

Convergence Analysis of Extended LOBPCG for Computing Extreme Eigenvalues

Peter Benner*

Xin Liang†

April 30, 2020

Abstract

This paper is concerned with the convergence analysis of an extended variation of the locally optimal preconditioned conjugate gradient method (LOBPCG) for the extreme eigenvalue of a Hermitian matrix polynomial which admits some extended form of Rayleigh quotient. This work is a generalization of the analysis by Ovtchinnikov (*SIAM J. Numer. Anal.*, 46(5):2567–2592, 2008). As instances, the algorithms for definite matrix pairs and hyperbolic quadratic matrix polynomials are shown to be globally convergent and to have an asymptotically local convergence rate. Also, numerical examples are given to illustrate the convergence.

Keywords. Extreme eigenvalue, convergence rate, LOBPCG, definite matrix pencil, hyperbolic quadratic eigenvalue problem

AMS subject classifications. 65F15, 65H17.

1 Introduction

Given a Hermitian matrix polynomial

$$F(\lambda) = \sum_{k=0}^m A_k \lambda^{m-k}, \quad (1)$$

of degree m , where $A_k \in \mathbb{C}^{n \times n}$ for $k = 0, \dots, m$, and an interval $I = (\lambda_-, \lambda_+)$. Suppose $F(\lambda_-)$ is negative definite. For some nonzero $x \in \mathbb{C}^n$, consider the equation

$$x^H F(\lambda)x = 0, \quad \lambda \in I. \quad (2)$$

Let \mathcal{D} denote the set of all x for which (2) has at least one root $\lambda = \rho(x)$ in I , while $\mathbb{C}^n \setminus \mathcal{D}$ is the set of all x for which (2) has no root in I . For any $x \in \mathcal{D}$, define

$$\sigma(x) := x^H F'(\rho(x))x = \sum_{k=0}^{m-1} (m-k) A_k \rho(x)^{m-k-1}.$$

Suppose that $\sigma(x) > 0$ for any $x \in \mathcal{D}$. Then (2) has only one root in I , which is called the Rayleigh quotient of $F(\lambda)$ at x . Suppose the matrix polynomial $F(\lambda)$ has ℓ eigenvalues in I , namely $\lambda_1 \leq \dots \leq \lambda_\ell$, while for any matrix $X \in \mathbb{C}^{n \times k}$ with a proper constraint, the projected polynomial $X^H F(\lambda)X$ has $\ell_X \leq \ell$ eigenvalues in I , namely $\lambda_{1,X} \leq \dots \leq \lambda_{\ell_X,X}$. Furthermore, suppose the eigenvalues of $F(\lambda)$ admit min-max principles, such as

1. the *Wielandt-Lidskii min-max principle*:

$$\min_{\substack{\mathcal{X}_1 \subset \dots \subset \mathcal{X}_k \\ \dim \mathcal{X}_j = i_j}} \max_{\substack{x_j \in \mathcal{X}_j \\ X = [x_1, \dots, x_k] \\ \text{rank}(X) = k \\ \text{proper } X}} \sum_{j=1}^k \lambda_{j,X} = \sum_{j=1}^k \lambda_{i_j}; \quad (3)$$

*Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, 39106 Magdeburg, Germany. E-mail: benner@mpi-magdeburg.mpg.de.

†Yau Mathematical Sciences Center, Tsinghua University, Beijing 100084, China. E-mail: liangxinslm@tsinghua.edu.cn.

2. the *Courant-Fischer min-max principle* obtained by setting $k = 1$ in (3) and noticing $\rho(x) = \lambda_{1,X}$:

$$\min_{\substack{\dim \mathcal{X}=i \\ \text{proper } \mathcal{X}}} \max_{\substack{x \in \mathcal{X} \\ \text{proper } x}} \rho(x) = \lambda_i; \quad (4)$$

3. the *Fan trace min principle* obtained by setting $i_j = j$ in (3):

$$\min_{\substack{\text{rank}(X)=k \\ \text{proper } X}} \sum_{j=1}^k \lambda_{j,X} = \sum_{j=1}^k \lambda_j; \quad (5)$$

4. or the extreme eigenvalue characterization obtained by setting $i = 1$ in (4) or $k = 1$ in (5):

$$\min_{\text{proper } x} \rho(x) = \lambda_1, \quad (6)$$

where the phrase ‘‘proper X ’’ in the min/max means that the minimum/maximum is obtained under some proper constraint.

These min-max principles motivate us to use the Rayleigh-Ritz procedure and gradient-type optimization methods, such as the steepest descent method (SD) or the conjugate gradient method (CG), to obtain several smallest eigenvalues and their corresponding eigenvectors. In this view, the *locally optimal block preconditioned (extended) conjugate gradient method* (LOBP(e)CG) has been developed to solve some kinds of eigenvalue problems. Locally optimal CG for nonlinear optimization was first described by Takahashi [25]. Later, Knyazev [7] established LOBPCG for the generalized Hermitian eigenvalue problem $A - \lambda B$, where $A \succ 0$. Because of its efficiency, this method has been used to solve different kinds of eigenvalue problems. Nevertheless, up to now, the convergence analysis of this method has been incomplete. As far as we know, current results on the estimate for the convergence rate fall into two categories. Ovtchinnikov [22, 23] dealt with the convergence rate of a standard form for LOBPCG applied to standard Hermitian eigenvalue problems and generalized Hermitian eigenvalue problems $(A - \lambda B)x = 0$ with a positive definite B . He analyzed the convergence rate of LOBPCG by constructing a relationship to SD and then bringing in the convergence rate of SD by Samokish [24]. On the other hand, also for those two types of eigenvalue problems, Neymeyr and his co-authors derived the convergence rate of a special form named ‘‘sharp estimate’’ for preconditioned inverse vector iteration (PINVIT) and (preconditioned) SD in a series of works [19, 8, 21, 20, 2]. In this paper, we will consider several instances of the generalized eigenvalue problem and try to apply the developed ideas to them for the algorithm LOBPCG for computing the extreme eigenvalue, which means the block size is 1, or equivalently, a vector version of LOBPCG. The problems are:

1. *Definite matrix pair* $F(\lambda) = \lambda B - A$, which means there exists $\lambda_0 \in \mathbb{R}$ such that $F(\lambda_0) \prec 0$. Let $\mathcal{I} = (\lambda_0, +\infty)$ and $\mathcal{D} = \{x \in \mathbb{C}^n : x^H B x > 0\}$, and let the proper constraint be $X^H B X = I$, satisfying the assumptions above (see, e.g. [10, 18, 16, 14]). Here, the investigated algorithm coincides with the algorithm given by Kressner et al [11, Algorithm 1].
2. *Hyperbolic quadratic matrix polynomial* $F(\lambda) = \lambda^2 A + \lambda B + C$, with $A \succ 0$ and assuming there exists $\lambda_0 \in \mathbb{R}$ such that $F(\lambda_0) \prec 0$. Let $\mathcal{I} = (\lambda_0, +\infty)$ and $\mathcal{D} = \mathbb{C}^n$, and let the proper constraint be $\text{rank}(X) = k$ or $X^H A X = I$, satisfying the assumptions above (see, e.g. [4, 17, 6, 15]). Here, the investigated algorithm coincides with the algorithm given by Liang and Li [15, Algorithm 11.2].

The rest of this paper is organized as follows. First, some notation is introduced. Section 2 presents the generic framework of LOBP(e)CG for any kind of Hermitian matrix polynomial satisfying the assumptions at the beginning of the paper, and also its convergence analysis. Section 3 applies this convergence analysis to the two problems listed above. In Section 4, two numerical examples are given to illustrate the convergence rate. Some conclusions are provided in Section 5. Appendices A and B are used to take care of detailed and difficult estimates in the proof of the convergence analysis in Section 2.

Notation. Throughout this paper, I_n (or simply I if its dimension is clear from the context) is the $n \times n$ identity matrix, and e_j is its j th column. $\mathbf{1}_n = \sum_{j=1}^n e_j$ (or also simply $\mathbf{1}$ if its dimension is clear from the context). $\text{diag}(\alpha_1, \dots, \alpha_n)$ is a diagonal matrix whose diagonal entries are $\alpha_1, \dots, \alpha_n$. X^H is the conjugate transpose of a vector or matrix X , and $\|X\|$ is its spectral norm, X^\dagger is the Moore-Penrose inverse of a matrix X .

Given a matrix A and a vector x , the $(m+1)$ -dimensional Krylov subspace is denoted by $\mathcal{K}_m(A, x) = \text{span}\{x, Ax, \dots, A^m x\}$, and $\mathcal{R}(A)$ denotes A 's column subspace.

We use $A > 0$ ($A \geq 0$) to indicate that A is Hermitian positive (semi-)definite, and $A < 0$ ($A \leq 0$) if $-A > 0$ ($-A \geq 0$). For $A \geq 0$, $A^{1/2}$ is the unique positive semidefinite square root of A .

For a Hermitian matrix A , its eigenvalues are denoted by

$$\lambda_{\min}(A) \leq \lambda_{\min}^{(2)}(A) \leq \dots \leq \lambda_{\min}^{(n)}(A), \quad \text{or} \quad \lambda_{\max}^{(n)}(A) \leq \dots \leq \lambda_{\max}^{(2)}(A) \leq \lambda_{\max}(A).$$

For any two functions $f(x), g(x)$, by $f(x) \sim g(x)$ we denote the case that $\tau_2 f(x) \leq g(x) \leq \tau_1 f(x)$ for some $\tau_1, \tau_2 > 0$ and all x in the joint domain of f and g . Similarly, by $f_i \sim g_i$ we denote the same situation for two sequences $\{f_i\}, \{g_i\}$. Clearly “ \sim ” is an equivalence relation.

Recall the matrix polynomial $F(\lambda)$ from (1). Define the corresponding residual vector $r(x) := F(\rho(x))x$. Then $x^H r(x) = 0$ and

$$r(x) = -\frac{1}{2}\sigma(x)\nabla\rho(x),$$

because

$$0 = \nabla(x^H F(\rho(x))x) = x^H F'(\rho(x))x \nabla\rho(x) + 2F(\rho(x))x = \sigma(x)\nabla\rho(x) + 2r(x).$$

Denote the divided difference by

$$\Phi(\rho_1, \rho_2) := \frac{F(\rho_1) - F(\rho_2)}{\rho_1 - \rho_2}.$$

Then for any nonzero x , define

$$P_{x, \rho_1, \rho_2} := \frac{xx^H \Phi(\rho_1, \rho_2)}{x^H \Phi(\rho_1, \rho_2)x},$$

and

$$\check{F}_{\rho_1, \rho_2}(\rho; x) := \left(I - P_{x, \rho_1, \rho_2}^H\right) F(\rho) \left(I - P_{x, \rho_1, \rho_2}\right).$$

It is easy to check that

$$P_{x, \rho_1, \rho_2} x = x, \quad x^H \Phi(\rho_1, \rho_2) P_{x, \rho_1, \rho_2} = x^H \Phi(\rho_1, \rho_2), \quad P_{x, \rho_1, \rho_2}^2 = P_{x, \rho_1, \rho_2},$$

i.e., P_{x, ρ_1, ρ_2} is an (oblique) projection.

2 Generic LOBPecG Framework

First we present a framework for LOBPecG, namely Algorithm 2.1. Note that in the shortcut LOCG(n_b, m_e), n_b represents the block size, i.e., the number the eigenpairs to compute simultaneously, while m_e indicates the size of the subspace extension so that $m_e + 1$ is the dimension of the Krylov subspace.

We will deal with LOCG(1, m_e) in the following. Since $j \equiv 1$, we can omit the index j safely.

In every iteration of the algorithm, computing the proper eigenpairs of $Z^H F(\lambda) Z$ is equivalent to solving the following optimization problem:

$$\rho_{i+1} = \rho(Z_i y_i) = \min_{\text{proper } y} \rho(Z_i y), \quad (7)$$

where Z_i is a basis of $\text{span}\{x_i, K_i F(\rho_i)x_i, \dots, (K_i F(\rho_i))^{m_e-1}x_i, x_{i-1}\}$.

Theorem 2.1. *Let the sequences $\{\rho_i\}, \{x_i\}, \{r_i := F(\rho_i)x_i\}$ be produced by LOCG(1, m_e). Suppose that for all i , y_i is a stationary point of $\rho(Z_i y)$.*

1. Only one of the following two mutually exclusive situations can occur:

Algorithm 2.1 Locally optimal block preconditioned extended conjugate gradient method: LOCG(n_b, m_e)

Given an initial proper approximation $X_0 \in \mathbb{C}^{n \times n_b}$, and an integer $m_e \geq 1$, and a series of preconditioners $\{K_{i;j}\}$, the algorithm computes the approximations of the eigenpairs (λ_j, u_j) for $j \in \mathbb{J}$, where $\mathbb{J} = \{1 \leq j \leq n_b\}$ for computing the few smallest eigenpairs.

- 1: solve the projected problem for $X_0^H F(\lambda) X_0$ to get its eigenpairs $(\rho_{0;j}, y_j)$;
 - 2: $X_0 (= [\dots, x_{0;j}, \dots]) = X_0[y_1, \dots, y_{n_b}]$, $X_{-1} = 0$, $\mathbb{J} = \{1 \leq j \leq n_b\}$;
 - 3: **for** $i = 0, 1, \dots$ **do**
 - 4: construct preconditioners $K_{i;j}$ for $j \in \mathbb{J}$;
 - 5: compute a basis matrix Z_i of the subspace $\sum_{j \in \mathbb{J}} \mathcal{K}_{m_e}(K_{i;j} F(\rho_{i;j}), x_{i;j}) + \mathcal{R}(X_{i-1})$;
 - 6: compute the n_b proper eigenpairs of $Z_i^H F(\lambda) Z_i$: $(\rho_{i+1;j}, y_{i;j})$ for $j \in \mathbb{J}$ and let $\Omega_{i+1} = \text{diag}(\dots, \rho_{i+1;j}, \dots)$ whose diagonal entries are those for $j \in \mathbb{J}$;
 - 7: $X_{i+1} (= [\dots, x_{i+1;j}, \dots]) = Z_i Y_i$, where $Y_i = [\dots, y_{i;j}, \dots]$ whose columns are those for $j \in \mathbb{J}$;
 - 8: **end for**
 - 9: **return** approximate eigenpairs to (λ_j, u_j) for $j \in \mathbb{J}$.
-

(a) For some i , $r_i = 0$, and then $\mathcal{K}_{m_e}(K_i F(\rho_i), x_i) = \text{span}\{x_i\}$ for $m_e \geq 2$. Then we have

$$\rho_i = \rho_{i+1} = \dots, \quad x_i = x_{i+1} = \dots, \quad r_i = r_{i+1} = \dots = 0, \quad (8)$$

and (ρ_i, x_i) is an eigenpair of $F(\lambda)$.

(b) ρ_i is strictly monotonically decreasing, and $\rho_i \rightarrow \hat{\rho} \in [\lambda_-, \lambda_+]$ as $i \rightarrow \infty$, and $r_i \neq 0$ for all i , and no two x_i are linearly dependent.

2. $x_i^H r_i = 0$, $Z_i^H r_{i+1} = 0$.

3. in the case of Item 1(b), if $\{x_i\}$ is bounded under the proper constraint, then

(a) $r_i \neq 0$ for all i but $r_i \rightarrow 0$ as $i \rightarrow \infty$,

(b) $\hat{\rho}$ is an eigenvalue of $F(\lambda)$, and any limit point \hat{x} of $\{x_i\}$ is a corresponding eigenvector, i.e., $F(\hat{\rho})\hat{x} = 0$.

Proof. The proof is nearly the same as its analogue by Liang and Li [15, Theorem 8.1]. First by (7), clearly $\rho_{i+1} \leq \rho_i$. There are only two possibilities: either $r_i = 0$ for some i or $r_i \neq 0$ for all i . If $r_i = F(\rho_i)x_i = 0$ for some i , then $\mathcal{R}(Z_i) = \text{span}\{x_i, x_{i-1}\}$. Note that $\mathcal{R}(Z_{i-1}) = \text{span}\{x_{i-1}, K_{i-1}F(\rho_i)x_{i-1}, \dots, (K_{i-1}F(\rho_i))^{m_e-1}x_{i-1}, x_{i-2}\}$ and $x_i = Z_{i-1}y_{i-1} \in \mathcal{R}(Z_{i-1})$. Then $\mathcal{R}(Z_i) \subset \mathcal{R}(Z_{i-1})$, which implies $\rho_{i+1} = \rho_i$ and $x_{i+1} = x_i$ and then $r_{i+1} = r_i = 0$. Thus, (8) holds. Now consider $r_i \neq 0$ for all i . Note that $r_i \neq 0$ implies $\nabla \rho_i \neq 0$, and so $\rho(x_i - v_1 K_i \nabla \rho_i) < \rho(x_i)$ for some v_1 with sufficiently tiny $|v_1|$. This in turn implies $\rho(x_i + v_2 r_i) < \rho(x_i)$ for some v_2 with sufficiently tiny $|v_2|$. Note that x_i satisfies the proper constraint and the constraint is continuous, which implies $x_i + v_2 r_i$ satisfies the proper constraint. Thus,

$$\rho_{i+1} = \min_i \rho(Z y_i) \leq \rho(x_i + v_2 r_i) < \rho(x_i).$$

Therefore ρ_i is strictly monotonically decreasing. Since ρ_i is strictly monotonically decreasing and bounded from below since $\rho_i \geq \lambda_-$, it is convergent and $\rho_i \rightarrow \hat{\rho} \in [\lambda_-, \lambda_+]$ because $\rho_i = \rho(x_i) \in [\lambda_-, \lambda_+]$ for all i . No two x_i are linear dependent because linear dependent x_i and x_j produce $\rho_i = \rho_j$. This proves Item 1.

For Item 2, easy to see $x_i^H r_i = x_i^H F(\rho_i)x_i = 0$. Since y_i is a stationary point,

$$Z_i^H r_{i+1} = -\frac{\sigma(x_{i+1})}{2} Z_i^H \nabla \rho(x_{i+1}) = -\frac{\sigma(x_{i+1})}{2} Z_i^H \nabla \rho(Z_i y_i) = -\frac{\sigma(x_{i+1})}{2} \frac{d\rho(Z_i y_i)}{dy} = 0.$$

For Item 3(a), we have $\|r_i\| = \|F(\rho_i)x_i\| \leq [\sum_{k=0}^{m_e} \|A_k\| |\lambda_{\ell}|^{m_e-k}] \|x_i\|$ so $\{r_i\}$ is a bounded sequence. It suffices to show that any limit point of $\{r_i\}$ is the zero vector. Assume, to the contrary, $\{r_i\}$ has a nonzero limit point \hat{r} , i.e., $r_{i_j} \rightarrow \hat{r}$, where $\{r_{i_j}\}$ is a subsequence of $\{r_i\}$. Since $\{x_{i_j}\}$ is bounded, it has a convergent subsequence. Without loss of generality, we may assume x_{i_j} itself is convergent and $x_{i_j} \rightarrow \hat{x}$ as $j \rightarrow \infty$. We have $\hat{r}^H \hat{x} = 0$ and \hat{x} satisfies the

proper constraint because $r_{i_j}^H x_{i_j} = 0$ and x_{i_j} satisfies the proper constraint. Now consider the projected problem for

$$F_{i_j}(\lambda) := Y_{i_j}^H F(\lambda) Y_{i_j} = \begin{bmatrix} x_{i_j}^H F(\lambda) x_{i_j} & x_{i_j}^H F(\lambda) r_{i_j} \\ r_{i_j}^H F(\lambda) x_{i_j} & r_{i_j}^H F(\lambda) r_{i_j} \end{bmatrix},$$

where $Y_{i_j} = [x_{i_j}, r_{i_j}]$. Since $r_{i_j}^H x_{i_j} = 0$, $\text{rank}(Y_{i_j}) = 2$, and thus $F_{i_j}(\lambda)$ still satisfies the assumptions at the beginning of the paper. Denote by $\mu_{j;k}$ its eigenvalues. It can be seen that

$$\lambda_- < \lambda_1 \leq \mu_{j;1} \leq \mu_{j;2} \leq \lambda_\ell. \quad (9)$$

Then $\lambda_1 \leq \rho_{i_j+1} \leq \mu_{j;1}$. Let

$$\hat{F}(\lambda) = \lim_{j \rightarrow \infty} F_{i_j}(\lambda)$$

whose eigenvalues are denoted by $\hat{\mu}_i$. By the continuity of the eigenvalues with respect to the entries of coefficient matrices, we know $\mu_{j;i} \rightarrow \hat{\mu}_i$ as $j \rightarrow \infty$, and thus

$$\lambda_- < \lambda_1 \leq \hat{\mu}_1 \leq \hat{\mu}_2 \leq \hat{\lambda}_\ell. \quad (10)$$

Notice by (9) and (10)

$$\lambda_1 \leq \rho_{i_j+1} \leq \mu_{j;1} \Rightarrow \lambda_- < \lambda_1 \leq \hat{\rho} \leq \hat{\mu}_1. \quad (11)$$

On the other hand, by (9), we have

$$\hat{F}(\hat{\rho}) = \lim_{j \rightarrow \infty} F_{i_j}(\rho_{i_j}) = \lim_{j \rightarrow \infty} \begin{bmatrix} 0 & r_{i_j}^H r_{i_j} \\ r_{i_j}^H r_{i_j} & r_{i_j}^H F(\rho_{i_j}) r_{i_j} \end{bmatrix} = \begin{bmatrix} 0 & \hat{r}^H \hat{r} \\ \hat{r}^H \hat{r} & \hat{r}^H F(\hat{\rho}) \hat{r} \end{bmatrix}$$

which is indefinite because $\hat{r}^H \hat{r} > 0$. But by (11), $\hat{F}(\hat{\rho}) \leq 0$, a contradiction. So $\hat{r} = 0$, as was to be shown.

For Item 3(b), since $\|x_i\| = 1$, $\{x_i\}$ has at least one limit point. Let \hat{x} be any limit point of x_i , i.e., $x_{i_j} \rightarrow \hat{x}$. Taking the limit on both sides of $F(\rho_{i_j})x_{i_j} = r_{i_j}$ yields $F(\hat{\rho})\hat{x} = 0$, i.e., $(\hat{\rho}, \hat{x})$ is an eigenpair. \square

Theorem 2.1 shows that $\text{LOCG}(1, m_e)$ converges globally, but provides no information on its convergence rate. In order to obtain such a rate, we proceed as follows: first, a relationship between the quantities of two successive iterations is established in Theorem 2.2; then, by this relationship, $\text{LOCG}(1, m_e)$ is compared with $\text{SD}(1, m_e)$ in Theorem 2.3, where $\text{SD}(1, m_e)$ is the block preconditioned steepest descent method; finally, the rate follows from this comparison in Theorem 2.4. These three theorems are reminiscent of the theorems by Ovtchinnikov [22, Theorem 2.6, Theorem 4.1, and Theorem 4.2], respectively. Our theorems are more general than those w.r.t. three aspects: they hold for any Hermitian matrix polynomial $F(\lambda)$ satisfying the assumptions in Section 1, other than only the standard Hermitian eigenvalue problem $F(\lambda) = \lambda I - A$; they allow for any m_e in $\text{LOCG}(1, m_e)$, other than only $m_e = 1$; the estimates are somewhat refined.

Theorem 2.2. *Let $x \neq 0$, $r(x) \neq 0$, $p \neq 0$, and $S = [s^{(1)} \ \dots \ s^{(k)}]$, which satisfy $p^H r(x) \neq 0$, $S^H r(x) = 0$. Suppose that $[x \ p \ S]$ is of full column rank, and $(\alpha_{\text{opt}}, b_{\text{opt}})$ is a stationary point of the function $\rho(x + \alpha(I - P_{x, \rho(x_{\text{opt}}), \rho(x)})[p + Sb])$. Write*

$$s = p + S b_{\text{opt}}, \quad d = \alpha_{\text{opt}}(I - P_{x, \rho(x_{\text{opt}}), \rho(x)})s, \quad x_{\text{opt}} = x + d.$$

Then, for the nontrivial case that $x_{\text{opt}} \neq x$,

$$\alpha_{\text{opt}} \neq 0, \quad r_{\text{opt}} \perp \text{span}\{x, p, S, s, d\}, \quad (12)$$

and

$$\alpha_{\text{opt}} = -\frac{p^H r(x)}{S^H \check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)s)} = -\frac{d^H F(\rho(x_{\text{opt}}))d}{r(x)^H p}, \quad (13)$$

$$\rho(x_{\text{opt}}) - \rho(x) = \frac{|r(x)^{\text{H}}p|^2}{\left[x^{\text{H}}\Phi(\rho(x_{\text{opt}}), \rho(x))x \right] \left[s^{\text{H}}\check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)s \right]} = \frac{d^{\text{H}}F(\rho(x_{\text{opt}}))d}{x^{\text{H}}\Phi(\rho(x_{\text{opt}}), \rho(x))x}, \quad (14)$$

$$r(x_{\text{opt}}) - r(x) = \check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)d, \quad (15)$$

$$b_{\text{opt}} = - \left[S^{\text{H}}\check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)S \right]^{\dagger} S^{\text{H}}\check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)p + v, \quad (16)$$

where v is a vector satisfying

$$\check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)Sv \perp \text{span}\{x, p, S, s, d\}, \quad (17)$$

as long as

$$x^{\text{H}}\Phi(\rho(x_{\text{opt}}), \rho(x))x \neq 0, \quad s^{\text{H}}\check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)s \neq 0,$$

Besides, (13)–(16) also holds for the trivial case that $\alpha_{\text{opt}} = 0, d = 0, x_{\text{opt}} = x, \rho(x_{\text{opt}}) = \rho(x), r(x_{\text{opt}}) = r(x)$.

Proof. Write

$$\Phi_{\text{opt}} = \Phi(\rho(x_{\text{opt}}), \rho(x)), \quad P_{\text{opt}} = P_{x, \rho(x_{\text{opt}}), \rho(x)} = \frac{xx^{\text{H}}\Phi_{\text{opt}}}{x^{\text{H}}\Phi_{\text{opt}}x}.$$

Recall from the end of Section 1 that we have

$$r(x_{\text{opt}})^{\text{H}}x_{\text{opt}} = 0, \quad r(x)^{\text{H}}x = 0, \quad r(x)^{\text{H}}P_{\text{opt}} = 0, \quad x^{\text{H}}\Phi_{\text{opt}}P_{\text{opt}} = x^{\text{H}}\Phi_{\text{opt}}.$$

Since $(\alpha_{\text{opt}}, b_{\text{opt}})$ is a stationary point of the function ρ ,

$$\begin{aligned} 0 &= \frac{\text{d}}{\text{d}b} \rho(x + \alpha_{\text{opt}}(I - P_{\text{opt}})(p + Sb_{\text{opt}})) = (\nabla \rho(x + \alpha_{\text{opt}}(I - P_{\text{opt}})s))^{\text{H}} \alpha_{\text{opt}}(I - P_{\text{opt}})S \\ &= -\frac{2\alpha_{\text{opt}}}{\sigma(x_{\text{opt}})} r(x_{\text{opt}})^{\text{H}}(I - P_{\text{opt}})S, \end{aligned} \quad (18)$$

and

$$\begin{aligned} 0 &= \frac{\text{d}}{\text{d}\alpha} \rho(x + \alpha_{\text{opt}}(I - P_{\text{opt}})s) = (\nabla \rho(x + \alpha_{\text{opt}}(I - P_{\text{opt}})s))^{\text{H}} (I - P_{\text{opt}})s \\ &= -\frac{2}{\sigma(x_{\text{opt}})} r(x_{\text{opt}})^{\text{H}}(I - P_{\text{opt}})s, \end{aligned} \quad (19)$$

which means $r(x_{\text{opt}})^{\text{H}}d = 0$. Then $r(x_{\text{opt}})^{\text{H}}x = r(x_{\text{opt}})^{\text{H}}(x_{\text{opt}} - d) = 0$ and $r(x_{\text{opt}})^{\text{H}}P_{\text{opt}} = 0$. Thus, $r(x_{\text{opt}})^{\text{H}}s = 0$ by (19) and $r(x_{\text{opt}})^{\text{H}}S = 0$ by (18), so that $r(x_{\text{opt}})^{\text{H}}p = r(x_{\text{opt}})^{\text{H}}(s - Sb_{\text{opt}}) = 0$. Then (12) holds. According to (19),

$$\begin{aligned} 0 &= x_{\text{opt}}^{\text{H}}F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s \\ &= x^{\text{H}}F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s + \overline{\alpha_{\text{opt}}} s^{\text{H}}\check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)s. \end{aligned} \quad (20)$$

Note that $d^{\text{H}}F(\rho(x_{\text{opt}}))d = |\alpha_{\text{opt}}|^2 s^{\text{H}}\check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)s$ and

$$\begin{aligned} x^{\text{H}}F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s &= x^{\text{H}} [F(\rho(x_{\text{opt}})) - F(\rho(x))] (I - P_{\text{opt}})s + x^{\text{H}}F(\rho(x))(I - P_{\text{opt}})s \\ &= [\rho(x_{\text{opt}}) - \rho(x)]x^{\text{H}}\Phi_{\text{opt}}(I - P_{\text{opt}})s + r(x)^{\text{H}}(I - P_{\text{opt}})s \\ &= r(x)^{\text{H}}s = r(x)^{\text{H}}p. \end{aligned} \quad (21)$$

Then by (20), we have (13). Since

$$\begin{aligned} r(x_{\text{opt}}) - r(x) &= F(\rho(x_{\text{opt}}))x_{\text{opt}} - F(\rho(x))x \\ &= F(\rho(x_{\text{opt}}))x_{\text{opt}} - F(\rho(x_{\text{opt}}))x + F(\rho(x_{\text{opt}}))x - F(\rho(x))x \\ &= \alpha_{\text{opt}}F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s + [\rho(x_{\text{opt}}) - \rho(x)]\Phi_{\text{opt}}x, \end{aligned} \quad (22)$$

by (21), we get

$$\rho(x_{\text{opt}}) - \rho(x) = \frac{x^{\text{H}}(r(x_{\text{opt}}) - r(x)) - \alpha_{\text{opt}}x^{\text{H}}F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s}{x^{\text{H}}\Phi_{\text{opt}}x} = -\frac{\alpha_{\text{opt}}r(x)^{\text{H}}p}{x^{\text{H}}\Phi_{\text{opt}}x}. \quad (23)$$

Together with (13), we obtain (14). Further,

$$\begin{aligned}
\check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)d &= \alpha_{\text{opt}}(I - P_{\text{opt}}^{\text{H}})F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s \\
&= \alpha_{\text{opt}} \left(F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s - \frac{\Phi_{\text{opt}} x x^{\text{H}}}{x^{\text{H}} \Phi_{\text{opt}} x} F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s \right) \\
&= \alpha_{\text{opt}} \left(F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s - \Phi_{\text{opt}} x \frac{r(x)^{\text{H}} p}{x^{\text{H}} \Phi_{\text{opt}} x} \right) \quad \text{by (21)} \\
&= \alpha_{\text{opt}} \left(F(\rho(x_{\text{opt}}))(I - P_{\text{opt}})s + \Phi_{\text{opt}} x \frac{\rho(x_{\text{opt}}) - \rho(x)}{\alpha_{\text{opt}}} \right) \quad \text{by (23)} \\
&= r(x_{\text{opt}}) - r(x), \quad \text{by (22)}
\end{aligned}$$

hence we obtain (15). Thus,

$$\begin{aligned}
(x_{\text{opt}} - x)^{\text{H}} \check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)(x_{\text{opt}} - x) &= (r(x_{\text{opt}}) - r(x))^{\text{H}}(x_{\text{opt}} - x) \\
&= -r(x)^{\text{H}}(x_{\text{opt}} - x) = -\alpha_{\text{opt}} r(x)^{\text{H}}(I - P_{\text{opt}})s = -\alpha_{\text{opt}} r(x)^{\text{H}} p.
\end{aligned}$$

Finally,

$$\begin{aligned}
0 &= S^{\text{H}}(I - P_{\text{opt}}^{\text{H}})(r(x_{\text{opt}}) - r(x)) \quad \text{by (18)} \\
&= S^{\text{H}}(I - P_{\text{opt}}^{\text{H}}) \check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x) \alpha_{\text{opt}}(I - P_{\text{opt}})(p + Sb) \quad \text{by (22)} \\
&= \alpha_{\text{opt}} S^{\text{H}} \check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x)(p + Sb), \quad \text{by the definition of } \check{F}
\end{aligned}$$

which implies (16), and $S^{\text{H}} \check{F}_{\rho(x_{\text{opt}}), \rho(x)}(\rho(x_{\text{opt}}); x) S v = 0$. Note that $S^{\text{H}} \check{F}_{\rho(x_{\text{opt}}), \rho(x)} d = S^{\text{H}}[r(x_{\text{opt}}) - r(x)] = 0$ by (15), and $\check{F}_{\rho(x_{\text{opt}}), \rho(x)} x = \check{F}(\rho(x_{\text{opt}}))(I - P_{\text{opt}})x = 0$. It is easy to obtain (17). \square

Theorem 2.3. Suppose $\lambda_1 < \rho_i < \lambda_2$. Assume that $K_i^{1/2} F'(\rho_i) K_i^{1/2}$ is positive definite in the search subspace, or equivalently, $Z_i^{\text{H}} K_i^{1/2} F'(\rho_i) K_i^{1/2} Z_i > 0$. If $\rho_{i-1} - \lambda_1$ is sufficiently small, then for LOCG(1, 1), either $\rho_i - \rho_{i+1} \geq \sqrt{\rho_{i-1} - \rho_i}$, or

$$\frac{1}{\rho_i - \rho_{i+1}} + \frac{1}{\rho_{i-1} - \rho_i} = \frac{1 + O(\sqrt{\rho_i - \rho_{i+1}}) + O(\rho_{i-1} - \rho_i)}{\rho_i - \rho_{i+1}^{\circ}}, \quad (24)$$

where ρ_{i+1}° is the minimal value of $\rho(x)$ in the subspace $\mathcal{K}_{m_e}(K_i F(\rho_i), x_i)$.

Remark 2.1. If the case that $\rho_i - \rho_{i+1} \geq \sqrt{\rho_{i-1} - \rho_i}$ occurs, the i th iteration improves the approximation a lot, so it is very exceptional.

Proof. Assume that $\rho_i - \rho_{i+1} \geq \sqrt{\rho_{i-1} - \rho_i}$ fails, namely

$$\rho_i - \rho_{i+1} < \sqrt{\rho_{i-1} - \rho_i}. \quad (25)$$

For a general $K_i > 0$, the i th iteration is just equivalent to the i th iteration of the algorithm applied to $K_i^{1/2} F(\lambda) K_i^{1/2}$ without a preconditioner, and then everything below can be easily examined. Thus, in the following we assume $K_i = I$.

To use Theorem 2.2, without loss of generality, suppose we normalize x_i in every iteration to make the first element of y_i (in Step 6 of Algorithm 2.1) be 1. Then in the i th iteration, write

$$\begin{aligned}
\varepsilon_i &= \rho_i - \lambda_1, \quad \delta_i = -(\rho_{i+1} - \rho_i) \geq 0, \quad d_i = x_{i+1} - x_i, \quad F_i = F(\rho_i), \quad F'_i = F'(\rho_i), \\
\Phi_i &= \Phi(\rho_{i+1}, \rho_i), \quad P_i = P_{x_i, \rho_{i+1}, \rho_i}, \quad \check{F}_i = \check{F}_{\rho_{i+1}, \rho_i}(\rho_{i+1}; x_i).
\end{aligned}$$

Clearly $d_{i-1}^H r_i = 0$. Note that $\sigma(x_i) = x_i^H F_i' x_i > 0$. Thus,

$$\frac{x_i^H \Phi_i x_i}{x_i^H x_i} = \frac{\sigma(x_i)}{x_i^H x_i} + \sum_{k=2}^m \frac{(-\delta_i)^{k-1}}{k!} \frac{x_i^H F^{(k)}(\rho_i) x_i}{x_i^H x_i} = \frac{\sigma(x_i)}{x_i^H x_i} + O(\delta_i) > 0.$$

Without loss of generality, we assume $x_i^H \Phi_i x_i = 1$.

If the notations in Theorem 2.2 are adopted, then

$$x_i = x, \quad r_i = r(x), \quad \rho_i = \rho(x), \quad x_{i+1} = x_{\text{opt}}, \quad r_{i+1} = r(x_{\text{opt}}), \quad \rho_{i+1} = \rho(x_{i+1}).$$

For

$$S_i := (I - P_i) \left(I - \frac{r_i r_i^H}{r_i^H r_i} \right) [F_i r_i \quad \dots \quad F_i^{m_e} r_i],$$

we obtain $r_i^H S_i = 0$. ρ_{i+1} can be recognized as ρ_{opt} in Theorem 2.2 as we let

$$p = r_i, \quad S = [x_{i-1} \quad S_i] =: \tilde{S}_i.$$

Without loss of generality, assume $[r_i \quad x_{i-1} \quad S_i]$ is of full column rank, otherwise we can delete the last several columns of S_i , which will not affect the search process. Thus, by (14) and (16),

$$\delta_i = \rho_i - \rho_{i+1} = -\frac{|r_i^H r_i|^2}{[x_i^H \Phi_i x_i][s_i^H \check{F}_i s_i]},$$

where

$$s_i = r_i - \tilde{S}_i (\tilde{S}_i^H \check{F}_i \tilde{S}_i)^\dagger \tilde{S}_i^H \check{F}_i r_i + \tilde{S}_i v_i, \quad \check{F}_i \tilde{S}_i v_i \perp \text{span}\{x_i, r_i, \tilde{S}_i, s_i, d_i\}.$$

To describe the search process in the subspace $\mathcal{K}_{m_e}(K_i F(\rho_i), x_i)$, we use the superscript “ \circ ” for certain terms, which gives

$$\begin{aligned} \delta_i^\circ = -(\rho_{i+1}^\circ - \rho_i) \geq 0, \quad F_{i+1}^\circ = F(\rho_{i+1}^\circ), \quad \Phi_i^\circ = \Phi(\rho_{i+1}^\circ, \rho_i), \quad P_i^\circ = P_{x_i, \rho_{i+1}^\circ, \rho_i}, \quad \check{F}_i^\circ = \check{F}_{\rho_{i+1}^\circ, \rho_i}(\rho_{i+1}^\circ; x_i). \\ x_{i+1}^\circ = x_{\text{opt}}, \quad r_{i+1}^\circ = r(x_{\text{opt}}), \quad \rho_{i+1}^\circ = \rho(x_{\text{opt}}), \end{aligned}$$

Similarly, ρ_{i+1}° can be recognized as ρ_{opt}° in Theorem 2.2 as we let

$$p^\circ = r_i, \quad S^\circ = S_i.$$

Thus, by (14) and (16),

$$\delta_i^\circ = \rho_i - \rho_{i+1}^\circ = -\frac{|r_i^H r_i|^2}{[x_i^H \Phi_i^\circ x_i][(s_i^\circ)^H \check{F}_i^\circ s_i^\circ]}. \quad (26)$$

where

$$s_i^\circ = r_i - S_i (S_i^H \check{F}_i^\circ S_i)^\dagger S_i^H \check{F}_i^\circ r_i + S_i v_i^\circ, \quad \check{F}_i^\circ S_i v_i^\circ \perp \text{span}\{x_i, r_i, S_i, s_i^\circ\}.$$

The rest of the proof is to estimate the ratio of δ_i° and δ_i . Let

$$\kappa := \frac{\delta_i^\circ}{\delta_i} = \frac{x_i^H \Phi_i x_i}{x_i^H \Phi_i^\circ x_i} \frac{s_i^H \check{F}_i s_i}{(s_i^\circ)^H \check{F}_i^\circ s_i^\circ}.$$

Clearly, $\kappa \leq 1$.

First, we prove that

$$S_i^H F_{i+1} S_i \text{ and } S_i^H F_{i+1}^\circ S_i \text{ are nonsingular.} \quad (27)$$

Write

$$\begin{aligned} T_i &= S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H \check{F}_i = S_i (S_i^H F_{i+1} S_i)^{-1} S_i^H F_{i+1} (I - P_i), \\ T_i^\circ &= S_i (S_i^H \check{F}_i^\circ S_i)^{-1} S_i^H \check{F}_i^\circ = S_i (S_i^H F_{i+1}^\circ S_i)^{-1} S_i^H F_{i+1}^\circ (I - P_i^\circ). \end{aligned}$$

Clearly, $P_i S_i = 0$, $P_i T_i = T_i P_i = 0$, $P_i^o T_i^o = T_i^o P_i^o = 0$, and

$$T_i^H \check{F}_i = T_i^H \check{F}_i T_i, \quad (I - T_i^H) \check{F}_i (I - T_i) = \check{F}_i (I - T_i) = (I - T_i^H) \check{F}_i.$$

We have $v_i^o = 0$ and

$$s_i^o = r_i - S_i (S_i^H \check{F}_i^o S_i)^{-1} S_i^H \check{F}_i^o r_i = (I - T_i^o) r_i.$$

On the other hand, it is easy to see that $\tilde{S}_i^H \check{F}_i \tilde{S}_i$ is nonsingular if and only if

$$\tau_i := x_{i-1}^H \check{F}_i (I - T_i) x_{i-1} \neq 0, \quad (28)$$

and when it is nonsingular, that

$$(\tilde{S}_i^H \check{F}_i \tilde{S}_i)^{-1} = \begin{bmatrix} x_{i-1}^H \check{F}_i x_{i-1} & x_{i-1}^H \check{F}_i S_i \\ S_i^H \check{F}_i x_{i-1} & S_i^H \check{F}_i S_i \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{\tau_i} & -\frac{1}{\tau_i} w_i^H \\ -\frac{1}{\tau_i} w_i & \frac{1}{\tau_i} w_i w_i^H + (S_i^H \check{F}_i S_i)^{-1} \end{bmatrix},$$

where $w_i = (S_i^H \check{F}_i S_i)^{-1} S_i^H \check{F}_i x_{i-1}$ satisfying $S_i w_i = T_i x_{i-1}$. Actually, (28) is guaranteed by the claim (31) below. Thus, $\tilde{S}_i^H \check{F}_i \tilde{S}_i$ is nonsingular,

$$\tilde{S} (\tilde{S}^H \check{F}_i \tilde{S})^{-1} \tilde{S}^H = S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H + \frac{1}{\tau_i} (I - T_i) x_{i-1} x_{i-1}^H (I - T_i^H),$$

and

$$\begin{aligned} s_i &= r_i - \tilde{S}_i (\tilde{S}_i^H \check{F}_i \tilde{S}_i)^{-1} \tilde{S}_i^H \check{F}_i r_i \\ &= r_i - S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H \check{F}_i r_i - \frac{1}{\tau_i} (I - T_i) x_{i-1} x_{i-1}^H (I - T_i^H) \check{F}_i r_i \\ &= (I - T_i) \left[r_i - \frac{x_{i-1}^H \check{F}_i (I - T_i) r_i}{\tau_i} x_{i-1} \right]. \end{aligned}$$

Write

$$e_i = T_i^o r_i - T_i r_i, \quad \beta_i = x_{i-1}^H \check{F}_i (I - T_i) r_i,$$

so that $s_i^o + e_i = (I - T_i) r_i$ and

$$s_i = s_i^o + e_i - \frac{\beta_i}{\tau_i} (I - T_i) x_{i-1}.$$

Let

$$\kappa = \frac{\delta_i^o}{\delta_i} = \frac{x_i^H \Phi_i x_i (s_i^o)^H \check{F}_i s_i^o (s_i^o + e_i)^H \check{F}_i (s_i^o + e_i) s_i^H \check{F}_i s_i}{x_i^H \Phi_i^o x_i (s_i^o)^H \check{F}_i^o s_i^o (s_i^o)^H \check{F}_i^o s_i^o (s_i^o + e_i)^H \check{F}_i (s_i^o + e_i)} =: \kappa_1 \kappa_2 \kappa_3 \kappa_4. \quad (29)$$

First, observe that

$$\kappa_1 = \frac{1}{x_i^H \Phi_i x_i} = \frac{1}{\sigma(x_i) + O(\delta_i^o)} = \frac{1}{1 + O(\delta_i)} = 1 + O(\delta_i).$$

We assume for now that

$$\kappa_2 = 1 + O(\delta_i), \quad \kappa_3 = 1 + O(\delta_i). \quad (30)$$

For κ_4 , since $(I - T_i^H) \check{F}_i (I - T_i) = \check{F}_i (I - T_i) = (I - T_i^H) \check{F}_i$, we get then

$$\kappa_4 = \frac{s_i^H \check{F}_i s_i}{(s_i^o + e_i)^H \check{F}_i (s_i^o + e_i)} = \frac{r_i^H \check{F}_i (I - T_i) r_i - \frac{\beta_i^2}{\tau_i}}{r_i^H \check{F}_i (I - T_i) r_i} = 1 - \frac{\beta_i^2}{\tau_i r_i^H \check{F}_i (I - T_i) r_i}.$$

We claim that

$$\tau_i = - \left[1 + O(\delta_{i-1}^{1/2}) + O(\delta_i) \right] \delta_{i-1}, \quad (31)$$

$$\beta_i = \left[1 + O(\delta_{i-1}) + O(\delta_i \delta_{i-1}^{1/2})\right] \|r_i\|^2 + \left[O(\delta_{i-1}) + O(\delta_i \delta_{i-1}^{1/2})\right] \|r_i\|, \quad (32)$$

and

$$-r_i^H \check{F}_i (I - T_i) r_i \sim r_i^H r_i = O(\delta_i). \quad (33)$$

Recall (25), namely $\delta_{i-1} > \delta_i^2$. Therefore,

$$\tau_i = - \left[1 + O(\delta_{i-1}^{1/2})\right] \delta_{i-1}, \quad \beta_i = \left[1 + O(\delta_{i-1})\right] \|r_i\|^2 + O(\delta_{i-1}) \|r_i\|.$$

Thus,

$$\begin{aligned} 1 - \kappa_4 &= \frac{\beta_i^2}{\tau_i r_i^H \check{F}_i (I - T_i) r_i} = \frac{(O(\delta_{i-1}) \|r_i\| + [1 + O(\delta_{i-1})] \|r_i\|^2)^2}{-\delta_{i-1} \left[1 + O(\delta_{i-1}^{1/2})\right] r_i^H \check{F}_i (I - T_i) r_i} \\ &= \frac{[1 + O(\delta_{i-1})] \|r_i\|^4 + O(\delta_{i-1}) \|r_i\|^3 + O(\delta_{i-1}^2) \|r_i\|^2}{-\delta_{i-1} \left[1 + O(\delta_{i-1}^{1/2})\right] r_i^H \check{F}_i (I - T_i) r_i} \\ &= \frac{[1 + O(\delta_{i-1}^{1/2})] \|r_i\|^4 + O(\delta_{i-1}) \|r_i\|^3 + O(\delta_{i-1}^2) \|r_i\|^2}{-\delta_{i-1} r_i^H \check{F}_i (I - T_i) r_i} \\ &= \frac{1 + O(\delta_{i-1}^{1/2})}{\delta_{i-1}} \frac{\|r_i\|^4}{r_i^H \check{F}_i (I - T_i) r_i} + O(\delta_i^{1/2}) + O(\delta_{i-1}). \end{aligned}$$

By (26) and (29),

$$\frac{\delta_i^o}{\kappa_1 \kappa_2 \kappa_3} = \frac{\|r_i\|^4}{r_i^H \check{F}_i (I - T_i) r_i},$$

which implies

$$1 - \kappa_4 = \frac{1 + O(\delta_{i-1}^{1/2})}{\delta_{i-1}} \frac{\delta_i^o}{\kappa_1 \kappa_2 \kappa_3} + O(\delta_i^{1/2}) + O(\delta_{i-1}).$$

Since $(1 - \kappa_4) \kappa_1 \kappa_2 \kappa_3 = \kappa_1 \kappa_2 \kappa_3 - \kappa = 1 - \kappa + O(\delta_i)$, we obtain

$$\frac{\delta_i^o}{\delta_{i-1}} + O(\delta_i^{1/2}) \sqrt{\frac{\delta_i^o}{\delta_{i-1}}} + O(\delta_i^{1/2}) + O(\delta_{i-1}) + O(\delta_i) - (1 - \kappa) = 0,$$

which implies

$$\begin{aligned} \frac{\delta_i^o}{\delta_{i-1}} &= \left(\frac{1}{2} \left[-O(\delta_i^{1/2}) \pm \sqrt{O(\delta_i) + O(\delta_i^{1/2}) + O(\delta_{i-1}) + 4(1 - \kappa)} \right] \right)^2 \\ &= O(\delta_i) + O(\delta_i^{1/2}) + O(\delta_{i-1}) + 4(1 - \kappa) + 2O(\delta_i^{1/2}) \sqrt{O(\delta_i^{1/2}) + O(\delta_{i-1}) + (1 - \kappa)} \\ &= 1 - \kappa + O(\delta_i^{1/2}) + O(\delta_{i-1}). \end{aligned}$$

With

$$\frac{1}{\delta_i} = \frac{1 + O(\delta_i^{1/2}) + O(\delta_{i-1})}{\delta_i^o} - \frac{1}{\delta_{i-1}},$$

we arrive at (24).

We defer the proofs of the claims (27), (30), (31), (32), and (33) to Appendix B, as these consist of rather technical calculations and estimations. \square

We summarize the findings of this section in the following theorem.

Theorem 2.4. Suppose $\lambda_1 \leq \rho_0 < \lambda_2$. Let $\{\rho_i\}$ and $\{\rho_i^0\}$ be produced by LOCG(1, m_e) and SD(1, m_e) with a fixed preconditioner $K > 0$, respectively. Assume that $Z_i^H K^{1/2} F'(\lambda_1) K^{1/2} Z_i > 0$. If $\rho_{i-1} - \lambda_1$ is sufficiently small, provided

$$\rho_{i+1}^0 - \lambda_1 \leq \eta_0(\rho_i^0 - \lambda_1) + O((\rho_i^0 - \lambda_1)^{3/2}), \quad \text{for all } i \text{ and a given } \eta_0 < 1,$$

then

$$\rho_{i+1} - \lambda_1 \leq \eta^2(\rho_{i-1} - \lambda_1) + O((\rho_{i-1} - \lambda_1)^{3/2}), \quad (34)$$

where

$$\eta = \frac{\eta_0}{2 - \eta_0}.$$

Proof. The proof is exactly the same as its analogue by Ovtchinnikov [22, Theorem 4.2]. \square

3 Application to Definite Pairs and Hyperbolic Quadratic Polynomials

3.1 Definite Matrix Pair

As we stated in Section 1, the definite pair $F(\lambda) = \lambda B - A$ for the special case that $F(\lambda_0) < 0$, $\mathcal{I} = (\lambda_0, +\infty)$, and the smallest positive-type eigenvalue is chosen here. This setting satisfies the assumptions needed to apply the results from the previous section. However, with little effort, we see that any definite pair or any type of eigenvalues could be transformed into the case mentioned before. For example, for $F(\lambda_0) < 0$, $\mathcal{I} = (-\infty, \lambda_0)$, we consider $\hat{F}(\lambda) = F(-\lambda)$ and $\hat{\mathcal{I}} = (-\lambda_0, +\infty)$; for $F(\lambda_0) > 0$, $\mathcal{I} = (\lambda_0, +\infty)$, we consider $\hat{F}(\lambda) = -F(\lambda)$ and $\hat{\mathcal{I}} = \mathcal{I}$.

Theorem 3.1. Let $\{\rho_i\}$, $\{x_i\}$ be produced by LOCG(1, m_e) with a fixed preconditioner $K > 0$ for the definite matrix pair $F(\lambda) = \lambda B - A$. Suppose $\lambda_1^+ \leq \rho_0 < \lambda_2^+$. Assume that $Z_i^H K^{1/2} F'(\lambda_1) K^{1/2} Z_i > 0$.

1. As $i \rightarrow \infty$, ρ_i monotonically converges to λ_1^+ , and x_i converges to the corresponding eigenvector in direction, i.e., $F(\rho_i)x_i \rightarrow 0$.
2. Denote by γ and Γ the smallest and largest positive eigenvalue of the matrix $-KF(\lambda_1)$. If $\rho_i - \lambda_1^+$ is sufficiently small, then

$$\rho_{i+1} - \lambda_1^+ \leq \eta^2(\rho_{i-1} - \lambda_1^+) + O((\rho_{i-1} - \lambda_1^+)^{3/2}), \quad (35)$$

where

$$\eta = \frac{2}{\Delta^{2m_e} + \Delta^{-2m_e}}, \quad \Delta = \frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1}, \quad \kappa = \frac{\Gamma}{\gamma}.$$

Proof. For a definite matrix pair, the optimization problem (7) is

$$\rho_{i+1} = \rho(Z_i y_i) = \min_{y^H Z_i^H B Z_i y = 1} y^H Z_i^H A Z_i y.$$

Using Lagrangian multipliers, it is equivalent to

$$\rho_{i+1} = \min \mathcal{L}(y, \mu) = \min y^H Z_i^H A Z_i y - \mu(y^H Z_i^H B Z_i y - 1).$$

The minimal point (y_i, μ_i) must satisfy:

$$\frac{\partial \mathcal{L}(y_i, \mu_i)}{\partial y} = 2Z_i^H A Z_i y_i - 2\mu_i Z_i^H B Z_i y_i = 0, \quad (36a)$$

$$\frac{\partial \mathcal{L}(y_i, \mu_i)}{\partial \mu} = y_i^H Z_i^H B Z_i y_i - 1 = 0. \quad (36b)$$

Left multiplying (36a) by y_i^H gives $\mu_i = \rho(Z_i y_i)$, and then $Z_i^H r(Z_i y_i) = Z_i^H F(\rho(Z_i y_i)) Z_i y_i = 0$. Thus, $\frac{d\rho(Z_i y_i)}{dy} = Z_i^H \nabla \rho(Z_i y_i) = 0$, which means y_i is a stationary point of $\rho(Z_i y)$. Besides, under the constraint $x_i^H B x_i = 1$,

$$x_i^H (\lambda_- B - A) x_i = (\lambda_- - \rho_i) x_i^H B x_i = \lambda_- - \rho_i.$$

Since $\lambda_- B - A < 0$, $\|x_i\| \leq \frac{\rho_i - \lambda_-}{\lambda_{\min}(A - \lambda_- B)} \leq \frac{\rho_0 - \lambda_-}{\lambda_{\min}(A - \lambda_- B)}$, which implies that $\|x_i\|$ is bounded. To sum up, by Theorem 2.1, Item 1 holds.

For Item 2, first, under the assumption $Z_i^H K^{1/2} F'(\lambda_1) K^{1/2} Z_i = Z_i^H K^{1/2} B K^{1/2} Z_i > 0$, it is easy to check that Theorem 3.4 in Golub and Ye [5] still holds, even if the matrix pair (A, B) is definite, rather than restricted to the case that $B > 0$. Then we choose the m th Chebyshev polynomial of the first kind as the polynomial p in the theorem. Similarly to the discussions by Li [12, Section 2], an upper bound of ϵ_m in the theorem results. Then, together with this theorem, by Theorem 2.4, Item 2 holds. \square

3.2 Hyperbolic Quadratic Eigenvalue Problems

As we stated in Section 1, the hyperbolic quadratic polynomial $F(\lambda) = \lambda^2 A + \lambda B + C$ for the special case that $\mathcal{I} = (\lambda_0, +\infty)$, and the smallest positive-type eigenvalue is chosen as what we need, satisfies the assumptions on a generic $F(\lambda)$. However, with little effort, we know the negative-type eigenvalue or the largest eigenvalue could be transformed into the case mentioned before. For example, for the largest eigenvalue lying in $\mathcal{I} = (-\infty, \lambda_0)$, we consider $\hat{F}(\lambda) = F(-\lambda)$ and $\hat{\mathcal{I}} = (-\lambda_0, +\infty)$; for the largest eigenvalue lying in $\mathcal{I} = (\lambda_0, +\infty)$, we consider $\hat{F}(\lambda) = -F(-\lambda)$ and $\hat{\mathcal{I}} = (-\infty, \lambda_0)$.

Theorem 3.2. *Theorem 3.1 holds for the hyperbolic quadratic polynomial*

$$F(\lambda) = \lambda^2 A + \lambda B + C.$$

Proof. The optimization problem (7) is

$$\rho_{i+1} = \rho(Z_i y_i) = \min_{y^H Z_i^H A Z_i y = 1} \rho(Z_i y).$$

Using Lagrangian multipliers, it is equivalent to

$$\rho_{i+1} = \min \mathcal{L}(y, \mu) = \min \rho(Z_i y) - \mu (y^H Z_i^H A Z_i y - 1).$$

The minimal point (y_i, μ_i) must satisfy:

$$\frac{\partial \mathcal{L}(y_i, \mu_i)}{\partial y} = -2 \frac{Z_i^H r(Z_i y_i)}{\sigma(Z_i y_i)} - 2\mu_i Z_i^H A Z_i y_i = 0, \quad (37a)$$

$$\frac{\partial \mathcal{L}(y_i, \mu_i)}{\partial \mu} = y_i^H Z_i^H A Z_i y_i - 1 = 0. \quad (37b)$$

Left multiplying (37a) by y_i^H gives $\mu_i = 0$, and then $Z_i^H r(Z_i y_i) = 0$. Thus, $\frac{d\rho(Z_i y_i)}{dy} = Z_i^H \nabla \rho(Z_i y_i) = 0$, which means y_i is a stationary point of $\rho(Z_i y)$. Besides, under the constraint $x_i^H A x_i = 1$, $\|x_i\| \leq \frac{1}{\lambda_{\min}(A)}$ and then $\|x_i\|$ is bounded. To sum up, by Theorem 2.1, Item 1 holds.

Item 2 holds by Theorem 2.4, together with a theorem by Liang and Li [15, Theorem 9.1]. \square

4 Numerical Examples

In the section, we will provide two examples to illustrate the proven convergence rate. We use the code by Li [13] and make small modifications to it to do calculations in the examples below. All experiments are done in MATLAB R2017a under the Windows 10 Professional 64-bit operating system on a PC with a Intel Core i7-8700 processor at 3.20GHz and 64GB RAM.

Example 4.1 ([15, Example 12.1]). This is the problem Wiresaw1 in the collection NLEVP [3]. It is actually a gyroscopic quadratic eigenvalue problem coming from the vibration analysis of a wiresaw [28], which we can transform to the following hyperbolic quadratic matrix polynomial:

$$A = \frac{1}{2} I_n, \quad C = \frac{(v^2 - 1)\pi^2}{2} \text{diag}(1^2, 2^2, \dots, n^2),$$

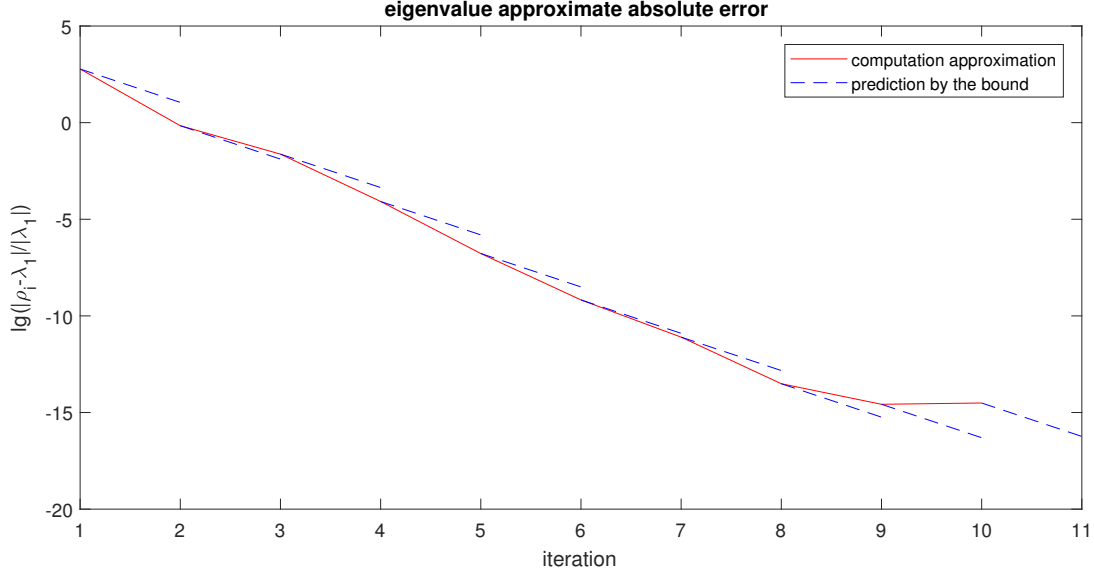


Figure 1: Example 4.1: calculation and prediction for LOCG(1, 1).

$$B = (b_{ij}) \quad \text{with} \quad b_{ij} = \begin{cases} \nu\sqrt{-1} \frac{4ij}{i^2 - j^2}, & \text{if } i + j \text{ is odd,} \\ 0, & \text{otherwise,} \end{cases}$$

where ν is a real nonnegative parameter related to the speed of the wire.

In this example, we use LOCG(1, 1) in Algorithm 2.1 with $X_0 = \text{randn}(n, 1)$ for $n = 1000$, $\nu = 0.1$, with the preconditioner $K = C^{-1}$ to get the smallest positive-type eigenvalue of the problem. For the projected problem in every step, the stopping criteria is that the normalized residual is no bigger than 0.1 or the number of CG steps reaches 10. In Figure 1, the final approximation is treated as the exact eigenvalue λ_1 , and then: the solid line is the real approximation error; the dash line is the result predicted by (compared with (35))

$$\rho_{i+1} - \lambda_1 = \frac{2}{\Delta^2 + \Delta^{-2}}(\rho_i - \lambda_1), \quad \Delta = \frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1}, \quad \kappa = \frac{\Gamma}{\gamma}.$$

At least we see that in this example, this kind of prediction is appropriate.

Example 4.2. This example is constructed by the MATLAB function `gen_hyper2` in the collection NLEVP [3]. Here, we generate a small-scale problem of size 10 with eigenvalues $\pm 1, \pm 2, \dots, \pm 10$, and a mid-scale problem of size 1000 with eigenvalues $\pm 1, \pm 2, \dots, \pm 1000$. The other parameters are chosen randomly. Thus, we know the exact eigenvalue $\lambda_1 = 1$.

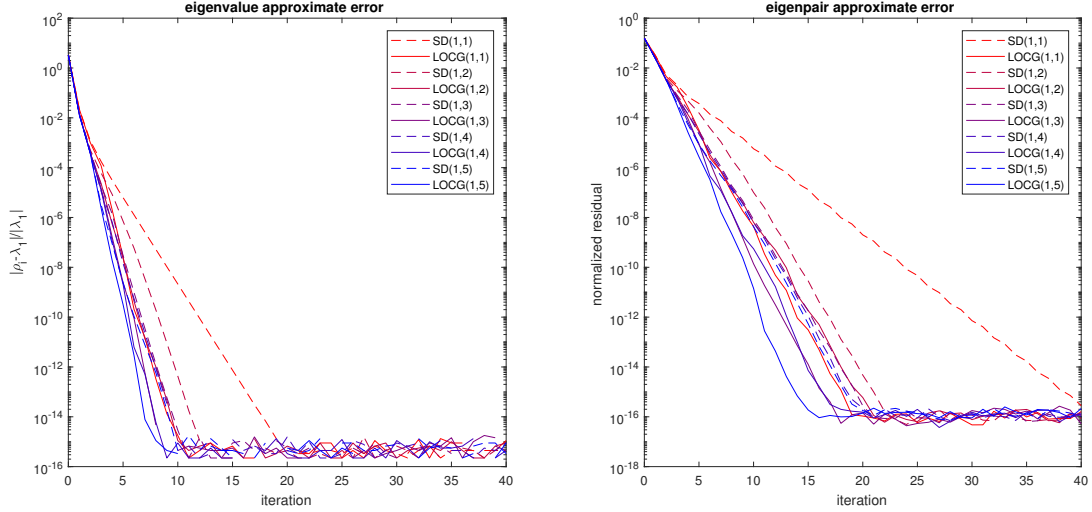
We use different values of m for SD(1, m) and LOCG(1, m) to calculate the smallest positive-type eigenvalue, with the preconditioner $K = C^{-1}$. For the projected problem in every step, the stopping criteria is that the normalized residual is no bigger than 0.1 or the number of CG steps reaches 10. In Figure 2, the left figure shows the relative error of the approximations; the right figure shows the normalized residuals

$$\frac{\|Q(\rho_i)x_i\|_2}{(\|A\|_1 \rho_i^2 + \|B\|_1 |\rho_i| + \|C\|_1) \|x_i\|_2}$$

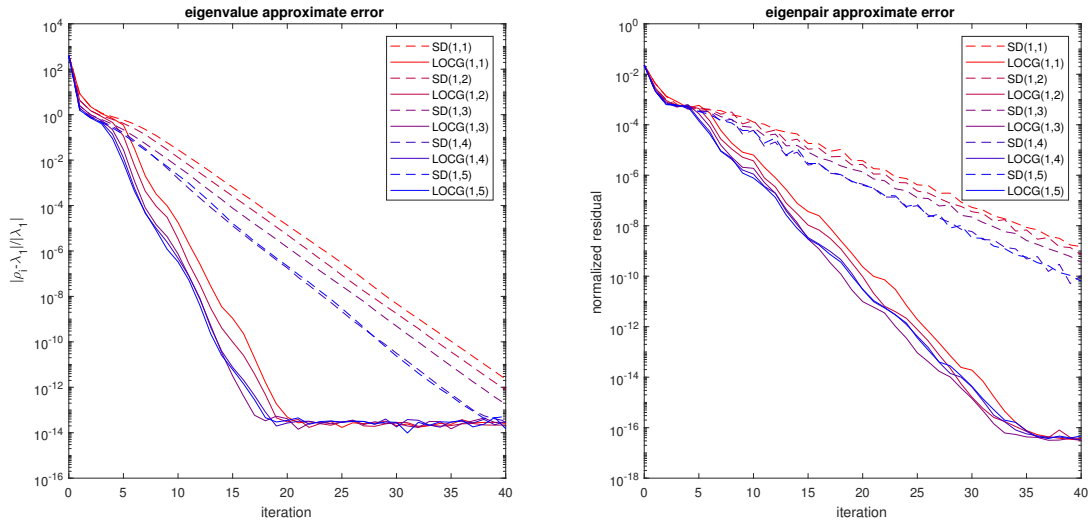
of the approximations.

In this example, we can see that

- LOCG is much better than SD, especially for mid/large-scale problems;
- increasing the dimension of the Krylov subspace indeed accelerates the convergence to the eigenvalue, though not so significantly;



(a) $n = 10$



(b) $n = 1000$

Figure 2: Example 4.2: different dimensions m of Krylov subspaces.

- increasing the dimension of the Krylov subspace perhaps slows down the convergence of the normalized residuals.

Thus, to balance the computational cost per step and the convergence, maybe the best choice is LOCG(1, 1).

5 Conclusions

We have performed the convergence analysis of an extended LOBPCG algorithm for computing the extreme eigenvalue of Hermitian matrix polynomials, including two common instances — definite matrix pairs and hyperbolic quadratic matrix polynomials. This analysis was considered out of reach by Kressner et al [11, Subsection 3.2] or by Liang and Li [15, Subsection 11.2] for the vector version of LOBPcCG. However, it is quite natural to ask whether there exists any kind of convergence analysis for the block version of LOBPcCG. It is likely that some analogues would hold, but this remains likely to be a difficult and complicated task for future work.

A A lemma on the inertia property

For any Hermitian matrix A , the inertia of A , denoted by $\text{inertia}(A)$, is a triple of integers which are the number of negative/zero/positive eigenvalues, respectively.

For any real λ , $F(\lambda)$ is a Hermitian matrix. So we can discuss its inertia, the result is Lemma A.1. Actually, the lemma is obvious for $\lambda B - A$ when $B > 0$; for a definite matrix pair or hyperbolic matrix polynomial $F(\lambda)$, it can be found in many works (see, e.g. [26, (0.7)], [1, Corollary 2.3.7], and [9, Section 3]).

Lemma A.1. *Given a Hermitian matrix polynomial $F(\lambda)$ satisfying the assumptions at the beginning of Section 1. Then*

$$\text{inertia}(F(\mu)) = (n - i, 0, i), \quad \text{for any } \mu \in (\lambda_i, \lambda_{i+1}), \quad (38)$$

where i is an index to make $\lambda_i < \lambda_{i+1}$.

Proof. First, for any $\mu \in (\lambda_i, \lambda_{i+1})$, $F(\lambda)$ is nonsingular. For μ_1 and μ_2 making $F(\mu_1)$ and $F(\mu)$ have different inertia, at least one positive (or negative) eigenvalue of $F(\mu_1)$ has to become a negative (or positive) eigenvalue of $F(\mu_2)$. Since the eigenvalues of a matrix, as functions of the matrix entries, are continuous, there exists μ_3 between μ_1 and μ_2 , such that $F(\mu_3)$ has at least one zero eigenvalue, or equivalently, there exists a nonzero vector x , such that $F(\mu_3)x = 0$. This implies μ_3 is an eigenvalue of $F(\lambda)$. Thus, for any interval in which no eigenvalue lies, the inertia is invariant.

Without loss of generality, we assume the eigenvalues are simple. Since $F(\lambda_1 - \varepsilon) < 0$, by the continuity of eigenvalues of a matrix, $\text{inertia}(F(\lambda_1)) = (n - 1, 1, 0)$. Write the corresponding eigenvector of λ_1 is u_1 , and then $u_1^H F(\lambda_1 + \varepsilon) u_1 > 0$. Then, also by the continuity, $\text{inertia}(F(\lambda_1 + \varepsilon)) = (n - 1, 0, 1)$. Similarly, we have (38) recursively. \square

B Claims in the proof of Theorem 2.3

Before proving the claims, we first establish two bound estimates, which will be used later.

One is that x_i is bounded. Note that

$$F_i = F(\lambda_1) + \sum_{k=1}^m \frac{\varepsilon_i^k}{k!} F^{(k)}(\lambda_1), \quad \Phi_i = F'(\lambda_1) + \sum_{k=2}^m \frac{\varepsilon_i^{k-1}}{k!} F^{(k)}(\lambda_1).$$

Since ε_i is sufficiently small, $Z_i^H F'(\rho_i) Z_i > 0$ implies $Z_i^H \Phi_i Z_i > 0$, $Z_i^H F'(\lambda_1) Z_i > 0$. Let $Q_i = Z_i (Z_i^H Z_i)^{-1/2}$ be the orthonormal basis of $\mathcal{R}(Z_i)$. Then $Q_i^H F'(\rho_i) Q_i > 0$, $Q_i^H \Phi_i Q_i > 0$, $Q_i^H F'(\lambda_1) Q_i > 0$. Write $x_i = Q_i \hat{x}_i$, and then

$$1 = x_i^H \Phi_i x_i = \hat{x}_i^H Q_i^H \Phi_i Q_i \hat{x}_i \geq \lambda_{\min}(Q_i^H \Phi_i Q_i) \|\hat{x}_i\|^2,$$

which implies

$$\|x_i\|^2 \leq \|\hat{x}_i\|^2 \leq \frac{1}{\lambda_{\min}(Q_i^H \Phi_i Q_i)} \leq \frac{1}{\lambda_{\min}(Q_i^H F_i Q_i)} + O(\delta_i).$$

The other is:

$$-t_i^H F_i t_i \sim t_i^H \Phi_i t_i \sim t_i^H t_i, \quad \text{for any } t_i = Q_i \hat{t}_i \neq 0 \text{ satisfying } t_i^H \Phi_i x_i = 0. \quad (39)$$

In fact, since $Q_i^H \Phi_i Q_i > 0$, $t_i^H \Phi_i t_i = \hat{t}_i^H Q_i^H \Phi_i Q_i \hat{t}_i \sim \hat{t}_i^H \hat{t}_i \sim t_i^H t_i$. For the rest, since $x_i^H \Phi_i x_i = 1$, $x_i^H F_i x_i = 0$, using the min-max principles (5) for the definite matrix pair $(-Q_i^H F_i Q_i, Q_i^H \Phi_i Q_i)$,

$$\begin{aligned} -\frac{\hat{t}_i^H Q_i^H F_i Q_i \hat{t}_i}{\hat{t}_i^H Q_i^H \Phi_i Q_i \hat{t}_i} &= \frac{\hat{t}_i^H (-Q_i^H F_i Q_i) \hat{t}_i}{\hat{t}_i^H Q_i^H \Phi_i Q_i \hat{t}_i} + \frac{\hat{x}_i^H (-Q_i^H F_i Q_i) \hat{x}_i}{\hat{x}_i^H Q_i^H \Phi_i Q_i \hat{x}_i} \\ &\geq \lambda_{\min}(-[Q_i^H \Phi_i Q_i]^{-1/2} Q_i^H F_i Q_i [Q_i^H \Phi_i Q_i]^{-1/2}) + \lambda_{\min}^{(2)}(-[Q_i^H \Phi_i Q_i]^{-1/2} Q_i^H F_i Q_i [Q_i^H \Phi_i Q_i]^{-1/2}) \\ &= 0 + \lambda_{\min}^{(2)}(-[Q_i^H F'(\lambda_1) Q_i]^{-1/2} Q_i^H F(\lambda_1) Q_i [Q_i^H F'(\lambda_1) Q_i]^{-1/2}) + O(\varepsilon_i). \end{aligned}$$

By (4),

$$\begin{aligned} &\lambda_{\min}^{(2)}(-[Q_i^H F'(\lambda_1) Q_i]^{-1/2} Q_i^H F(\lambda_1) Q_i [Q_i^H F'(\lambda_1) Q_i]^{-1/2}) \\ &= \min_{\dim \mathcal{U}=2} \max_{u \in \mathcal{U}} \frac{-u^H [Q_i^H F'(\lambda_1) Q_i]^{-1/2} Q_i^H F(\lambda_1) Q_i [Q_i^H F'(\lambda_1) Q_i]^{-1/2} u}{u^H u} \\ &\quad (\text{write } v = [Q_i^H F'(\lambda_1) Q_i]^{-1/2} u, \text{ and then } u = [Q_i^H F'(\lambda_1) Q_i]^{1/2} v) \end{aligned}$$

$$\begin{aligned}
&= \min_{\dim \mathcal{V}=2} \max_{v \in \mathcal{V}} \frac{-v^H Q_i^H F(\lambda_1) Q_i v}{v^H Q_i^H Q_i v} \frac{v^H v}{v^H Q_i^H F'(\lambda_1) Q_i v} \quad (\text{write } w = Q_i^H v) \\
&= \min_{\dim \mathcal{W}=2} \max_{w \in \mathcal{W}} \frac{-w^H F(\lambda_1) w}{w^H w} \frac{v^H v}{v^H Q_i^H F'(\lambda_1) Q_i v} \\
&\geq \min_{\dim \mathcal{V}=2} \max_{v \in \mathcal{V}} \frac{-v^H F(\lambda_1) v}{v^H v} \frac{1}{\lambda_{\max}(Q_i^H F'(\lambda_1) Q_i)} \\
&= \frac{\lambda_{\min}^{(2)}(-F(\lambda_1))}{\lambda_{\max}(Q_i^H F'(\lambda_1) Q_i)} \\
&\geq \frac{-\lambda_{\max}^{(2)}(F(\lambda_1))}{\lambda_{\max}(F'(\lambda_1))} =: \omega.
\end{aligned}$$

Thus,

$$\frac{-t_i^H F_i t_i}{t_i^H \Phi_i t_i} = -\frac{\hat{t}_i^H Q_i^H F_i Q_i \hat{t}_i}{\hat{t}_i^H Q_i^H \Phi_i Q_i \hat{t}_i} \geq \omega + O(\varepsilon_i) > 0. \quad (40)$$

On the other hand, $-t_i^H F_i t_i \leq \|F_i\| t_i^H t_i \sim t_i^H \Phi_i t_i$. In total, $-t_i^H F_i t_i \sim t_i^H \Phi_i t_i$.

Now we can begin to prove those claims.

Proof of (27). Note that $\mathcal{R}(S_i) \subset \mathcal{R}(Z_i)$ and $S_i^H \Phi_i x_i = 0$. By (40), $-\hat{t}_i^H S_i^H F_i S_i \hat{t}_i \geq (\omega + O(\varepsilon_i)) \hat{t}_i^H S_i^H \Phi_i S_i \hat{t}_i$. Hence

$$\lambda_{\min}(-S_i^H F_i S_i) \geq (\omega + O(\varepsilon_i)) \lambda_{\min}(S_i^H \Phi_i S_i) \geq (\omega + O(\varepsilon_i)) \lambda_{\min}(Q_i^H \Phi_i Q_i) \lambda_{\min}(S_i^H S_i) > 0.$$

Note that $S_i^H F_{i+1} S_i = S_i^H F_i S_i - \delta_i S_i^H \Phi_i S_i$. It is clear that $\lambda_{\min}(-S_i^H F_{i+1} S_i) \geq \omega \lambda_{\min}(Q_i^H F'(\lambda_1) Q_i) + O(\varepsilon_i) > 0$, which implies that $S_i^H F_{i+1} S_i$ is nonsingular. It is similar that $S_i^H F_{i+1}^0 S_i$ is nonsingular. \square

Proof of (33). Since $(I - P_i)(I - T_i)r_i \in \mathcal{R}(Z_i)$ and $x_i^H \Phi_i (I - P_i)(I - T_i)r_i = 0$, by (39),

$$-r_i^H \check{F}_i (I - T_i)r_i = -r_i^H (I - T_i^H) \check{F}_i (I - T_i)r_i \sim r_i^H r_i.$$

For the rest, let ρ_{i+1}^{SD} be the minimal value of $\rho(x)$ in the subspace $\text{span}\{x_i, r_i\}$, then

$$\delta_i^{\text{SD}} = -\frac{|r_i^H r_i|^2}{[x_i^H \Phi_i^{\text{SD}} x_i][r_i^H \check{F}_i^{\text{SD}} r_i]} \Rightarrow r_i^H r_i = -\delta_i^{\text{SD}} [x_i^H \Phi_i^{\text{SD}} x_i] \frac{r_i^H \check{F}_i^{\text{SD}} r_i}{r_i^H r_i} = O(\delta_i). \quad \square$$

Proof of (30). Consider κ_2 .

$$\begin{aligned}
\kappa_2 &= \frac{(s_i^0)^H \check{F}_i s_i^0}{(s_i^0)^H \check{F}_i^0 s_i^0} = \frac{(s_i^0)^H (I - P_i^H) F_{i+1} (I - P_i) s_i^0}{(s_i^0)^H (I - (P_i^0)^H) F_{i+1}^0 (I - P_i^0) s_i^0} \\
&= \frac{(s_i^0)^H (I - P_i^H) F_i (I - P_i) s_i^0 - \delta_{i+1} (s_i^0)^H (I - P_i^H) \Phi_i (I - P_i) s_i^0}{(s_i^0)^H (I - (P_i^0)^H) F_i (I - P_i^0) s_i^0 - \delta_{i+1}^0 (s_i^0)^H (I - (P_i^0)^H) \Phi_i^0 (I - P_i^0) s_i^0}.
\end{aligned}$$

Since $(I - P_i^H) s_i^0 \in \mathcal{R}(Z_i)$ and $(I - P_i^H) \Phi_i x_i = 0$, by (39),

$$-(s_i^0)^H (I - P_i^H) F_i (I - P_i) s_i^0 \sim (s_i^0)^H (I - P_i^H) \Phi_i (I - P_i) s_i^0;$$

since $(I - (P_i^0)^H) s_i^0 \in \mathcal{R}(Z_i)$ and $(I - (P_i^0)^H) \Phi_i^0 x_i = 0$, then similarly to (39), we have

$$-(s_i^0)^H (I - (P_i^0)^H) F_i (I - P_i^0) s_i^0 \sim (s_i^0)^H (I - (P_i^0)^H) \Phi_i^0 (I - P_i^0) s_i^0.$$

Thus

$$\kappa_2 = \frac{[1 + O(\delta_i)] (s_i^0)^H (I - P_i^H) F_i (I - P_i) s_i^0}{[1 + O(\delta_i^0)] (s_i^0)^H (I - (P_i^0)^H) F_i (I - P_i^0) s_i^0}.$$

Note that

$$\begin{aligned} 0 &\geq (s_i^0)^H (I - P_i^H) F_i (I - P_i) s_i^0 = (s_i^0)^H F_i s_i^0 - 2\Re(s_i^0)^H \Phi_i x_i x_i^H F_i s_i^0 + (s_i^0)^H \Phi_i x_i x_i^H F_i x_i x_i^H \Phi_i s_i^0 \\ &= (s_i^0)^H F_i s_i^0 - 2r_i^H r_i \Re(s_i^0)^H \Phi_i x_i, \end{aligned}$$

and a similar expansion of $(s_i^0)^H (I - (P_i^0)^H) F_i (I - P_i^0) s_i^0$ holds. Then

$$\begin{aligned} \kappa_2 &= [1 + O(\delta_i)] \frac{(s_i^0)^H F_i s_i^0 - 2r_i^H r_i \Re(s_i^0)^H \Phi_i x_i}{(s_i^0)^H F_i s_i^0 - 2r_i^H r_i \Re(s_i^0)^H \Phi_i^0 x_i} \\ &= [1 + O(\delta_i)] \left[1 + \frac{2r_i^H r_i \Re(s_i^0)^H [\Phi_i^0 - \Phi_i] x_i}{(s_i^0)^H F_i s_i^0 - 2r_i^H r_i \Re(s_i^0)^H \Phi_i^0 x_i} \right] \\ &= [1 + O(\delta_i)] \left[1 + \frac{2r_i^H r_i \Re(s_i^0)^H [\Phi_i^0 - \Phi_i] x_i}{[1 + O(\delta_i^0)] (s_i^0)^H \check{F}_i^0 s_i^0} \right]. \end{aligned}$$

It is easy to see that

$$(s_i^0)^H \check{F}_i^0 s_i^0 = r_i^H (I - (T^0)^H) \check{F}_i^0 (I - T^0) r_i = r_i^H \check{F}_i^0 r_i - r_i^H \check{F}_i^0 S_i (S_i^H \check{F}_i^0 S_i)^{-1} S_i^H \check{F}_i^0 r_i.$$

Similarly to the proof of (27), we know $-[S_i \ r_i]^H \check{F}_i^0 [S_i \ r_i] = -[S_i \ (I - P_i^0)r_i]^H F_{i+1}^0 [S_i \ (I - P_i^0)r_i]$ is positive definite. Thus, since $r_i^H S_i = 0$, by a matrix version of the Wielandt inequality (see Wang and Ip [27, Theorem 1]),

$$-r_i^H \check{F}_i^0 S_i (S_i^H \check{F}_i^0 S_i)^{-1} S_i^H \check{F}_i^0 r_i \leq -[\chi + O(\varepsilon_i)] r_i^H \check{F}_i^0 r_i, \quad \chi = \left(\frac{\lambda_{\max}(-F(\lambda_1)) - \lambda_{\min}^{(2)}(-F(\lambda_1))}{\lambda_{\max}(-F(\lambda_1)) + \lambda_{\min}^{(2)}(-F(\lambda_1))} \right)^2.$$

which gives $-(s_i^0)^H \check{F}_i^0 s_i^0 \sim -r_i^H \check{F}_i^0 r_i$. Note that by (39), $-r_i^H \check{F}_i^0 r_i \sim r_i^H r_i$, $-(s_i^0)^H \check{F}_i^0 s_i^0 \sim (s_i^0)^H s_i^0$. Thus,

$$-r_i^H \check{F}_i^0 r_i \sim r_i^H r_i \sim (s_i^0)^H s_i^0 \sim -(s_i^0)^H \check{F}_i^0 s_i^0, \quad (41)$$

and

$$\kappa_2 = [1 + O(\delta_i)] (1 + O(1) \Re(s_i^0)^H [\Phi_i^0 - \Phi_i] x_i).$$

Noticing that

$$\left| (s_i^0)^H [\Phi_i^0 - \Phi_i] x_i \right| \leq \|s_i\| (\delta_i - \delta_i^0) [\|F''(\rho_i)\| + O(\delta_i)] \|x_i\| = O(\delta_i^{3/2}),$$

we have

$$\kappa_2 = [1 + O(\delta_i)] (1 + O(\delta_i^{3/2})) = 1 + O(\delta_i).$$

Consider κ_3 . By the Sherman-Morrison-Woodbury formula, letting $D_i = \check{F}_i^0 - \check{F}_i$,

$$\begin{aligned} e_i &= S_i (S_i^H \check{F}_i^0 S_i)^{-1} S_i^H \check{F}_i^0 r_i - S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H \check{F}_i r_i, \\ &= S_i [(S_i^H \check{F}_i^0 S_i)^{-1} S_i^H \check{F}_i^0 - (S_i^H \check{F}_i S_i)^{-1} S_i^H \check{F}_i] r_i \\ &= S_i [((S_i^H \check{F}_i S_i)^{-1} - (S_i^H \check{F}_i S_i)^{-1} S_i^H D_i S_i (S_i^H \check{F}_i^0 S_i)^{-1}) S_i^H \check{F}_i^0 - (S_i^H \check{F}_i S_i)^{-1} S_i^H \check{F}_i] r_i \\ &= S_i [(S_i^H \check{F}_i S_i)^{-1} S_i^H D_i - (S_i^H \check{F}_i S_i)^{-1} S_i^H D_i S_i (S_i^H \check{F}_i^0 S_i)^{-1} S_i^H \check{F}_i^0] r_i \\ &= S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H D_i [I - S_i (S_i^H \check{F}_i^0 S_i)^{-1} S_i^H \check{F}_i^0] r_i \\ &= S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H D_i s_i^0. \end{aligned}$$

Since $S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H \check{F}_i (s_i^0 + e_i) = T_i (I - T_i) r_i = 0$, we have $e_i^H \check{F}_i (s_i^0 + e_i) = 0$. Thus,

$$\kappa_3 = \frac{(s_i^0 + e_i)^H \check{F}_i (s_i^0 + e_i)}{(s_i^0)^H \check{F}_i s_i^0} = 1 - \frac{e_i^H \check{F}_i e_i}{(s_i^0)^H \check{F}_i s_i^0} = 1 - \frac{(s_i^0)^H D_i S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H D_i s_i^0}{(s_i^0)^H \check{F}_i s_i^0}.$$

First we estimate $S_i(S_i^H \check{F}_i S_i)^{-1} S_i^H$. Let $S_i = Q_S R_S$ be its QR factorization, and then

$$S_i(S_i^H \check{F}_i S_i)^{-1} S_i^H = Q_S(Q_S^H \check{F}_i Q_S)^{-1} Q_S^H = Q_S(Q_S^H(I - P_i^H)F_{i+1}(I - P_i)Q_S)^{-1} Q_S^H.$$

Since $\mathcal{R}((I - P_i)Q_S) \subset \mathcal{R}(Z_i)$, similarly to the proof of (27), we have

$$\|S_i(S_i^H \check{F}_i S_i)^{-1} S_i^H\| \leq \frac{1}{\omega \lambda_{\min}(Q_S^H F'(\lambda_1) Q_S) + O(\varepsilon_i)}. \quad (42)$$

Then turn to D_i . Noticing $(I - P_i)Q_S = Q_S$,

$$\begin{aligned} Q_S^H D_i &= Q_S^H [(I - (P_i^0)^H)F_{i+1}^0(I - P_i^0) - (I - P_i^H)F_{i+1}(I - P_i)] \\ &= Q_S^H [(P_i^H - (P_i^0)^H)F_{i+1}^0(I - P_i^0) + F_{i+1}^0(I - P_i^0) - F_{i+1}(I - P_i)] \\ &= Q_S^H [(P_i^H - P_i^0)^H F_{i+1}^0(I - P_i^0) + F_{i+1}^0(P_i - P_i^0) + (F_{i+1}^0 - F_{i+1})(I - P_i)] \\ &= Q_S^H [(\Phi_i - \Phi_i^0)x_i x_i^H F_{i+1}^0(I - P_i^0) + F_{i+1}^0 x_i x_i^H (\Phi_i - \Phi_i^0) + (F_{i+1}^0 - F_{i+1})(I - P_i)] \end{aligned}$$

and then

$$\|Q_S^H D_i\| \leq (\delta_i - \delta_i^0) [(\|F''(\rho_i)\| + O(\delta_i)) \|x_i\|^2 \|F_{i+1}^0\| (\|I - P_i^0\| + 1) + (\|F'(\rho_i)\| + O(\delta_i)) \|I - P_i\|] = O(\delta_i).$$

Thus, to sum up, together with (41),

$$\begin{aligned} \kappa_3 &= 1 - \frac{(s_i^0)^H D_i Q_S Q_S^H S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H Q_S Q_S^H D_i s_i^0}{(s_i^0)^H \check{F}_i s_i^0} \\ &= 1 + \frac{O(1) \|Q_S^H D_i\|^2 \|s_i^0\|^2}{\|s_i^0\|^2} = 1 - O(\delta_i^2). \end{aligned} \quad \square$$

Proof of (31). Since $\check{F}_i x_{i-1} = \check{F}_i(x_i - d_{i-1}) = -\check{F}_i d_{i-1}$ and $\check{F}_i(I - T_i) = (I - T_i^H)\check{F}_i$,

$$\tau_i = x_{i-1}^H \check{F}_i(I - T_i)x_{i-1} = d_{i-1}^H \check{F}_i(I - T_i)d_{i-1}.$$

First

$$\begin{aligned} \check{F}_i &= (I - P_i^H)F_{i+1}(I - P_i) \\ &= P_i^H F_{i+1} P_i - P_i^H F_{i+1} - F_{i+1} P_i + F_{i+1} - F_i + F_i \\ &= F_{i+1} - F_i + \Phi_i x_i x_i^H F_{i+1} x_i x_i^H \Phi_i - \Phi_i x_i x_i^H F_{i+1} - F_{i+1} x_i x_i^H \Phi_i + F_i \\ &= -\delta_i \Phi_i - \delta_i \Phi_i x_i x_i^H \Phi_i - \Phi_i x_i x_i^H (F_i - \delta_i \Phi_i) - (F_i - \delta_i \Phi_i) x_i x_i^H \Phi_i + F_i \\ &= F_i - \Phi_i x_i r_i^H - r_i x_i^H \Phi_i - \delta_i \Phi_i [I - x_i x_i^H \Phi_i]. \end{aligned} \quad (43)$$

Since $r_i^H d_{i-1} = 0$ by (12),

$$\begin{aligned} d_{i-1}^H \check{F}_i d_{i-1} &= d_{i-1}^H F_i d_{i-1} - d_{i-1}^H \Phi_i x_i r_i^H d_{i-1} - d_{i-1}^H r_i x_i^H \Phi_i d_{i-1} - \delta_i d_{i-1}^H \Phi_i (I - P_i) d_{i-1} \\ &= d_{i-1}^H F_i d_{i-1} - \delta_i d_{i-1}^H \Phi_i (I - P_i) d_{i-1} \\ &= d_{i-1}^H F_i d_{i-1} + O(\delta_i) \|d_{i-1}\|^2. \end{aligned}$$

Then, noticing that $x_{i-1}^H \Phi_{i-1} d_{i-1} = x_{i-1}^H \Phi_{i-1} (I - P_{i-1}) d_{i-1} = 0$, by (14),

$$\begin{aligned} d_{i-1}^H F_i d_{i-1} &= -\delta_{i-1} x_{i-1}^H \Phi_{i-1} x_{i-1} = -\delta_{i-1} (x_i - d_{i-1})^H \Phi_{i-1} (x_i - d_{i-1}) \\ &= -\delta_{i-1} (x_i^H \Phi_{i-1} x_i - d_{i-1}^H \Phi_{i-1} d_{i-1}) \\ &= -\delta_{i-1} (x_i^H \Phi_{i-1} x_i - d_{i-1}^H \Phi_{i-1} d_{i-1} + O(\delta_{i-1})) \\ &= -\delta_{i-1} (1 - d_{i-1}^H \Phi_{i-1} d_{i-1} + O(\delta_{i-1})). \end{aligned}$$

Similarly to (39), $-d_{i-1}^H F_i d_{i-1} \sim d_{i-1}^H \Phi_{i-1} d_{i-1}$, which implies

$$d_{i-1}^H F_i d_{i-1} = -\frac{\delta_{i-1}}{1 + O(\delta_{i-1})} + O(\delta_{i-1}^2) = -\delta_{i-1} + O(\delta_{i-1}^2),$$

and $\delta_{i-1} \sim d_{i-1}^H \Phi_{i-1} d_{i-1} \sim d_{i-1}^H d_{i-1}$. Thus

$$d_{i-1}^H \check{F}_i d_{i-1} = -\delta_{i-1}[1 + O(\delta_{i-1}) + O(\delta_i)]. \quad (44)$$

Then, by (43),

$$\begin{aligned} d_{i-1}^H \check{F}_i T_i d_{i-1} &= d_{i-1}^H F_i T_i d_{i-1} - d_{i-1}^H \Phi_i x_i r_i^H T_i d_{i-1} - d_{i-1}^H r_i x_i^H \Phi_i T_i d_{i-1} - \delta_i d_{i-1}^H \Phi_i [I - x_i x_i^H \Phi_i] T_i d_{i-1} \\ &= d_{i-1}^H F_i T_i d_{i-1} - \delta_i d_{i-1}^H \Phi_i [I - x_i x_i^H \Phi_i] T_i d_{i-1}. \end{aligned}$$

Since $\|T_i\| \leq \|S_i(S_i^H \check{F}_i S_i)^{-1} S_i^H\| \|F_i\| \|I - P_i\|^2$, by (42),

$$d_{i-1}^H \check{F}_i T_i d_{i-1} = d_{i-1}^H F_i T_i d_{i-1} + O(\delta_i \delta_{i-1}).$$

Then, also using (42),

$$\begin{aligned} d_{i-1}^H F_i T_i d_{i-1} &= [x_i - x_{i-1}]^H F_i S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H F_{i+1} (I - P_i) [x_i - x_{i-1}] \\ &= [x_i - x_{i-1}]^H F_i S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H F_{i+1} [x_i (x_i^H \Phi_i x_{i-1}) - x_{i-1}] \\ &= [r_i - (F_{i-1} - \delta_{i-1} \Phi_{i-1}) x_{i-1}]^H S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H [(F_i - \delta_i \Phi_i) x_i (x_i^H \Phi_i x_{i-1}) - (F_{i-1} - \delta_{i-1} \Phi_{i-1} - \delta_i \Phi_i) x_{i-1}] \\ &= [r_i^H - r_{i-1}^H + \delta_{i-1} x_{i-1}^H \Phi_{i-1}] S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H [(r_i - \delta_i \Phi_i x_i)(1 + O(\delta_{i-1}^{1/2})) - r_{i-1} + \delta_{i-1} \Phi_{i-1} x_{i-1} + \delta_i \Phi_i x_{i-1}] \\ &= [-r_{i-1}^H + \delta_{i-1} x_{i-1}^H \Phi_{i-1}] S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H [-r_{i-1} + \delta_{i-1} \Phi_{i-1} x_{i-1} - \delta_i \Phi_i (d_{i-1} + x_i O(\delta_{i-1}^{1/2}))] \\ &= r_{i-1}^H S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H r_{i-1} + O(\delta_{i-1}^{3/2}). \end{aligned}$$

Since $r_{i-1}^H F_{i-1}^j r_{i-1} = 0$ for $j = 1, \dots, m_e$ by (12) and then

$$\begin{aligned} r_{i-1}^H F_i^j r_i &= r_{i-1}^H [F_{i-1}^j - \delta_{i-1} F_{i-1}^{j-1} \Phi_{i-1} - \delta_{i-1} \Phi_{i-1} F_{i-1}^{j-1} + \delta_{i-1}^2 F_{i-1}^{j-2} \Phi_{i-1}^2 + \dots] r_i \\ &= r_{i-1}^H F_{i-1}^j r_i + O(\delta_{i-1}) \|r_{i-1}\| \|r_i\| = O(\delta_{i-1}^{3/2}) \|r_i\|, \end{aligned}$$

together with

$$r_{i-1}^H x_i = r_{i-1}^H (x_{i-1} + d_{i-1}) = r_{i-1}^H d_{i-1} = O(\delta_{i-1}),$$

we have

$$\|r_{i-1}^H S_i\| = \|r_{i-1}^H (I - x_i x_i^H \Phi_i - r_i r_i^H (r_i^H r_i)^{-1}) [F_i r_i \quad \dots \quad F_i^{m_e} r_i]\| = O(\delta_{i-1}) \|r_i\|. \quad (45)$$

Similarly to the proof of (27),

$$\|(S_i^H \check{F}_i S_i)^{-1}\| = O(\|r_i\|^{-2}). \quad (46)$$

Thus, $r_{i-1}^H S_i (S_i^H \check{F}_i S_i)^{-1} S_i^H r_{i-1} = O(\delta_{i-1}^2)$ and $d_{i-1}^H F_i T_i d_{i-1} = O(\delta_{i-1}^{3/2})$. Thus,

$$d_{i-1}^H \check{F}_i T_i d_{i-1} = \delta_{i-1} [O(\delta_{i-1}^{1/2}) + O(\delta_i)]. \quad (47)$$

Then (44) and (47) give (31). \square

Proof of (32). Since $\check{F}_i x_{i-1} = \check{F}_i (x_i - d_{i-1}) = -\check{F}_i d_{i-1}$ and $\check{F}_i (I - T_i) = (I - T_i^H) \check{F}_i$,

$$\beta_i = x_{i-1}^H \check{F}_i (I - T_i) r_i = d_{i-1}^H \check{F}_i (I - T_i) r_i.$$

By (43),

$$\begin{aligned} d_{i-1}^H \check{F}_i (I - T_i) r_i &= d_{i-1}^H F_i (I - T_i) r_i - d_{i-1}^H \Phi_i x_i r_i^H (I - T_i) r_i - d_{i-1}^H r_i x_i^H \Phi_i (I - T_i) r_i - \delta_i d_{i-1}^H \Phi_i (I - P_i) (I - T_i) r_i \\ &= d_{i-1}^H F_i (I - T_i) r_i - d_{i-1}^H \Phi_i x_i r_i^H r_i - \delta_i d_{i-1}^H \Phi_i (I - P_i) (I - T_i) r_i \end{aligned}$$

$$= d_{i-1}^H \check{F}_{i-1} (I - T_i) r_i + d_{i-1}^H F_i P_{i-1} (I - T_i) r_i - d_{i-1}^H \Phi_i x_i r_i^H r_i + O(\delta_i \delta_{i-1}^{1/2}) \|r_i\|.$$

By (15), $d_{i-1}^H \check{F}_{i-1} (I - T_i) r_i = (r_i - r_{i-1})^H (I - T_i) r_i = r_i^H r_i + r_{i-1}^H T_i r_i$. Note that

$$\begin{aligned} d_{i-1}^H F_i P_{i-1} (I - T_i) r_i &= d_{i-1}^H F_i x_{i-1} \frac{x_{i-1}^H \Phi_{i-1} (I - T_i) r_i}{x_{i-1}^H \Phi_{i-1} x_{i-1}} \\ &= (x_i - x_{i-1})^H F_i x_{i-1} \frac{x_{i-1}^H \Phi_{i-1} (I - T_i) r_i}{x_{i-1}^H \Phi_{i-1} x_{i-1}} \\ &= -x_{i-1}^H F_i x_{i-1} \frac{x_{i-1}^H \Phi_{i-1} (I - T_i) r_i}{x_{i-1}^H \Phi_{i-1} x_{i-1}} \\ &= -x_{i-1}^H (F_{i-1} - \delta_{i-1} \Phi_{i-1}) x_{i-1} \frac{x_{i-1}^H \Phi_{i-1} (I - T_i) r_i}{x_{i-1}^H \Phi_{i-1} x_{i-1}} \\ &= \delta_{i-1} x_{i-1}^H \Phi_{i-1} (I - T_i) r_i \\ &= O(\delta_{i-1}) \|r_i\|. \end{aligned}$$

Thus,

$$d_{i-1}^H \check{F}_i (I - T_i) r_i = r_{i-1}^H T_i r_i + (1 - d_{i-1}^H \Phi_i x_i) r_i^H r_i + [O(\delta_{i-1}) + O(\delta_i \delta_{i-1}^{1/2})] \|r_i\|.$$

Note that $\delta_{i-1} \sim d_{i-1}^H \Phi_i d_{i-1} \sim d_{i-1}^H d_{i-1}$ and then $\|x_{i-1}\| = \|x_i - d_{i-1}\| \leq \|x_i\| + O(\delta_{i-1})$ which means x_{i-1} is bounded. Also, note that $r_i^H r_i = O(\delta_i)$ and $x_{i-1}^H \Phi_{i-1} d_{i-1} = 0$. Thus,

$$\begin{aligned} x_i^H \Phi_i d_{i-1} &= d_{i-1}^H \Phi_i d_{i-1} + x_{i-1}^H \Phi_i d_{i-1} \\ &= O(\delta_{i-1}) + x_{i-1}^H \Phi_{i-1} d_{i-1} + (\delta_{i-1} - \delta_i) x_{i-1}^H F''(\lambda_1) d_{i-1} \\ &= O(\delta_{i-1}) + O(\delta_i \delta_{i-1}^{1/2}). \end{aligned}$$

By (45) and (46), noticing that $\|S_i\| \leq \left\| \begin{bmatrix} F_i r_i & \dots & F_i^{m_e} r_i \end{bmatrix} \right\| = O(1) \|r_i\|$, we have

$$\begin{aligned} |r_{i-1}^H T_i r_i| &= |r_{i-1}^H S_i (S_i^H F_{i+1} S_i)^{-1} S_i^H F_{i+1} (I - P_i) r_i| \\ &\leq \|r_{i-1}^H S_i\| \|(S_i^H F_{i+1} S_i)^{-1}\| \|S_i^H F_{i+1} (I - P_i) r_i\| = O(\delta_{i-1}) \|r_i\|. \end{aligned}$$

Then, to sum up, we have (32). □

Acknowledgement. The authors thank Prof. Ren-Cang Li for his MATLAB code and helpful discussions.

References

- [1] Maha Al-Ammari. *Analysis of structured polynomial eigenvalue problems*. Ph.d. thesis, University of Manchester, Manchester, UK, 2011.
- [2] Merico E. Argentati, Andrew V. Knyazev, Klaus Neymeyr, Evgueni E. Ovtchinnikov, and Ming Zhou. Convergence theory for preconditioned eigenvalue solvers in a nutshell. *Foundations of Computational Mathematics*, pages 1–15, 2015.
- [3] Timo Betcke, Nicholas J. Higham, Volker Mehrmann, Christian Schröder, and Françoise Tisseur. NLEVP: A collection of nonlinear eigenvalue problems. MIMS Eprint 2011.116, Manchester Institute for Mathematical Sciences, The University of Manchester, Manchester, UK, 2011.
- [4] R. Duffin. A minimax theory for overdamped networks. *Indiana Univ. Math. J.*, 4:221–233, 1955.
- [5] Gene H. Golub and Qiang Ye. An inverse free preconditioned Krylov subspace method for symmetric generalized eigenvalue problems. *SIAM J. Sci. Comput.*, 24(1):312–334, 2002.
- [6] C.-H. Guo and P. Lancaster. Algorithms for hyperbolic quadratic eigenvalue problems. *Math. Comp.*, 74:1777–1791, 2005.

- [7] Andrew V. Knyazev. Toward the optimal preconditioned eigensolver: Locally optimal block preconditioned conjugate gradient method. *SIAM J. Sci. Comput.*, 23(2):517–541, 2001.
- [8] Andrew V. Knyazev and Klaus Neymeyr. A geometric theory for preconditioned inverse iteration III: A short and sharp convergence estimate for generalized eigenvalue problems. *Linear Algebra Appl.*, 358(1-3):95–114, 2003.
- [9] Aleksandra Kostić and Heinrich Voss. On Sylvester’s law of inertia for nonlinear eigenvalue problems. *Electron. Trans. Numer. Anal.*, 40:82–93, 2013.
- [10] J. Kovač-Striko and K. Veselić. Trace minimization and definiteness of symmetric pencils. *Linear Algebra Appl.*, 216:139–158, 1995.
- [11] Daniel Kressner, Marija Miloloža Pandur, and Meiyue Shao. An indefinite variant of LOBPCG for definite matrix pencils. *Numer. Alg.*, 66:681–703, 2014.
- [12] Ren-Cang Li. On Meinardus’ examples for the conjugate gradient method. *Math. Comp.*, 77(261):335–352, 2008.
- [13] Ren-Cang Li. Lobpcghqep.m. <http://www.uta.edu/faculty/rccli/G2S3/g2s3.html>, July 2013. Programming assignment of the lecture for 4th Gene Golub SIAM Summer School.
- [14] Xin Liang and Ren-Cang Li. Extensions of Wielandt’s min-max principles for positive semi-definite pencils. *Lin. Multilin. Alg.*, 62(8):1032–1048, 2014.
- [15] Xin Liang and Ren-Cang Li. The hyperbolic quadratic eigenvalue problem. *Forum of Mathematics, Sigma*, 3(e13), 2015. 93 pages, doi:10.1017/fms.2015.14.
- [16] Xin Liang, Ren-Cang Li, and Zhaojun Bai. Trace minimization principles for positive semi-definite pencils. *Linear Algebra Appl.*, 438(7):3085–3106, 2013.
- [17] A.S. Markus. *Introduction to the Spectral Theory of Polynomial Operator Pencils*. Translations of mathematical monographs, vol. 71. AMS, Providence, RI, 1988.
- [18] I. Nakić and K. Veselić. Wielandt and Ky-Fan theorem for matrix pairs. *Linear Algebra Appl.*, 369:77–93, 2003.
- [19] Klaus Neymeyr. A geometric theory for preconditioned inverse iteration, i: Extrema of the Rayleigh quotient. *Linear Algebra Appl.*, 332:61–85, 2001.
- [20] Klaus Neymeyr. A geometric convergence theory for the preconditioned steepest descent iteration. *SIAM J. Numer. Anal.*, 50:3188–3207, 2012.
- [21] Klaus Neymeyr, E. E. Ovtchinnikov, and Ming Zhou. Convergence analysis of gradient iterations for the symmetric eigenvalue problem. *SIAM J. Matrix Anal. Appl.*, 32:443–456, 2011.
- [22] E. E. Ovtchinnikov. Jacobi correction equation, line search, and conjugate gradients in Hermitian eigenvalue computation I: computing an extreme eigenvalue. *SIAM J. Numer. Anal.*, 46(5):2567–2592, 2008.
- [23] E. E. Ovtchinnikov. Jacobi correction equation, line search, and conjugate gradients in Hermitian eigenvalue computation II: computing several extreme eigenvalues. *SIAM J. Numer. Anal.*, 46(5):2593–2619, 2008.
- [24] B. Samokish. The steepest descent method for an eigenvalue problem with semi-bounded operators. *Izv. Vyssh. Uchebn. Zaved. Mat.*, 5:105–114, 1958. in Russian.
- [25] I. Takahashi. A note on the conjugate gradient method. *Inform. Process. Japan*, 5:45–49, 1965.
- [26] Krešimir Veselić. Note on interlacing for hyperbolic quadratic pencils. In Jussi Behrndt, Karl-Heinz Förster, and Carsten Trunk, editors, *Recent Advances in Operator Theory in Hilbert and Krein Spaces*, volume 198 of *Oper. Theory: Adv. Appl.*, pages 305–307. Birkhäuser, Boston, 2010.
- [27] Song-Gui Wang and Wai-Cheung Ip. A matrix version of the wielandt inequality and its applications to statistics. *Linear Algebra Appl.*, 296:171–181, 1999.
- [28] Songbin Wei and Imin Kao. Vibration analysis of wire and frequency response in the modern wiresaw manufacturing process. *J. Sound and Vibration*, 231(5):1383–1395, 2000.