylov subspace method, we can apply Rayleigh-Ritz projections directly on (A, B) but replace the Krylov subspace $\mathcal{K}_m(A-\rho_kB, x_k)$ by the projected subspace

$$\mathcal{K}_m((I - V_\ell V_\ell^TB)(A - \rho_kB), (I - V_\ell V_\ell^TB)x_k) \tag{4}$$

This enforces that all approximate eigenvectors obtained are in the B-orthogonal complement of $\mathcal{V}_\ell$ but the resulting algorithm is no longer equivalent to the original one and there is no guarantee on the convergence of the new process. Note that the spectral projection $I - V_\ell V_\ell^TB$ does not generally diagonalize the matrix $A - \rho_kB$ (for $B \neq I$) and hence the projected subspace (4) is not equivalent to the one produced by $A - \rho_kB$ and a projected initial vector $(I - V_\ell V_\ell^TB)x_k$. Nevertheless, this deflation strategy is implemented in [8] for the singular value problem and it is reported numerically that it has a convergence characteristics similar to the original process.

In this paper, we will show that the original convergence theory in [5] can be generalized to the algorithm modified with the deflation by restriction scheme based on (4). We will show that the algorithm with deflation by restriction still converges globally and under some conditions converge locally at least linearly. However, the rate of convergence is now determined by the eigenvalues of $(I - BV_\ell V_\ell^T)(A - \rho_kB)(I - V_\ell V_\ell^TB)$ as illustrated in Section 3. Numerical experiments will be given to demonstrate our theoretical results.

The paper is organized as follows. We briefly review the inverse-free preconditioned Krylov subspace method in Section 2. In Section 3 we introduce the new deflation strategy and prove some global and local convergence results that are similar to the ones in [5]. We will present some numerical examples in Section 4 to illustrate the convergence properties. We conclude the paper with some remarks in Section 5. Throughout the paper, we use $\|\cdot\|$ to denote 2-norm.

2. Inverse-free Preconditioned Krylov Subspace Method.

Given a vector x, the Rayleigh quotient $\rho(x) = (x^TAx)/(x^TBx)$ is the best approximation to an eigenvalue in the sense that $\alpha = \rho(x)$ minimizes the 2-norm of the residual $Ax - \alpha Bx$.

Since $r = (Ax - \rho(x)Bx)/x^TBx$ is the gradient of $\rho(x)$, the well-known steepest descent method aims to minimize the Rayleigh quotient over $\text{span}\{x, r\}$. Noticing that it can be viewed as a Rayleigh-Ritz orthogonal projection method on the Krylov subspace $\mathcal{K}_1(A - \rho(x)B, x) = \text{span}\{x, (A - \rho(x)B)x\}$, the inverse-free Krylov subspace method improves this by considering the Rayleigh-Ritz orthogonal projection on a larger Krylov subspace $\mathcal{K}_m(A - \rho(x)B, x) = \text{span}\{x, (A - \rho(x)B)x, \ldots, (A - \rho(x)B)^m x\}$. Namely, assume that x_k is the approximate eigenvector at step k in an iterative procedure of finding the smallest eigenvalue of the pair (A, B), [5] obtains a new approximation through the Rayleigh-Ritz orthogonal projection on

$$\mathcal{K}_m(A - \rho_k B, x_k) = \text{span}\{x_k, (A - \rho_k B)x_k, \ldots, (A - \rho_k B)^m x_k\}$$

where

$$\rho_k = \rho(x_k) = \frac{x_k^T A x_k}{x_k^T B x_k} \tag{5}$$

and m is a parameter to be chosen. Suppose Z_m is a matrix whose columns are basis vectors of $\mathcal{K}_m(A - \rho_k B, x_k)$. Let $A_m = Z_m^T(A - \rho_k B)Z_m$ and $B_m = Z_m^T B Z_m$. The smallest eigenvalue μ_1 of (A_m, B_m) and a corresponding eigenvector h can be obtained by any state-of-the-art eigensolver. Then the new approximation x_{k+1} is

$$x_{k+1} = Z_m h \tag{6}$$

and, correspondingly, the Rayleigh quotient

$$\rho_{k+1} = \rho_k + \mu_1 \tag{7}$$

is a new approximate eigenvalue. The choices of Z_m are not unique and it can be constructed by either the Lanczos method or the Arnoldi method with the B-inner product; see [5] for a more detailed discussion. Throughout this paper, we will only consider the case when the columns of Z_m are B-orthonormal, i.e. $Z_m^T B Z_m = I$. Then the basic procedure of inverse-free Krylov subspace method is given in Algorithm 2.1.

Algorithm 2.1 Inverse-free Krylov subspace method for (A, B)

1: **Input:** $m \geq 1$ and an initial approximate eigenvector x_0 with $\|x_0\| = 1$;
2: $\rho_0 = \rho(x_0)$;
3: **for** $k = 0, 1, 2, \ldots$ until convergence **do**
4: Construct a B-orthonormal basis $Z_m = [z_0, z_1, \ldots, z_m]$ for $\mathcal{K}_m(A - \rho_k B, x_k)$;
5: Form $A_m = Z_m^T(A - \rho_k B)Z_m$;
6: Find the smallest eigenpair (μ_1, h) of A_m;
7: $\rho_{k+1} = \rho_k + \mu_1$ and $x_{k+1} = Z_m h$.
8: **end for**

The following theorem states that Algorithm 2.1 always converges to an eigenpair of (A, B).

Theorem 2.1. ([5, Proposition 3.1 and Theorems 3.2]) *Let λ_1 be the smallest eigenvalue of (A, B) and (ρ_k, x_k) be the eigenpair approximation of Algorithm 2.1 at step k. Then*

1. $\lambda_1 \leq \rho_{k+1} \leq \rho_k$;
2. ρ_k *converges to some eigenvalue* $\hat{\lambda}$ *of* (A, B) *and* $\|(A - \hat{\lambda}B)x_k\| \to 0$.

Theorem 2.1 shows that x_k in Algorithm 2.1 always converges in direction to an eigenvector of (A, B). Through a local analysis, we have that Algorithm 2.1 converges linearly under some conditions with a rate bounded below.

Theorem 2.2. ([5, Theorems 3.4]) *Let $\lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$ be the eigenvalues of (A, B). Let (ρ_{k+1}, x_{k+1}) be the approximate eigenpair obtained by Algorithm 2.1 at step $k+1$ from (ρ_k, x_k). Let $\sigma_1 < \sigma_2 \leq \cdots \leq \sigma_n$ be the eigenvalues of $A - \rho_k B$ and u_1 be a unit eigenvector corresponding to σ_1. Assume $\lambda_1 < \rho_k < \lambda_2$. Then*

$$\rho_{k+1} - \lambda_1 \leq (\rho_k - \lambda_1)\epsilon_m^2 + 2(\rho_k - \lambda_1)^{3/2}\epsilon_m \left(\frac{\|B\|}{\sigma_2}\right)^{\frac{1}{2}} + \mathcal{O}\left((\rho_k - \lambda_1)^2\right) \quad (8)$$

where

$$\epsilon_m = \min_{p \in \mathcal{P}_m, p(\sigma_1)=1} \max_{i \neq 1} |p(\sigma_i)|$$

and $\mathcal{P}_m$ denote the set of all polynomials of degree not greater than m.

Theorem 2.2 shows that ρ_k converges at least at the rate of ϵ_m^2 which is bounded in terms of σ_i as

$$\epsilon_m \leq 2\left(\frac{1-\sqrt{\phi}}{1+\sqrt{\phi}}\right)^m \text{ with } \phi = \frac{\sigma_2 - \sigma_1}{\sigma_n - \sigma_1}.$$

It illustrates an interesting fact that the speed of convergence of ρ_k depends on the distribution of eigenvalues of $A - \rho_k B$ rather than those of (A, B). It leads to some equivalent transformations of the problem, called preconditioning, that changes the spectrum of $A - \rho_k B$ to accelerate the convergence of Algorithm 2.1. In particular, suppose $\lambda_1 < \rho_k < \lambda_2$ and let $A - \rho_k B = L_k D_k L_k^T$ be the LDL^T factorization with $D_k = \text{diag}\{-1, 1, \ldots, 1\}$. Then the transformed pair $(\hat{A}_k, \hat{B}_k) \equiv (L_k^{-1} A L_k^{-T}, L_k^{-1} A L_k^{-T})$ will have the same eigenvalues as (A, B) and the convergence of Algorithm 2.1 will depend on the spectral gap of $L_k^{-1}(A - \rho_k B)L_k^{-T}$ in which case $\epsilon_m = 0$. Then, by Theorem 2.2, the preconditioned Algorithm converges quadratically. However, this is an ideal situation since we assume a complete LDL^T factorization and L_k is computed for each iteration which is not practical. In practice, we use an approximate LDL^T factorization through an incomplete factorization for example. This usually leads to a small ϵ_m and hence accelerates convergence; see [5] for more discussions.

3. Analysis of Deflation Algorithms.

Algorithm 2.1 computes the smallest eigenvalue of (A, B) only. When the smallest eigenvalue has been computed, we can use a deflation procedure to compute additional eigenvalues. While both the deflation by restriction method and the Wielandt deflation can be used in most other iterative methods, the Wielandt deflation is the only one that can be directly used for Algorithm 2.1. We first briefly describe this process as presented in [14].

Suppose that ℓ eigenpairs (λ_i, v_i)(for $1 \leq i \leq \ell$) of (A, B) have been found and let $V_\ell = [v_1, ..., v_l]$ with $V_\ell^T B V_\ell = I$ and $\Lambda_\ell = \text{diag}\{\lambda_1, \ldots, \lambda_\ell\}$. Then $AV_\ell = BV_\ell\Lambda_\ell$. In the Wielandt deflation method, we apply Algorithm 2.1 to

$$(A_\ell, B) := (A + (BV_\ell)\Sigma(BV_\ell)^T, B) \text{ where } \Sigma = \text{diag}\{\alpha - \lambda_i\}$$

with α any value chosen to be greater than $\lambda_{\ell+2}$. Since $\lambda_{\ell+1}$ is the smallest eigenvalue of (A_ℓ, B), Algorithm 2.1 will converge to $\lambda_{\ell+1}$ under the conditions of Theorem 2.2.

As discussed in the introduction, the Wielandt deflation changes the structure of the problem and this may be undesirable in certain applications such as the

singular value computations (see [8]). In such problems, it is of interest to consider the deflation by restriction, namely, by projecting the subspaces involved to the B-orthogonal complement of $\mathcal{V}_\ell := \text{span}\{v_1, \cdots, v_\ell\}$. This can be done by simply using $(I - V_\ell V_\ell^T B)\mathcal{K}_m(A - \rho_k B, x_k)$, but this does not lead to a convergent algorithm. A more appropriate approach is to apply the projection on the matrix or on every step of the basis construction; namely we use $\mathcal{K}_m((I - V_\ell V_\ell^T B)(A - \rho_k B), (I - V_\ell V_\ell^T B)x_k)$; This also changes subspaces and the existing convergence theory does not apply. However, it has been observed numerically in [8] that such a deflation scheme appears to work in practice.

In this section, we formulate a deflation by restriction method for the inverse-free Krylov subspace method (Algorithm 2.1) and present a convergence theory that generalizes the convergence results of Section 2. We first state the deflation by restriction method in the following algorithm.

Algorithm 3.2 Inverse-free Krylov subspace method with deflation by restriction

1: **Input**: $V_\ell = [v_1, \cdots, v_\ell]$ satisfying $Av_i = \lambda_i Bv_i$ (for $1 \le i \le \ell$) and $V_\ell^T B V_\ell = I$; m and x_0 with $\|x_0\| = 1$ and $V_\ell^T B x_0 = 0$;
2: $\rho_0 = \rho(x_0)$;
3: **for** $k = 0, 1, 2, \ldots$ until convergence **do**
4: Construct a basis $\{z_1, z_2, \ldots, z_m\}$ for $\mathcal{K}_m((I - V_\ell V_\ell^T B)(A - \rho_k B), x_k)$;
5: $A_m = Z_m^T (A - \rho_k B) Z_m$ and $B_m = Z_m^T B Z_m$ where $Z_m = [z_1, z_2, \ldots, z_m]$;
6: Find the smallest eigenvalue μ_1 and a unit eigenvector v for (A_m, B_m);
7: $\rho_{k+1} = \rho_k + \mu_1$ and $x_{k+1} = Z_m v$.
8: **end for**

Note that if there is no converged eigenpairs available, V_ℓ in the algorithm is empty. Then the algorithm is the same as the standard Algorithm 2.1. When we have ℓ eigenpairs available as given in V_ℓ, the difference from Algorithm 2.1 is the use of the projected Krylov subspace $\mathcal{K}_m(P_V(A-\rho_k B), x_k)$ where $P_V = I - V_\ell V_\ell^T B$. We can easily show by induction that $P_V x_k = x_k$ for all k. Then

$$\mathcal{K}_m(P_V(A - \rho_k B), x_k) = \mathcal{K}_m(P_V(A - \rho_k B)P_V, x_k).$$

However, since the columns of V_ℓ are generally not eigenvectors of $A - \rho_k B$ (when $B \neq I$), $P_V(A - \rho_k B)P_V$ does not lead to a deflated operator (i.e. a spectral restriction of $A-\rho_k B$). Indeed, with P_V a B-orthogonal projection, $P_V(A-\rho_k B)P_V$ is not even symmetric. However, the following lemma expresses the Krylov subspace as one generated by a symmetric matrix, which is key in our analysis of Algorithm 3.2.

Lemma 3.1. *Let $V_\ell = [v_1, \cdots, v_\ell]$ be such that $Av_i = \lambda_i Bv_i$ (for $1 \le i \le \ell$) and $V_\ell^T B V_\ell = I$. Let $P_V = I - V_\ell V_\ell^T B$. Then we have*

$$(A - \rho_k B)P_V = P_V^T (A - \rho_k B) \tag{9}$$

and for any x_k with $P_V x_k = x_k$,

$$\mathcal{K}_m(P_V(A - \rho_k B), x_k) = P_V \mathcal{K}_m(P_V^T (A - \rho_k B)P_V, x_k). \tag{10}$$

Proof. First we have $AV_\ell = BV_\ell\Lambda$, where $\Lambda = \mathrm{diag}\{\lambda_1, \cdots, \lambda_\ell\}$. Then $V_\ell^T A = \Lambda V_\ell^T B$. It follows that

$$\begin{aligned} P_V^T(A-\rho_k B) &= (A-\rho_k B) - (BV_\ell V_\ell^T A - \rho_k BV_\ell V_\ell^T B) \\ &= (A-\rho_k B) - (BV_\ell \Lambda V_\ell^T B - \rho_k BV_\ell V_\ell^T B) \\ &= (A-\rho_k B) - (AV_\ell V_\ell^T B - \rho_k BV_\ell V_\ell^T B) \\ &= (A-\rho_k B)P_V, \end{aligned}$$

which proves (9). From this and $P_V^2 = P_V$, we have

$$P_V^T(A-\rho_k B)P_V = (A-\rho_k B)P_V P_V = (A-\rho_k B)P_V.$$

Thus, it follows from $P_V x_k = x_k$ that for all $i = 1, \cdots, m-1$,

$$\begin{aligned} (P_V(A-\rho_k B))^i x_k &= (P_V(A-\rho_k B))^i P_V x_k \\ &= P_V((A-\rho_k B)P_V)^i x_k \\ &= P_V(P_V^T(A-\rho_k B)P_V)^i x_k. \end{aligned}$$

Hence $\mathcal{K}_m(P_V(A-\rho_k B), x_k) = P_V\mathcal{K}_m(P_V^T(A-\rho_k B)P_V, x_k)$. □

With the above characterization of the projection subspace used in Algorithm 3.2, the convergence properties described in Section 2 can be generalized following similar lines of proofs in [5, Theorem 3.2] with careful analysis of some subtle effects of the projection that are highly nontrivial. We first present a generalization of the global convergence result (Theorem 2.1).

Theorem 3.2. *Let $V_\ell = [v_1, \cdots, v_\ell]$ be such that $Av_i = \lambda_i Bv_i$ (for $1 \le i \le \ell$) and $V_\ell^T BV_\ell = I$. Let $\lambda_{\ell+1} \le \lambda_{\ell+2} \le \cdots \le \lambda_n$ together with $\lambda_1, \cdots, \lambda_\ell$ be the eigenvalues of (A, B). Let (ρ_k, x_k) be the eigenpair approximation obtained at step k of Algorithm 3.2 with V_ℓ. Then*

$$\lambda_{\ell+1} \le \rho_{k+1} \le \rho_k.$$

Furthermore, ρ_k converges to some eigenvalue $\hat{\lambda} \in \{\lambda_{\ell+1}, \cdots, \lambda_n\}$ of (A, B) and $\|(A-\hat{\lambda}B)x_k\| \to 0$ (i.e., x_k converges in direction to a corresponding eigenvector).

Proof. From Algorithm 3.2, we have

$$\rho_{k+1} = \rho_k + \min_{w\in\mathcal{W}, w\neq 0} \frac{w^T(A-\rho_k B)w}{w^T Bw} = \min_{w\in\mathcal{W}} \frac{w^T Aw}{w^T Bw}$$

where $\mathcal{W} = \mathcal{K}_m(P_V(A-\rho_k B), x_k)$ and $P_V = I - V_\ell V_\ell^T B$. Since $x_k \in \mathcal{W}$, we have $\rho_{k+1} \le \rho_k$. On the other hand, it follows from Lemma 3.1 that $\mathcal{W} = P_V\mathcal{K}_m(P_V^T(A-\rho_k B)P_V, x_k) \subset \mathcal{R}(P_V)$ (the range space of P_V). Then

$$\rho_{k+1} \ge \min_{V_\ell^T Bw=0, w\neq 0} \frac{w^T Aw}{w^T Bw} = \lambda_{\ell+1}.$$

It follows that ρ_k is convergent. Since $\{x_k\}$ is bounded, there is a convergent subsequence $\{x_{n_k}\}$. Let

$$\lim \rho_k = \hat{\lambda}, \text{ and } \lim x_{n_k} = \hat{x}.$$

Write $\hat{r} = (A-\hat{\lambda}B)\hat{x}$. Then it follows from $x_k^T(A-\rho_k B)x_k = 0$ that

$$\hat{x}^T\hat{r} = \hat{x}^T(A-\hat{\lambda}B)\hat{x} = 0.$$

Suppose now $\hat{r} \neq 0$. Using Lemma 3.1 and the fact that $P_V\hat{x} = \hat{x}$ which follows from $P_V x_k = x_k$, we obtain

$$P_V^T\hat{r} = P_V^T(A - \hat{\lambda}B)\hat{x} = (A - \hat{\lambda}B)P_V\hat{x} = (A - \hat{\lambda}B)\hat{x} = \hat{r}. \tag{11}$$

We now show that $\hat{x}$ and $P_V\hat{r}$ are linearly independent. If they are linearly dependent, we have $P_V\hat{r} = \gamma\hat{x}$ for some scaler γ. Then by (11), $\hat{r}^T P_V P_V^T\hat{r} = \hat{r}^T P_V\hat{r} = \gamma\hat{r}^T\hat{x} = 0$. Thus $P_V^T\hat{r} = 0$ or by (11) again, $\hat{r} = 0$, which is a contradiction. Therefore, $\hat{x}$ and $P_V\hat{r}$ are linearly independent. We next consider the projection of (A, B) onto $\text{span}\{\hat{x}, P_V\hat{r}\}$ by defining

$$\hat{A} = [\hat{x}, P_V\hat{r}]^T A[\hat{x}, P_V\hat{r}] \text{ and } \hat{B} = [\hat{x}, P_V\hat{r}]^T B[\hat{x}, P_V\hat{r}].$$

Clearly, $\hat{B} > 0$. Furthermore,

$$\hat{A} - \hat{\lambda}\hat{B} = \begin{pmatrix} 0 & \hat{r}^T P_V\hat{r} \\ \hat{r}^T P_V^T\hat{r} & \hat{r}^T P_V^T(A - \hat{\lambda}B)P_V\hat{r} \end{pmatrix}$$

is indefinite because, by (11), $\hat{r}^T P_V\hat{r} = (P_V^T\hat{r})^T\hat{r} = \hat{r}^T\hat{r} \neq 0$. Thus the smallest eigenvalue of $(\hat{A}, \hat{B})$, denoted by $\tilde{\lambda}$, is less than $\hat{\lambda}$, i.e.

$$\tilde{\lambda} < \hat{\lambda}. \tag{12}$$

Furthermore, let $r_k = (A - \rho_k B)x_k$,

$$\hat{A}_k = [x_k, P_V r_k]^T A[x_k, P_V r_k] \text{ and } \hat{B}_k = [x_k, P_V r_k]^T B[x_k, P_V r_k].$$

Let $\tilde{\lambda}_{k+1}$ be the smallest eigenvalue of $(\hat{A}_k, \hat{B}_k)$. Clearly, as $n_k \to \infty$, $\hat{A}_{n_k} \to \hat{A}$ and $\hat{B}_{n_k} \to \hat{B}$. Hence by the continuity property of the eigenvalue, we have

$$\tilde{\lambda}_{n_k+1} \to \tilde{\lambda}.$$

On the other hand, ρ_{k+1} is the smallest eigenvalue of the projection of (A, B) on $K_m = \text{span}\{x_k, P_V(A - \rho_k B)x_k, \cdots, (P_V(A - \rho_k B))^m x_k\}$, which implies

$$\rho_{k+1} \leq \tilde{\lambda}_{k+1}.$$

Finally, combining the above together, we have obtained

$$\tilde{\lambda} = \lim \tilde{\lambda}_{n_k+1} \geq \lim \rho_{n_k+1} = \hat{\lambda}$$

which is a contradiction to (12). Therefore, $\hat{r} = (A - \hat{\lambda}B)\hat{x} = 0$, i.e. $\hat{\lambda}$ is an eigenvalue and $\|(A - \hat{\lambda}B)x_{n_k}\| \to 0$.

Now, to show $\|(A - \hat{\lambda}B)x_k\| \to 0$, suppose there is a subsequence m_k such that $\|(A - \hat{\lambda}B)x_{m_k}\| \geq \alpha > 0$. From the subsequence m_k, there is a subsequence n_k for which x_{n_k} is convergent. Hence by virtue of the above proof, $\|(A - \hat{\lambda}B)x_{n_k}\| \to 0$, which is a contradiction. Therefore $\|(A - \hat{\lambda}B)x_k\| \to 0$, i.e. x_k approaches in direction an eigenvector corresponding to $\hat{\lambda}$. Since x_k is B-orthogonal to $\{v_1, \cdots, v_\ell\}$, we have $\hat{\lambda} \in \{\lambda_{\ell+1}, \cdots, \lambda_n\}$. This completes the proof. □

Next we present a lemma and then our main result concerning local linear convergence of ρ_k that generalizes Theorem 2.2.

Lemma 3.3. *Let $V_\ell = [v_1, \cdots, v_\ell]$ be such that $Av_i = \lambda_i Bv_i$ (for $1 \leq i \leq \ell$) and $V_\ell^T BV_\ell = I$ and let $P_V = I - V_\ell V_\ell^T B$ and $\mathcal{V}_\ell = \text{span}\{v_1, \cdots, v_\ell\}$. Let $\lambda_{\ell+1} < \lambda_{\ell+2} \leq \cdots \leq \lambda_n$ together with $\lambda_1, \cdots, \lambda_\ell$ be the eigenvalues of (A, B). Let (ρ_k, x_k) be the eigenpair approximation obtained at step k of Algorithm 3.2 with V_ℓ and assume that $\lambda_{\ell+1} \leq \rho_k < \lambda_{\ell+2}$. Let $P_V^T(A - \rho_k B)P_V = WSW^T$ be the eigenvalue decomposition of $P_V^T(A - \rho_k B)P_V$ where $S = \text{diag}\{0, 0, \cdots, 0, s_{\ell+1}, \cdots, s_n\}$ with*

$s_{\ell+1} \le s_{\ell+2} \le \cdots \le s_n$, and $W = [w_1, \cdots, w_\ell, w_{\ell+1}, \cdots, w_n]$ with $w_i \in \mathcal{V}_\ell$ (for $i = 1, \cdots, \ell$), and $w_i \perp \mathcal{V}_\ell$ (for $i = \ell+1, \cdots, n$). Then we have $s_{\ell+1} \le 0 < s_{\ell+2}$, $P_V w_{\ell+1} \neq 0$ and

$$\frac{|s_{\ell+1}|}{w_{\ell+1}^T P_V^T B P_V w_{\ell+1}} \le \rho_k - \lambda_{\ell+1}. \tag{13}$$

Furthermore, $\rho_k \to \lambda_{\ell+1}$ and

$$\frac{s_{\ell+1}}{w_{\ell+1}^T P_V^T B P_V w_{\ell+1}} = (\lambda_{\ell+1} - \rho_k) + \mathcal{O}((\lambda_{\ell+1} - \rho_k)^2). \tag{14}$$

Proof. First, by Theorem 3.2 and the assumption $\lambda_{\ell+1} \le \rho_k < \lambda_{\ell+2}$, we have the convergence of ρ_k to $\lambda_{\ell+1}$.

Let $\tilde{V} = [v_{\ell+1}, v_{\ell+2}, \cdots, v_n]$ be such that $Av_i = \lambda_i B v_i$ (for $\ell+1 \le i \le n$) and $\tilde{V}^T B \tilde{V} = I$. Let $V = [V_\ell, \tilde{V}]$ and $P_V V = [P_V V_\ell, P_V \tilde{V}] = [0, \tilde{V}]$ and hence

$$V^T P_V^T (A - \rho_k B) P_V V = \begin{pmatrix} 0 & 0 \\ 0 & \tilde{V}^T (A - \rho_k B) \tilde{V} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \tilde{\Lambda} - \rho_k I \end{pmatrix}$$

where $\tilde{V}^T (A - \rho_k B) \tilde{V} = \tilde{V}^T B \tilde{V} (\tilde{\Lambda} - \rho_k I) = \tilde{\Lambda} - \rho_k I$ and $\tilde{\Lambda} = \mathrm{diag}\{\lambda_{\ell+1}, \cdots, \lambda_n\}$. By Sylvester's law of inertia and $\lambda_{\ell+1} - \rho_k \le 0 < \lambda_{\ell+2} - \rho_k$, $P_V^T (A - \rho_k B) P_V$ has exactly $n-\ell-1$ negative, ℓ zero, and 1 nonpositive eigenvalues, i.e., $s_{\ell+1} \le 0 < s_{\ell+2}$.

Let $\tilde{w}_{\ell+1} = P_V w_{\ell+1}$ and suppose $\tilde{w}_{\ell+1} = 0$. Then $w_{\ell+1} = V_\ell V_\ell^T B w_{\ell+1} \in \mathcal{V}_\ell$. This implies $w_{\ell+1} = 0$ as $w_{\ell+1} \perp \mathcal{V}_\ell$. This is a contradiction. Therefore, $\tilde{w}_{\ell+1} \neq 0$.

Furthermore, $\tilde{w}_{\ell+1} \perp_B \mathcal{V}_\ell$, i.e. $V_\ell^T B \tilde{w}_{\ell+1} = 0$. Then

$$\begin{aligned}
\lambda_{\ell+1} &= \min_{V_\ell^T B w = 0, w \neq 0} \frac{w^T A w}{w^T B w} \\
&\le \frac{\tilde{w}_{\ell+1}^T A \tilde{w}_{\ell+1}}{\tilde{w}_{\ell+1}^T B \tilde{w}_{\ell+1}} \\
&= \rho_k + \frac{\tilde{w}_{\ell+1}^T (A - \rho_k B) \tilde{w}_{\ell+1}}{\tilde{w}_{\ell+1}^T B \tilde{w}_{\ell+1}} \\
&= \rho_k + \frac{w_{\ell+1}^T P_V^T (A - \rho_k B) P_V w_{\ell+1}}{\tilde{w}_{\ell+1}^T B \tilde{w}_{\ell+1}} \\
&= \rho_k + \frac{s_{\ell+1}}{w_{l+1}^T P_V^T B P_V w_{l+1}}.
\end{aligned}$$

where we have used $P_V^T (A - \rho_k B) P_V w_{\ell+1} = s_{\ell+1} w_{\ell+1}$ in the last equation. This proves (13).

Finally, to prove the asymptotic expansion, let $s(t)$ be the smallest eigenvalue of $P_V^T (A - tB) P_V$. Then $s(\rho_k) = s_{\ell+1}$. It is easy to check that $s(\lambda_{\ell+1}) = 0$. Using the analytic perturbation theory, we obtain $s'(\rho_k) = -\tilde{w}_{\ell+1}^T B \tilde{w}_{\ell+1}$ and hence

$$\begin{aligned}
s(t) &= s(\rho_k) + s'(\rho_k)(t - \rho_k) + \mathcal{O}((t - \rho_k)^2) \\
&= s_{\ell+1} - \tilde{w}_{\ell+1}^T B \tilde{w}_{\ell+1} (t - \rho_k) + \mathcal{O}((t - \rho_k)^2)
\end{aligned}$$

Choosing $t = \lambda_{\ell+1}$, we have

$$0 = s(\lambda_{\ell+1}) = s_{\ell+1} - \tilde{w}_{\ell+1}^T B \tilde{w}_{\ell+1} (\lambda_{\ell+1} - \rho_k) + \mathcal{O}((\lambda_{\ell+1} - \rho_k)^2)$$

from which the expansion follows. □

Theorem 3.4. *Let $V_\ell = [v_1, \cdots, v_\ell]$ be such that $Av_i = \lambda_i Bv_i$ (for $1 \le i \le \ell$) and $V_\ell^T BV_\ell = I$ and write $P_V = I - V_\ell V_\ell^T B$ and $\mathcal{V}_\ell = \text{span}\{v_1, \cdots, v_\ell\}$. Let $\lambda_{\ell+1} < \lambda_{\ell+2} \le \cdots \le \lambda_n$ together with $\lambda_1, \cdots, \lambda_\ell$ be the eigenvalues of (A, B). Let (ρ_k, x_k) be the eigenpair approximation obtained at step k of Algorithm 2.1 with V_ℓ and assume that $\lambda_{\ell+1} \le \rho_k < \lambda_{\ell+2}$. Let $P_V^T(A - \rho_k B)P_V = WSW^T$ be the eigenvalue decomposition of $P_V^T(A - \rho_k B)P_V$ where $S = diag\{0, 0, \cdots, 0, s_{\ell+1}, \cdots, s_n\}$ with $s_{\ell+1} \le s_{\ell+2} \le \cdots \le s_n$, and $W = [w_1, \cdots, w_\ell, w_{\ell+1}, \cdots, w_n]$ with $w_i \in \mathcal{V}_\ell$ (for $i = 1, \cdots, \ell$), and $w_i \perp \mathcal{V}_\ell$ (for $i = \ell + 1, \cdots, n$). Then ρ_k converges to $\lambda_{\ell+1}$ and*

$$\rho_{k+1} - \lambda_{\ell+1} \le (\rho_k - \lambda_{\ell+1})\epsilon_m^2 + 2(\rho_k - \lambda_{\ell+1})^{3/2}\epsilon_m \left(\frac{\|B\|}{s_{\ell+2}}\right)^{1/2} + \delta_k, \tag{15}$$

where

$$0 \le \delta_k := \rho_k - \lambda_{\ell+1} + \frac{s_{\ell+1}}{w_{\ell+1}^T P_V^T B P_V w_{\ell+1}} = \mathcal{O}((\rho_k - \lambda_{\ell+1})^2)$$

and

$$\epsilon_m = \min_{\substack{p \in \mathcal{P}_m, \\ p(s_{\ell+1})=1}} \max_{i \ge 1} |p(s_{\ell+i})|$$

with $\mathcal{P}_m$ denoting the set of all polynomials of degree not greater than m.

Proof. First, it follows from Lemma 3.3 that ρ_k converges to $\lambda_{\ell+1}$, $s_{\ell+1} \le 0 < s_{\ell+2}$ and $P_V w_{\ell+1} \ne 0$.

Let $\tilde{H}_k := P_V^T(A - \rho_k B)P_V$. From Lemma 3.1, $\mathcal{K}_m(P_V(A - \rho_k B), x_k) = P_V \mathcal{K}_m(\tilde{H}_k, x_k) = \{P_V p(\tilde{H}_k)x_k, p \in \mathcal{P}_m\}$. At step k of the algorithm, we have

$$\begin{aligned}
\rho_{k+1} &= \min_{\substack{u \in \mathcal{K}_m(P_V(A-\rho_k B), x_k), \\ u \ne 0}} \frac{u^T A u}{u^T B u} \\
&= \rho_k + \min_{\substack{u \in \mathcal{K}_m(P_V(A-\rho_k B), x_k), \\ u \ne 0}} \frac{u^T (A - \rho_k B) u}{u^T B u} \\
&= \rho_k + \min_{\substack{p \in \mathcal{P}_m, \\ P_V p(\tilde{H}_k)x_k \ne 0}} \frac{x_k^T p(\tilde{H}_k) P_V^T (A - \rho_k B) P_V p(\tilde{H}_k) x_k}{x_k^T p(\tilde{H}_k) P_V^T B P_V p(\tilde{H}_k) x_k} \\
&= \rho_k + \min_{\substack{p \in \mathcal{P}_m, \\ P_V p(\tilde{H}_k)x_k \ne 0}} \frac{x_k^T p(\tilde{H}_k) \tilde{H}_k p(\tilde{H}_k) x_k}{x_k^T p(\tilde{H}_k)(P_V^T B P_V) p(\tilde{H}_k) x_k}
\end{aligned}$$

Let q be the minimizing polynomial in ϵ_m with $q(s_{\ell+1}) = 1$ and $\max_{i \ge l+2} |q(s_i)| = \epsilon_m < 1$. Let

$$\hat{S} = \text{diag}[s_{\ell+1}, \cdots, s_n] \quad \text{and} \quad \hat{W} = [w_{\ell+1}, \cdots, w_n].$$

Then $W = [V_\ell T, \hat{W}]$ for some $T \in \mathbb{R}^{\ell \times n}$. Since $x_k^T \tilde{H}_k x_k = x_k^T (A - \rho_k B) x_k = 0$ and $x_k^T \tilde{H}_k x_k = x_k^T W S W^T x_k = \sum_{i=\ell+1}^n s_i (w_i^T x_k)^2$ with $s_i > 0$ for $i \ge \ell + 2$, we have $w_{\ell+1}^T x_k \ne 0$. Hence $P_V q(\tilde{H}_k) x_k = P_V W q(S) W^T x_k = [0, P_V \hat{W}] q(S) W^T x_k \ne 0$ where we note that $V_\ell^T \hat{W} = 0$ and hence $P_V \hat{W}$ has full column rank. Let $B_1 =$

$\hat{W}^T P_V^T B P_V \hat{W}$ and $y = \hat{W}^T x_k$. Then

$$\begin{aligned}
\rho_{k+1} &\leq \rho_k + \frac{x_k^T q(\tilde{H}_k)\tilde{H}_k q(\tilde{H}_k) x_k}{x_k^T q(\tilde{H}_k)(P_V^T B P_V) q(\tilde{H}_k) x_k} \\
&= \rho_k + \frac{x_k^T W q(S) S q(S) W^T x_k}{x_k^T W q(S) W^T P_V^T B P_V W q(S) W^T x_k} \\
&= \rho_k + \frac{x_k^T \hat{W} q^2(\hat{S}) \hat{S} \hat{W}^T x_k}{x_k^T \hat{W} q(\hat{S}) \hat{W}^T P_V^T B P_V \hat{W} q(\hat{S}) \hat{W}^T x_k} \\
&= \rho_k + \frac{y^T q^2(\hat{S}) \hat{S} y}{y^T q(\hat{S}) B_1 q(\hat{S}) y}. \qquad (16)
\end{aligned}$$

where we have used

$$W q(S) S q(S) W^T = \hat{W} q^2(\hat{S}) \hat{S} \hat{W}^T$$

and

$$P_V W q(S) W^T = [0, P_V \hat{W}] q(S) W^T = P_V \hat{W} q(\hat{S}) \hat{W}^T.$$

Let $y = [y_1, y_2, \ldots, y_{n-\ell}]^T$, $\hat{y} = [0, y_2, \ldots, y_{n-\ell}]^T$, and $e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^{n-\ell}$. Then,

$$\begin{aligned}
y^T q(\hat{S}) B_1 q(\hat{S}) y &= (y_1 e_1 + \hat{y})^T q(\hat{S}) B_1 q(\hat{S}) (y_1 e_1 + \hat{y}) \\
&= y_1^2 q(s_{\ell+1})^2 e_1^T B_1 e_1 + 2 y_1 q(s_{\ell+1}) e_1^T B_1 q(\hat{S}) \hat{y} + \hat{y}^T q(\hat{S}) B_1 q(\hat{S}) \hat{y} \\
&= y_1^2 \beta_1^2 + 2 y_1 \beta_2 + \beta_3^2,
\end{aligned}$$

where $\beta_1 \geq 0, \beta_2$ and $\beta_3 \geq 0$ are defined such that

$$\begin{aligned}
\beta_1^2 &= e_1^T B_1 e_1 = w_{\ell+1}^T P_V^T B P_V w_{\ell+1}, \\
\beta_3^2 &= \hat{y}^T q(\hat{S}) B_1 q(\hat{S}) \hat{y} \\
&\leq \max_{l+1 \leq i \leq n} q(s_i)^2 \|B_1\| \|\hat{y}\|^2 \\
&= \epsilon_m^2 \|B\| \|\hat{y}\|^2
\end{aligned}$$

and

$$|\beta_2| = |e_1^T B_1 q(\hat{S}) \hat{w}| \leq \beta_1 \beta_3.$$

Since $y^T \hat{S} y = x_k^T \hat{W} \hat{S} \hat{W}^T x_k = x_k^T \tilde{H}_k x_k = 0$, we have $\sum_{i=1}^{n-\ell} s_{\ell+i} y_i^2 = 0$. Then

$$|s_{\ell+1}| y_1^2 = \sum_{i=2}^{n-\ell} s_{\ell+i} y_i^2 \geq s_{\ell+2} \|\hat{y}\|^2, \qquad (17)$$

and hence

$$\beta_3 \leq \epsilon_m \|B\|^{1/2} \left(\frac{|s_{\ell+1}|}{s_{\ell+2}} \right)^{1/2} |y_1|. \qquad (18)$$

On the other hand, we also have

$$y^T q^2(\hat{S}) \hat{S} y = \sum_{i=1}^{n-\ell} s_{\ell+i} q^2(s_{\ell+i}) y_i^2 \leq \sum_{i=1}^{n-\ell} s_{\ell+i} y_i^2 = y^T \hat{S} y = 0$$

and

$$0 \leq \hat{y}^T q^2(\hat{S}) \hat{S} \hat{y} = \sum_{i=2}^{n-\ell} s_{\ell+i} q^2(s_{\ell+i}) y_i^2 \leq \epsilon_m^2 \sum_{i=2}^{n-\ell} s_{\ell+i} y_i^2 = \epsilon_m^2 |s_{\ell+1}| y_1^2, \qquad (19)$$

where we have used that $q(s_{\ell+1}) = 1$, $|q(s_{\ell+i})| \le \epsilon_m < 1$ for $i > 1$ and (17). Thus

$$\begin{aligned}
\frac{y^T q^2(\hat{S})\hat{S}y}{y^T q(\hat{S})B_1 q(\hat{S})y} &\le \frac{y_1^2 s_{\ell+1} + \hat{y}^T q(\hat{S})^2 \hat{S}\hat{y}}{y_1^2\beta_1^2 + 2|y_1|\beta_1\beta_3 + \beta_3^2} \\
&= \frac{s_{\ell+1}}{\beta_1^2} - \frac{s_{\ell+1}}{\beta_1^2}\frac{2|y_1|\beta_1\beta_3 + \beta_3^2}{y_1^2\beta_1^2 + 2|y_1|\beta_1\beta_3 + \beta_3^2} \\
&\quad + \frac{\hat{y}^T q(\hat{S})^2 \hat{S}\hat{y}}{y_1^2\beta_1^2 + 2|y_1|\beta_1\beta_3 + \beta_3^2} \\
&\le \frac{s_{\ell+1}}{\beta_1^2} - \frac{s_{\ell+1}}{\beta_1^2}\frac{2|y_1|\beta_1\beta_3}{y_1^2\beta_1^2} + \frac{\hat{y}^T q(\hat{S})^2 \hat{S}\hat{y}}{y_1^2\beta_1^2} \\
&\le \frac{s_{\ell+1}}{\beta_1^2} + 2\left(\frac{|s_{\ell+1}|}{\beta_1^2}\right)^{3/2}\epsilon_m\left(\frac{\|B\|}{s_{\ell+2}}\right)^{1/2} + \frac{|s_{\ell+1}|}{\beta_1^2}\epsilon_m^2, \quad (20)
\end{aligned}$$

where we have used (18) and (19). Finally, combining (16), (20), and Lemma 3.3, we have

$$\begin{aligned}
0 \le \rho_{k+1} - \lambda_{\ell+1} &\le \rho_k - \lambda_{\ell+1} + \frac{s_{\ell+1}}{\beta_1^2} + 2(\rho_k - \lambda_{\ell+1})^{3/2}\epsilon_m\left(\frac{\|B\|}{s_{\ell+2}}\right)^{1/2} + (\rho_k - \lambda_{\ell+1})\epsilon_m^2 \\
&\le \delta_k + 2(\rho_k - \lambda_{\ell+1})^{3/2}\epsilon_m\left(\frac{\|B\|}{s_{\ell+2}}\right)^{1/2} + (\rho_k - \lambda_{\ell+1})\epsilon_m^2,
\end{aligned}$$

where $\delta_k = \rho_k - \lambda_{\ell+1} + \frac{s_{\ell+1}}{\beta_1^2} = \mathcal{O}((\rho_k - \lambda_{\ell+1})^2)$ by Lemma 3.3. The proof is complete. □

Remark 1. ϵ_m in the theorem can be bounded by the Chebyshev polynomials as

$$\epsilon_m \le \frac{1}{T_m\left(\frac{1+\psi}{1-\psi}\right)}, \quad \text{where} \quad \psi = \frac{s_{l+2} - s_{l+1}}{s_n - s_{l+1}} \quad (21)$$

and T_m is the Chebyshev polynomial of degree m. This bound can be further simplified to

$$\epsilon_m \le 2\left(\frac{1+\sqrt{\psi}}{1-\sqrt{\psi}}\right)^m \quad (22)$$

to show the dependence on the spectral separation ψ. Thus, the speed of convergence of the deflation algorithm depends on the spectral gap of the smallest nonzero eigenvalue of $P_V^T(A - \rho_k B)P_V$, rather than that of $A - \rho_k B$ in the original algorithm. In particular, this may have a different convergence characteristic from the Wielandt deflation (3).

We also note that for small m, the bound (21) may be significantly stronger than (22), but when m is sufficiently large, (22) is almost as good as (21). It is also easy to see that, asymptotically, we can use the eigenvalues of $P_V^T(A - \lambda_{\ell+1}B)P_V$ in the place of $s_{\ell+1} \le s_{\ell+2} \le \cdots \le s_n$ without changing the first order term of the bound; see [5] for more discussions.

As in [5], a congruence transformation can be used in Algorithm 3.2 to reduce ϵ_m to 0 so as to accelerate convergence. Consider the ideal situation that we compute the LDL^T-decomposition of $P_V^T(A - \rho_k B)P_V = L_k D_k L_k^T$ with D_k being a diagonal matrix of 0 and ± 1. Then the congruence transformation

$$(\hat{A}_k, \hat{B}_k) := (L_k^{-1} A L_k^{-T}, L_k^{-1} B L_k^{-T})$$

does not change the spectrum of (A, B). Applying Algorithm 3.2 to the transformed problem, we use

$$\hat{V}_\ell := L_k V_\ell$$

to construct the projection $P_{\hat{V}} := I - \hat{B}\hat{V}_\ell\hat{V}_\ell^T$, as $\hat{A}_k\hat{v}_i = \lambda_i\hat{B}_k\hat{v}_i (1 \le i \le \ell)$ and $\hat{V}_\ell^T\hat{B}_k\hat{V}_\ell = I$. Then, by Theorem 3.4, the convergence rate is determined by the eigenvalues of $P_{\hat{V}}^T(\hat{A} - \rho_k\hat{B})P_{\hat{V}}$. It is easy to see that

$$P_{\hat{V}}^T(\hat{A} - \rho_k\hat{B})P_{\hat{V}} = L_k^{-1}P_V^T(A - \rho_k B)P_V L_k^{-T} = D_k. \tag{23}$$

Then at the convergence stage with $\lambda_{l+1} < \rho_k < \lambda_{l+2}$, we have $s_1 = \cdots = s_l = 0$ and $s_{l+1} = -1$, $s_{l+2} = \ldots = s_n = 1$, which implies, for $m \ge 1$, $\epsilon_m = 0$, and hence by Theorem 3.4,

$$\rho_k - \lambda_{l+1} \le \delta_k = \mathcal{O}((\rho_k - \lambda_{l+1})^2).$$

The above is an ideal situation that requires computing the LDL^T-decomposition. In practice, we can use an incomplete LDL^T-decomposition of $P_V^T(A - \mu B)P_V = L_k D_k L_k^T$ with a shift $\mu \approx \rho_k$ (or $\lambda_{\ell+1}$), which would reduce ϵ_m and hence accelerate convergence.

4. **Numerical Examples.** In this section, we present two numerical examples to demonstrate the convergence properties of the deflation by restriction for the inverse free Krylov subspace method. All computations were carried out using MATLAB version 8.0.0.783 from MathWorks on a PC with an Intel quad-core i7-2670QM @ 2.20GHz and 12 GB of RAM running Ubuntu Linux 12.04. The machine epsilon is $\mathbf{u} \approx 2.2 \cdot 10^{-16}$.

Our implementation is based on the MATLAB program `eigifp` of [14]. In particular, the basis of the projected Krylov subspace is constructed using the Arnoldi method. In both examples, we compute the three smallest eigenvalues and use the deflation algorithm in computing the second and the third smallest eigenvalues. The initial vectors are generated by `randn(n,3)` and we fix the number of inner iterations as $m = 20$. Note that m can be set to be chosen adaptively in `eigifp`, but here we consider a fixed m for the demonstration of the convergence bound by ϵ_m. The stopping criterion is set as $\|r_k\| \le 10^{-8}$, where $r_k = (Ax_k - \rho_k Bx_k)/\|x_k\|$.

Example 1. Consider the Laplace eigenvalue problem with the Dirichlet boundary condition on an L-shaped domain. A definite symmetric generalized eigenvalue problem $Ax = \lambda Bx$ is obtained by a finite element discretization on a mesh with 20,569 interior nodes using PDE toolbox of MATLAB. Three iterations of deflation algorithms are carried out to compute the three smallest eigenvalues and we plot the convergence history of the residuals $\|r_k\|$ against the number of iterations for the three eigenvalues $\lambda_i (1 \le i \le 3)$ together in Figure 1. To illustrate Theorem 3.4, we also plot in Figure 2 the convergence rate $(\rho_{k+1} - \lambda_i)/(\rho_k - \lambda_i)$ and compare it with the upper bound (21) of ϵ_m^2. For the purpose of simplicity, the bound (21) is computed from the eigenvalues of the projected matrix $P_V^T(A - \lambda_i B)P_V$. The top straight lines are the upper bounds of ϵ_m^2 and the bottom three lines are the corresponding actual error ratios $(\rho_{k+1} - \lambda_i)/(\rho_k - \lambda_i)$.

We observe that the deflation algorithm converges indeed linearly and (21) provides a good bound on the rate of convergence. We note that λ_1 takes more iterations overall than the other two eigenvalues. This is due to the use of initial random vector for λ_1, but to compute λ_2 and λ_3 in the `eigifp` implementation, initial approximate eigenvectors are computed from the projection used to compute

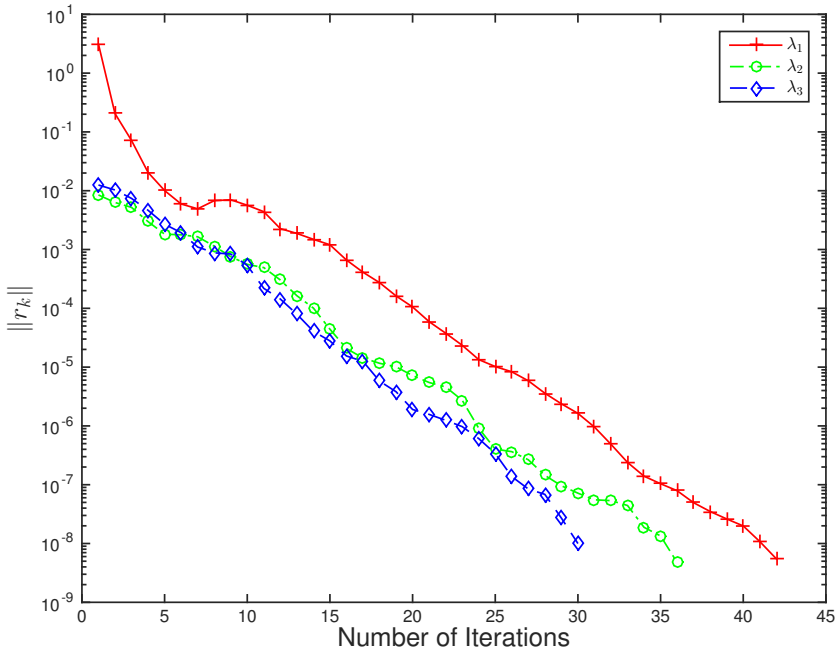

FIGURE 1. Convergence History of Residuals for three eigenvalues $\lambda_1, \lambda_2, \lambda_3$

λ_1. As a result, λ_2 and λ_3 have smaller initial errors, but their overall convergence rates are still comparable as suggested by their bounds. Finally, we list all the converged eigenvalues, the number of iterations used to reduce the residuals below the threshold, and their final residuals in Table 1.

TABLE 1. 3 smallest eigenvalues of Laplacian eigenvalue problem on L-shaped domain

λ_l	Number of Iterations	Residual $\|r_k\|$
23.3876	42	5.50e-09
37.9873	36	4.76e-09
47.4515	30	9.98e-09

We also run the original implementation of `eigifp` which uses Wielandt deflation to compute additional eigenvalues with the same setting. The numbers of iterations are 42, 37, 33 for $\lambda_1, \lambda_2, \lambda_3$ respectively. It shows that these two deflation schemes are comparable in computational cost which we expect to be the case. However, as we discussed earlier, Algorithm 3.2 is superior to `eigifp` with Wielandt deflation as it can handle the singular values computation; see [8] for more details.

EXAMPLE 2. In this example, we consider the deflation algorithm when used with preconditioning. A and B are the same finite element matrices as in Example 1. For preconditioning, we use a constant L as obtained by the threshold incomplete LDL^T factorization of $A-\mu_i B$ with the drop tolerance 10^{-2}, where the shift μ_i is an

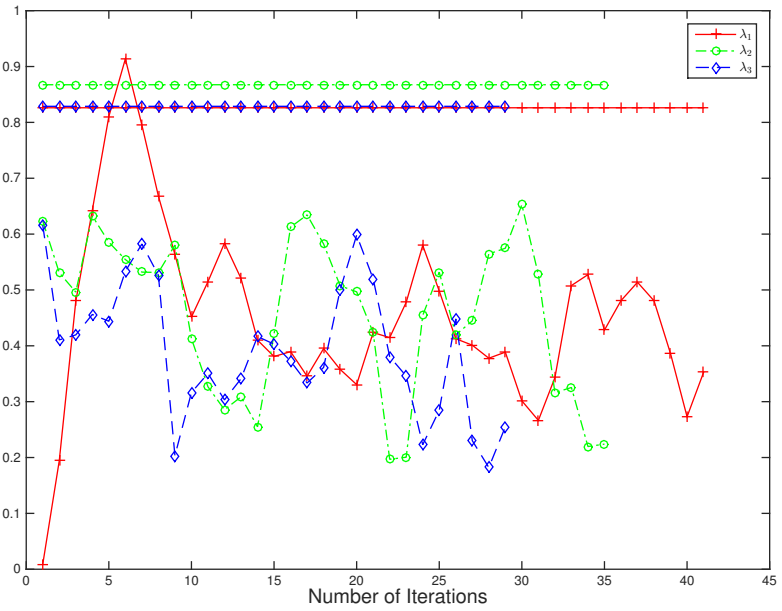

FIGURE 2. Top: bound ϵ_m^2; Bottom: error ratio $(\rho_{k+1} - \lambda_i)/(\rho_k - \lambda_i)$.

approximation of the desired eigenvalue λ_i. We use $\mu_1 = 0$ for λ_1 and $\mu_i = \lambda_{i-1}$ for $i > 1$. Then, the convergence rate is given by ϵ_m as determined by the eigenvalues of $L^{-1}P_V^T(A - \lambda_i B)P_V L^{-T}$ as in (21).

As in Example 1, three iterations of deflation algorithms with preconditioning are carried out to compute the three smallest eigenvalues. We plot the convergence history of the residuals $\|r_k\|$ in Figure 3 and the convergence rate $(\rho_{k+1} - \lambda_i)/(\rho_k - \lambda_i)$ as well as its upper bound (21) in Figure 4. We also list all the converged eigenvalues, the number of iterations used to reduce the residuals below the threshold, and their final residuals in Table 2.

TABLE 2. 3 smallest eigenvalues of Laplacian eigenvalue problem on L-shaped domain

λ_l	Number of Iterations	Residual $\|r_k\|$
23.3876	18	1.54e-09
37.9873	14	1.73e-09
47.4515	12	7.63e-09

We observe that the deflation algorithm with preconditioning converges linearly and (21) provides a very good bound on the rate of convergence. In particular, with the preconditioning, the convergence bounds are significantly improved and correspondingly, the actual convergence rates are also improved demonstrating the effects of preconditioning.

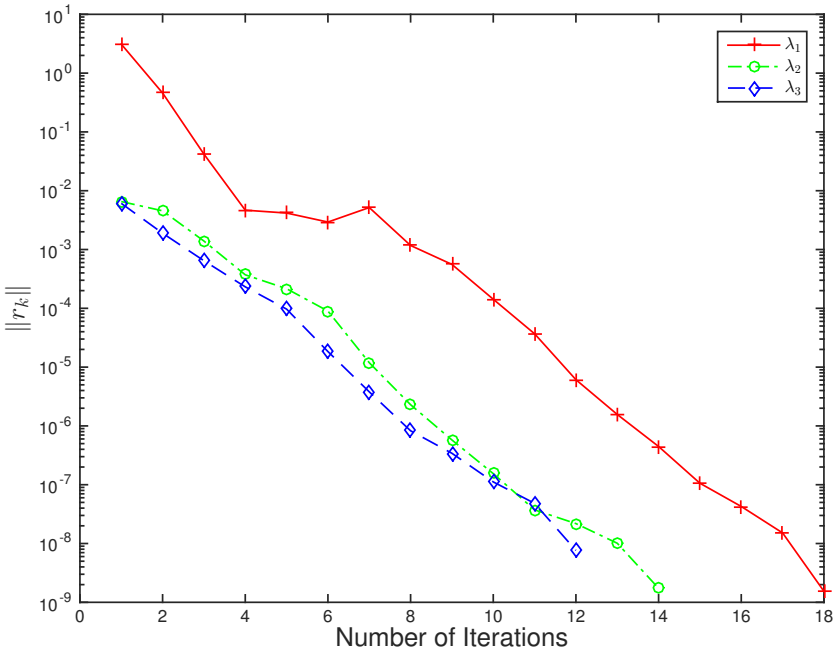

FIGURE 3. Convergence History of Residuals for three eigenvalues $\lambda_1, \lambda_2, \lambda_3$

5. **Conclusion Remarks.** We have incorporated the deflation by restriction method into the inverse-free preconditioned Krylov subspace method to find several eigenvalues of the generalized symmetric definite eigenvalue problem. We extend the convergence analysis in [5] to justify the deflation scheme. Numerical examples confirm the convergence properties as revealed by the new theory. This deflation scheme allows implementation of the inverse-free preconditioned Krylov subspace method without using perturbations to the original problems as in the Wielandt deflation. This may be important in applications such as the singular value computation where the structure of the problems needs to be preserved.

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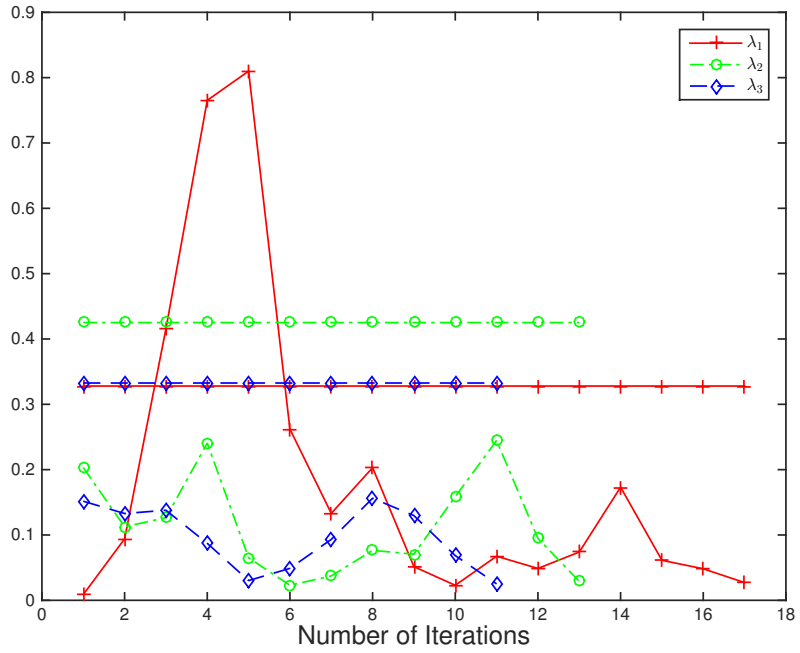

FIGURE 4. Top: bound ϵ_m^2; Bottom: error ratio $(\rho_{k+1} - \lambda_i)/(\rho_k - \lambda_i)$.

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