On Convergence of the Inexact Rayleigh Quotient Iteration with the Lanczos Method Used for Solving Linear Systems

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Abstract

For the Hermitian inexact Rayleigh quotient iteration (RQI), the author has established new general convergence results, independent of iterative solvers for inner linear systems. The theory shows that the method converges at least quadratically under a new condition, called the uniform positiveness condition, that may allow inner tolerance \( \xi_k \geq 1 \) at outer iteration \( k \) and is fundamentally different from the condition \( \xi_k \leq \xi < 1 \) with \( \xi \) a constant not near one commonly used in literature. In this paper we first consider the convergence of the inexact RQI with the unpreconditioned Lanczos method for the linear systems. Some attractive properties are derived for the residuals of the linear systems obtained by the Lanczos method. Based on them and the new general convergence results, we make a more refined analysis and establish convergence results. It is proved that the inexact RQI with Lanczos converges quadratically provided that \( \xi_k \leq \xi \) with a constant \( \xi > 1 \), that is, the linear systems are allowed to be solved with no accuracy in the sense of solving the linear systems. The results are fundamentally different from the existing quadratic convergence results and have an impact on effective implementations of the method. We extend the new theory to the inexact RQI with a tuned preconditioned Lanczos for the linear systems. Based on the new theory, we can design practical criteria to best control \( \xi_k \) to achieve quadratic convergence and implement the method more effectively than ever before. Numerical experiments confirm our theory.

Keywords. Hermitian, inexact RQI, convergence, quadratic, inner iteration, outer iteration, unpreconditioned Lanczos, tuned preconditioned Lanczos

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1 Introduction

We consider the problem of computing an eigenvalue \( \lambda \) and the associated eigenvector \( x \) of a large and possibly sparse Hermitian matrix \( A \in \mathbb{C}^{n \times n} \), i.e.,

\[
Ax = \lambda x.
\]

Throughout the paper, we are interested in the eigenvalue \( \lambda_1 \) closest to a target \( \sigma \) and its corresponding eigenvector \( x_1 \) in the sense that

\[
|\lambda_1 - \sigma| < |\lambda_2 - \sigma| \leq \cdots \leq |\lambda_n - \sigma|.
\]
Suppose that $\sigma$ is between $\lambda_1$ and $\lambda_2$. Then we have

$$|\lambda_1 - \sigma| < \frac{1}{2}|\lambda_1 - \lambda_2|.$$  (3)

We denote by $x_1, x_2, \ldots, x_n$ are the unit length eigenvectors associated with $\lambda_1, \lambda_2, \ldots, \lambda_n$. For brevity we denote $(\lambda_1, x_1)$ by $(\lambda, x)$. There are a number of methods for solving this kind of problem, such as the inverse iteration [13], the Rayleigh quotient iteration (RQI) [13], the Lanczos method and its shift-invert variant [13], the Davidson method and the Jacobi–Davidson method [20, 22]. However, except the standard Lanczos method, these methods and shift-invert Lanczos require the exact solution of a possibly ill-conditioned linear system at each iteration. This is generally very difficult and even impractical by a direct solver since a factorization of a shifted $A$ may be too expensive. So one generally resorts to iterative methods to solve inner linear systems, called inner iterations. We call updates of approximate eigenpairs outer iterations. A combination of inner and outer iterations yields an inner-outer iterative eigensolver, also called an inexact eigensolver.

The inexact inverse iteration and the inexact RQI are the simplest and most basic inexact eigensolvers. They not only have their own rights, but also are key ingredients of some other more sophisticated and practical inexact solvers, such as subspace iteration [15] and the Jacobi–Davidson method. So one must first analyze their convergence. This is the first step towards better understanding and analyzing those more practical inexact solvers.

For $A$ Hermitian or non-Hermitian, general theory on the inexact RQI can be found in Berns-Müller and Spence [1], Simoncini and Eldén [16], Smit [18], van den Eshof [21] and Xue and Elman [23]. Let $\|r_k\|$ be the residual norm of the approximate eigenpair at outer iteration $k$. They prove that the inexact RQI converges cubically if $\xi_k = O(\|r_k\|)$ and quadratically if $\xi_k \leq \xi < 1$ with a constant $\xi$ not near one. For the inexact RQI, to the author’s best knowledge, there is no result available on linear convergence and its conditions. However, the condition $\xi_k \leq \xi < 1$, though seemingly natural, is generally stringent. The author in [8] has revisited the convergence of the inexact RQI independent of iterative solvers and presents a new general convergence theory. It has been proved that the inexact RQI converges quadratically under a so-called uniform positiveness condition which is fundamentally different from and weaker than the condition $\xi_k \leq \xi < 1$. Based on it, the author has established a number of new results on the inexact RQI with MINRES. It appears that the method generally converges cubically for $\xi_k \leq \xi < 1$ once $\xi$ is not near one, converges quadratically provided that $\xi_k = 1 - O(\|r_k\|)$ and converges linearly provided that $\xi_k = 1 - O(\|r_k\|^2)$. In comparisons with the existing ones, these conditions are much more relaxed and can be exploited to implement the method more effectively than ever before.

RQI and the inexact RQI are closely related to the simplified exact JD method without subspace acceleration and its inexact version for Hermitian and non-Hermitian cases, respectively; see [11, 16, 17, 19, 21]. The two exact versions are mathematically equivalent [16, 17], and the two inexact versions are equivalent too if an $m + 1$-step and $m$-step Galerkin–Krylov type method without preconditioner, e.g., the conjugate gradient method and the Lanczos (Arnoldi) method, is used for solving the linear systems arising in the inexact RQI and the inexact JD method at each outer iteration [16], respectively. The simplified inexact JD method with a preconditioned Galerkin–Krylov solver is equivalent to the inexact RQI when the preconditioner is modified by a rank-1 matrix [4]. This equivalence is generalized to the exact and inexact two sided RQI and the simplified exact and inexact two-sided JD method [7] if the biconjugate gradient (BiCG) method without preconditioner is used to solve inner linear systems.

In this paper, we revisit the inexact RQI with the (unpreconditioned and tuned pre-
have been established for the inexact RQI with Lanczos in the literature, one treats the residuals obtained by the Lanczos method as general ones and simply takes their norms but ignores their directions. A direct consequence is that all existing convergence results require $\xi_k \leq \xi < 1$, and fundamental effects of residual directions on convergence may have not been reasonably exposed. Remarkably, we first establish some attractive properties of the residuals obtained by the Lanczos method for the linear systems. By fully exploiting them, we take a different analysis approach to consider the convergence of the inexact RQI with Lanczos. Based on the new general convergence theory, we derive a number of insightful results that are not only stronger than but also fundamentally different from the ones available in the literature.

For the inexact RQI with the unpreconditioned Lanczos, the most remarkable results we will prove are that the inexact RQI with Lanczos converges quadratically provided that $\xi_k \leq \xi$ with a constant $\xi$ that is allowed to be bigger than one and it converges linearly even if $\xi_k \gg 1$ and is up to as large as $O(\frac{1}{\|r_k\|})$. Therefore, in order to achieve quadratic convergence, we allow the Lanczos method to solve the linear systems with no accuracy in the sense of solving the linear systems. These results have a strong impact on effective implementations of the method. For quadratic convergence, compared with prevailing implementations of the method, they indicate that the method now converges much more easily and the computational cost of solving the linear systems is generally reduced much more considerably. Numerical experiments demonstrate that our new implementation is twice to four times as fast as the prevailing implementations and the method still converges smoothly and quickly when $\xi_k$ increases up to $10^4 \sim 10^7$.

As byproducts, similar to those done in [8, 16], we establish lower bounds on the norms of approximate solutions $w_{k+1}$ of the linear systems obtained by the unpreconditioned Lanczos. We show that $\|w_{k+1}\|$ is always $O(\frac{1}{\|r_k\|^2})$ no matter the inexact RQI with Lanczos converges cubically or quadratically. Therefore, it is distinctive that $\|w_{k+1}\|$ itself obtained by Lanczos cannot reveal the convergence behavior of the inexact RQI and cannot be used to design stopping criteria for inner iterations. Making use of these bounds, we present a simpler but weaker quadratic convergence result. Finally, as a global result, similar to that for the inexact RQI with MINRES [16], we derive a relationship between $\|r_k\|$ and $\|r_{k+1}\|$, starting with an arbitrary vector instead of a reasonably good one. We will see that, unlike the exact RQI, the inexact RQI with Lanczos loses the residual monotonic decreasing property for an arbitrary starting vector.

It appears [8, 5, 23] that it is beneficial to precondition each shifted inner linear system with a tuned preconditioner, which can be much more effective than a usual one. We study the convergence of the inexact RQI with a tuned preconditioned Lanczos and show that our main theory in the unpreconditioned case can be nontrivially extended to the tuned preconditioned case.

The paper is organized as follows. In Section 2, we review the inexact RQI and the new general convergence theory of [8] on the inexact RQI. In Section 3, we present convergence results on the inexact RQI with the unpreconditioned Lanczos Lanczos for solving inner linear systems. In Section 4, we extend the theory to the inexact RQI with a tuned preconditioned Lanczos method for solving inner linear systems. We perform numerical experiments to confirm our results in Section 5. Finally, we end up with some concluding remarks in Section 6.

Throughout the paper, denote by the superscript * the conjugate transpose of a matrix or vector, by $I$ the identity matrix of order $n$, by $\parallel \cdot \parallel$ the vector 2-norm and the matrix spectral norm, and by $\lambda_{\min}, \lambda_{\max}$ the smallest and largest eigenvalues of $A$, respectively.
2 The inexact RQI and general convergence theory

RQI is a famous iterative algorithm and its locally cubic convergence for Hermitian problems is very attractive [13]. It plays a crucial role in some practical effective algorithms, e.g., the QR algorithm, [6, 13]. Assume that the unit length $u_k$ is a reasonably good approximation to $x$. Then the Rayleigh quotient $\theta_k = u_k^* A u_k$ is a good approximation to $\lambda$ too. RQI [6, 13] computes a new approximation $u_{k+1}$ to $x$ by solving the shifted inner linear system

$$(A - \theta_k I)w = u_k$$

for $w_{k+1}$ and updating $u_{k+1} = w_{k+1}/\|w_{k+1}\|$ and iterates until convergence. It is known [1, 10, 13] that if $|\lambda - \theta_0| < \frac{1}{2} \min_{j=2,3,...,n} |\lambda - \lambda_j|$ then RQI (asymptotically) converges to $\lambda$ and $x$ cubically. So we can assume that the eigenvalues of $A$ are ordered as

$$|\lambda - \theta_k| < |\lambda_2 - \theta_k| \leq \cdots \leq |\lambda_n - \theta_k|.$$  

(5)

With this ordering and $\lambda_{\min} \leq \theta_k \leq \lambda_{\max}$, we have

$$|\lambda - \theta_k| < \frac{1}{2} |\lambda - \lambda_2|.$$  

(6)

An obvious drawback of RQI is that at each iteration $k$ we need the exact solution $w_{k+1}$ of $(A - \theta_k I)w = u_k$. For a large $A$, it is generally very expensive and even impractical to solve it by a direct solver due to excessive memory and/or computational cost. So we must resort to iterative solvers to get an approximate solution of it. This leads to the inexact RQI. (4) is solved by an iterative solver and an approximate solution $w_{k+1}$ satisfies

$$(A - \theta_k I)w_{k+1} = u_k + \xi_k d_k, \quad u_{k+1} = w_{k+1}/\|w_{k+1}\|$$  

(7)

with $0 < \xi_k \leq \xi$, where $\xi_k d_k$ with $\|d_k\| = 1$ is the residual of $(A - \theta_k I)w = u_k$, $d_k$ is the residual direction vector and $\xi_k$ is the relative residual norm (inner tolerance) as $\|u_k\| = 1$ and may change at every outer iteration $k$. This process is summarized as Algorithm 1. If $\xi_k = 0$ for all $k$, Algorithm 1 becomes the exact RQI.

**Algorithm 1** The inexact RQI

1: Choose a unit length $u_0$, an approximation to $x$.
2: for $k = 0, 1, \ldots$ do
3: \hspace{1em} $\theta_k = u_k^* A u_k$.
4: \hspace{1em} Solve $(A - \theta_k I)w = u_k$ for $w_{k+1}$ by an iterative solver with
5: \hspace{2em} $\|(A - \theta_k I)w_{k+1} - u_k\| = \xi_k \leq \xi$.
6: $u_{k+1} = w_{k+1}/\|w_{k+1}\|$.
7: If convergence occurs, stop.
8: end for

There are a number of general quadratic convergence results in the literature, e.g., [1, 16, 18, 21], all under the same condition on $\xi_k \leq \xi < 1$ that is seemingly a very natural requirement. In [8], new general convergence results have been given under a new condition.
that is fundamentally different and can relax $\xi_k$ very much. To present the results, we decompose $u_k$ and $d_k$ into the orthogonal direct sums

\begin{align}
  u_k &= x \cos \phi_k + e_k \sin \phi_k, \quad e_k \perp x, \\
  d_k &= x \cos \psi_k + f_k \sin \psi_k, \quad f_k \perp x
\end{align}

with $\|e_k\| = \|f_k\| = 1$ and $\phi_k = \angle(u_k, x)$, $\psi_k = \angle(d_k, x)$. Here without loss of generality and for brevity, we suppose that $\theta_k$ is the acute angle between $u_k$ and $x$. Given this, we should stress that $\cos \psi_k$ is either positive or negative depending on $d_k$. Note that (7) can be written as

$$
(A - \theta_k I)w_{k+1} = (\cos \phi_k + \xi_k \cos \psi_k) x + (e_k \sin \phi_k + \xi_k f_k \sin \psi_k).
$$

Inverting $A - \theta_k I$ gives

$$
w_{k+1} = (\lambda - \theta_k)^{-1} (\cos \phi_k + \xi_k \cos \psi_k) x + (A - \theta_k I)^{-1} (e_k \sin \phi_k + \xi_k f_k \sin \psi_k).
$$

Define $\|r_k\| = \|(A - \theta_k I)u_k\|$. Then by (6) we get $|\lambda_2 - \theta_k| > \frac{\lambda_2 - \lambda}{2}$. So it is known from [13] Theorem 11.7.1 that

$$
\frac{\|r_k\|}{\lambda_{\text{max}} - \lambda_{\text{min}}} \leq \sin \phi_k \leq \frac{2\|r_k\|}{|\lambda_2 - \lambda|},
$$

We comment that $\lambda_{\text{max}} - \lambda_{\text{min}}$ is the spectrum spread of $A$ and $|\lambda_2 - \lambda|$ is the gap or separation of $\lambda$ and the other eigenvalues of $A$.

Before proceeding, we define

$$
\beta = \frac{\lambda_{\text{max}} - \lambda_{\text{min}}}{|\lambda_2 - \lambda|}
$$

throughout the paper.

**Theorem 1.** If the uniform positiveness condition

$$
|\cos \phi_k + \xi_k \cos \psi_k| \geq c
$$

is satisfied with a constant $c > 0$ uniformly independent of $k$, then

$$
\tan \phi_{k+1} \leq 2\beta \frac{\sin \phi_k + \xi_k \sin \psi_k}{|\cos \phi_k + \xi_k \cos \psi_k|}\cos^2 \phi_k
$$

that is, the inexact RQI converges quadratically at least for uniformly bounded $\xi_k \leq \xi$ with $\xi$ a moderate constant.

**Theorem 2.** If the uniform positiveness condition [13] holds, then

$$
\|r_{k+1}\| \leq \frac{8\beta^2 \xi_k}{c|\lambda_2 - \lambda|}\|r_k\|^2 + O(\|r_k\|/3).
$$

We make some comments on the above two theorems.

**Remark 1.** They illustrate that it is the size of $|\cos \phi_k + \xi_k \cos \psi_k|$ other than $\xi_k \leq \xi < 1$ that is critical in convergence.

**Remark 2.** If $\xi_k = 0$ for all $k$, then the inexact RQI reduces to the exact RQI and Theorems [14] show the cubic convergence: $\tan \phi_{k+1} \leq \frac{2\beta}{\cos \phi_k} \sin^3 \phi_k$ and $\|r_{k+1}\| = O(\|r_k\|^3)$.
If the linear systems are solved with decreasing tolerance \( \xi_k = O(\sin \phi_k) = O(\|r_k\|) \), then we have the cubic convergence: \( \tan \phi_{k+1} = O(\sin^3 \phi_k) \) and \( \|r_{k+1}\| = O(\|r_k\|^3) \).

**Remark 3.** If \( \cos \psi_k \) is positive, the uniform positiveness condition holds for any uniformly bounded \( \xi_k \leq \xi \) with \( \xi \) a moderate constant. So we may have \( \xi \geq 1 \) considerably. If \( \cos \psi_k \) is negative, the uniform positiveness condition \( |\cos \phi_k + \xi_k \cos \psi_k| \geq c \) means that

\[
\xi_k \leq \frac{c - \cos \phi_k}{\cos \psi_k}
\]

if \( \cos \phi_k + \xi_k \cos \psi_k \geq c \) with \( c \leq 1 \) is required and

\[
\xi_k \geq \frac{c + \cos \phi_k}{-\cos \psi_k}
\]

if \( -\cos \phi_k - \xi_k \cos \psi_k \geq c \) is required. So the size of \( \xi_k \) critically depends on that of \( \cos \psi_k \), and for a given \( c \) we may have \( \xi_k \approx 1 \) and even \( \xi_k > 1 \). Obviously, without the information on \( \cos \psi_k \), it would be impossible to access or estimate \( \xi_k \). As a general convergence result, however, its significance and importance consist in that it reveals a new remarkable fact: It appears first time that (13) may allow \( \xi_k \) to be relaxed (much) more than that used in all known literatures and meanwhile preserves the same convergence rate of outer iteration. As a result, the condition \( \xi_k \leq \xi < 1 \) with constant \( \xi \) not near one may be stringent and unnecessary for the quadratic convergence of the inexact RQI, independent of iterative solvers for the linear systems. The new condition has a strong impact on practical implementations as we must use a certain iterative solver, e.g., the very popular MINRES method and the Lanczos method (SYMMLQ) for solving \((A - \theta_k I)w = u_k\). We will see that \( \cos \psi_k \) is critically iterative solver dependent. For Lanczos, \( \cos \psi_k \) has some very attractive properties, by which we can precisely determine bounds for \( \xi_k \) in Section 3 which are much more relaxed than those in the literature. For MINRES, we refer to [8] for \( \cos \psi_k \) and \( \xi_k \), where \( \cos \psi_k \) and \( \xi_k \) are fundamentally different from those obtained by Lanczos.

### 3 Convergence of the inexact RQI with the unpreconditioned Lanczos

The previous results and discussions are for general purpose, independent of iterative solvers for \((A - \theta_k I)w = u_k\). Since we have \( \lambda_{\min} \leq \theta_k \leq \lambda_{\max} \), the matrix \( A - \theta_k I \) is Hermitian indefinite. The Lanczos method is a popular Krylov subspace iterative solver for Hermitian linear systems [14]. The method fits into the inexact RQI nicely, leading to the inexact RQI with Lanczos.

We briefly review the Lanczos method for solving [4]. At outer iteration \( k \), taking the starting vector \( v_1 \) to be \( u_k \), the \( m \)-step Lanczos process on \( A - \theta_k I \) can be written as

\[
(A - \theta_k I)V_m = V_mT_m + t_{m+1}v_{m+1}e_m^*,
\]

where the columns of \( V_m = (v_1, \ldots, v_m) \) form an orthonormal basis of the Krylov subspace \( K_m(A, \theta_k I, u_k) = K_m(A, u_k) \) and \( T_m = (t_{ij}) = V_m^*(A - \theta_k I)V_m \) is an \( m \times m \) Hermitian tridiagonal matrix [13, 14].

Taking the zero vector as an initial guess to the solution of \((A - \theta_k I)w = u_k\), the Lanczos method [6, 12, 14] extracts the approximate solution \( w_{k+1} = V_m\hat{y} \) to \((A - \theta_k I)w = u_k\) from \( K_m(A, u_k) \), where \( \hat{y} \) is the solution of the Hermitian tridiagonal linear system \( T_m\hat{y} = e_1 \) with \( e_1 \) being the first coordinate vector of dimension \( m \).

The Lanczos method is mathematically equivalent to the conjugate gradient method and has the optimality that the error of the approximate solution is minimal with respect
to the energy norm over the given Krylov subspace when the linear system is Hermitian positive definite [13]. For indefinite linear systems, it does not have any kind of optimality. For our case, the linear system \((A - \theta_k I)w = u_k\) is not only indefinite but also increasingly ill conditioned as \(\theta_k \to \lambda\). The system is typically ill conditioned and \(T_m\) can be singular or nearly so, so that the Lanczos method may converge slowly and irregularly and \(\xi_k\) can be typically big for \(m\) small. For more details, we refer to [12, 14].

It is worth noting that we should naturally take \(m > 1\); otherwise we would have \(K_1(A, u_k) = \text{span}\{u_k\}\) and \(T_1 = 0\), so that the Lanczos method would break down and \(w_{k+1}\) would not exist.

We will present convergence results on the inexact RQI with Lanczos. First of all, we present the following results.

**Theorem 3.** It holds that

\[
|\cos \psi_k| \leq \tan \phi_k, \tag{18}
\]

and asymptotically

\[
\sin \psi_k \geq 1 - \frac{1}{2} \sin^2 \phi_k \tag{19}
\]

by ignoring the higher order term \(O(\sin^4 \phi_k)\).

**Proof.** Recall that the Lanczos method requires that its residual \(\xi_k d_k\) satisfies \(\xi_k d_k \perp \mathcal{K}_m(A, u_k)\). So, we specially have \(d_k \perp u_k\). Therefore, from (8) and (9) we get

\[
\cos \phi_k \cos \psi_k + e_k^* f_k \sin \phi_k \sin \psi_k = 0,
\]

which means

\[
\frac{|\cos \psi_k|}{\sin \psi_k} = |e_k^* f_k \tan \phi_k| \leq \tan \phi_k.
\]

From the above it follows that (18) holds. By the Taylor expansion, from (19) we get asymptotically

\[
\sin \psi_k = \sqrt{1 - \cos^2 \psi_k} = 1 - \frac{1}{2} |\cos \psi_k| + O(\cos^4 \psi_k) \geq 1 - \frac{1}{2} \tan^2 \phi_k = 1 - \frac{1}{2} \sin^2 \phi_k
\]

by dropping the higher order term \(O(\sin^4 \phi_k)\).

Combining this theorem with (14) of Theorem 1, we can establish one of our main results for the inexact RQI with the preconditioned Lanczos.

**Theorem 4.** If \(\xi_k \leq \xi\) is uniformly bounded and satisfies

\[
\xi \sin \phi_k \leq \alpha < 1 \tag{20}
\]

with \(\alpha\) a constant, then the uniform positiveness condition (13) holds and the inexact RQI with Lanczos asymptotically converges quadratically at least:

\[
\tan \phi_{k+1} \leq \frac{2\beta \xi}{1 - \alpha^2} \sin^2 \phi_k. \tag{21}
\]

It converges cubically if

\[
\xi_k = O(\sin \phi_k); \tag{22}
\]

it converges at linear factor \(\gamma\) at least:

\[
\tan \phi_{k+1} \leq \gamma \sin \phi_k \tag{23}
\]

if

\[
\xi_k \leq \frac{\gamma - 2\beta \sin^2 \phi_k}{(2\beta + \gamma) \sin \phi_k} \leq \frac{\gamma}{(2\beta + \gamma) \sin \phi_k} \tag{24}
\]

with \(\gamma < 1\) independent of \(k\).
Proof. By (19), we get
\[ \sin \phi_k + \xi_k \sin \psi_k \leq \sin \phi_k + \xi \leq \sin \phi_k + \xi. \]

On the other hand, we get asymptotically from (18)
\[ \left| \cos \phi_k + \xi_k \cos \psi_k \right| \geq \left| \cos \phi_k - \xi \right| \cos \psi_k \]
\[ \geq \left| 1 - \frac{1}{2} \sin^2 \phi_k + O(\sin^4 \phi_k) - \xi \tan \phi_k \right| \]
\[ \geq 1 - \xi \sin \phi_k \]
\[ \geq 1 - \alpha, \] (25)

by dropping the higher order term \( O(\sin^2 \phi_k) \), which is uniformly away from zero by assumption. So the uniform positiveness condition (13) holds. We then derive asymptotically from (14) that
\[ \tan \phi_{k+1} \leq 2\beta \left( \frac{\sin \phi_k + \xi}{\sin^2 \phi_k} \right) \left( \frac{\sin \phi_k + \xi}{1 - \xi \sin \phi_k} \right) \]
\[ \leq 2\beta \frac{\sin \phi_k + \xi}{1 - \alpha} \]
\[ \leq 2\beta \frac{\xi}{1 - \alpha} \sin^2 \phi_k + O(\sin^3 \phi_k) \] (26)

which is just (21) by ignoring \( O(\sin^3 \phi_k) \).

Cubic convergence is direct from (25) if \( \xi_k = O(\sin \phi_k) \).

It follows from (26) that the inexact RQI with Lanczos converges at linear factor \( \gamma \) at least if for all \( k \) it holds that \( \xi_k \sin \phi_k < 1 \) and
\[ 2\beta \frac{\sin \phi_k + \xi}{1 - \xi \sin \phi_k} \leq \gamma < 1, \]
from which we get condition (24) by manipulation.

Theorem 4 presents the conditions on cubic, quadratic and linear convergence in terms of a priori uncomputable \( \sin \phi_k \). We next give alternatives of them in terms of the computable \( \|r_k\| \), so that they are of practical value as much as possible and can be used to control inner tolerance to achieve a desired convergence rate.

**Theorem 5.** If \( \xi_k \leq \xi \) is uniformly bounded and satisfies
\[ \frac{2\xi \|r_k\|}{|\lambda_2 - \lambda|} \leq \alpha < 1 \] (27)

with \( \alpha \) a constant, the uniform positiveness condition holds and the inexact RQI with Lanczos asymptotically converges quadratically at least:
\[ \|r_{k+1}\| \leq \frac{8\beta^2 (2\|r_k\| + \xi \lambda_2 - \lambda) \|r_k\|^2}{|\lambda_2 - \lambda| (|\lambda_2 - \lambda| - 2\xi \|r_k\|^2)}, \] (28)
\[ \leq \frac{8\beta^2 (2\|r_k\| + \xi \lambda_2 - \lambda) \|r_k\|^2}{(\lambda_2 - \lambda)^2 (1 - \alpha)} \] (29)
It converges cubically if
\[ \xi_k = O(\|r_k\|); \quad (30) \]
it converges linearly:
\[ \|r_{k+1}\| \leq \gamma \|r_k\| \quad \text{if} \]
\[ \xi_k \leq \frac{\gamma(\lambda_2 - \lambda)^2 - 16\beta^2\|r_k\|^2}{2|\lambda_2 - \lambda|(4\beta^2 + \gamma)\|r_k\|} < \frac{\gamma|\lambda_2 - \lambda|}{(8\beta^2 + 2\gamma)\|r_k\|}. \quad (32) \]
with \( \gamma < 1 \) independent of \( k \).

**Proof.** Making use of (12) gives
\[ \frac{\|r_{k+1}\|}{\lambda_{\text{max}} - \lambda_{\text{min}}} \leq \sin \phi_{k+1} \leq \tan \phi_{k+1}, \]
\[ 1 - \xi_k \sin \phi_k \geq 1 - \xi_k \frac{2\|r_k\|}{|\lambda_2 - \lambda|} \geq 1 - \frac{2\xi_k\|r_k\|}{|\lambda_2 - \lambda|} \geq 1 - \alpha > 0 \]
and
\[ \sin \phi_k + \xi_k \leq \frac{2\|r_k\|}{|\lambda_2 - \lambda|} + \xi_k. \]
Substituting the above relations into (26) and (21) establishes (28) and (29), respectively. It is clear from (28) that the inexact RQI with Lanczos converges cubically once \( \xi_k = O(\|r_k\|) \).

In order to make \( \|r_k\| \) linearly converge to zero monotonically, from (28) we simply set
\[ \frac{8(\lambda_2 - \phi_k)^2 2\|r_k\| + \xi_k|\lambda_2 - \lambda|}{|\lambda_2 - \lambda|^3 |\lambda_2 - \lambda| - 2\xi_k\|r_k\|\|r_k\|} \leq \gamma < 1 \]
with \( \gamma \) independent of \( k \). Solving it for \( \xi_k \) gives
\[ \xi_k \leq \frac{\gamma(\lambda_2 - \lambda)^2 - 16\beta^2\|r_k\|^2}{2|\lambda_2 - \lambda|(4\beta^2 + \gamma)\|r_k\|} < \frac{\gamma|\lambda_2 - \lambda|}{(8\beta^2 + 2\gamma)\|r_k\|}. \]

We make some comments on Theorems 4–5.

**Remark 1.** The quadratic convergence condition (20) in Theorem 4 is sufficient and it indicates that \( \xi > 1 \) considerably is allowed. Noting that (20) is assumed to satisfy for all \( k \), it is sufficient that \( \xi < \frac{1}{\sin \phi_0} \). So the old requirement \( \xi_k \leq 1 < 1 \) is stringent and not necessary for quadratic convergence. The comments apply to (27) in Theorem 5 as well. Note that these two conditions are only sufficient but not necessary. Actually, it can be seen from (26) that \( \xi \leq \frac{c}{\sin \phi_0} \) with a moderate constant \( c \), say, \( 1 \leq c \leq 5 \) also works well for quadratic convergence. The numerical experiments in Section 5 have confirmed this.

Since the initial residual norm is \( \|u_k\| = 1 \) before performing the Lanczos method, in order to make the inexact RQI with Lanczos converge quadratically, we do not need to solve the inner linear systems \( (A - \theta_k)w = u_k \)'s with any accuracy at all in the sense of solving the linear systems.

**Remark 2.** Conditions (24) and (32) for linear convergence show that \( \xi_k \) can be as big as \( O\left(\frac{1}{\sin \phi_0}\right) \) and \( O\left(\frac{1}{\|r_k\|}\right) \) as outer iterations proceed. More precisely, (24) indicates that the inexact RQI with Lanczos still converges linearly at least even if \( \xi_k \) is as big as \( O\left(\frac{1}{\sin \phi_0}\right) \) with the order constant \( \frac{2\gamma}{2\beta + \gamma} < 1 \) smaller than one.
Below, as done in [8, 16], we estimate \( \|w_{k+1}\| \) in (7) obtained by Lanczos and present more results. Note that the exact solution of \((A - \theta_k I)w = u_k\) is \(w_{k+1} = (A - \theta_k I)^{-1}u_k\), which corresponds to \(\xi_k = 0\) in (11). Therefore, we have from (11) and (12)

\[
\|w_{k+1}\| = \frac{\cos \phi_k}{|\theta_k - \lambda|} + O(\sin \phi_k)
\]

\[
\approx \frac{1}{|\theta_k - \lambda|} = \|(A - \theta_k I)^{-1}\|
\]

\[
= O \left( \frac{1}{\sin^2 \phi_k} \right) = O \left( \frac{1}{\|r_k\|^2} \right).
\]

From (11) and (12), we also see that these estimates hold for \(\xi_k = O(\sin \phi_k) = O(\|r_k\|)\). So \(\|w_{k+1}\|\) is also \(O(\|r_k\|^2)\) when the inexact RQI with Lanczos converges cubically.

**Theorem 6.** Assume that \(\xi_k \leq \xi\) is uniformly bounded and satisfies \(\sin \phi_k \leq \alpha < 1\) with \(\alpha\) a constant. Then asymptotically we have

\[
\|w_{k+1}\| \geq \frac{(1 - \alpha)|\lambda_2 - \lambda|}{4\beta\|r_k\|^2}, \quad (33)
\]

\[
\|r_{k+1}\| \leq \frac{\sqrt{1 + \xi^2}}{\|w_{k+1}\|}, \quad (34)
\]

\[
\|r_{k+1}\| \leq \frac{4\beta \sqrt{1 + \xi^2}}{|\lambda_2 - \lambda|(1 - \alpha)} \|r_k\|^2, \quad (35)
\]

where (34) holds strictly.

**Proof.** As \(\xi_k d_k \perp u_k\) and \((A - \theta_k I)w_{k+1} = u_k + \xi_k d_k\), we have

\[
\|(A - \theta_k I)w_{k+1}\|^2 = \|u_k\|^2 + \|\xi_k d_k\|^2 = 1 + \xi_k^2.
\]

So we get from \(u_{k+1} = w_{k+1}/\|w_{k+1}\|\) that

\[
\|(A - \theta_k I)u_{k+1}\| = \frac{\sqrt{1 + \xi_k^2}}{\|w_{k+1}\|} \leq \frac{\sqrt{1 + \xi^2}}{\|w_{k+1}\|}, \quad (36)
\]

By the optimality of Rayleigh quotient we obtain

\[
\|r_{k+1}\| = \|(A - \theta_k I)u_{k+1}\| \leq \|(A - \theta_k I)u_{k+1}\| = \frac{\sqrt{1 + \xi_k^2}}{\|w_{k+1}\|} \leq \frac{\sqrt{1 + \xi^2}}{\|w_{k+1}\|}, \quad (37)
\]

which shows (34). It is easy to verify (cf. [13, p. 77]) that

\[
|\lambda_2 - \lambda| \sin^2 \phi_k \leq |\lambda - \theta_k| \leq (\lambda_{\text{max}} - \lambda_{\text{min}}) \sin^2 \phi_k. \quad (38)
\]

By using (11), (25), (38) and (12) in turn, we obtain

\[
\|w_{k+1}\| \geq \frac{|\cos \phi_k + \xi_k \cos \psi_k|}{|\theta_k - \lambda|}
\]

\[
\geq \frac{|1 - \xi_k \sin \phi_k|}{|\theta_k - \lambda|}
\]

\[
\geq \frac{1 - \alpha}{|\theta_k - \lambda|}
\]

\[
\geq \frac{1 - \alpha}{(\lambda_{\text{max}} - \lambda_{\text{min}}) \sin^2 \phi_k}
\]

\[
\geq \frac{(1 - \alpha)|\lambda_2 - \lambda|}{4\beta \|r_k\|^2}
\]

\[
\geq \frac{(1 - \alpha)|\lambda_2 - \lambda|}{4\beta \|r_k\|^2},
\]
which proves (33). Substituting (33) into (34) establishes (35).

(35) indicates that the inexact RQI with Lanczos converges quadratically if $\alpha$ is not near one. By combining this theorem with Theorems 4–5, (33) shows that $\|w_{k+1}\|$ is always no less than $O(\|r_k\|^2)$ when the inexact RQI with Lanczos converges quadratically provided that $\alpha$ is not near one. Noting that the inexact RQI with Lanczos for $\xi_k = O(\sin \phi_k) = O(\|r_k\|)$ converges cubically and $\|w_{k+1}\|$ is also $O(\|r_k\|^2)$ (cf. the comments before Theorem 6), this illustrates that the size of $\|w_{k+1}\|$ itself cannot reveal cubic and quadratic convergence rates of the inexact RQI with Lanczos. However, we cannot recover the cubic convergence of the exact RQI and the inexact RQI when $\xi_k = 0$ and $\xi_k = O(\|r_k\|)$, respectively. So (35) is weaker than Theorems 4–5. This is because $\|r_{k+1}\| \leq \|(A - \theta_k I)u_{k+1}\|$ is not sharp in the proof.

So far, all the convergence results are local, that is, they care how the exact and inexact RQI behaves only from the current outer iteration to the next one, assuming that current $(\theta_k, u_k)$ is already a reasonably good approximation to $(\lambda, x)$. As is well known, one of the important properties of the exact RQI is its global residual monotonic decreasing property, i.e., $\|r_{k+1}\| \leq \|r_k\|$, for any (poor) starting vector $u_0$; see Theorem 4.8.1 of [13, p. 79]. We now present a global property to the inexact RQI with Lanczos.

**Theorem 7.** For the inexact RQI with Lanczos starting with any starting vector $u_0$, we have

$$\|r_{k+1}\| \leq \sqrt{1 + \xi_k^2} \|r_k\|, \quad k = 0, 1, \ldots$$

**Proof.** From (7), we have

$$w_{k+1} = (A - \theta_k I)^{-1}(u_k + \xi_k d_k).$$

Again, note that for the Lanczos method its residual $\xi_k d_k$ satisfies $\xi_k d_k^* u_k = 0$. Then from (37) and the Cauchy–Schwarz inequality, we get

$$\frac{\|r_{k+1}\|}{\|r_k\|} \leq \frac{\|(A - \theta_k I)u_{k+1}\|}{\|r_k\|} \leq \sqrt{1 + \xi_k^2} \|w_{k+1}\| \|r_k\|$$

$$= \frac{\|(A - \theta_k I)^{-1}(u_k + \xi_k d_k)\|}{\|r_k\|} \|r_k\|$$

$$\leq \sqrt{1 + \xi_k^2} \|\|(A - \theta_k I)^{-1}(A - \theta_k I)u_k\|\|$$

$$= \sqrt{1 + \xi_k^2} \|\|(A - \theta_k I)^{-1}(A - \theta_k I)u_k\|\|$$

which proves (39).
4 The inexact RQI with a tuned preconditioned Lanczos

We have found that for a given $\xi$ satisfying our convergence conditions, we may still need quite many inner iteration steps at each outer iteration. This is especially the case for difficult problems, i.e., big $\beta$’s, or for computing an interior eigenvalue $\lambda$ since it leads to a highly Hermitian indefinite matrix $(A - \theta_k I)$ at each outer iteration. So, in order to improve the overall performance, preconditioning may be necessary to speed up the Lanczos method. Some preconditioning techniques have been proposed in e.g., [1, 16]. In the unpreconditioned case, the right-hand side $u_k$ of (4) is rich in the direction of the desired $x$. We can benefit much from this property when solving the linear system. Actually, if the right-hand side is an eigenvector of the coefficient matrix, Krylov subspace type methods will find the exact solution in one step. However, a usual preconditioner loses this important property, so that inner iteration steps may not be reduced [1, 3, 5]. A preconditioner with tuning is necessary to recover this property and meanwhile attempts to improve the conditioning of the preconditioned system, so that considerable improvement over a usual preconditioner is possible [3, 5, 23]. In what follows we show how to extend our previous theory to the inexact RQI with a tuned preconditioned Lanczos.

Let $Q = LL^*$ be a Cholesky factorization of some Hermitian positive definite matrix which is an approximation to $A - \theta_k I$ in some sense [1, 5, 23]. A tuned preconditioner $Q = LL^*$ can be constructed by adding a rank-1 or rank-2 modification to $Q$, so that

$$Q u_k = A u_k;$$

(40) see [3, 5, 23] for details. Using the tuned preconditioner $Q$, the shifted inner linear system (4) is equivalently transformed to the preconditioned one

$$B \hat{w} = L^{-1}(A - \theta_k I)L^{-*} \hat{w} = L^{-1} u_k,$$

(41)

with the original $w = L^{-*} \hat{w}$. Once the Lanczos method is used to solve it, we are led to the inexact RQI with a tuned preconditioned Lanczos. A power of the tuned preconditioner $Q$ is that the right-hand side $L^{-1} u_k$ is rich in the eigenvector of $B$ associated with its smallest eigenvalue and has the same quality as $u_k$ as an approximation the eigenvector $x$ of $A$, while for the usual preconditioner $Q$ the right-hand side $L^{-1} u_k$ does not possess this property.

Take the zero vector as an initial guess to the solution of (41) and let $\hat{w}_{k+1}$ be the approximate solution obtained by the $m$-step Lanczos method applied to it. Then we have

$$L^{-1}(A - \theta_k I)L^{-*} \hat{w}_{k+1} = L^{-1} u_k + \hat{\xi}_k \hat{d}_k,$$

(42)

where $\hat{w}_{k+1} \in K_m(B, L^{-1} u_k)$, $\hat{\xi}_k \hat{d}_k$ with $\|\hat{d}_k\| = 1$ is the residual and $\hat{d}_k$ is the residual direction vector. Keep in mind that $w_{k+1} = L^{-*} \hat{w}_{k+1}$. We then get

$$(A - \theta_k I) w_{k+1} = u_k + \hat{\xi}_k L \hat{d}_k = u_k + \hat{\xi}_k \|L \hat{d}_k\| \frac{L \hat{d}_k}{\|L \hat{d}_k\|}.$$

(43)

So $\hat{\xi}_k$ and $d_k$ in (7) are $\hat{\xi}_k \|L \hat{d}_k\|$ and $\frac{L \hat{d}_k}{\|L \hat{d}_k\|}$, respectively. Hence our general Theorems [1, 2] apply and is not repeated here.

How to extend Theorem [3] to the preconditioned case is nontrivial and need more work. Let $(\mu_i, y_i)$, $i = 1, 2, \ldots, n$ be the eigenpairs of $B$ with

$$| \mu_1 | < | \mu_2 | \leq \cdots \leq | \mu_n |.$$

Define $\hat{u}_k = L^{-1} u_k / \|L^{-1} u_k\|$. Similar to (8) and (9), let

$$\hat{u}_k = y_1 \cos \hat{\phi}_k + \hat{e}_k \sin \hat{\phi}_k, \quad \hat{e}_k \perp y_1, \quad \|\hat{e}_k\| = 1,$$

(44)

$$\hat{d}_k = y_1 \cos \hat{\psi}_k + \hat{f}_k \sin \hat{\psi}_k, \quad \hat{f}_k \perp y_1, \quad \|\hat{f}_k\| = 1,$$

(45)
be the orthogonal direct sum decompositions. Then it is known \[^{5}\] that

\[
|\mu_1| = O(\sin \phi_k), \tag{46}
\]

\[
\sin \hat{\phi}_k \leq c_1 \sin \phi_k \tag{47}
\]

with \(c_1\) a constant.

From Theorem \[^{3}\] and \(^{(47)}\), the following results are direct.

**Lemma 1.** It holds that

\[
|\cos \hat{\psi}_k| \leq \tan \hat{\phi}_k, \tag{48}
\]

and asymptotically

\[
\sin \hat{\psi}_k \geq 1 - \frac{1}{2} \sin^2 \hat{\phi}_k \tag{49}
\]

by ignoring the higher order term \(O(\sin^4 \hat{\phi}_k)\).

**Remark.** Combining with \(^{(47)}\), this theorem means

\[
|\cos \hat{\psi}_k| = O(\sin \phi_k), \quad \sin \hat{\psi}_k = 1 - O(\sin^2 \phi_k). \tag{50}
\]

**Theorem 8.** It holds that

\[
|\cos \psi_k| = O(\sin \phi_k), \tag{51}
\]

\[
\sin \psi_k = 1 - O(\sin^2 \phi_k). \tag{52}
\]

**Proof.** From the requirement of the \(m\)-step Lanczos for \(^{(42)}\), we have \(\hat{\xi}_k \hat{d}_k \perp K_m(B, L^{-1}u_k)\). Particularly, it holds that

\[
\hat{d}_k L^{-1} u_k = \hat{d}_k L^{-1} u_k = 0,
\]

from which and \(\hat{u}_k = L^{-1} u_k / \|L^{-1} u_k\|\) it follows that \(\hat{d}_k \hat{u}_k = 0\). Therefore, from \(d_k = \frac{L \hat{d}_k}{\|L \hat{d}_k\|}\) we have

\[
0 = \hat{d}_k \hat{u}_k = \hat{d}_k L \hat{u}_k L^{-1} u_k = \|L \hat{d}_k\| \|L^{-1} u_k\| d_k^{\ast} L^{-\ast} \hat{u}_k = 0,
\]

i.e.,

\[
d_k^{\ast} L^{-\ast} \hat{u}_k = 0. \tag{53}
\]

By definition, we have

\[
L^{-1} (A - \theta_k I) L^{-\ast} y_1 = \mu_1 y_1,
\]

from which it follows that

\[
(A - \theta_k I) \hat{u}_k = \mu_1 \frac{L y_1}{\|L \hat{u}_k\|}
\]

with \(\hat{u}_k = L^{-\ast} y_1 / \|L^{-\ast} y_1\|\). Therefore, by standard perturbation theory and \(^{(46)}\), we get

\[
\sin \angle(\hat{u}_k, x) = O(\mu_1 \frac{\|L y_1\|}{\|L \hat{u}_k\|}) = O(|\mu_1|) = O(\sin \phi_k). \tag{54}
\]

On the other hand, from \(^{(47)}\), we have

\[
\sin \hat{\phi}_k = \sin \angle(\hat{u}_k, y_1) = \sin \angle(L^{-1} u_k, y_1) = O(\sin \phi_k).
\]

Therefore, we can write

\[
\hat{u}_k = y_1 + O(\sin \phi_k),
\]

...
which leads to
\[ \mathcal{L}^{-*} \hat{u}_k = \mathcal{L}^{-*} y_1 + O(\sin \phi_k). \]
Thus, we have
\[ \sin \angle(\mathcal{L}^{-*} \hat{u}_k, \mathcal{L}^{-*} y_1) = \sin \angle(\mathcal{L}^{-*} \hat{u}_k, \bar{u}_k) = O(\sin \phi_k). \] (55)

Since
\[ \angle(\mathcal{L}^{-*} \hat{u}_k, x) \leq \angle(\mathcal{L}^{-*} \hat{u}_k, \tilde{u}_k) + \angle(\tilde{u}_k, x), \]
combining (54) and (55), we get
\[ \sin \angle(\mathcal{L}^{-*} \hat{u}_k, x) \leq \sin \angle(\mathcal{L}^{-*} \hat{u}_k, \tilde{u}_k) + \sin \angle(\tilde{u}_k, x) = O(\sin \phi_k). \] (56)

Recall that
\[ d_k = x \cos \psi_k + e_k \sin \psi_k \]
and substituting it and the orthogonal direct sum decomposition
\[ \mathcal{L}^{-*} \hat{u}_k = \| \mathcal{L}^{-*} \hat{u}_k \| (x \cos \angle(\mathcal{L}^{-*} \hat{u}_k, x) + g_k \sin \angle(\mathcal{L}^{-*} \hat{u}_k, x)) \]
with \( g_k \perp x \) into (53). Then based on (53) and following the proof of Theorem 8 we get
\[ | \cos \psi_k | \leq | \tan \angle(\mathcal{L}^{-*} \hat{u}_k, x) |, \]
\[ \sin \psi_k = 1 - O(\sin^2 \angle(\mathcal{L}^{-*} \hat{u}_k, x)). \]
Combining them with (56) yields (51) and (52).

Using this theorem and writing (51) as \( | \cos \psi_k | \leq c_2 \sin \phi_k \) with \( c_2 \) a constant, it is direct to extend Theorems 4–5 in the unpreconditioned Lanczos case to the tuned preconditioned Lanczos case. We have made preliminary numerical experiments and confirmed the theory. Since our concerns in this paper are the convergence theory of the inexact RQI with the unpreconditioned and tuned preconditioned Lanczos and the pursuit of effective tuned preconditioners are beyond the scope of the current paper, we will only report numerical results on the inexact RQI with the unpreconditioned Lanczos.

5 Numerical experiments

Our numerical experiments were performed on an Intel (R) Core (TM) 2 Quad CPU Q9400 2.66GHz with main memory 2 GB using Matlab 7.8.0 with the machine precision \( \epsilon = 2.22 \times 10^{-16} \) under the Microsoft Windows XP operating system.

We report numerical experiments made by the inexact RQI with the unpreconditioned Lanczos on four symmetric (Hermitian) matrices: BCSPWR08 of order 1624, CAN1054 of order 1054, DWT2680 of order 3025 and LSHP3466 of order 3466 [2]. Note that the bigger the factor \( \beta \) is, the worse conditioned \( x \) is. At the meanwhile, for \( \beta \) big, Theorem 4 and Theorem 7 show that although RQI and the inexact RQI can still converge cubically and quadratically, they may converge more slowly and needs more outer iterations as the factors \( 2\beta \) and \( \frac{2\beta}{1-\sigma} \) in (14) and (21) are big. As a reference, we use the Matlab function \texttt{eig.m} to compute \( \beta \). We find that DWT2680 and LSHP3466 are considerably more difficult than the two others. We only report the results on the computation of the smallest eigenpair.

Remembering that the cubic convergence of the inexact RQI with Lanczos for \( \xi_k = O(\| r_k \|) \) occurs when updating \( (\theta_k, u_k) \) to get \( (\theta_{k+1}, u_{k+1}) \), in the experiments we take
\[ \xi_k = \frac{\| r_k \|}{\| A \|_1}. \] (57)
We construct the same initial \( u_0 \) for each matrix that is \( x \) plus a reasonably small perturbation generated randomly in a uniform distribution, such that \( |\lambda - \theta_0| < \frac{\lambda_2 - \lambda_1}{2} \).

The algorithm stops whenever \( \|r_k\| = \|(A - \theta_k I)u_k\| \leq \|A\|_1 \text{tol} \), where \( \text{tol} = 10^{-14} \) unless stated otherwise. In the experiments, we use the Matlab function \texttt{symmlq.m} to solve the inner linear systems with \( \xi_k \leq \xi < 1 \). We should notice that for \( \xi_k \geq 1 \) the Matlab function \texttt{symmlq.m} cannot be applied. Since the Lanczos method behaves irregularly and may nearly break down or break down for indefinite linear systems, that is, \( T_m \in \mathbb{R} \) is ill conditioned and can be nearly singular and even numerically singular, it may produce bad approximate solutions with large norms and large residual norms \( \xi_k \)'s for some steps \( m \).

As far as solving the linear systems is concerned, such approximate solutions have no accuracy and no practical value. In \texttt{symmlq.m}, if such a bad approximate solution emerges, it always outputs the approximate solution as zero and the residual norm \( \xi_k = 1 \) simply, telling us nothing! However, we have seen that in the inexact RQI with Lanczos, \( \xi_k \geq 1 \) is allowed.

So for our purpose, we have worked out a Lanczos code that uses the Gram–Schmidt with iterative refinement \cite{20} to generate a numerically orthonormal basis of the Krylov subspace \( \mathcal{K}_m(A, u_k) \) and delivers 'correct' results that the Lanczos method should produce. We point out that our Lanczos code is not optimized but numerically stable.

We test the inexact RQI with Lanczos by choosing \( \xi_k \) as in \cite{57} and a few fixed \( \xi_k = \xi = 0.1, 1, 5, 20 \). Based on our theory, the method should converge quadratically for the \( \xi = 1, 5, 20 \) and use almost the same outer iterations as those for \( \xi = 0.1 \). Therefore, the total computational cost may be reduced considerably. For the inexact RQI with Lanczos, the total inner iteration steps, i.e., the total matrix-vector products in inner iterations, is a good measure of overall performance of the method.

Tables \ref{1}–\ref{4} list the computed results, where \( \text{iters} \) denotes the number of total inner iteration steps and \( \text{iter}^{(k-1)} \) is the number of inner iteration steps when computing \( (\theta_k, u_k) \), the "-" denotes the stagnation of \texttt{symmlq.m} at the \( \text{iter}^{(k-1)} \)-th step, and \( \text{res}^{(k-1)} \) is the actual relative residual norm of the inner linear system. Clearly, \( \text{iters} \) is a reasonable measure of the overall efficiency of the inexact RQI with Lanczos. We comment that in \texttt{symmlq.m} the output \( \text{iter}^{(k-1)} = m - 1 \), where \( m \) is the steps of the Lanczos process.

Before commenting the experiments, we should remind that in finite precision arithmetic \( \|r_k\|/\|A\|_1 \) can not decline further whenever it reaches a moderate multiple of \( \epsilon = 2.2 \times 10^{-16} \). Therefore, assuming that the algorithm stops at outer iteration \( k \), if \( \sin \phi_{k-1} \) or \( \|r_{k-1}\| \leq 10^{-6} \) or \( 10^{-9} \), then the algorithm may not continue converging cubically or quadratically at the final outer iteration \( k \). Another point is that when judging convergence rates, we must take the factor \( \beta \) into account. The smaller it is, the more clearly cubic and quadratic convergence exhibits, as indicated by \cite{20} and \cite{28}; the bigger it is, the less apparent cubic and quadratic convergence is. So we should precisely base \cite{20} or \cite{28} to judge cubic and quadratic convergence of \( \sin \phi_k \) or \( \|r_k\| \). In this sense, we see from Tables \ref{1}–\ref{4} that the exact RQI and the inexact RQI with Lanczos for decreasing \( \xi_k \) converge cubically and the method starts to converge quadratically for the given fixed \( \xi \)'s after very few outer iterations. But for \( \xi \geq 1 \), the method is much more efficient than that for \( \xi = 0.1 \) and for decreasing \( \xi \); the method with \( \xi \geq 1 \) is four times and twice as fast as that with \( \xi = 0.1 \) for BCSPWR08 and for CAN1054 and DWT2680, respectively. For LSHP3466, the gain is not so great, but the method with \( \xi \geq 1 \) is still one and a half times as fast as the method with \( \xi = 0.1 \). With the fixed \( \xi = 1, 5, 20 \), it is always three to ten times as fast as that with decreasing \( \xi_k = O(\|r_k\|) \) for the four test matrices. It is seen that for a bigger \( \xi \) the method may need a little more outer iterations but it does indeed converge quadratically and is in agreement with quadratic convergence bound \cite{20}. Why the method with fixed bigger \( \xi_k \)'s converges a little more slowly is due to the bigger convergence factor \( \frac{2\xi}{1-\xi} \) in \cite{21}.

Note that the linear systems \( (A - \theta_k)w = u_k \)'s are Hermitian indefinite and become
increasingly worse conditioned and even numerically singular as \( \theta_k \to \lambda \) with increasing \( k \). So, more inner iteration steps are needed generally for a fixed \( \xi \) as \( k \) increases. We find that for the difficult DTW2680 and LSHP3466, many more iters's are used than those for BCSPWR08 and CAN1054. We have tested many fixed \( \xi \)'s ranging from 1 to 50 for each matrix and found that the method asymptotically converges quadratically. \( \xi \geq 10 \) does not satisfy the sufficient condition (20) for quadratic convergence but is a moderate multiple of \( \frac{1}{\sin(\phi_0)} \). The algorithm with these \( \xi \) behaves almost the same as that with \( \xi = 1, 5 \) and uses a little more outer iterations and comparable total inner iteration steps iters.

For linear convergence, we see that conditions (24) and (32) depend on \( \beta \), which is unknown a priori. So it appears impossible to design a practical criterion robustly and reliably unless a rough estimate on \( \beta \) is available in advance. Note that the convergence of the method allows \( \xi_k \) to increase up to \( \frac{1}{O(\|r_k\|)} \) as outer iterations proceed. Therefore, we may not care \( \xi_k \)'s themselves but implement the inexact RQI with Lanczos for certain

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
\xi_{k-1} \leq \xi & k & \|r_k\| & \sin \phi_k & \text{res}^{(k-1)} & \text{iter}^{(k-1)} & \text{iters} \\
\hline
0 \ (\text{RQI}) & 1 & 0.0124 & 0.0036 & & & \\
& 2 & 3.1e-8 & 8.5e-8 & & & \\
& 3 & 2.0e-15 & 6.6e-15 & & & \\
\hline
\frac{\|r_{k-1}\|}{\|A\|_1} & 1 & 0.0071 & 0.0029 & 0.0367 & 7 & 1003 \\
& 2 & 3.7e-8 & 1.2e-7 & 4.1e-4 & 40 & \\
& 3 & 3.0e-15 & 3.0e-15 & - & 956 & \\
\hline
0.1 & 1 & 0.0090 & 0.0045 & 0.0950 & 5 & 300 \\
& 2 & 2.1e-5 & 3.7e-5 & 0.0847 & 24 & \\
& 3 & 3.3e-13 & 3.2e-13 & 0.0754 & 44 & \\
\hline
1 & 1 & 0.0462 & 0.0165 & 0.7161 & 3 & 87 \\
& 2 & 5.1e-4 & 8.9e-4 & 0.8505 & 11 & \\
& 3 & 2.3e-7 & 2.9e-7 & 0.9829 & 26 & \\
& 4 & 1.1e-14 & 1.3e-14 & - & 47 & \\
\hline
5 & 1 & 0.1259 & 0.0332 & 2.0694 & 2 & 87 \\
& 2 & 0.0107 & 0.0064 & 3.0112 & 4 & \\
& 3 & 1.9e-4 & 2.5e-4 & 4.2267 & 13 & \\
& 4 & 1.2e-7 & 1.6e-7 & 4.8117 & 25 & \\
& 5 & 5.7e-14 & 3.5e-14 & 4.8558 & 43 & \\
\hline
20 & 1 & 0.1259 & 0.0332 & 2.0694 & 2 & 90 \\
& 2 & 0.0546 & 0.0178 & 17.7245 & 2 & \\
& 3 & 0.0100 & 0.0062 & 14.0583 & 3 & \\
& 4 & 6.0e-4 & 9.0e-4 & 12.7284 & 7 & \\
& 5 & 4.6e-6 & 4.4e-6 & 15.4553 & 18 & \\
& 6 & 1.6e-10 & 2.2e-10 & 13.9482 & 31 & \\
& 7 & 3.3e-14 & 3.5e-14 & 19.9337 & 27 & \\
\hline
\end{array}
\]

Table 1: BCSPWR08, \( \beta = 40.19 \), \( \sin \phi_0 = 0.1020 \).
| $\xi_{k-1} \leq \xi$ | $k$ | $\|r_k\|$ | $\sin \phi_k$ | $res^{(k-1)}$ | $iter^{(k-1)}$ | iters |
|---------------------|-----|--------|---------|-------------|-------------|------|
| 0 (RQI)             | 1   | 0.0269 | 0.0110  |             |             |      |
|                     | 2   | $1.1e-7$ | $2.1e-7$ |             |             |      |
|                     | 3   | $3.2e-15$ | $5.0e-15$ |             |             |      |
|                     | 4   | $2.5e-15$ | $4.7e-15$ |             |             |      |
| $\|r_{k-1}\|$      | 1   | 0.0155 | 0.0038  | 0.0403      | 8            | 432  |
| $\|A\|$            | 2   | $1.4e-7$ | $3.1e-7$ | $3.1e-4$    | 45           |      |
|                     | 3   | $1.4e-14$ | $5.0e-15$ | -           | 379          |      |
| $0.1$               | 1   | 0.0181 | 0.0055  | 0.0796      | 6            | 207  |
|                     | 2   | $3.8e-6$ | $2.2e-5$ | 0.0679      | 30           |      |
|                     | 3   | $4.7e-13$ | $2.0e-13$ | 0.0969      | 51           |      |
|                     | 4   | $6.0e-15$ | $5.0e-15$ | -           | 120          |      |
| $1$                 | 1   | 0.0624 | 0.0132  | 0.4376      | 4            | 107  |
|                     | 2   | $5.7e-4$ | $9.7e-4$ | 0.9980      | 14           |      |
|                     | 3   | $2.4e-7$ | $1.3e-7$ | 0.9561      | 30           |      |
|                     | 4   | $1.7e-14$ | $8.0e-14$ | 0.9952      | 53           |      |
| $5$                 | 1   | 0.2238 | 0.0454  | 1.7072      | 2            | 101  |
|                     | 2   | 0.0310 | 0.00946 | 3.7008      | 4            |      |
|                     | 3   | $8.3e-4$ | 0.0012  | 4.5335      | 11           |      |
|                     | 4   | $1.7e-6$ | $1.1e-6$ | 3.6374      | 26           |      |
|                     | 5   | $4.0e-12$ | $1.5e-12$ | 3.9095      | 45           |      |
|                     | 6   | $3.4e-15$ | $2.0e-14$ | 4.5305      | 13           |      |
| $20$                | 1   | 0.2238 | 0.0454  | 1.7072      | 2            | 102  |
|                     | 2   | 0.0661 | 0.0146  | 8.5434      | 3            |      |
|                     | 3   | 0.0119 | 0.0050  | 16.0483     | 4            |      |
|                     | 4   | $6.7e-4$ | $4.1e-4$ | 18.7495     | 9            |      |
|                     | 5   | $2.8e-6$ | $1.9e-6$ | 18.7545     | 23           |      |
|                     | 6   | $5.1e-11$ | $2.7e-11$ | 15.5764     | 40           |      |
|                     | 7   | $5.9e-14$ | $6.2e-14$ | 14.4397     | 21           |      |

| $m$ | outer iterations | iters |
|-----|------------------|-------|
| 5   | 110              | 550   |
| 10  | 21               | 210   |
| 15  | 10               | 150   |
| 20  | 7                | 140   |
| 30  | 5                | 150   |

Table 2: CAN1054, $\beta = 88.28$, $\sin \phi_0 = 0.1008$. 
\[
\xi_{k-1} \leq \xi_k
\]

| \(\xi_k\) | \(k\) | \(\|r_k\|\) | \(\sin \phi_k\) | \(\text{res}(k-1)\) | \(\text{iter}(k-1)\) | \(\text{iters}\) |
|---|---|---|---|---|---|---|
| 0 (RQI) | 1 | 0.0144 | 0.1188 | | | |
| | 2 | 1.6e - 4 | 0.0018 | | | |
| | 3 | 5.1e - 10 | 2.6e - 8 | | | |
| | 4 | 1.0e - 15 | 6.7e - 13 | | | |
| \(\|r_{k-1}\|\) \(\|A\|_1\) | 1 | 0.0143 | 0.0121 | 0.1171 | 5 | 1512 |
| | 2 | 4.8e - 5 | 5.1e - 4 | 0.0019 | 167 | |
| | 3 | 4.2e - 11 | 9.9e - 10 | - | 424 | |
| | 4 | 6.1e - 15 | 6.6e - 13 | - | 916 | |
| 5 | 1 | 0.0123 | 0.0104 | 0.0830 | 6 | 955 |
| | 2 | 5.1e - 5 | 1.1e - 4 | 0.0972 | 93 | |
| | 3 | 1.3e - 11 | 1.5e - 10 | 0.0986 | 267 | |
| | 4 | 5.0e - 15 | 6.6e - 13 | 0.1109(*) | 589 | |
| 0.1 | 1 | 0.0419 | 0.0265 | 0.4842 | 3 | 402 |
| | 2 | 6.7e - 4 | 0.0041 | 0.9424 | 15 | |
| | 3 | 8.6e - 7 | 1.2e - 5 | 0.9667 | 117 | |
| | 4 | 1.9e - 12 | 2.2e - 11 | 0.9276 | 267 | |
| 5 | 1 | 0.0851 | 0.0387 | 1.0223 | 2 | 535 |
| | 2 | 0.0092 | 0.0125 | 3.8250 | 5 | |
| | 3 | 2.8e - 4 | 0.0027 | 4.8280 | 19 | |
| | 4 | 1.1e - 6 | 1.3e - 5 | 4.7719 | 108 | |
| | 5 | 1.3e - 11 | 2.6e - 10 | 4.8329 | 238 | |
| | 6 | 7.0e - 15 | 5.8e - 13 | 4.9521 | 163 | |
| 20 | 1 | 0.0877 | 0.0400 | 1.0123 | 2 | 520 |
| | 2 | 0.0249 | 0.0200 | 12.2984 | 3 | |
| | 3 | 0.0040 | 0.0095 | 14.3550 | 5 | |
| | 4 | 2.9e - 4 | 0.0031 | 16.3542 | 14 | |
| | 5 | 5.2e - 6 | 9.7e - 6 | 19.9212 | 86 | |
| | 6 | 2.7e - 9 | 2.1e - 9 | 18.9912 | 175 | |
| | 7 | 4.0e - 14 | 1.2e - 12 | 19.0863 | 232 | |

| \(m\) | outer iterations | \(\text{iters}\) |
|---|---|---|
| 10 | 268 | 2680 |
| 20 | 55 | 1100 |
| 30 | 30 | 900 |
| 40 | 17 | 680 |
| 50 | 11 | 550 |
| 60 | 11 | 660 |

Table 3: DWT2680, \(tol = 10^{-12}\), \(\beta = 2295.6\), \(\sin \phi_0 = 0.1095\).
| $\xi_{k-1} \leq \xi$ | $k$ | $\|r_k\|$ | $\sin \phi_k$ | $\text{res}^{(k-1)}$ | $\text{iter}^{(k-1)}$ | iters |
|-----------------|-----|----------------|----------------|-----------------|----------------|-------|
| 0 (RQI)         | 1   | 0.0149        | 0.1716         |                 |                 |       |
|                 | 2   | 4.0e - 4      | 0.0056         |                 |                 |       |
|                 | 3   | 1.2e - 8      | 8.9e - 7       |                 |                 |       |
|                 | 4   | 2.0e - 15     | 4.0e - 13      |                 |                 |       |
| $\frac{\|r_{k-1}\|}{\|A\|_1}$ | 1   | 0.0102        | 0.0097         | 0.0874          | 6               | 1717 |
|                 | 2   | 3.9e - 5      | 1.2e - 4       | 0.0014          | 201             |       |
|                 | 3   | 1.2e - 9      | 4.5e - 8       | -               | 497             |       |
|                 | 4   | 5.2e - 15     | 6.1e - 13      | -               | 1013            |       |
| 0.1             | 1   | 0.0102        | 0.0098         | 0.0874          | 6               | 651  |
|                 | 2   | 4.2e - 4      | 5.4e - 4       | 0.0990          | 102             |       |
|                 | 3   | 4.5e - 8      | 2.8e - 7       | 0.0948          | 256             |       |
|                 | 4   | 5.3e - 13     | 5.6e - 11      | 0.0965          | 287             |       |
| 1               | 1   | 0.0408        | 0.0251         | 0.5335          | 3               | 424  |
|                 | 2   | 6.4e - 4      | 0.0036         | 0.9685          | 15              |       |
|                 | 3   | 7.6e - 7      | 1.9e - 5       | 0.9770          | 123             |       |
|                 | 4   | 2.7e - 12     | 2.9e - 11      | 0.9907          | 283             |       |
| 5               | 1   | 0.0779        | 0.0370         | 1.0528          | 2               | 444  |
|                 | 2   | 0.0088        | 0.0128         | 4.2424          | 5               |       |
|                 | 3   | 2.4e - 4      | 0.0021         | 4.4646          | 21              |       |
|                 | 4   | 7.0e - 7      | 2.8e - 5       | 4.6415          | 121             |       |
|                 | 5   | 1.9e - 11     | 2.4e - 10      | 4.6506          | 146             |       |
|                 | 6   | 1.0e - 14     | 3.8e - 13      | 4.6805          | 149             |       |
| 20              | 1   | 0.0779        | 0.0370         | 1.0528          | 2               | 427  |
|                 | 2   | 0.0245        | 0.0195         | 12.8944         | 3               |       |
|                 | 3   | 0.0041        | 0.0089         | 15.1663         | 5               |       |
|                 | 4   | 3.4e - 4      | 0.0030         | 19.9916         | 16              |       |
|                 | 5   | 4.7e - 6      | 8.6e - 5       | 19.3891         | 92              |       |
|                 | 6   | 1.9e - 9      | 5.6e - 8       | 19.9778         | 145             |       |
|                 | 7   | 1.5e - 14     | 4.7e - 13      | 19.7118         | 164             |       |

| $m$ | outer iterations | iters |
|-----|-----------------|-------|
| 10  | 278             | 2780  |
| 20  | 54              | 1080  |
| 30  | 32              | 960   |
| 40  | 19              | 760   |
| 50  | 13              | 650   |
| 60  | 11              | 660   |

Table 4: LSHP3466, $tol = 10^{-12}$, $\beta = 2613.1$, $\sin \phi_0 = 0.1011$. 
fixed small inner iteration steps $m$’s, expecting that resulting $\xi_k$’s are not too large and at least obey one of (24) and (32). Of course, if $T_m$ is too ill conditioned, it is possible for $\xi_k$ to be too large. We have tested several $m$’s for each test matrix; see Tables 1–4. Figure 1 displays convergence processes of the inexact RQI with Lanczos for various fixed $m$’s.

We find that the method works very well and robustly. In terms of iters, it is seen from the tables that the overall efficiency of the inexact RQI with Lanczos for fixed small $m$’s is comparable to that of the method with given fixed $\xi$’s, except for $m = 5$ for BCSPWR08 and CAN1054 and $m = 10$ for DWT2680 and LSHP3466. Furthermore, we observe that for BCSPWR08 and CAN1054 the inexact RQI with Lanczos converges almost as fast as the exact RQI for $m = 30$, and for the difficult problems DWT2680 and LSHP3466 we need to properly increase $m$ to achieve fast outer convergence. As explained, it is not surprising from the figures that a five-step and at most ten-step Lanczos method for the inner linear systems is enough to ensure the convergence of the inexact RQI with Lanczos. However, for the difficult BWT2680 and LSHP3466, the inexact RQI with Lanczos fails to converge when $m = 5$. The reason is that some $\xi_k$’s are too big and violate the linear convergence conditions. Finally, we should point out that although Lanczos with a smaller $m$ usually produces a bigger $\xi_k$ and thus makes the inexact RQI use more outer iterations than Lanczos with a bigger $m$, the total inner iteration steps iters used by the former is not necessarily more than that by the latter.

To see how big $\xi_k$’s may be as outer iterations converge, we display the curves of $\xi_k$’s versus $\sin \phi_k$’s for some fixed $m$’s in Figure 2. We remark that $\xi_k$ in the figure should correspond to $\xi_{k-1}$ in our context.

It is clear from Figure 2 that the inexact RQI with Lanczos works very well and $\sin \phi_k$

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{example.png}
\caption{The inexact RQI with Lanczos for varying inner iteration steps}
\end{figure}
tends to zero smoothly and quickly, that is, $\frac{1}{\sin \phi_k}$ tends to infinity smoothly and quickly, though most of $\xi_k$'s are much bigger than one and some of them are near $\frac{1}{\sin \phi_k}$ and can be as big as $10^4 \sim 10^7$! Furthermore, we observe that almost all $\xi_k$'s are smaller than $\frac{1}{\sin \phi_k}$ and the only exception is $\xi_6 > \frac{1}{\sin \phi_6}$ for BWT2680.

We also computed some other eigenpairs of each test matrix. We observed similar behavior and confirmed our theory. However, when an interior eigenpair was required, we often needed much more iters. This is because the shifted inner linear systems can be highly indefinite (i.e., each shifted matrix has many positive and negative eigenvalues) and may be hard to solve. If the smallest or largest eigenpair is required, then $A - \theta_k I$ has only one negative or positive eigenvalue, assuming that $A$ only has simple eigenvalues. As a consequence, after the smallest Ritz value converges to the smallest eigenvalue $\lambda - \theta_k$ of $A - \theta_k I$, the Lanczos method will behave as if $A - \theta_k I$ is positive or negative definite, so that it converges smoothly after the smallest Ritz value converges. Comparing with the computation of the smallest or largest eigenpair, we found that we must take a considerably bigger fixed inner iteration steps $m$ to make the method converge correctly when an interior eigenpair was desired. For a descriptive analysis, see, e.g., [3, 5, 12, 23].

6 Conclusions

We have considered the convergence of the inexact RQI with the unpreconditioned and tuned preconditioned Lanczos methods and have established a number of results. These results show how inner tolerance affects accuracy of outer iterations and provide practical
criteria on how to best control inner tolerance to achieve quadratic convergence of the inexact RQI. It is the first time to appear surprisingly that the inexact RQI with Lanczos converge quadratically provided $\xi_k \leq \xi$ with $\xi$ a constant being allowed bigger than one. This is both attractive and exciting as we can implement the method much more effectively than ever before. Numerical experiments have confirmed our theory.

Perspectively, since the inexact RQI has intimate relations with the simplified Jacobi-Davidson method and the former is mathematically equivalent to the latter when a Galerkin-Krylov type solver, e.g., the Lanczos method, is used for solving the linear systems, we can use the convergence theory developed here for the inexact RQI to help understand the inexact simplified JD method. Meanwhile, the inexact inverse iteration is a simpler variation of the inexact RQI, where varying $\theta_k$'s are fixed to be a constant $\sigma$, leading to different convergence behavior. Thus, a specific analysis is needed. It is likely to exploit the analysis approach used in this paper to study the inexact inverse iteration. Finally, although we have restricted to the Hermitian case, the analysis approach in this paper might be applied to the inexact RQI for the non-Hermitian eigenvalue problem, where the Arnoldi method is used for non-Hermitian inner linear systems.

We have only considered the standard Hermitian eigenvalue problem $Ax = \lambda x$ in this paper. For the Hermitian definite generalized eigenvalue problem $Ax = \lambda Mx$ with $A$ Hermitian and $M$ Hermitian positive definite, if the $M$-inner product, the $M$-norm and the $M^{-1}$-norm, the angle induced from the $M$-inner product are properly placed in positions of the usual Euclidean inner product, the Euclidean norm and the usual angle, then based on the underlying $M$-orthogonality of eigenvectors of the matrix pair $(A, M)$ we are able to extend our theory developed in the paper to the inexact RQI with the unpreconditioned and tuned preconditioned Lanczos for the generalized problem. This work is under research.

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