# THE CONVERGENCE OF THE GENERALIZED LANCZOS TRUST-REGION METHOD FOR THE TRUST-REGION SUBPROBLEM\*

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Abstract. Solving the trust-region subproblem (TRS) plays a key role in numerical optimization and many other applications. The generalized Lanczos trust-region (GLTR) method is a well-known Lanczos type approach for solving a large-scale TRS. The method projects the original large-scale TRS onto a k dimensional Krylov subspace, whose orthonormal basis is generated by the symmetric Lanczos process, and computes an approximate solution from the underlying subspace. There have been some a-priori error bounds for the optimal solution and the optimal objective value in the literature, but no a-priori result exists on the convergence of Lagrangian multipliers involved in projected TRS's and the residual norm of approximate solution. In this paper, a general convergence theory of the GLTR method is established, and a-priori bounds are derived for the errors of the optimal Lagrangian multiplier, the optimal solution, the optimal objective value and the residual norm of approximate solution. Numerical experiments demonstrate that our bounds are realistic and predict the convergence rates of the three errors and residual norms accurately.

Key words. trust-region subproblem, GLTR method, a-priori bound, Lagrangian multiplier, Chebyshev polynomial, eigenvalue problem, symmetric Lanczos process, Krylov subspace

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**1.** Introduction. Consider the solution of the trust-region subproblem (TRS)

(1.1) 
$$\min_{\|s\| \le \Delta} q(s) = g^T s + \frac{1}{2} s^T A s,$$

where  $A \in \mathbb{R}^{n \times n}$  is symmetric and nonsingular, the nonzero  $g \in \mathbb{R}^n$ ,  $\Delta > 0$  is the trust-region radius, and the norm  $\|\cdot\|$  is the 2-norm of a matrix or vector. Problem (1.1) arises from nonlinear numerical optimization [3, 21], where q(s) is a quadratic model of min f(s) at the current approximate solution, A is Hessian and g is the gradient of f at the current approximate solution, and many others, e.g., Tikhonov regularization of ill-posed problems [23, 24], graph partitioning problems [14], the constrained eigenvalue problem [10], and the Levenberg–Marquardt algorithm for solving nonlinear least squares problems [21].

The following results [3, 20] provide a theoretical basis for a TRS algorithm and give necessary and sufficient conditions, called the optimal conditions, for the solution of TRS (1.1).

THEOREM 1.1. A vector  $s_{opt}$  is a solution to (1.1) if and only if there exists the optimal Lagrangian multiplier  $\lambda_{opt} \geq 0$  such that

 $(1.2) ||s_{opt}|| \leq \Delta,$ 

(1.3) 
$$(A + \lambda_{opt}I)s_{opt} = -g_{s}$$

(1.4) 
$$\lambda_{opt}(\Delta - \|s_{opt}\|) = 0,$$

(1.5)  $A + \lambda_{opt} I \succeq 0,$ 

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where  $\|\cdot\|$  is the 2-norm of a matrix or vector, and the notation  $\succeq 0$  indicates that a symmetric matrix is semi-positive definite.

TRS algorithms for solving (1.1) have been extensively studied for a few decades and can be classified as the following four categories, in which most of the algorithms in the first three categories are mentioned in [1].

- Accurate methods for dense problems. The Moré-Sorensen method [20] iteratively solves symmetric positive definite linear systems by the Cholesky factorizations. It is highly efficient and accurate for small to medium sized dense problems.
- Accurate methods for large sparse problems. Algorithms in [23, 24, 26] iteratively compute the smallest eigenvalue of the matrix  $\begin{pmatrix} \alpha & g^T \\ g & A \end{pmatrix}$ , where  $\alpha$  is a adjusted parameter. Another approach due to [22] solves TRS via semidefinite programming, and a modification of the Moré-Sorensen method using Taylor series is presented in [9]. The generalized Lanczos trust-region(GLTR) method [8] solves the TRS by a Lanczos type approach. Other accurate methods include subspace projection methods; see, e.g., [6, 13].
- Approximate methods. Steihaug and Toint independently propose a Truncated Conjugate Gradient (TCG) method [27, 29], and Yuan [30] proves that the function reduction obtained at the point produced by this method is at least half of that obtained at the function minimizer when the function q(s) is convex, i.e., A is symmetric positive definite. If A is symmetric indefinite, an approximate solution must reach the trust-region boundary and TCG only solves (1.1) approximately.
- Eigenvalue based methods. The method due to Gander, Golub and von Matt [10] reduces TRS (1.1) to a single quadratic eigenvalue problem, which is linearized to a standard eigenvalue problem of size 2n. Using a different derivation, Adachi et al. [1] extend the method in [10] to a more general TRS (1.6) and formulate it as a generalized eigenvalue problem of size 2n. A solution to (1.1) can be determined by the rightmost eigenvalue and the associated eigenvector of the resulting  $2n \times 2n$  matrix. The eigenvalue problem is solved by the QR algorithm for A small or moderate and by iterative projection methods for A large [25].

In applications, rather than simply using the 2-norm, some methods (see, e.g., [1, 8, 22, 26]) focus on the following more general TRS

(1.6) 
$$\min_{\|s\|_B \le \Delta} q(s),$$

where B is symmetric positive definite and the norm  $||s||_B = \sqrt{s^T B s}$ . In light of [23], the matrix B is often constructed to impose a smoothness condition on a solution to (1.6) for the ill-posed problem and to incorporate scaling of variables in optimization. For instance, it is argued in [3] that a good choice is  $B = J^{-T}J^{-1}$  for some invertible matrix J or the Hermitian polar factor [15] of A.

Notice that the problem (1.6) is mathematically equivalent to a standard TRS (1.1) through the following substitutions

$$A \leftarrow B^{-\frac{1}{2}}AB^{-\frac{1}{2}}, \quad g \leftarrow B^{-\frac{1}{2}}g.$$

Therefore, we assume that B = I, the identity matrix, and just consider TRS (1.1) without loss of generality when considering the convergence of the GLTR method.

The GLTR method and other projection methods avoid the high overhead of computing a series of Cholesky factorizations and have shown to be efficient for a large-scale TRS; see, e.g., [2, 5, 8]. Let  $s_{opt}$  be a solution to TRS (1.1) and  $s_k$  be the approximate solution from the underlying k + 1 dimensional Krylov subspace  $\mathcal{K}_k(g, A) = span\{g, Ag, \dots, A^kg\}$  obtained by the GLTR method. By Theorem 1.1, there is an optimal Lagrangian multiplier  $\lambda_k$  for each projected TRS problem onto  $\mathcal{K}_k(g, A)$ . Then four central convergence problems are: how fast the three errors  $|\lambda_{opt} - \lambda_k|, \|s_k - s_{opt}\|, q(s_k) - q(s_{opt})$  and the residual norm  $\|(A + \lambda_k I)s_k + g\|$  of the approximate solution  $\lambda_k, s_k$  of (1.3) decrease as k increases. Regarding  $||s_k - s_{opt}||$ and  $q(s_k) - q(s_{opt})$ , some a-priori bounds have been derived in [31]. However, for  $|\lambda_{opt} - \lambda_k|$  and  $||(A + \lambda_k I)s_k + g||$ , there have been no a-priori bounds to show how they converge and tend to zero as k increases. The only known result on  $\lambda_k$  is that  $\lambda_k$ increases monotonically with k and is bounded from above by  $\lambda_{opt}$  [18]. Therefore, we always have  $|\lambda_{opt} - \lambda_k| = \lambda_{opt} - \lambda_k \ge 0$ . The residual norm is important in both theory and practice as it is computable and its size is commonly used to measure the convergence of the GLTR method. We mention that a mixed bound is given for  $|\lambda_{opt} - \lambda_k|$  in [32, Lemma 3.4]. However, it is easy to check that the mixed bound in [32] does not exhibit any decreasing tendency and even can never be small unless the symmetric Lanczos process breaks down, in which case the bound is trivially zero.

Remarkably, it has recently been shown that, under certain mild conditions, the solution of (1.1) is mathematically equivalent to solving a certain matrix eigenvalue problem of size 2n [1]. This equivalence provides us a new approach to efficiently solve (1.1). Among others, such mathematical equivalence makes us realize that, at iteration k, the GLTR method amounts to solving a certain eigenvalue problem of size 2(k+1) by projecting the  $2n \times 2n$  matrix eigenvalue problem onto a special 2(k+1) dimensional subspace in  $\mathbb{R}^{2n}$  constructed by  $\mathcal{K}_k(g, A)$  used in the GLTR method. At iteration k, unlike the GLTR method, one can simultaneously obtain the optimal  $\lambda_k$  and the solution  $s_k$  to the projected TRS. Such key observation is our starting point to study the convergence of the GLTR method. A note is that we are mainly concerned with  $\sin \angle (s_k, s_{opt})$  other than the error  $||s_k - s_{opt}||$ . The sine is a standard measure when considering the error of an eigenvector and its approximations in the context of the matrix eigenvalue problem [28]. The authors of [1] measure the error of  $s_k$  and  $s_{opt}$  by the sine of angle  $\angle (s_k, s_{opt})$  in their experiments.

The importance of the contributions in this paper is, in turn, the establishment of the two a-priori bounds for  $\lambda_{opt} - \lambda_k$  for the first time, that of the bound for  $\sin \angle (s_k, s_{opt})$ , that of the bounds for the residual norm  $||(A + \lambda_k I)s_k + g||$  for the first time, and finally that of a new sharp bound for  $q(s_k) - q(s_{opt})$ . The bound for  $q(s_k) - q(s_{opt})$  is different from the two ones presented in [31], and its proof is also simpler than those in [31]. The first a-priori bound for  $\lambda_{opt} - \lambda_k$ , though a considerable overestimate, is the background for establishing the second much sharper one. With the bounds for  $\lambda_{opt} - \lambda_k$  and  $\sin \angle (s_k, s_{opt})$  or  $||s_k - s_{opt}||$ , we are able to derive apriori bounds for  $||(A + \lambda_k I)s_k + g||$ . When establishing the first a-priori bound for  $\lambda_{opt} - \lambda_k$  and the a-priori bound for  $\sin \angle (s_k, s_{opt})$ , we need to solve the problem of the polynomial best uniform approximation to the rational function  $\frac{1}{(x-\eta)^2}$  with  $x \in [-1, 1]$  and  $\eta > 1$ . We will exploit a generating function of  $\frac{1}{(x-\eta)^2}$  with Chebyshev polynomials of the second kind [4] to handle this best uniform approximation problem by obtaining a suboptimal approximation polynomial. Numerical results demonstrate that our a-priori bounds predict the convergence rates of the three errors and residual norms and estimate their values accurately.

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This paper is organized as follows. In section 2, we give some preliminaries and introduce the equivalence of the solution of (1.1) and a certain  $2n \times 2n$  matrix eigenvalue problem. We review the GLTR method in section 3. Section 4 is devoted to a-priori bounds for  $\lambda_{opt} - \lambda_k$  and  $q(s_k) - q(s_{opt})$ . A-priori bounds for  $\sin \angle (s_k, s_{opt})$ and  $||(A + \lambda_k I)s_k + g||$  are presented in section 5. In section 6, we report numerical experiments to confirm that our bounds estimate the convergence rates and behavior of the GLTR method accurately. Finally, we conclude the paper in section 7.

Throughout this paper, denote by the superscript T the transpose of a matrix or vector, by  $\|\cdot\|$  the 2-norm of a matrix or vector, by I the identity matrix with order clear from the context, and by  $e_i$  the *i*th column of I. All vectors are column vectors and are typeset in lower case letters.

## 2. Preliminaries.

**2.1.** A solution to TRS (1.1). Suppose that  $A = S\Lambda S^T$  is the eigendecomposition of A, where S is orthogonal and  $\Lambda = diag(\alpha_1, \alpha_2, \ldots, \alpha_n)$  with the  $\alpha_i$  being the eigenvalues of A labeled as  $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n$ .

If  $A + \lambda_{opt}I \succ 0$ , then the solution  $s_{opt}$  to TRS (1.1) is unique and  $s_{opt} = -(A + \lambda_{opt}I)^{-1}g$ . If (1.1) has no solution  $s_{opt}$  with  $||s_{opt}|| = \Delta$ , then A is positive definite and  $s_{opt} = -A^{-1}g$  with  $||s_{opt}|| < \Delta$  and  $\lambda_{opt} = 0$ . All these correspond to the so-called "easy case" [3, 8, 20, 21] or "nondegenerate case" [13].

If A is indefinite and

$$g \perp \mathcal{N}(A - \alpha_n I),$$

the null space of  $A - \alpha_n I$ , then we have the following definition [3, 8, 21].

DEFINITION 2.1 (Hard Case). The solution of TRS (1.1) is a hard case if g is orthogonal to the eigenspace corresponding to the eigenvalue  $\alpha_n$  of A and the optimal Lagrangian multiplier is  $\lambda_{opt} = -\alpha_n$ .

The hard case is also called the "degenerate case" [13]. In this case, (1.1) may have multiple optimal solutions [21, p.87-88], which can be characterized as

$$s_{opt} = -(A - \alpha_n I)^{\dagger}g + \eta u_n$$

where  $u_n \in \mathcal{N}(A - \alpha_n I)$  and  $||u_n|| = 1$ ,  $||(A - \alpha_n I)^{\dagger}g|| \leq \Delta$ , and the superscript  $\dagger$  denotes the Moore-Penrose generalized inverse.  $s_{opt}$  with  $||s_{opt}|| = \Delta$  is unique if and only if  $\alpha_n$  is a simple eigenvalue of A and the scalar  $\eta$  satisfies

$$\eta^2 = \Delta^2 - ||(A - \alpha_n I)^{\dagger}g||^2 \ge 0.$$

As we can see, in the hard case, we not only need to solve a singular system but also need to compute the eigenspace of A associated with the smallest eigenvalue  $\alpha_n$ . The hard case has been studied for years; see, e.g., [7, 8, 20, 21, 22]. An eigensolver is proposed in [1] to detect and handle the hard case theoretically and numerically.

As has been addressed in [3], the hard case rarely occurs in practice, as it requires that both A be indefinite and g be orthogonal to  $\mathcal{N}(A - \alpha_n I)$ . In the sequel, we are only concerned with the easy case.

2.2. The equivalence of the TRS and a matrix eigenvalue problem. Adachi et al. [1] prove that TRS (1.6) can be treated by solving a certain generalized eigenvalue problem of order 2n. For B = I, the generalized eigenvalue problem in [1] reduces to the standard eigenvalue problem of the augmented matrix

(2.1) 
$$M = \begin{pmatrix} -A & \frac{gg^{T}}{\Delta^{2}} \\ I & -A \end{pmatrix} \in \mathbb{R}^{2n \times 2n}.$$

Let  $\mu_1, \mu_2, \ldots, \mu_{2n}$  be the eigenvalues of M labeled as

(2.2) 
$$Re(\mu_1) \ge Re(\mu_2) \ge \dots \ge Re(\mu_{2n})$$

where  $Re(\cdot)$  is the real part of a scalar. The following result in [1] establishes a key relationship between the TRS solution and the eigenpair of M.

THEOREM 2.2 ([1]). Let  $(\lambda_{opt}, s_{opt})$  satisfy Theorem 1.1 with  $||s_{opt}|| = \Delta$ . Then the rightmost eigenvalue  $\mu_1$  of M is real and simple, and  $\mu_1 = \lambda_{opt}$ . Let  $y^T = (y_1^T, y_2^T)^T$  be the unit length eigenvector of M associated with the eigenvalue  $\mu_1$ , i.e.,

(2.3) 
$$M\left(\begin{array}{c}y_1\\y_2\end{array}\right) = \mu_1\left(\begin{array}{c}y_1\\y_2\end{array}\right), \quad \left\|\left(\begin{array}{c}y_1\\y_2\end{array}\right)\right\| = 1,$$

and suppose that  $g^T y_2 \neq 0$ . Then the unique TRS solution is

(2.4) 
$$s_{opt} = -\frac{\Delta^2}{g^T y_2} y_1.$$

REMARK 2.1. Adachi et al. [1] have proved that  $g^T y_2 = 0$  corresponds to the hard case, i.e.,  $\lambda_{opt} = -\alpha_n$  and  $g \perp \mathcal{N}(A - \alpha_n I)$ . Therefore, in the easy case,  $g^T y_2 \neq 0$  is guaranteed, and (2.4) holds.

**3.** The generalized Lanczos trust-region (GLTR) method [8]. For (1.1) large, an effective approach is to iteratively solve a sequence of smaller projected problems

(3.1) 
$$\min_{s \in \mathcal{S}_k, \|s\| \le \Delta} q(s),$$

where  $S_k \subset \mathbb{R}^n$  is some specially chosen k + 1 dimensional subspace, and we use the solution  $s_k$  to TRS (3.1) to approximate  $s_{opt}$ .

A most commonly used  $S_k$  is the k + 1 dimensional Krylov subspace

(3.2) 
$$\mathcal{S}_k = \mathcal{K}_k(g, A) \doteq span\{g, Ag, A^2g, \dots, A^kg\}$$

generated by g and A. The GLTR method starts with the TCG method [27, 29]. When A is positive definite and  $||A^{-1}g|| \leq \Delta$ , which corresponds to  $\lambda_{opt} = 0$ , the method returns a *converged* approximate solution  $s_k$  to  $s_{opt} = -A^{-1}g$ . In this case, the convergence theory of the standard conjugate gradient method is directly applicable. The GLTR method switches to the Lanczos method to accurately solve the projected problem (3.1) whenever a negative curvature is present or the solution norm by the TCG method exceeds the trust-region radius  $\Delta$ , which corresponds to an indefinite A or  $\lambda_{opt} > 0$ . It proceeds in such a way until  $s_k$  converges to  $s_{opt}$ .

In the sequel, without loss of generality we always assume that the TCG method does not solve (3.1) exactly and one must use the Lanczos method starting from the first iteration, so as to compute the solution  $s_k$  to (3.1) with  $||s_k|| = \Delta$ , meaning that  $\lambda_k > 0$  for  $k = 0, 1, \ldots$ 

In the following, we describe the GLTR method. At iteration k, mathematically, the GLTR method exploits the symmetric Lanczos process to generate an orthonormal basis  $\{q_i\}_{i=0}^k$  of  $\mathcal{S}_k$  defined by (3.2), which can be written in matrix form

(3.3) 
$$AQ_k = Q_k T_k + \beta_{k+1} q_{k+1} e_{k+1}^T,$$

- (3.4)  $Q_k^T g = \beta_0 e_1, \ \beta_0 = ||g||,$
- $(3.5) g = \beta_0 q_0,$

where  $Q_k = (q_0, q_1, \dots, q_k)$  is orthonormal and the matrix

(3.6) 
$$T_k = Q_k^T A Q_k = \begin{pmatrix} \delta_0 & \beta_1 & & \\ \beta_1 & \delta_1 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \delta_{k-1} & \beta_k \\ & & & & \beta_k & \delta_k \end{pmatrix} \in \mathbb{R}^{(k+1) \times (k+1)}$$

is symmetric tridiagonal, which is called the orthogonal projection matrix of A onto  $S_k$  in the orthonormal basis  $\{q_i\}_{i=0}^k$ .

We shall consider vectors of form

$$(3.7) s = Q_k h \in \mathcal{S}_k.$$

Let  $s_k = Q_k h_k$  solve the projected problem

(3.8) 
$$\min_{s \in S_k, \|s\| \le \Delta} q(s) = g^T s + \frac{1}{2} s^T A s.$$

It then follows from (3.7) and the Lanczos process that  $h_k$  solves the reduced TRS

(3.9) 
$$\min_{\|h\| \le \Delta} \phi(h) = \beta_0 e_1^T h + \frac{1}{2} h^T T_k h$$

and  $q(s_k) = \phi(h_k)$ .

From Theorem 1.1, the vector  $h_k$  is a solution to (3.9) if and only if there exists the optimal Lagrangian multiplier  $\lambda_k \geq 0$  such that

$$(3.10) ||h_k|| \leqslant \Delta,$$

$$(3.11) (T_k + \lambda_k I)h_k = -\beta_0 e_1,$$

(3.12) 
$$\lambda_k(\Delta - \|h_k\|) = 0,$$

$$(3.13) T_k + \lambda_k I \succeq 0.$$

As  $T_k$  is tridiagonal, we can use the Moré-Sorensen method to efficiently solve (3.8) even if n is large and then obtain  $s_k$  from  $s_k = Q_k h_k$ . The resulting method is the GLTR method for solving (1.1). It has been shown in [1] that TRS (3.9) is always the easy case provided that the symmetric Lanczos process does not break down at iteration k. Under the assumption that  $||s_k|| = ||h_k|| = \Delta$ , this means that we always  $\lambda_k > 0$  for all  $k \leq k_{\max}$ , where  $k_{\max}$  is the first iteration at which the symmetric Lanczos process breaks down, i.e.,  $\beta_{k_{\max}+1} = 0$ .

The authors of [8] prove that the residual norm of  $\lambda_k$  and  $s_k$  as approximate solutions of (1.3) satisfies

(3.14) 
$$||(A + \lambda_k I)s_k + g|| = \beta_{k+1}|e_{k+1}^T h_k|,$$

from which it is known that if the symmetric Lanczos process breaks down at iteration  $k_{\max}$  for the first time, then  $s_{k_{\max}} = s_{opt}$  and  $\lambda_{k_{\max}} = \lambda_{opt}$ . This result indicates that we can efficiently measure the residual norm by exploiting the last entry of  $h_k$  without explicitly forming  $s_k = Q_k h_k$  before a prescribed convergence tolerance is achieved.

In the next two sections we shall consider the convergence of the GLTR method, and establish a-priori bounds for the errors  $\lambda_{opt} - \lambda_k$ ,  $q(s_k) - q(s_{opt})$ ,  $\sin \angle (s_k, s_{opt})$ and the residual norm  $||(A + \lambda_k I)s_k + g||$ . We will prove how they decrease as k increases. We point out that, unlike  $||s_k - s_{opt}||$ , which is concerned with in [31, 32], we consider the error  $\sin \angle (s_k, s_{opt})$ .

4. A-priori bounds for  $\lambda_{opt} - \lambda_k$  and  $q(s_k) - q(s_{opt})$ . We establish a-priori bounds for  $\lambda_{opt} - \lambda_k$  in this section. It is known from [18] that  $\lambda_k$  increases monotonically with k and is bounded from above by  $\lambda_{opt}$ . Precisely, suppose that the symmetric Lanczos process breaks down at some  $k_{\max} \leq n-1$ . Then for  $k \leq k_{\max}$  it holds that

$$0 \leq \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{k_{\max}} = \lambda_{opt}.$$

Under the assumption that  $||s_k|| = ||h_k|| = \Delta$ , we have  $\lambda_k > 0$  for  $k = 0, 1, \dots, k_{\max}$ , but there has been no quantitative result on how fast  $\lambda_k$  converges to  $\lambda_{opt}$ .

Define the  $2(k+1) \times 2(k+1)$  matrix

(4.1) 
$$M_k = \tilde{Q}_k^T M \tilde{Q}_k$$

with M defined by (2.1) and

(4.2) 
$$\widetilde{Q}_k = \begin{pmatrix} Q_k \\ Q_k \end{pmatrix},$$

with the columns of the orthonormal  $Q_k$  defined by (3.3). It is straightforward that

(4.3) 
$$M_k = \begin{pmatrix} -T_k & \frac{\beta_0^2 e_1 e_1^T}{\Delta^2} \\ I & -T_k \end{pmatrix}$$

with  $T_k$  defined by (3.6) and  $\beta_0 = ||g||$ .

Obviously,  $Q_k$  is column orthonormal, and its columns span the 2(k+1) dimensional subspace

(4.4) 
$$\widetilde{\mathcal{S}}_k = \begin{pmatrix} \mathcal{S}_k & 0\\ 0 & \mathcal{S}_k \end{pmatrix} \subset \mathbb{R}^{2n}$$

Therefore,  $M_k$  is the orthogonal projection matrix of M onto  $\widetilde{\mathcal{S}}_k$  in the orthonormal basis  $\{(q_i^T, 0)^T\}_{i=0}^k$  and  $\{(0, q_i^T)^T\}_{i=0}^k$ . Let  $\mu_i^{(k)}$ ,  $i = 1, 2, \ldots, 2(k+1)$ , be the eigenvalues of  $M_k$ , which, similarly to (2.2),

are labeled as

$$Re(\mu_1^{(k)}) \ge Re(\mu_2^{(k)}) \ge \dots \ge Re(\mu_{2(k+1)}^{(k)}).$$

From Theorem 2.2 it is known that

(4.5) 
$$\mu_1^{(k)} = \lambda_k$$

is real and simple.

Let 
$$z^{(k)} = \begin{pmatrix} z_1^{(k)} \\ z_2^{(k)} \end{pmatrix}$$
 be the unit length eigenvector of  $M_k$  associated with  $\mu_1^{(k)}$ ,

i.e.,

(4.6) 
$$M_k \begin{pmatrix} z_1^{(k)} \\ z_2^{(k)} \end{pmatrix} = \mu_1^{(k)} \begin{pmatrix} z_1^{(k)} \\ z_2^{(k)} \end{pmatrix}, \quad \left\| \begin{pmatrix} z_1^{(k)} \\ z_2^{(k)} \end{pmatrix} \right\| = 1.$$

Then the vector

$$(4.7) \quad y^{(k)} = \widetilde{Q}_k \begin{pmatrix} z_1^{(k)} \\ z_2^{(k)} \end{pmatrix} = \begin{pmatrix} Q_k \\ Q_k \end{pmatrix} \begin{pmatrix} z_1^{(k)} \\ z_2^{(k)} \end{pmatrix} = \begin{pmatrix} Q_k z_1^{(k)} \\ Q_k z_2^{(k)} \end{pmatrix} = \begin{pmatrix} y_1^{(k)} \\ y_2^{(k)} \end{pmatrix}$$

is the Ritz vector of A from the subspace  $\widetilde{\mathcal{S}}_k$  and approximates the unit length eigenvector  $y^T = (y_1^T, y_2^T)^T$  of M associated with its rightmost real eigenvalue  $\mu_1 = \lambda_{opt}$ .

From the structure (4.3) of  $M_k$  and the definition (4.6) of  $z^{(k)}$ , it is easy to show that

$$\left(\begin{array}{c}z_2^{(k)}\\z_1^{(k)}\end{array}\right)$$

is the left eigenvector of  $M_k$  corresponding to the real simple eigenvalue  $\mu_1^{(k)} = \lambda_k$ . and from (4.6) it is straightforward to verify that

(4.8) 
$$z_2^{(k)} = (T_k + \lambda_k I)^{-1} z_1^{(k)}$$

Therefore, by definition (cf. [28, p.186]), the spectral condition number of  $\mu_1^{(k)}$  is

(4.9) 
$$s(\lambda_k) = \frac{1}{2|(z_2^{(k)})^T z_1^{(k)}|} = \frac{1}{2(z_1^{(k)})^T (T_k + \lambda_k I)^{-1} z_1^{(k)}}.$$

Similarly, by the structure (2.1) of M and the definition (2.3) of y, the vector  $(y_2^T, y_1^T)^T$  is the left eigenvector of M associated with the eigenvalue  $\mu_1$ . As a result, the spectral condition number of  $\mu_1$  is

(4.10) 
$$s(\lambda_{opt}) = \frac{1}{2|y_2^T y_1|} = \frac{1}{2y_1^T (A + \lambda_{opt}I)^{-1} y_1}$$

By Theorem 2.2, the unique solution  $h_k$  to (3.9) is

(4.11) 
$$h_k = -\frac{\Delta^2}{(\beta_0 e_1)^T z_2^{(k)}} z_1^{(k)},$$

and the unique solution  $s_k$  to TRS (3.8) is

(4.12) 
$$s_k = Q_k h_k = -\frac{\Delta^2}{(\beta_0 e_1)^T z_2^{(k)}} Q_k z_1^{(k)} = -\frac{\Delta^2}{(\beta_0 e_1)^T z_2^{(k)}} y_1^{(k)}.$$

Denote by  $\angle(u, \mathcal{S}_k)$  the acute angle between a nonzero vector u and  $\mathcal{S}_k$ . Then

(4.13) 
$$\sin \angle (u, \mathcal{S}_k) = \frac{\|(I - \pi_k)u\|}{\|u\|},$$

where  $\pi_k$  is the orthogonal projector onto  $S_k$ . In terms of Theorem 2.2 and (4.5), we have

(4.14) 
$$\lambda_{opt} - \lambda_k = \mu_1 - \mu_1^{(k)},$$

where  $\mu_1$  is the rightmost eigenvalue of M.

Let  $\tilde{\pi}_k = \tilde{Q}_k \tilde{Q}_k^T$  be the orthogonal projector onto  $\tilde{\mathcal{S}}_k$ . Then  $\tilde{\pi}_k M \tilde{\pi}_k$  is the restriction of M to the subspace  $\tilde{\mathcal{S}}_k$  and its matrix representation is  $M_k$  in the orthonormal basis  $\{(q_i^T, 0)^T\}_{i=0}^k$  and  $\{(0, q_i^T)^T\}_{i=0}^k$ . The eigenvalues of  $\tilde{\pi}_k M \tilde{\pi}_k$  restricted to  $\tilde{\mathcal{S}}_k$  are the eigenvalues of  $M_k$ , and the eigenvectors are the Ritz vectors of M from  $\tilde{\mathcal{S}}_k$ ; see

[25] for details. Therefore, a direct application of Theorem 3.8 in [16] to our context gives the following result.

LEMMA 4.1. Let  $\mu_1^{(k)} = \lambda_k$  and  $\mu_1 = \lambda_{opt}$  be the rightmost eigenvalues of  $M_k$  and M, respectively, and suppose that  $\|s_{opt}\| = \|s_k\| = \Delta$ . Then for  $\sin \angle (y, \tilde{\mathcal{S}}_k)$  small it holds that

(4.15) 
$$\lambda_{opt} - \lambda_k \le s(\lambda_k) \widetilde{\gamma}_k \sin \angle (y, \widetilde{\mathcal{S}}_k) + \mathcal{O}(\sin^2 \angle (y, \widetilde{\mathcal{S}}_k)),$$

where  $s(\lambda_k)$  is defined by (4.9) and  $\widetilde{\gamma}_k = \|\widetilde{\pi}_k M(I - \widetilde{\pi}_k)\|$ .<sup>1</sup>

From (4.7) and (4.9), we obtain

$$s(\lambda_k) = \frac{1}{2|(y_2^{(k)})^T y_1^{(k)}|},$$

which converges to  $s(\lambda_{opt})$  defined by (4.10) when  $y^{(k)} \to y$ . This is indeed the case, as will be shown in the next section. In the meantime,  $\tilde{\gamma}_k \leq ||M||$ . As a result, by this lemma, the convergence problem of  $\lambda_k$  to  $\lambda_{opt}$  becomes to analyze how fast  $\sin \angle (y, \tilde{S}_k)$  decreases as k increases.

Notice that

(4.16) 
$$\sin^2 \angle (y, \widetilde{\mathcal{S}}_k) = \left\| (I - \widetilde{\pi}_k) \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \right\|^2 = \| (I - \pi_k) y_1 \|^2 + \| (I - \pi_k) y_2 \|^2$$

Therefore, in order to bound  $\lambda_{opt} - \lambda_k$  and to show how it converges to zero as k increases, we need to analyze  $||(I - \pi_k)y_1||$  and  $||(I - \pi_k)y_2||$  separately.

We first consider  $||(I - \pi_k)y_1||$ . Throughout the paper, we denote by  $P_k$  the set of polynomials of degree not exceeding k + 1. We first present the following result.

LEMMA 4.2. The distance  $||(I - \pi_k)s_{opt}||$  between  $s_{opt}$  and  $S_k = \mathcal{K}_k(g, A)$  satisfies

(4.17) 
$$\|(I - \pi_k)s_{opt}\| = \min_{p_k \in \bar{P}_k, p_k(0) = 1} \|p_k(A + \lambda_{opt}I)s_{opt}\|$$

and

(4.18) 
$$\|(I - \pi_k)s_{opt}\| \le \|s_{opt}\|\epsilon_1^{(k)},$$

where

(4.19) 
$$\epsilon_1^{(k)} = \min_{p \in \bar{P}_k, p(0)=1} \max_{1 \le i \le n} \|p(\alpha_i + \lambda_{opt})\|$$

with  $\alpha_1 \geq \alpha_{n-1} \geq \cdots \geq \alpha_n$  being the eigenvalues of A. Moreover,

(4.20) 
$$\epsilon_1^{(k)} \le 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{k+1},$$

where  $\kappa = \frac{\alpha_1 + \lambda_{opt}}{\alpha_n + \lambda_{opt}}$  is the condition number of  $A + \lambda_{opt}I$ .

<sup>&</sup>lt;sup>1</sup>In Theorem 3.8 of [16],  $\tan \angle (y, \widetilde{S}_k)$  in the right-hand side of (4.15) is  $\sin \angle (y, \widetilde{S}_k)$ , but it is obvious that the sine and tangent can be replaced each other in the right-hand side when  $\sin \angle (y, \widetilde{S}_k)$  becomes small.

*Proof.* Theorem 1.1 has shown that  $s_{opt}$  satisfies the linear system  $(A + \lambda_{opt})s_{opt} =$ -g. Therefore, exploiting the shift invariance  $\mathcal{K}_k(g, A) = \mathcal{K}_k(g, A + \lambda_{opt}I)$  and the eigendecomposition  $A = S\Lambda S^T$ , we have

$$\begin{aligned} \|(I - \pi_k)s_{opt}\| &= \min_{s \in \mathcal{K}_k(g, A + \lambda_{opt}I)} \|s_{opt} - s\| \\ &= \min_{q \in \bar{P}_{k-1}} \|s_{opt} - q(A + \lambda_{opt}I)g\| \\ &= \min_{q \in \bar{P}_{k-1}} \|s_{opt} - q(A + \lambda_{opt}I)g\| \\ &= \min_{q \in \bar{P}_{k-1}} \|s_{opt} + q(A + \lambda_{opt}I)(A + \lambda_{opt})s_{opt}\| \\ &= \min_{p_k \in \bar{P}_k, p_k(0) = 1} \|p_k(A + \lambda_{opt}I)s_{opt}\| \\ &\leq \|s_{opt}\| \min_{p_k \in \bar{P}_k, p_k(0) = 1} \|p_k(\Lambda + \lambda_{opt}I)\| \\ &= \|s_{opt}\| \epsilon_1^{(k)} \end{aligned}$$

with the polynomial  $p_k(\lambda) = 1 + \lambda q(\lambda) \in \overline{P}_k$  and  $p_k(0) = 1$ .

Note that  $A + \lambda_{opt}I$  is symmetric positive definite. Applying a standard estimate (cf. the book [11, p.51, Theorem 3.1.1] to  $\epsilon_1^{(k)}$ , we obtain (4.20). 

Relation (2.4) shows that  $y_1$  is the same as  $s_{opt}$  up to a scaling. Therefore, replacing  $s_{opt}$  in (4.17) and (4.18) by  $y_1$  and exploiting (4.20), we have established the following upper bound for  $||(I - \pi_k)y_1||$ . THEOREM 4.3. Let  $y^T = (y_1^T, y_2^T)^T$  be the unit length eigenvector of M associated

with its rightmost eigenvalue  $\mu_1$ . Then

(4.21) 
$$\|(I - \pi_k)y_1\| \le 2\|y_1\| \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{k+1},$$

where  $\kappa = \frac{\alpha_1 + \lambda_{opt}}{\alpha_n + \lambda_{opt}}$ . As it will turn out, an estimation of  $||(I - \pi_k)y_2||$  is much more involved. THEOREM 4.4. With the notation previously, we have

(4.22) 
$$\|(I - \pi_k)y_2\| \le \frac{4(\alpha_1 + \lambda_{opt})}{(\alpha_1 - \alpha_n)^2} \|y_1\|\epsilon_2^{(k)},$$

where  $\alpha_1$  and  $\alpha_n$  are the largest and smallest eigenvalues of A, and

(4.23) 
$$\epsilon_2^{(k)} = \min_{q \in \bar{P}_{k-1}} \max_{x \in [-1,1]} \left| \frac{1}{(x-\eta)^2} - q(x) \right|$$

with

(4.24) 
$$\eta = \frac{\alpha_1 + \alpha_n + 2\lambda_{opt}}{\alpha_1 - \alpha_n} = \frac{\kappa + 1}{\kappa - 1} > 1,$$

where  $\kappa = \frac{\alpha_1 + \lambda_{opt}}{\alpha_n + \lambda_{opt}}$ .

*Proof.* Recall that  $A = S\Lambda S^T$  is the eigendecomposition of A, where S is orthogonal and  $\Lambda = diag(\alpha_1, \alpha_2, \ldots, \alpha_n)$  with  $\alpha_1 \ge \alpha_2 \ge \cdots \ge \alpha_n$  the eigenvalues.

From  $(A + \lambda_{opt}I)s_{opt} = -g$  and (2.4), we obtain

$$\frac{\Delta^2}{g^T y_2} (A + \lambda_{opt} I) y_1 = g.$$

From (2.3), we have

(4.25) 
$$y_2 = (A + \lambda_{opt}I)^{-1}y_1$$

Making use of  $\mathcal{K}_k(g, A) = \mathcal{K}_k(g, A + \lambda_{opt}I)$ , (4.25) and the orthogonality of S, we then obtain

$$\begin{split} \|(I - \pi_{k})y_{2}\| &= \min_{z \in \mathcal{K}_{k}(g, A + \lambda_{opt}I)} \|y_{2} - z\| \\ &= \min_{q \in \bar{P}_{k-1}} \|y_{2} - q(A + \lambda_{opt}I)g\| \\ &= \min_{q \in \bar{P}_{k-1}} \|(A + \lambda_{opt}I)^{-1}y_{1} - \frac{\Delta^{2}}{g^{T}y_{2}}(A + \lambda_{opt}I)q(A + \lambda_{opt}I)y_{1}\| \\ &= \min_{p \in \bar{P}_{k-1}} \|(A + \lambda_{opt}I)[(A + \lambda_{opt}I)^{-2} - p(A + \lambda_{opt}I)]y_{1}\| \\ &\leq \|A + \lambda_{opt}I\| \min_{q \in \bar{P}_{k-1}} \|[(A + \lambda_{opt}I)^{-2} - p(A + \lambda_{opt}I)]y_{1}\| \\ &= \|A + \lambda_{opt}I\| \min_{p \in \bar{P}_{k-1}} \|S[(A + \lambda_{opt}I)^{-2} - p(A + \lambda_{opt}I)]S^{T}y_{1}\| \\ &\leq (\alpha_{1} + \lambda_{opt})\|y_{1}\| \min_{p \in \bar{P}_{k-1}} \max_{z \in [\alpha_{n}, \alpha_{1}]} \left|\frac{1}{(z + \lambda_{opt})^{2}} - p(z)\right|. \end{split}$$

Consider the variable transformation

$$z = \frac{\alpha_1 - \alpha_n}{2}x + \frac{\alpha_n + \alpha_1}{2},$$

which maps  $x \in [-1, 1]$  to  $z \in [\alpha_n, \alpha_1]$  in one-to-one correspondence. Then

$$\begin{split} \min_{p \in \bar{P}_{k-1}} \max_{z \in [\alpha_n, \alpha_1]} \left| \frac{1}{(z + \lambda_{opt})^2} - p(z) \right| \\ &= \min_{p \in \bar{P}_{k-1}} \max_{x \in [-1, 1]} \left| \frac{4}{(\alpha_1 - \alpha_n)^2 (x - \eta)^2} - p(x) \right| \\ &= \frac{4}{(\alpha_1 - \alpha_n)^2} \min_{p \in \bar{P}_{k-1}} \max_{x \in [-1, 1]} \left| \frac{1}{(x - \eta)^2} - \frac{(\alpha_1 - \alpha_n)^2}{4} p(x) \right| \\ &= \frac{4}{(\alpha_1 - \alpha_n)^2} \min_{q \in \bar{P}_{k-1}} \max_{x \in [-1, 1]} \left| \frac{1}{(x - \eta)^2} - q(x) \right| \\ &= \frac{4}{(\alpha_1 - \alpha_n)^2} \epsilon_2^{(k)}. \quad \Box \end{split}$$

(4.26)

 $\epsilon_2^{(k)}$  is the error of the best or optimal uniform polynomial approximation from  $\overline{P}_{k-1}$  to the rational function  $\frac{1}{(x-\eta)^2}$  over the interval [-1,1] with  $\eta > 1$ . To our best knowledge, there seems no known explicit solution to such approximation problem. However, recall from (4.16) that  $\sin \angle (y, \widetilde{S}_k) > ||(I - \pi)y_1||$ . Therefore, it is enough to prove that  $\epsilon_2^{(k)}$  is of the same order as bound (4.21) because this means that  $\sin \angle (y, \widetilde{S}_k)$  is at least as small as bound (4.21) for  $||(I - \pi)y_1||$ . To this end, exploiting Chebyshev polynomials of the second kind and one of its fundamental properties, we will establish a desired bound for  $\epsilon_2^{(k)}$ , which is indeed as small as bound (4.21).

THEOREM 4.5. The approximation error

(4.27) 
$$\epsilon_2^{(k)} \le \left(1 + \frac{k+2}{|\ln t|}\right) \frac{4}{1-t^2} \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{k+3},$$

and

(4.28) 
$$\|(I - \pi_k)y_2\| \le \frac{16(\alpha_1 + \lambda_{opt})\|y_1\|}{(\alpha_1 - \alpha_n)^2(1 - t^2)} \left(1 + \frac{k+2}{|\ln t|}\right) \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{k+3}$$

where  $t = \eta - \sqrt{\eta^2 - 1}$  and  $\kappa = \frac{\alpha_1 + \lambda_{opt}}{\alpha_n + \lambda_{opt}}$ . *Proof.* For any  $t \in (-1, 1)$  and  $x \in [-1, 1]$  there is the following generating function [4, p.215]:

(4.29) 
$$\sum_{j=0}^{\infty} (j+1)t^j U_j(x) = \frac{1-t^2}{(1+t^2-2tx)^2},$$

where  $U_j(x) = \sin(j \arccos x)$  is the *j*th degree Chebyshev polynomial of the second kind [4, p.212].

For  $t = \eta - \sqrt{\eta^2 - 1}$ , it is easily justified that  $1 + t^2 = 2\eta t$ . Therefore, the identity (4.29) becomes

(4.30) 
$$\sum_{j=0}^{\infty} (j+1)t^j U_j(x) = \frac{1-t^2}{4t^2(x-\eta)^2},$$

from which it follows that

$$\frac{1}{(x-\eta)^2} = \frac{4t^2}{1-t^2} \sum_{j=0}^{\infty} (j+1)t^j U_j(x).$$

Taking the kth degree polynomial

$$p_k(x) = \frac{4t^2}{1 - t^2} \sum_{j=0}^k (j+1)t^j U_j(x) \in \bar{P}_{k-1}$$

and noting that  $-\ln t = |\ln t|$  for 0 < t < 1 and  $|U_j(x)| \le 1$  for  $x \in [-1, 1]$ , we have

$$\epsilon_{2}^{(k)} \leq \max_{x \in [-1,1]} \left| \frac{1}{(x-\eta)^{2}} - p_{k}(x) \right|$$

$$= \max_{x \in [-1,1]} \left| \frac{4t^{2}}{1-t^{2}} \sum_{j=k+1}^{\infty} (j+1)t^{j}U_{j}(x) \right|$$

$$\leq \frac{4t^{2}}{1-t^{2}} \sum_{j=k+1}^{\infty} (j+1)t^{j}$$

$$= \frac{4t^{2}}{1-t^{2}} \int_{k+1}^{\infty} (z+1)t^{z}dz$$

$$= \frac{4t^{2}}{1-t^{2}} \left( \frac{z+1}{\ln t}t^{z} \Big|_{k+1}^{\infty} - t^{z} \Big|_{k+1}^{\infty} \right)$$

$$= \left( 1 - \frac{k+2}{\ln t} \right) \frac{4t^{k+3}}{1-t^{2}} = \left( 1 + \frac{k+2}{\ln t} \right) \frac{4t^{k+3}}{1-t^{2}}.$$
(4.31)

From (4.24), it is straightforward to justify that

(4.32) 
$$t = \eta - \sqrt{\eta^2 - 1} = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}.$$

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Therefore, from (4.22), (4.26) and (4.31) it follows that (4.27) and (4.28) hold. 

Combining Lemma 4.1, (4.16), Theorem 4.3 and Theorem 4.5, by a simple manipulation, we achieve the following bounds for  $\sin \angle (y, \mathcal{S}_k)$  and  $\lambda_{opt} - \lambda_k$ .

THEOREM 4.6. Suppose that  $||s_{opt}|| = ||s_k|| = \Delta$ . Then

(4.33) 
$$\sin \angle (y, \widetilde{\mathcal{S}}_k) \le c_k \|y_1\| \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{k+1}$$

and asymptotically

(4.34) 
$$\lambda_{opt} - \lambda_k \le c_k s(\lambda_k) \widetilde{\gamma}_k \|y_1\| \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{k+1},$$

where

(4.35) 
$$c_k = 2 + \frac{16(\alpha_1 + \lambda_{opt})}{(\alpha_1 - \alpha_n)^2 (1 - t^2)} \left(1 + \frac{k+2}{|\ln t|}\right) \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^2,$$

 $\widetilde{\gamma}_k = \|\widetilde{\pi}_k M(I - \widetilde{\pi}_k)\|$  with  $\widetilde{\pi}_k$  the orthogonal projector onto  $\widetilde{\mathcal{S}}_k$  defined by (4.4), and  $s(\lambda_k)$  and t are defined by (4.9) and (4.32).

A-priori bound (4.34), for the first time, proves that  $\lambda_{opt} - \lambda_k$  converges to zero as k increases. As a matter of fact, based on this bound, we can further establish a much sharper bound for  $\lambda_{opt} - \lambda_k$ . Before proceeding, we first derive the following result, which will play a key role in establishing the sharper a-priori bound for  $\lambda_{opt} - \lambda_k$ .

THEOREM 4.7. For  $k = 0, 1, \ldots, k_{max}$ , the following a-priori bound holds:

(4.36) 
$$e_1^T (T_{k_{\max}} + \lambda_{opt} I)^{-1} e_1 - e_1^T (T_k + \lambda_{opt} I)^{-1} e_1 \le \frac{4\Delta}{\beta_0} \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2(k+1)},$$

where  $\kappa = \frac{\alpha_1 + \lambda_{opt}}{\alpha_n + \lambda_{opt}}$  and  $\beta_0 = ||g||$ . *Proof.* Consider the symmetric positive definite linear system

(4.37) 
$$(T_{k_{\max}} + \lambda_{opt}I)h = -\beta_0 e_1$$

with  $\beta_0 = ||g||$ , which is (3.11) for  $k = k_{\text{max}}$  and has the solution  $h_{k_{\text{max}}}$ . When taking  $e_1$  as the starting vector, i.e., taking the zero vector as an initial guess to  $h_{k_{\text{max}}}$ , the symmetric Lanczos process generates an orthonormal basis  $\{e_i\}_{i=1}^{k+1}$  of the (k+1)dimensional Krylov subspace

$$\mathcal{K}_{k+1}(e_1, T_{k_{\max}} + \lambda_{opt}I) = span\{e_1, (T_{k_{\max}} + \lambda_{opt}I)e_1, \dots, (T_{k_{\max}} + \lambda_{opt}I)^k e_1\}$$

and the symmetric tridiagonal  $T_k + \lambda_{opt}I$ . Define  $E_k = (e_1, e_2, \dots, e_{k+1})$ . Then  $T_k + \lambda_{opt}I = E_k^T (T_{k_{max}} + \lambda_{opt}I)E_k$ . Applying the symmetric Lanczos method to solving (4.37), at iteration  $k \leq k_{\text{max}}$  we obtain the projected problem

$$(T_k + \lambda_{opt}I)\tilde{y} = -\beta_0 e_1.$$

Write its solution as  $\tilde{y}_k$ . Then the symmetric Lanczos method computes the approximation  $h_k = E_k \tilde{y}_k$  of  $h_{k_{\max}}$ .

Define the error  $\varepsilon_k = \tilde{h}_{k_{\text{max}}} - \tilde{h}_k$  and the residual  $r_k = -\beta_0 e_1 - (T_{k_{\text{max}}} + \lambda_{opt} I)\tilde{h}_k$ of (4.37). Note that the initial residual  $r_0 = -\beta_0 e_1$ . Then  $||r_0||^2 = \beta_0^2$  and

$$(T_{k_{\max}} + \lambda_{opt}I)\varepsilon_k = r_k,$$

from which and [19, Theorem 2.11] it follows that the square of  $(T_{k_{\max}} + \lambda_{opt}I)$ -norm error satisfies

$$\begin{split} \|\varepsilon_k\|_{(T_{k_{\max}}+\lambda_{opt}I)}^2 &= \varepsilon_k^T (T_{k_{\max}}+\lambda_{opt}I)\varepsilon_k^T \\ &= r_k^T (T_{k_{\max}}+\lambda_{opt}I)^{-1}r_k \\ &= \beta_0^2 \left(e_1^T (T_{k_{\max}}+\lambda_{opt}I)^{-1}e_1 - e_1^T (T_k+\lambda_{opt}I)^{-1}e_1\right). \end{split}$$

As a result, we obtain

(4.38) 
$$e_1^T (T_{k_{\max}} + \lambda_{opt}I)^{-1} e_1 - e_1^T (T_k + \lambda_{opt}I)^{-1} e_1 = \frac{\|\varepsilon_k\|_{(T_{k_{\max}} + \lambda_{opt}I)}^2}{\beta_0^2}.$$

Notice that the eigenvalues of  $T_{k_{\max}}$  are the exact eigenvalues of A, which means that the smallest and largest eigenvalues of  $T_{k_{\max}} + \lambda_{opt}I$  lie in  $[\alpha_n + \lambda_{opt}, \alpha_1 + \lambda_{opt}]$ . Since the symmetric Lanczos method is mathematically equivalent to the conjugate gradient method at the same iteration when the same initial guess on  $h_{k_{\max}}$  is used, applying a standard estimate (cf. [11, Theorem 3.1.1] and [19, Theorem 2.30]) to  $\|\varepsilon_k\|_{(T_{k_{\max}} + \lambda_{opt}I)}^2$  gives rise to

$$\|\varepsilon_k\|_{(T_{k_{\max}}+\lambda_{opt}I)}^2 \le 4\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{2(k+1)} \|\varepsilon_0\|_{(T_{k_{\max}}+\lambda_{opt}I)}^2$$

Since  $r_0 = -\beta_0 e_1$ , the squared initial error

$$\|\varepsilon_0\|_{(T_{k_{\max}}+\lambda_{opt}I)}^2 = r_0^T (T_{k_{\max}}+\lambda_{opt}I)^{-1} r_0 = \beta_0^2 e_1^T (T_{k_{\max}}+\lambda_{opt}I)^{-1} e_1$$

Exploiting  $\beta_0 \| (T_{k_{\max}} + \lambda_{opt}I)^{-1} e_1 \| = \| h_{k_{\max}} \| = \Delta$ , we obtain

$$\beta_0^2 e_1^T (T_{k_{\max}} + \lambda_{opt} I)^{-1} e_1 \le \beta_0 ||e_1|| \Delta = \beta_0 \Delta.$$

Substituting the above three relations into (4.38) yields (4.36).

THEOREM 4.8. Assume that the symmetric Lanczos process breaks down at iteration  $k_{\max}$  and  $||s_{opt}|| = ||s_k|| = \Delta$  for  $k = 0, 1, \ldots, k_{\max}$ . Then for k suitably large we have the asymptotic a-priori bound

(4.39)  

$$\lambda_{opt} - \lambda_k \leq \eta_{k1} \left( e_1^T (T_{k_{\max}} + \lambda_{opt} I)^{-1} e_1 - e_1^T (T_k + \lambda_{opt} I)^{-1} e_1 \right) + \eta_{k2} \left( q(s_k) - q(s_{opt}) \right),$$

where the factors

(4.40) 
$$\eta_{k1} = \frac{\beta_0^2}{\Delta^2 + \beta_0^2 e_1^T (T_k + \lambda_{opt}I)^{-2} e_1} \le \frac{\beta_0^2 (\alpha_1 + \lambda_{opt})^2}{\beta_0^2 + (\alpha_1 + \lambda_{opt})^2 \Delta^2}$$

(4.41) 
$$\eta_{k2} = \frac{2}{\Delta^2 + \beta_0^2 e_1^T (T_k + \lambda_{opt} I)^{-2} e_1} \le \frac{2(\alpha_1 + \lambda_{opt})^2}{\beta_0^2 + (\alpha_1 + \lambda_{opt})^2 \Delta^2}$$

with  $\beta_0 = ||g||$ .

*Proof.* From (3.11), we obtain

$$h_k = -\beta_0 (T_k + \lambda_k I)^{-1} e_1$$

and  $||h_k|| = \beta_0 ||(T_k + \lambda_k I)^{-1} e_1|| = \Delta$ . Therefore, by (3.9) we have  $q(s_k) = \phi(h_k)$  and  $q(s_k) = -\beta_0^2 e_1^T (T_k + \lambda_k I)^{-1} e_1 + \frac{1}{2} \beta_0^2 e_1^T (T_k + \lambda_k I)^{-1} T_k (T_k + \lambda_k I)^{-1} e_1$   $= -\beta_0^2 e_1^T (T_k + \lambda_k I)^{-1} e_1 + \frac{1}{2} \beta_0^2 e_1^T (T_k + \lambda_k I)^{-1} (T_k + \lambda_k I - \lambda_k I) (T_k + \lambda_k I)^{-1} e_1$   $= -\beta_0^2 e_1^T (T_k + \lambda_k I)^{-1} e_1 + \frac{1}{2} \beta_0^2 e_1^T (T_k + \lambda_k I)^{-1} e_1 - \frac{1}{2} \lambda_k \beta_0^2 e_1^T (T_k + \lambda_k I)^{-2} e_1$   $= -\frac{1}{2} \beta_0^2 e_1^T (T_k + \lambda_k I)^{-1} e_1 - \frac{1}{2} \lambda_k \beta_0^2 e_1^T (T_k + \lambda_k I)^{-2} e_1$ (4.42)

$$= -\frac{1}{2}\beta_0^2 e_1^T (T_k + \lambda_k I)^{-1} e_1 - \frac{1}{2}\lambda_k \Delta^2.$$

By assumption and (3.9), we have

$$s_{k_{\max}} = Q_{k_{\max}} h_{k_{\max}} = s_{opt}, \quad \lambda_{k_{\max}} = \lambda_{opt}, \quad q(s_{k_{\max}}) = q(s_{opt}) = \phi(h_{k_{max}})$$

with  $||h_{k_{max}}|| = \Delta$ , and the eigenvalues  $T_{k_{max}}$  are the exact eigenvalues of A. Similarly to the above derivation, we obtain

(4.43) 
$$q(s_{opt}) = -\frac{1}{2}\beta_0^2 e_1^T (T_{k_{\max}} + \lambda_{opt}I)^{-1} e_1 - \frac{1}{2}\lambda_{opt}\Delta^2.$$

Subtracting the two hand sides of (4.42) and (4.43) yields

(4.44)

$$(\lambda_{opt} - \lambda_k)\Delta^2 = \beta_0^2 \left( e_1^T (T_k + \lambda_k I)^{-1} e_1 - e_1^T (T_{k_{\max}} + \lambda_{opt} I)^{-1} e_1 \right) + 2 \left( q(s_k) - q(s_{opt}) \right).$$

Since  $||(T_k + \lambda_{opt}I)^{-1}|| \leq \frac{1}{\alpha_n + \lambda_{opt}}$  and (4.33) has proved that  $\lambda_{opt} - \lambda_k$  is nonnegative and tends to zero as k increases, we must have  $(\lambda_{opt} - \lambda_k)||(T_k + \lambda_{opt}I)^{-1}|| < 1$ , i.e.,  $\lambda_{opt} - \lambda_k \leq \alpha_n + \lambda_{opt}$ , for k suitably large. Precisely, by (4.34), a sufficient condition is to choose k such that

$$c_k s(\lambda_k) \widetilde{\gamma}_k \|y_1\| \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{k+1} \le \alpha_n + \lambda_{opt}.$$

Moreover, since  $\lambda_k \to \lambda_{opt}$ , by continuity argument, we have

$$e_{1}^{T}(T_{k}+\lambda_{k}I)^{-1}e_{1}-e_{1}^{T}(T_{k_{\max}}+\lambda_{opt}I)^{-1}e_{1} \to e_{1}^{T}(T_{k}+\lambda_{opt}I)^{-1}e_{1}-e_{1}^{T}(T_{k_{\max}}+\lambda_{opt}I)^{-1}e_{1}$$

where the quantity in the right hand side has been shown by (4.38) to be strictly negative for all  $k = 0, 1, ..., k_{\max} - 1$ . Therefore,  $e_1^T (T_k + \lambda_k I)^{-1} e_1 - e_1^T (T_{k_{\max}} + \lambda_{opt} I)^{-1} e_1$  must become nonpositive for k suitably large, that is, the first term in the right hand side of (4.44) becomes nonpositive as k increases. As a result, from (4.44) we obtain the inequality (4.45)

$$(\lambda_{opt} - \lambda_k)\Delta^2 \le \beta_0^2 \left( e_1^T (T_{k_{\max}} + \lambda_{opt}I)^{-1} e_1 - e_1^T (T_k + \lambda_k I)^{-1} e_1 \right) + 2 \left( q(s_k) - q(s_{opt}) \right)$$

when k is suitably large.

Let us analyze  $e_1^T (T_k + \lambda_k I)^{-1} e_1$ . Since  $(\lambda_{opt} - \lambda_k) ||(T_k + \lambda_{opt} I)^{-1}|| < 1$  for k suitably large, exploiting the series expansion of  $((I - (\lambda_{opt} - \lambda_k)(T_k + \lambda_{opt} I)^{-1}))^{-1}$ ,

we obtain

$$(T_k + \lambda_k I)^{-1} = (T_k + \lambda_{opt}I + (\lambda_k - \lambda_{opt})I)^{-1}$$
  
=  $((T_k + \lambda_{opt}I)(I - (\lambda_{opt} - \lambda_k)(T_k + \lambda_{opt}I)^{-1}))^{-1}$   
=  $((I - (\lambda_{opt} - \lambda_k)(T_k + \lambda_{opt}I)^{-1}))^{-1}(T_k + \lambda_{opt}I)^{-1}$   
=  $(I + (\lambda_{opt} - \lambda_k)(T_k + \lambda_{opt}I)^{-1} + \mathcal{O}((\lambda_{opt} - \lambda_k)^2))(T_k + \lambda_{opt}I)^{-1}$   
=  $(T_k + \lambda_{opt}I)^{-1} + (\lambda_{opt} - \lambda_k)(T_k + \lambda_{opt}I)^{-2} + \mathcal{O}((\lambda_{opt} - \lambda_k)^2).$ 

Therefore, we have

$$(4.46) e_1^T (T_{k_{\max}} + \lambda_{opt}I)^{-1} e_1 - e_1^T (T_k + \lambda_k I)^{-1} e_1 = e_1^T (T_{k_{\max}} + \lambda_{opt}I)^{-1} e_1 - e_1^T (T_k + \lambda_{opt}I)^{-1} e_1 - (\lambda_{opt} - \lambda_k) e_1^T (T_k + \lambda_{opt}I)^{-2} e_1 - \mathcal{O}((\lambda_{opt} - \lambda_k)^2),$$

which is *nonnegative* provided that k is suitably large. Substituting this relation into (4.45) and dropping the nonnegative higher small term  $\mathcal{O}((\lambda_{opt} - \lambda_k)^2)$  in the resulting left-hand side give rise to

$$\lambda_{opt} - \lambda_k \le \eta_{k1} \left( e_1^T (T_{k_{\max}} + \lambda_{opt} I)^{-1} e_1 - e_1^T (T_k + \lambda_{opt} I)^{-1} e_1) \right) + \eta_{k2} \left( q(s_k) - q(s_{opt}) \right)$$

with  $\eta_{k1}$  and  $\eta_{k2}$  defined by (4.40) and (4.41), respectively, which proves (4.39).

Since  $T_k + \lambda_{opt}I$  is symmetric positive definite and its eigenvalues lie between  $\alpha_n + \lambda_{opt}$  and  $\alpha_1 + \lambda_{opt}$ , the smallest and largest ones of  $A + \lambda_{opt}I$ , respectively, we have  $\frac{1}{(\alpha_1 + \lambda_{opt})^2} \leq e_1^T (T_k + \lambda_{opt}I)^{-2} e_1 \leq \frac{1}{(\alpha_n + \lambda_{opt})^2}$ . As a result, from the forms of  $\eta_{k1}$  and  $\eta_{k2}$ , it is straightforward to obtain

$$\eta_{k1} \le \frac{\beta_0^2 (\alpha_1 + \lambda_{opt})^2}{\beta_0^2 + (\alpha_1 + \lambda_{opt})^2 \Delta^2}, \quad \eta_{k2} \le \frac{2(\alpha_1 + \lambda_{opt})^2}{\beta_0^2 + (\alpha_1 + \lambda_{opt})^2 \Delta^2}.$$

independent of iteration k.

Relation (4.39) shows that bounding  $\lambda_{opt} - \lambda_k$  amounts to bounding  $e_1^T(T_{k_{\max}} + \lambda_{opt}I)^{-1}e_1 - e_1^T(T_k + \lambda_{opt}I)^{-1}e_1$  and  $q(s_k) - q(s_{opt})$  separately. We have established an a-priori bound (4.36) for the former one. Now we investigate  $q(s_k) - q(s_{opt})$ . Steihaug [27] has proved that the error  $q(s_k) - q(s_{opt})$  of the optimal objective value monotonically decreases with respect to k. Zhang et al. [31, Theorem 4.3] have given the following result. Starting with it, we can derive a new a-priori bound for  $q(s_k) - q(s_{opt})$ , whose proof is much shorter than those in [31].

LEMMA 4.9 ([31]). Suppose  $||s_{opt}|| = ||s_k|| = \Delta$ . Then

(4.47) 
$$0 \le q(s_k) - q(s_{opt}) \le 2(\alpha_1 + \lambda_{opt}) \|\tilde{s} - s_{opt}\|^2$$

for any nonzero  $\tilde{s} \in \mathcal{K}_k(g, A)$ .

THEOREM 4.10. Suppose  $||s_{opt}|| = ||s_k|| = \Delta$ . Then

(4.48) 
$$0 \le q(s_k) - q(s_{opt}) \le 8(\alpha_1 + \lambda_{opt})\Delta^2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2(k+1)}$$

where  $\kappa = \frac{\alpha_1 + \lambda_{opt}}{\alpha_n + \lambda_{opt}}$ .

*Proof.* Relation (4.47) has shown that

(4.49) 
$$q(s_k) - q(s_{opt}) \le 2(\alpha_1 + \lambda_{opt}) \min_{\tilde{s} \in \mathcal{K}_k(g,A)} \|\tilde{s} - s_{opt}\|^2.$$

By definition, we have

(4.50) 
$$\min_{\tilde{s}\in\mathcal{K}_k(g,A)} \|\tilde{s} - s_{opt}\|^2 = \|(I - \pi_k)s_{opt}\|^2,$$

where  $\pi_k$  is the orthogonal projector onto  $\mathcal{K}_k(g, A)$ . From the above relation and Lemma 4.2, it is immediate that

(4.51) 
$$\min_{\tilde{s} \in \mathcal{K}_{k}(g,A)} \|\tilde{s} - s_{opt}\|^{2} \leq 4 \|s_{opt}\|^{2} \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2(k+1)} = 4\Delta^{2} \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2(k+1)}.$$

Substituting it into (4.49) yields (4.48).

By a comparison, we find that bound (4.48) is as sharp as (4.24a) and (4.26a) in [31] but has a simpler form than the latter two, and its proof is also simpler.

Substituting bound (4.48) for  $q(s_k) - q(s_{opt})$  into (4.39) and bound (4.36) into (4.39) ultimately leads to the following a-priori bound for  $\lambda_{opt} - \lambda_k$ .

THEOREM 4.11. Suppose  $||s_{opt}|| = ||s_k|| = \Delta$ . Then for k suitably large we have

(4.52) 
$$\lambda_{opt} - \lambda_k \le \left(\frac{4\eta_{k1}\Delta}{\beta_0} + 8(\alpha_1 + \lambda_{opt})\eta_{k2}\Delta^2\right) \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2(k+1)}$$

with the factors  $\eta_{k1}$  and  $\eta_{k2}$  defined by (4.40) and (4.41), respectively.

This theorem clearly indicates that, except for the bounded factor,  $\lambda_{opt} - \lambda_k$  converges at least as fast as  $\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{2(k+1)}$ , and bound (4.52) is much sharper than bound (4.34) and is roughly square of the latter.

5. A-priori bounds for  $\sin \angle (s_k, s_{opt})$  and  $||(A + \lambda_k I)s_k + g||$ . Suppose that  $||s_{opt}|| = ||s_k|| = \Delta$ . Then  $s_k/||s_{opt}||$  and  $s_{opt}/||s_{opt}||$  have unit length. It is worthwhile to notice that the measures  $\sin \angle (s_k, s_{opt})$  and  $||s_k - s_{opt}||/||s_{opt}||$  are equivalent once they start to become fairly small. In fact, for  $\angle (s_k, s_{opt})$  fairly small we have

(5.1)  
$$\frac{\|s_k - s_{opt}\|^2}{\|s_{opt}\|^2} = \frac{s_k^T s_k}{\|s_{opt}\|^2} + \frac{s_{opt}^T s_{opt}}{\|s_{opt}\|^2} - 2\frac{s_k^T s_{opt}}{\|s_{opt}\|^2} = 1 + 1 - 2\cos \angle (s_k, s_{opt}) = 4\sin^2 \frac{\angle (s_k, s_{opt})}{2} \approx \sin^2 \angle (s_k, s_{opt}).$$

It is seen from (4.12) and (2.4) that  $s_k$  and  $s_{opt}$  are the same as  $y_1^{(k)}$  and  $y_1$  up to scaling, respectively. As a result, we have

(5.2) 
$$\sin \angle (s_k, s_{opt}) = \sin \angle (y_1^{(k)}, y_1).$$

We take two steps to estimate  $\sin \angle (s_k, s_{opt})$ . Firstly, we bound  $\sin \angle (y_1^{(k)}, y_1)$  in terms of  $\sin \angle (y^{(k)}, y)$  with y and  $y^{(k)}$  defined by (2.3) and (4.7), respectively.

Secondly, we establish an a-priori bound for  $\sin \angle (y^{(k)}, y)$ , showing how it converges to zero as k increases. To this end, we need the following result [12, Lemma 2.3].

LEMMA 5.1 ([12]). Let  $u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$  and  $\tilde{u} = \begin{pmatrix} \tilde{u}_1 \\ \tilde{u}_2 \end{pmatrix}$  where  $u_i$ ,  $\tilde{u}_i \in \mathbb{C}^n$  for i = 1, 2, and  $||u_1|| = ||\tilde{u}_1|| = 1$ . Then

 $\sin \angle (u_1, \tilde{u}_1) \le \min \left\{ \|u\|, \|\tilde{u}\| \right\} \sin \angle (u, \tilde{u}).$ 

With this lemma, we can present the following bound.

THEOREM 5.2. For the unit length eigenvector  $y^T = (y_1^T, y_2^T)^T$  of M associated with the eigenvalue  $\lambda_{opt}$  and  $y^{(k)}$  defined by (4.7), we have

(5.3) 
$$\sin \angle (s_k, s_{opt}) \le \frac{1}{\|y_1\|} \sin \angle (y^{(k)}, y).$$

*Proof.* From (2.4) and (4.12), since

$$\sin \angle (s_k, s_{opt}) = \sin \angle (y_1^{(k)}, y_1) = \sin \angle \left(\frac{y_1^{(k)}}{\|y_1^{(k)}\|}, \frac{y_1}{\|y_1\|}\right)$$

with the unit length vectors  $y_1^{(k)}/||y_1^{(k)}||$  and  $y_1/||y_1||$ , by definition (4.7) of  $y^{(k)}$  and Lemma 5.1 we obtain

$$\sin \angle (s_k, s_{opt}) = \sin \angle \left(\frac{y_1^{(k)}}{\|y_1^{(k)}\|}, \frac{y_1}{\|y_1\|}\right)$$

$$\leq \min \left\{\frac{1}{\|y_1\|}, \frac{1}{\|y_1^{(k)}\|}\right\} \sin \angle \left(\frac{y^{(k)}}{\|y_1^{(k)}\|}, \frac{y}{\|y_1\|}\right)$$

$$= \min \left\{\frac{1}{\|y_1\|}, \frac{1}{\|y_1^{(k)}\|}\right\} \sin \angle \left(\frac{y^{(k)}}{\|y_1^{(k)}\|}, \frac{y}{\|y_1\|}\right)$$

$$\leq \frac{1}{\|y_1\|} \sin \angle (y^{(k)}, y). \quad \Box$$

Bound (5.3) indicates that how fast  $\sin \angle (s_k, s_{opt})$  converges amounts to how fast  $\sin \angle (y^{(k)}, y)$  tends to zero as k increases. In what follows, we derive an a-priori bound for  $\sin \angle (y^{(k)}, y)$ .

As has been seen,  $(\mu_1, y)$  and  $(\mu_1^{(k)}, z^{(k)})$  are simple eigenpairs of M and  $M_k$ , respectively, and  $(\mu_1^{(k)}, y^{(k)})$  is the Ritz pair approximating the eigenpair  $(\mu_1, y)$  of M. Let  $(y, Y_{\perp})$  be orthogonal. Then the columns of  $Y_{\perp}$  form an orthonormal basis of the orthogonal complement of the subspace spanned by y. It follows from the relation  $My = \mu_1 y$  that

(5.5) 
$$\begin{pmatrix} y^T \\ Y_{\perp}^T \end{pmatrix} M(y, Y_{\perp}) = \begin{pmatrix} \mu_1 & f^T \\ 0 & L \end{pmatrix},$$

where  $f^T = y^T M Y_{\perp}$  and  $L = Y_{\perp}^T M Y_{\perp}$ .

Because the right hand side of (5.5) is block triangular, the eigenvalues of M consist of  $\mu_1$  and the eigenvalues of L. Since  $\mu_1$  is simple,  $L - \mu_1 I$  is nonsingular. The quantity

(5.6) 
$$sep(\mu_1, L) = \|(L - \mu_1 I)^{-1}\|^{-1}$$

(5.4)

is called the separation of  $\mu_1$  and L, and  $sep(\mu_1, L) = \sigma_{\min}(L - \mu_1 I)$ , the smallest singular value of  $L - \mu_1 I$  [28].

Let the columns of  $Z_{\perp}^{(k)}$  be an orthonormal basis of the orthogonal complement of the subspace spanned by  $z^{(k)}$  and  $(z^{(k)}, Z_{\perp}^{(k)})$  be orthogonal. From (4.6) we have  $M_k z^{(k)} = \mu_1^{(k)} z^{(k)}$ , from which it follows that

(5.7) 
$$\begin{pmatrix} (z^{(k)})^T \\ (Z^{(k)}_{\perp})^T \end{pmatrix} M_k(z^{(k)}, Z^{(k)}_{\perp}) = \begin{pmatrix} \mu_1^{(k)} & f_k^T \\ 0 & C_k \end{pmatrix},$$

where  $f_k^T = (z^{(k)})^T M_k Z_{\perp}^{(k)}$  and  $C_k = (Z_{\perp}^{(k)})^T M_k Z_{\perp}^{(k)}$ . Note that the eigenvalues of  $C_k$  are the Ritz values but  $\mu_1^{(k)}$  of M with respect to the subspace  $\widetilde{\mathcal{S}}_k$  defined by (4.4). As a result, by (4.5),  $\mu_1^{(k)}$  is a simple eigenvalue of  $M_k$  and  $sep(\mu_1^{(k)}, C_k) > 0$ . Since  $\mu_1 - \mu_1^{(k)} = \lambda_{opt} - \lambda_k \ge 0, \lambda_k \to \lambda_{opt}$  and  $sep(\mu_1, C_k) \ge sep(\mu_1^{(k)}, C_k) - |\mu_1 - \mu_1^{(k)}|$ , we must have  $sep(\mu_1, C_k) > 0$  for k suitably large.

In our notation, the following result is established in [17].

LEMMA 5.3 ([17]). With the previous notation, let  $\varepsilon_k = \sin \angle (y, \tilde{\mathcal{S}}_k)$ , assume that  $sep(\mu_1, C_k) > 0$ . Then

(5.8) 
$$\sin \angle (y^{(k)}, y) \le \left(1 + \frac{\|M\|}{\sqrt{1 - \varepsilon_k^2} sep(\mu_1, C_k)}\right) \varepsilon_k.$$

Combining (5.3) and (5.8) with (4.33) yields the following result immediately.

THEOREM 5.4. For the unit length eigenvector  $y^T = (y_1^T, y_2^T)^T$  of M associated with its rightmost eigenvalue  $\mu_1$ , assume that  $sep(\mu_1, C_k) > 0$ . Then it holds that

(5.9) 
$$\sin \angle (s_k, s_{opt}) \le c_k \left( 1 + \frac{\|M\|}{\sqrt{1 - \varepsilon_k^2} sep(\mu_1, C_k)} \right) \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^{k+1}$$

where  $\kappa = \frac{\alpha_1 + \lambda_{opt}}{\alpha_n + \lambda_{opt}}$ ,

$$c_k = 2 + \frac{16(\alpha_1 + \lambda_{opt})}{(\alpha_1 - \alpha_n)^2 (1 - t^2)} \left(1 + \frac{k+2}{|\ln t|}\right) \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^2$$

and  $t = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$  (cf. (4.35) and (4.32)).

This theorem indicates that  $s_k$  converges to  $s_{opt}$  at least as fast as  $\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{k+1}$ . Finally, we establish a-priori bounds for the residual norm  $||(A + \lambda_k I)s_k + g||$ . THEOREM 5.5. Suppose  $||s_{opt}|| = ||s_k|| = \Delta$ . Then for  $k = 0, 1, \ldots, k_{\max}$  we have

(5.10) 
$$\|(A+\lambda_k I)s_k + g\| \le (\lambda_{opt} - \lambda_k)\Delta + (\alpha_1 + \lambda_{opt})\|s_{opt} - s_k\|$$

by dropping the higher order small term  $(\lambda_{opt} - \lambda_k) ||s_{opt} - s_k||$ . Proof. From (1.3), we have

$$0 = (A + \lambda_{opt}I)s_{opt} + g = (A + \lambda_kI + (\lambda_{opt} - \lambda_k)I)(s_k + s_{opt} - s_k) + g$$
$$= (A + \lambda_kI)s_k + g + (\lambda_{opt} - \lambda_k)s_k$$
$$+ (A + \lambda_kI)(s_{opt} - s_k) + (\lambda_{opt} - \lambda_k)(s_{opt} - s_k).$$

Therefore, from  $||s_k|| = \Delta$ ,  $\lambda_{opt} - \lambda_k \ge 0$ , and  $\lambda_{opt} \ge 0$ , noting that  $||A + \lambda_{opt}I|| = \alpha_1 + \lambda_{opt}$ , we obtain

$$\begin{aligned} \|(A + \lambda_k I)s_k + g\| &= \|(\lambda_{opt} - \lambda_k)s_k + (A + \lambda_{opt}I)(s_{opt} - s_k)\| \\ &+ (\lambda_{opt} - \lambda_k)\|s_{opt} - s_k\| \\ &\leq (\lambda_{opt} - \lambda_k)\Delta + \|A + \lambda_{opt}I\|\|s_{opt} - s_k\| \\ &+ (\lambda_{opt} - \lambda_k)\|s_{opt} - s_k\| \\ &= (\lambda_{opt} - \lambda_k)\Delta + (\alpha_1 + \lambda_{opt})\|s_{opt} - s_k\| \end{aligned}$$

by dropping the higher order small term  $(\lambda_{opt} - \lambda_k) \|s_{opt} - s_k\|$ .

Keep (5.1) in mind. By substituting bound (4.52) for  $\lambda_{opt} - \lambda_k$  and bound (5.9) for  $\sin \angle (s_k, s_{opt})$ , which is approximately equal to  $||s_{opt} - s_k|| / ||s_{opt}||$  for k sufficiently large, into (5.10), we obtain an *approximate* a-priori bound for  $||(A + \lambda_k I)s_k + g||$ . They illustrate that  $||(A + \lambda_k I)s_k + g||$  is dominated by  $||s_k - s_{opt}||$  and tends to zero at least as fast as  $\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{k+1}$ . Since the resulting bound is not rigorous, we do not write it explicitly.

As a by-product, by exploiting some of the previous results, it is easy to establish an a-priori bound for  $||s_k - s_{opt}||$ , as shown below. With it, we will establish a rigorous a-priori bound for  $||(A + \lambda_k I)s_k + g||$ .

THEOREM 5.6. Suppose  $||s_{opt}|| = ||s_k|| = \Delta$ . Then

(5.11) 
$$\|s_k - s_{opt}\| \le 4\sqrt{\kappa}\Delta\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{k+1},$$

where  $\kappa = \frac{\alpha_1 + \lambda_{opt}}{\alpha_n + \lambda_{opt}}$ .

*Proof.* It follows from [31, Theorem 4.3] and (4.50) that

$$\|s_k - s_{opt}\| \le 2\sqrt{\kappa} \|(I - \pi_k)s_{opt}\|,$$

where  $\pi_k$  is the orthogonal projector onto  $\mathcal{K}_k(g, A)$ . Therefore, (5.11) follows from the above relation and (4.51) directly.  $\square$ 

This theorem is the same as (4.18b) in [31]. With it, by substituting bound (4.52) for  $\lambda_{opt} - \lambda_k$  and bound (5.6) for  $||s_k - s_{opt}||$  into (5.10), it is straightforward to obtain the following rigorous a-priori bound for  $||(A + \lambda_k I)s_k + g||$ .

THEOREM 5.7. Suppose  $||s_{opt}|| = ||s_k|| = \Delta$ , and let  $||r_k|| = ||(A + \lambda_k I)s_k + g||$ . Then for k suitably large we have

$$\|r_k\| \le \left(\frac{4\eta_{k1}\Delta^2}{\beta_0} + 8(\alpha_1 + \lambda_{opt})\eta_{k2}\Delta^3\right) \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2(k+1)} + 4\sqrt{\kappa}\Delta(\alpha_1 + \lambda_{opt}) \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{k+1}$$

with the factors  $\eta_{k1}$  and  $\eta_{k2}$  defined by (4.40) and (4.41), respectively.

Clearly, the second term of the right hand side in (5.12) dominates the bound soon as k increases.

Summarizing the results obtained in these two sections, we conclude that the convergence rates of  $\lambda_{opt} - \lambda_k$  and  $q(s_k) - q(s_{opt})$  are the squares of  $\sin \angle (s_k, s_{opt})$ ,  $||s_k - s_{opt}||$  and  $||(A + \lambda_k I)s_k + g||$ . This means that the convergence of  $q(s_k)$  and  $\lambda_k$  uses roughly half of the iterations as needed for  $s_k$  and  $||(A + \lambda_k I)s_k + g||$  when the three errors and  $||(A + \lambda_k I)s_k + g||$  are reduced to about the same level.

6. Numerical examples. In this section, we compare our a-priori bounds in this paper with the four errors in the GLTR method:  $\lambda_{opt} - \lambda_k$ ,  $\sin \angle (s_k, s_{opt})$ ,  $q(s_k) - q(s_{opt})$  and  $||(A + \lambda_k I)s_k + g||$ , respectively. In order to give a full justification on our a-priori bounds, we test TRS's with A having different representative eigenvalue distributions and various condition numbers  $\kappa$ 's.

All the experiments were performed on an Intel Core (TM) i7, CPU 3.6GHz, 8 GB RAM using MATLAB 2017A under the Microsoft Windows 10 64 bit.

Throughout this section, we always take n = 10000 and a fixed trust-region radius  $\Delta = 1$ , and the vector g is a unit length vector generated by the Matlab builtin function randn(n, 1). Since the uncomputable  $\varepsilon_k$  tends to zero as k increases, we take  $\varepsilon_k = 0$  in the denominator of the bound of Theorem 5.4. We exploit the Matlab functions eigs and svds with the stopping tolerance  $10^{-14}$  to compute  $\lambda_{opt}$ ,  $s_{opt}$  and ||M||, respectively, use them as the "exact" ones, and then compute  $q(s_{opt})$ . To maintain the numerical orthogonality of the Lanczos basis vectors, in finite precision arithmetic, we use the symmetric Lanczos process with complete reorthogonalization.

When assessing our a-priori bounds, we should note that the bounds may be often large overestimates of the true errors, but that there are cases where the actual errors and their bounds become close to each other when k increases. However one cannot say that a certain kind of bound is the sharpest in all cases. Possible overestimates of our bounds are not surprising, since the bounds are established in the worst case and the factors in front of  $\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{k+1}$  or  $\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{2(k+1)}$  are the largest possible. Our aim consists in giving a-priori bounds which may yield sharp estimates of the asymptotic convergence rates even if those factors in front of the bounds are large.

**Example 1.** This example is randomly generated, where the symmetric indefinite sparse matrix is generated by the Matlab function

(6.1) 
$$A = sprandsym(n, density, rc)$$

where rc is a vector of A's eigenvalues, and we take density = 0.01. We construct two A's by taking two different rc's.

**Example 1a.** The elements of rc are evenly distributed among [-2, 2]:

$$\operatorname{rc}(i) = \begin{cases} -2 + \frac{4}{n}(i-1), & i \leq \frac{n}{2} \\ 2 - \frac{4}{n}(n-i), & i > \frac{n}{2} \end{cases}$$

**Example 1b.** We take the *i*th element rc(i) of rc as

$$\operatorname{rc}(i) = \begin{cases} -e^{\frac{2i}{n}}, & i \leq \frac{n}{2} \\ e^{\frac{2i-n}{n}}, & i > \frac{n}{2}. \end{cases}$$

Therefore, the eigenvalues of A lies in the union  $[-e, -1.0002] \cup [1.0002, e]$ , and their magnitudes monotonically increases at the rate  $e^{2/n}$  at each subinterval.

In Tables 1–2 and Figures 1–2, we list the results and compare the a-priori bounds with  $\lambda_{opt} - \lambda_k$ ,  $\sin \angle (s_k, s_{opt})$ ,  $q(s_k) - q(s_{opt})$  and  $||(A + \lambda_k I)s_k + g||$ , respectively.

**Example 2.** We take A to be diagonal with translated Chebyshev nodes on the diagonal. This problem is tested in [31]. The zero nodes of the *n*th Chebyshev polynomial in [-1, 1] are given by

$$t_{jn} = \cos \frac{(2j-1)\pi}{2n}, \ 1 \le j \le n.$$

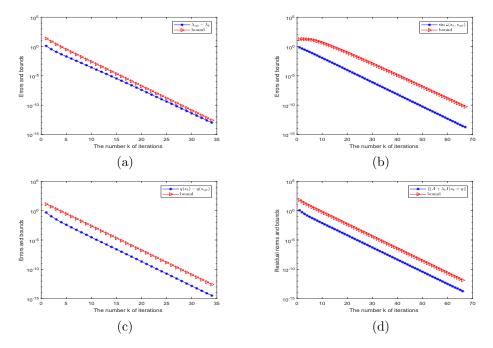


FIG. 1. Example 1a. (a):  $\lambda_{opt} - \lambda_k$  and its bound (4.52); (b):  $\sin \angle (s_k, s_{opt})$  and its bound (5.9); (c):  $q(s_k) - q(s_{opt})$  and its bound (4.48); (d):  $||(A + \lambda_k I)s_k + g||$  and its bound (5.12).

TABLE 1 $Example \ 1a.$ 

Para	meters in Exam	ple 1a, where	$t = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$ (cf	(4.32)) in all	the tables.	
$\alpha_1$	$lpha_n$	$\kappa$	t	$\lambda_{opt}$	$q(s_{opt})$	
2.0000	-2.0000	18.1481	0.6198	2.2333	-1.4770	
		$\lambda_{opt} - \lambda_k$ and	d its bound (4	4.52).		
k	X	$\lambda_{opt} - \lambda_k$		boun	d	
34	1	.0658e - 13		2.670	8e - 13	
	s	$\operatorname{in} \angle(s_k, s_{opt})$	and its bound	l (5.9).		
k	$\sin \angle (s_k, s_{opt})$			bound		
67	1	.8249e - 14		5.462	2e - 11	
	$\ (A$	$+\lambda_k I)s_k + g$	and its boun	nd $(5.12)$ .		
k		$(A + \lambda_k I)s_k +$	$\vdash g \parallel$	boun	d	
66	1.8928e - 14			1.3984e - 12		
	q(	$(s_k) - q(s_{opt})$	and its bound	(4.48).		
k	q	$(s_k) - q(s_{opt})$		boun	d	
34	3	.3307e - 15		2.521	9e - 13	

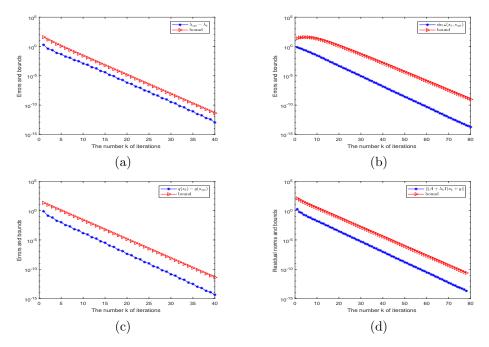


FIG. 2. Example 1b. (a):  $\lambda_{opt} - \lambda_k$  and its bound (4.52); (b):  $\sin \angle (s_k, s_{opt})$  and its bound (5.9); (c):  $q(s_k) - q(s_{opt})$  and its bound (4.48); (d):  $||(A + \lambda_k I)s_k + g||$  and its bound (5.12).

TABLE 2 Example 1b.

		Parameters	in Example	1b.			
$\alpha_1$	$\alpha_n$	$\kappa$	t	$\lambda_{opt}$	$q(s_{opt})$		
2.7183	-2.7183	29.0828	0.6872	2.9119	-1.7907		
		$\lambda_{opt} - \lambda_k$ and	l its bound (4	.52).			
k	$\lambda_{opt} - \lambda_k$			bound			
40	1	.1013e - 13		4.33	4.3314e - 12		
	s	$\operatorname{in} \angle(s_k, s_{opt})$ a	and its bound	(5.9).			
k	$\sin \angle (s_k, s_{opt})$			bound			
80	1	1.8667e - 14			9.6252e - 10		
	$\ (A$	$+\lambda_k I)s_k + g $	and its bour	nd $(5.12)$ .			
k	$\ (A+\lambda_k I)s_k+g\ $			bound			
78	2.0334e - 14			2.3683e - 11			
	q(	$(s_k) - q(s_{opt})$ a	and its bound	(4.48).			
k	q	$q(s_k) - q(s_{opt})$			bound		
40	4	.4409e - 15		4.14	72e - 12		

Given an interval [a, b], the linear transformation

$$y = \left(\frac{b-a}{2}\right) \left(x + \left(\frac{a+b}{b-a}\right)\right)$$

maps  $x \in [-1, 1]$  to  $y \in [a, b]$ . The *n*th translated Chebyshev zero nodes on [a, b] are

$$t_{jn}^{[a,b]} = \left(\frac{b-a}{2}\right) \left(t_{jn} + \left(\frac{a+b}{b-a}\right)\right),$$

which monotonically decreases for j = 1, 2, ..., n/2 and increases for j = n/2, ..., n, respectively, and cluster at [a,b] = [-5,5] and  $A = diag\{t_{jn}^{[a,b]}\}, j = 1, 2, \dots, n$ .

In Figure 3 and Table 3, we draw and list the results.

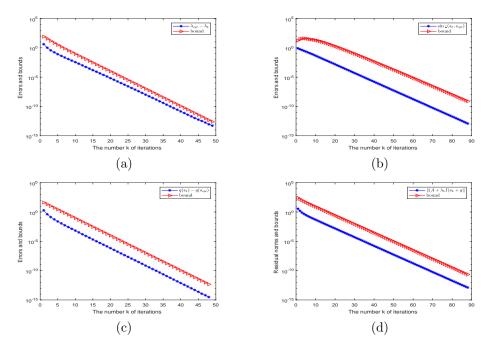


FIG. 3. Example 2. (a):  $\lambda_{opt} - \lambda_k$  and its bound (4.52); (b):  $\sin \angle (s_k, s_{opt})$  and its bound (5.9); (c):  $q(s_k) - q(s_{opt})$  and its bound (4.48); (d):  $||(A + \lambda_k I)s_k + g||$  and its bound (5.12).

**Example 3.** We use the Strakoš matrix [19, p.16], which is used to test the behavior of the symmetric Lanczos method for the eigenvalue problem. The matrix A is diagonal with the eigenvalues

$$\alpha_i = \alpha_1 + \left(\frac{i-1}{n-1}\right)(\alpha_n - \alpha_1)\rho^{n-i},$$

 $i = 1, 2, \ldots, n$ . The parameter  $\rho$  controls the eigenvalue distribution. The large eigenvalues of A are well separated for  $\rho < 1$ . We take  $\alpha_1 = 8$ ,  $\alpha_n = -2$  and  $\rho = 0.99$ .

In Figure 4 and Table 4, we depict and list the results.

Example 4. We take

TABLE 3 Example 2.

		Parameter	s in Example	2.		
$\alpha_1$	$\alpha_n$	$\kappa$	t	$\lambda_{opt}$	$q(s_{opt})$	
5.0000	-5.0000	34.9455	0.7106	5.2946	-2.9367	
		$\lambda_{opt} - \lambda_k$ and	l its bound (4	.52).		
k	$\lambda_{opt} - \lambda_k$			bound		
49	5	.4197e - 14		2.4375e - 13		
	S	$\operatorname{in} \angle(s_k, s_{opt})$	and its bound	(5.9).		
k	$\sin \angle (s_k, s_{opt})$			bound		
88	1	.2208e - 13		7.768	88e - 10	
	$\ (A$	$+\lambda_k I)s_k + g$	and its boun	d $(5.12)$ .		
k	$\ (A+\lambda_k I)s_k+g\ $			bound		
88	1.3066e - 13 $2.1418e - 11$		1.3066e - 13		18e - 11	
	q(	$(s_k) - q(s_{opt}) =$	and its bound	(4.48).		
k	q	$q(s_k) - q(s_{opt})$		bound		
48	3	.1086e - 15		4.712	24e - 13	

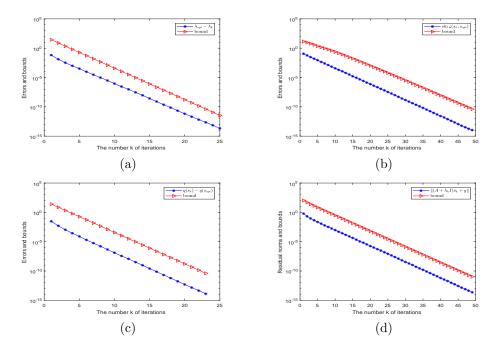


FIG. 4. Example 3. (a):  $\lambda_{opt} - \lambda_k$  and its bound (4.52); (b):  $\sin \angle (s_k, s_{opt})$  and its bound (5.9); (c):  $q(s_k) - q(s_{opt})$  and its bound (4.48); (d):  $||(A + \lambda_k I)s_k + g||$  and its bound (5.12).

TABLE 4 Example 3.

$\alpha_1$	$\alpha_n$	$\kappa$	t	$\lambda_{opt}$	$q(s_{opt})$	
8.0000	-2.0000	11.1518	0.5391	2.9850	-1.9893	
		$\lambda_{opt} - \lambda_k$ and	l its bound (4	.52).		
k	λ	$\lambda_{opt} - \lambda_k$		bound		
25	2	2.0872e - 14 $3.4477e -$			77e - 12	
	S	$\operatorname{in} \angle(s_k, s_{opt})$ a	and its bound	(5.9).		
k	$\sin \angle (s_k, s_{opt})$			bound		
49	1	.0765e - 14		4.126	58e - 11	
	$\ (A$	$+\lambda_k I)s_k + g $	and its bour	nd $(5.12)$ .		
k	$\ (A+\lambda_k I)s_k+g\ $		bound			
49	2	2.2856e - 14 $1.0440e - 11$		40e - 11		
	q(	$(s_k) - q(s_{opt})$ a	and its bound	(4.48).		
k	q	$q(s_k) - q(s_{opt})$ bound		ıd		
23	-	.2879e - 14		0.000	06e - 11	

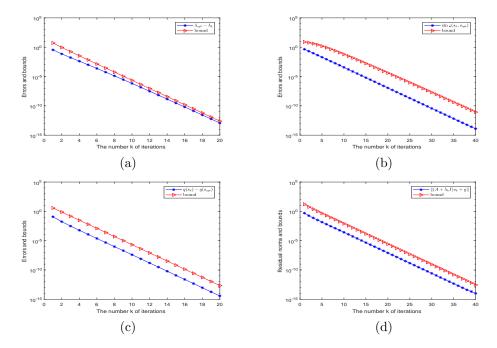


FIG. 5. Example 4. (a):  $\lambda_{opt} - \lambda_k$  and its bound (4.52); (b):  $\sin \angle (s_k, s_{opt})$  and its bound (5.9); (c):  $q(s_k) - q(s_{opt})$  and its bound (4.48); (d):  $||(A + \lambda_k I)s_k + g||$  and its bound (5.12).

## TABLE 5 Example 4.

$\alpha_1$	$\alpha_n$	$\kappa$	t	$\lambda_{opt}$	$q(s_{opt})$	
1.0000	-0.9997	6.9000	0.4485	1.3386	-1.1155	
		$\lambda_{opt} - \lambda_k$ an	d its bound (4	.52).		
k	λ	$\lambda_{opt} - \lambda_k$		bour	ıd	
20	1.1702e - 13 $2.4462e - 13$			52e - 13		
	S	$\operatorname{in} \angle(s_k, s_{opt})$	and its bound	(5.9).		
k	$\sin \angle (s_k, s_{opt})$			bound		
40	1	1.2388e - 14		8.458	8.4588e - 12	
	$\ (A$	$+\lambda_k I)s_k + g$	$\parallel$ and its bour	nd $(5.12)$ .		
k	$\ (A+\lambda_k I)s_k+g\ $			bound		
40	1	1.0193e - 14 $2.9026e - 13$				
	q(	$(s_k) - q(s_{opt})$	and its bound	(4.48).		
k	$q(s_k) - q(s_{opt})$ bound		nd			
20	3	.7748e - 15		1 116	63e - 14	

with G generated by randn(n) and A := A/||A||. The eigenvalues of A exhibit normal distribution characteristics. Figure 5 and Table 5 give the results.

We have observed from the figures and tables that, for all the test problems, (i) the corresponding bounds predict the convergence rates of  $\lambda_{opt} - \lambda_k$ ,  $\sin \angle (s_k, s_{opt})$ ,  $q(s_k) - q(s_{opt})$  and  $||(A + \lambda_k I)s_k + g||$  accurately and (ii) the bounds are very close to their values in most of the cases, especially for  $\lambda_{opt} - \lambda_k$  and  $q(s_k) - q(s_{opt})$ .

The tables and figures also indicate that (i) the errors  $\lambda_{opt} - \lambda_k$  and  $q(s_k) - q(s_{opt})$ as well as their bounds use roughly half of the iterations needed for  $\sin \angle (s_k, s_{opt})$ and  $||(A + \lambda_k I)s_k + g||$  as well as their bounds to achieve approximately the same tolerance and (ii) the condition number  $\kappa$  affects the convergence of the GLTR method: the bigger  $\kappa$  is, the more iterations the method needs to reduce each of  $\lambda_{opt} - \lambda_k$ ,  $\sin \angle (s_k, s_{opt}), q(s_k) - q(s_{opt})$  and  $||(A + \lambda_k I)s_k + g||$  to approximately the same level.

7. Conclusion. The GLTR method has been receiving high attention both theoretically and numerically. Some a-priori bounds have been obtained for  $q(s_k) - q(s_{opt})$ and  $||s_k - s_{opt}||$  in the literature, but there has been no quantitative analysis and result on  $\lambda_{opt} - \lambda_k$  and  $||(A + \lambda_k I)s_k + g||$ . Starting with the mathematical equivalence of the solution of TRS (1.1) and the eigenvalue problem of the augmented matrix M, we have established a-priori bounds for  $\lambda_{opt} - \lambda_k$ ,  $\sin \angle (s_k, s_{opt}), q(s_k) - q(s_{opt})$ , and the residual norm  $||(A + \lambda_k I)s_k + g||$ . The results prove how the three errors and the residual norm decrease as the subspace dimension increases. Numerical results have confirmed that our bounds are realistic and they accurately predict the true convergence rates of the three errors and the residual norm in the GLTR method.

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