On Inner Iterations in the Shift-Invert Residual Arnoldi Method and the Jacobi–Davidson Method

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Abstract

Using a new analysis approach, we establish a general convergence theory of the Shift-Invert Residual Arnoldi (SIRA) method for computing a simple eigenvalue nearest to a given target \( \sigma \) and the associated eigenvector. In SIRA, a subspace expansion vector at each step is obtained by solving a certain inner linear system. We prove that the inexact SIRA method mimics the exact SIRA well, that is, the former uses almost the same outer iterations to achieve the convergence as the latter does if all the inner linear systems are iteratively solved with low or modest accuracy during outer iterations. Based on the theory, we design practical stopping criteria for inner solves. Our analysis is on one step expansion of subspace and the approach applies to the Jacobi–Davidson (JD) method with the fixed target \( \sigma \) as well, and a similar general convergence theory is obtained for it. Numerical experiments confirm our theory and demonstrate that the inexact SIRA and JD are similarly effective and are considerably superior to the inexact SIA.

Keywords. Subspace expansion, expansion vector, inexact, low or modest accuracy, the SIRA method, the JD method, inner iteration, outer iteration.

AMS subject classifications. 65F15, 15A18, 65F10.

1 Introduction

Consider the large and possibly sparse matrix eigenproblem

\[ \mathbf{A}\mathbf{x} = \lambda \mathbf{x}, \tag{1} \]

with \( \mathbf{A} \in \mathbb{C}^{n \times n} \), the 2-norm \( \|\mathbf{x}\| = 1 \) and the eigenvalues labeled as

\[ 0 < |\lambda_1 - \sigma| < |\lambda_2 - \sigma| \leq \cdots \leq |\lambda_n - \sigma| \]

for a given target \( \sigma \in \mathbb{C} \). We are interested in the eigenvalue \( \lambda_1 \) closest to the target \( \sigma \) and/or the associated eigenvector \( \mathbf{x}_1 \). We denote \((\lambda_1, \mathbf{x}_1)\) by \((\lambda, \mathbf{x})\) for simplicity. A number of numerical methods \([2, 14, 15, 20, 21]\) are available for solving this kind of problems. The Residual Arnoldi (RA) method and Shift-Invert Residual Arnoldi (SIRA) method are new ones that have their origins in the Jacobi–Davidson (JD) method \([18]\). RA was initially proposed by van der Vorst and Stewart in 2001; see \([11]\). The methods were then studied and developed by Lee \([10]\) and Lee and Stewart \([11]\). We briefly describe RA now.

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Given a starting vector $v_1$ with $\|v_1\| = 1$, suppose an orthonormal $V_m = (v_1, \ldots, v_m)$ has been constructed by the Arnoldi process. Then the columns of $V_m$ form a basis of the $m$-dimensional Krylov subspace $K_m(A, v_1) = \text{span}\{v_1, Av_1, \ldots, A^{m-1}v_1\}$, and the next basis vector $v_{m+1}$ is obtained by orthogonalizing $Av_m$ against $V_m$. Let $(\lambda, y)$ be the candidate Ritz pair of $A$ for a desired eigenpair of $A$ with respect to $K_m(A, v_1)$, and define the residual $r = Ay - \lambda y$. Then the RA method orthogonalizes $r$ against $V_m$ to get the next basis vector, which, in exact arithmetic, is just $v_{m+1}$ obtained by the Arnoldi process \cite{10,11}. So the Arnoldi method is mathematically equivalent to the RA method. However, van der Vorst and Stewart discovered a striking phenomenon that $r$ in the RA method may allow much larger errors or perturbations than $Av_m$ in the Arnoldi method.

The Shift-Invert Arnoldi (SIA) method is the Arnoldi method applied to the shift-invert matrix $B = (A - \sigma I)^{-1}$ and finds a few eigenvalues nearest to $\sigma$ and the associated eigenvectors. It computes $v_{m+1}$ by orthogonalizing $u = Bh_m$ against $V_m$, whose columns now form a basis of $K_m(B, v_1)$. So at step $m$ one has to solve the linear system

$$\label{eq:2}(A - \sigma I)u = v_m$$

for $u$. The SIRA method \cite{10,11} is an alternative of the RA method applied to $B$. At each step one has to solve the linear system

$$\label{eq:3}(A - \sigma I)u = r$$

for $u$, where $r = Ay - \nu y$ is the residual of the current approximate eigenpair $(\nu, y)$ obtained by SIRA. Then the SIRA method computes the next basis vector $v_{m+1}$ by orthogonalizing $u$ against $V_m$. A mathematical difference between SIA and SIRA is that the SIA method computes Ritz pairs of the shift-invert $B$ with respect to $K_m(B, v_1)$ and recovers an approximation to $(\lambda, x)$, while the SIRA method computes the Ritz pairs of the original $A$ with respect to the same $K_m(B, v_1)$ and gets an approximation to $(\lambda, x)$. So SIA and SIRA generally obtain different approximations to $(\lambda, x)$ with respect to the same subspace $K_m(B, v_1)$.

However, for large $m$, only iterative solvers are generally viable. This leads to the inexact SIRA, an inner-outer iterative method, built-up by outer iteration as the eigensolver and inner iteration as the solver of \cite{3}. Inexact eigensolvers have attracted much attention over the last two decades, and among them inexact SIA type methods \cite{3,16,17,23} are closely related to the work in the current paper. Central concerns on all inexact eigensolvers are how the accuracy of inner iterations ensures and affects the convergence of outer iterations and how to choose the accuracy requirements of inner iterations so that each inexact eigensolver mimics its corresponding exact counterpart very well in the sense that the two eigensolvers use almost the same or very comparable outer iterations to achieve the convergence.

The JD method with fixed or variable targets \cite{18} is a very popular inexact eigensolver, in which a correction equation (inner linear system) is solved iteratively at each outer iteration; see, e.g., \cite{2,20,21} and more recent \cite{4,13,19,22}. Hitherto, however, there has been no result on the accuracy requirement of inner iterations involved in the standard JD method. Existing work only focuses on the simplified (or single-vector) JD method without subspace acceleration. One hopes that the results on the accuracy requirement of inner iterations developed for the simplified JD may help understand the standard JD. Nevertheless, such treatment may be too inaccurate and far from the essence of the standard JD. As is well known, the standard JD is much more complicated than the simplified JD, and the convergence of its outer iterations is much more involved; see \cite{9} and also \cite{2,20,21} for details. Therefore, the standard JD method lacks a general theory on inner iterations, and a rigorous and insightful analysis is necessary and very appealing.

For the inexact SIA method, Simoncini \cite{17} has established a relaxation theory on the accuracy requirements of inner iterations of \cite{2} as $m$ increases. She proved that the accuracy...
of approximate solution of (2) should be very high initially and is relaxed as the approximate eigenpairs start converging. Freitag and Spence [3] have extended Simoncini’s relaxation theory to the inexact implicitly restarted Arnoldi method. Xue and Elman [23] have made a refined analysis on the relaxation strategy. So it may be very costly to implement the inexact SIA type methods.

For the SIRA method, it has been reported by Lee [10] and Lee and Stewart [11] that when the accuracy of approximate solutions of (3) is low or modest at each step, the method may still work well. Lee and Stewart [11] have made some analysis on the RA and SIRA methods but they did not derive any quantitative and explicit bounds for the accuracy requirements of inner iterations.

In this paper, we take a different approach from that in [10,11] to giving a rigorous one-step analysis of the inexact SIRA method and establish a general and quantitative theory of the accuracy requirements of inner iterations. Our analysis approach applies to the JD method with the fixed target \( \sigma \) as well. We first show that the exact SIRA and JD methods are mathematically equivalent. We then focus on a detailed quantitative analysis of the inexact SIRA and JD methods. Let \( \varepsilon \) be the relative error of the approximate solution of the inner linear system. We prove that a modestly small \( \varepsilon \), e.g., \( \varepsilon \in [10^{-4}, 10^{-3}] \), is generally enough to make the inexact SIRA and JD use almost the same outer iterations as the exact ones to achieve the convergence. As a result, one only needs to solve all inner linear systems with low or modest accuracy in the inexact SIRA and the JD methods, and both methods are expected to be considerably more effective than the inexact SIA method. We should point out that our work is locally an one step analysis. A global analysis involving subspaces accumulating all previous perturbations is much harder and seems impossible. Actually, an one step local analysis is typical in the field of inexact eigensolvers, and it indeed sheds lights on the behavior of the inexact solvers.

The paper is organized as follows. In Section 2, we review the SIRA and JD methods and show the equivalence of two exact versions. In Section 3, we derive some relationships between \( \varepsilon \) and subspace expansions and show that the inexact SIRA and methods behave very similar when their respective inner linear systems are solved with the same accuracy. In Section 4, we consider subspace improvement and the selection of \( \varepsilon \) and prove that the inexact SIRA mimics the exact SIRA very well when \( \varepsilon \) is modestly small at all steps. In Section 5, we consider some practical issues and design practical stopping criteria for inner solves in the inexact SIRA and JD. In Section 6, we report numerical experiments to confirm our theory and the considerable superiority of the inexact SIRA and JD algorithms to the inexact SIA algorithm. Meanwhile, we show that the inexact SIRA and JD are similarly effective. Finally, we conclude the paper and point out future work in Section 7.

Throughout the paper, denote by \( \| \cdot \| \) the 2-norm of a vector or matrix, by \( I \) the identity matrix with the order clear from the context, by the superscript \( H \) the conjugate transpose of a vector or matrix, and by \( \kappa(Q) = \|Q\|\|Q^{-1}\| \) the condition number of a nonsingular matrix \( Q \). We measure the distance between a nonzero vector \( y \) and a subspace \( \mathcal{V} \) by

\[
\sin \angle(\mathcal{V}, y) = \frac{\| (I - P_{\mathcal{V}}) y \|}{\| y \|} = \frac{\| V^*_H y \|}{\| y \|},
\]

where \( P_{\mathcal{V}} \) is the orthogonal projector onto \( \mathcal{V} \) and the columns of \( V_{\perp} \) form an orthonormal basis of the orthogonal complement of \( \mathcal{V} \).

2 Equivalence of the exact SIRA and JD methods

Algorithms [11,2] describe the SIRA algorithm and the JD algorithm with the fixed target \( \sigma \), respectively (for brevity we drop iteration subscript). Comparing them, we observe that the
only seemingly differences between them are the linear systems to be solved (step 4) and
the expansion vectors to be orthogonalized against the initial subspace \( V \). In fact, they are
equivalent, as the following theorem shows.

**Algorithm 1** SIRA method with the target \( \sigma \)

Given the target \( \sigma \) and a user-prescribed convergence tolerance \( tol \), suppose the columns
of \( V \) form an orthonormal basis of an initial subspace \( V \).

repeat
1. Compute the Rayleigh quotient \( H = V^H A V \).
2. Let \( (\nu, z) \) be an eigenpair of \( H \), where \( \nu \cong \lambda \).
3. Compute the residual \( r_S = Ay - \nu y \), where \( (\nu, y) = (\nu, Vz) \).
4. Solve the linear system
   \[
   (A - \sigma I)u = r_S. \tag{5}
   \]
5. Orthonormalize \( u \) against \( V \) to get \( v \).
6. Expand the subspace as \( V = [ V \ v ] \) and update \( H \).
until \( \|r_S\| < tol \).

**Algorithm 2** Jacobi–Davidson method with the fixed target \( \sigma \)

Given the target \( \sigma \) and a user-prescribed convergence tolerance \( tol \), suppose the columns
of \( V \) form an orthonormal basis of an initial subspace \( V \).

repeat
1. Compute the Rayleigh quotient \( H = V^H A V \).
2. Let \( (\nu, z) \) be an eigenpair of \( H \), where \( \nu \cong \lambda \).
3. Compute the residual \( r_J = Ay - \nu y \), where \( (\nu, y) = (\nu, Vz) \).
4. Solve the correction equation for \( u \perp y \),
   \[
   (I - yy^H)(A - \sigma I)(I - yy^H)u = -r_J. \tag{6}
   \]
5. Orthonormalize \( u \) against \( V \) to get \( v \).
6. Expand the subspace as \( V = [ V \ v ] \) and update \( H \).
until \( \|r_S\| < tol \).

**Theorem 1.** For the same initial \( V \), if \( \sigma \neq \nu \), then the SIRA method and the JD method
are mathematically equivalent when inner linear systems (5) and (6) are solved exactly.

**Proof.** For the same initial \( V \), the two methods share the same \( H, \nu \) and \( y \), leading to the
same \( r_S \) and \( r_J \). Let \( u_S \) and \( u_J \) be the exact solutions of (5) and (6), respectively. Since
\( B = (A - \sigma I)^{-1} \), we get
\[
   u_S = Br_S = (\sigma - \nu)By + y. \tag{7}
\]
From (6), we have
\[
   (A - \sigma I)u_J = (y^H(A - \sigma I)u_J)y = r_J = \gamma y - (A - \sigma I)y, \tag{8}
\]
where \( \gamma = y^H(A - \sigma I)u_J - \sigma + \nu \). Premultiplying two sides of (8) by \( B \), we obtain
\[
   u_J = \gamma By - y. \tag{9}
\]
Since \( u_J \perp y \), we get \( \gamma = \frac{1}{y^H By} \). Since \( y \in V \), we have \((I - P_V)y = 0\). So from (7) and (9), we get
\[
(I - P_V)By = \frac{1}{\sigma - \nu}(I - P_V)u_S = \frac{1}{\gamma}(I - P_V)u_J.
\]
(10)

Note that \((I - P_V)u_S\) and \((I - P_V)u_J\) (after normalization) are the subspace expansion vectors in SIRA and JD, respectively. The two methods generate the same subspace in the next iteration and \((\nu, y)\) obtained by them are thus identical.

From (8), define
\[
r'_J = Ay - (\sigma + \gamma)y,
\]
where
\[
\gamma = y^H (A - \sigma I)u_J - \sigma + \nu = \frac{1}{y^H By}.
\]
Then (8) and thus (6) become
\[
(A - \sigma I)u = r'_J,
\]
(11)
whose solution is \(-u_J\) and is the same as \(u_J\) up to the sign \(-1\). So mathematically, hereafter we use (11) as the inner linear system in the JD method. Since \(y^H By\) approximates the eigenvalue \( \frac{1}{\lambda - \sigma} \) of \(B\), \( \gamma + \sigma = \frac{1}{y^H By} + \sigma \) approximates \(\lambda\). So \(r'_J\) is a residual associated with the desired eigenpair \((\lambda, x)\), just like \(r_S\) in (5).

3 Relationships between the accuracy of inner iterations and subspace expansions

We observe that (5) and (11) fall into the category of
\[
(A - \sigma I)u = \alpha_1 y + \alpha_2 (A - \sigma I)y,
\]
(12)
where specifically \(\alpha_1 = \sigma - \nu\) and \(\alpha_2 = 1\) in SIRA and \(\alpha_1 = -\frac{1}{y^H By}\) and \(\alpha_2 = 1\) in JD. The exact solution \(u\) of (12) is
\[
u = \alpha_1 By + \alpha_2 y.
\]
(13)
Since \((I - P_V)y = 0\), the (unnormalized) subspace expansion vector is \((I - P_V)u = \alpha_1 (I - P_V)By\). Let \(\tilde{u}\) be an approximate solution of (12), whose relative error is defined by
\[
\varepsilon = \frac{\|\tilde{u} - u\|}{\|u\|}.
\]
(14)
Then we can write
\[
\tilde{u} = u + \varepsilon\|u\|f
\]
with \(f\) the normalized error direction vector. So we get
\[
(I - P_V)\tilde{u} = (I - P_V)u + \varepsilon\|u\|f_\perp.
\]
(15)
where
\[
f_\perp = (I - P_V)f.
\]
(16)
Define
\[
\tilde{v} = \frac{(I - P_V)\tilde{u}}{\|(I - P_V)\tilde{u}\|}, \quad v = \frac{(I - P_V)u}{\|(I - P_V)u\|}.
\]
(17)
which are the normalized subspace expansion vectors in the inexact and exact methods, respectively. We measure the difference between \((I - P_V)\hat{u}\) and \((I - P_V)u\) by the relative error

\[
\hat{\varepsilon} = \frac{\|(I - P_V)\hat{u} - (I - P_V)u\|}{\|(I - P_V)u\|} \tag{18}
\]

or by \(\sin \angle(\hat{v}, v)\). Two quantities \(\hat{\varepsilon}\) and \(\sin \angle(\hat{v}, v)\) are two valid measures for the difference. Next we establish a relationship between \(\hat{\varepsilon}\) and \(\sin \angle(\hat{v}, v)\), which will be used in proving our final result in this paper.

**Lemma 1.** With the notations defined above, it holds that

\[
\sin \angle(\hat{v}, v) = \hat{\varepsilon} \sin \angle(\hat{v}, f_\perp). \tag{19}
\]

**Proof.** Let \(U_\perp\) be an orthonormal basis of the orthogonal complement of \(\text{span} \{(I - P_V)\hat{u}\}\) with respect to \(C^n\). Since \(U_\perp\) is the normalized subspace expansion vector in the exact methods, we have

\[
\begin{align*}
\sin \angle(\hat{v}, v) &= \sin \angle((I - P_V)\hat{u}, (I - P_V)u) \\
&= \frac{\|U_\perp(I - P_V)u\|}{\|(I - P_V)u\|} \\
&= \frac{\|U_\perp(I - P_V)\hat{u} - U_\perp(I - P_V)u\|}{\|(I - P_V)u\|} \\
&= \frac{\|U_\perp((I - P_V)\hat{u} - (I - P_V)u)\|}{\|(I - P_V)u\|}. \tag{20}
\end{align*}
\]

From (15) we have \((I - P_V)\hat{u} - (I - P_V)u = \varepsilon \|u\|f_\perp\). Substituting it into (20) gives

\[
\sin \angle(\hat{v}, v) = \hat{\varepsilon} \sin \angle(\hat{v}, f_\perp).
\]

\(\Box\)

In order to make the inexact SIRA method mimic the SIRA method well, we must require that \(\hat{v}\) approximates \(v\) with certain accuracy, i.e., \(\hat{\varepsilon}\) suitably small, so that the two expanded subspaces have comparable quality. We will come back to this key point and estimate \(\hat{\varepsilon}\) quantitatively in Section 3.

In what follows we establish an important relationship between \(\varepsilon\) and \(\hat{\varepsilon}\), and based on it we analyze how \(\varepsilon\) varies with \(\alpha_1\) and \(\alpha_2\) for a given \(\hat{\varepsilon}\).

**Theorem 2.** Let \(y\) be the current approximate eigenvector and \(\alpha = -\frac{\alpha_2}{\alpha_1}\) with \(\alpha_1, \alpha_2\) in (12). We have

\[
\varepsilon \leq \frac{2\|B\| \sin \angle(y, x)}{\|By - \alpha y\| \sin \angle(V, f)} \hat{\varepsilon}. \tag{21}
\]

**Proof.** By definition (16), we have

\[
\|f_\perp\| = \|(I - P_V)f\| = \sin \angle(V, f).
\]

From (15), we get

\[
\begin{align*}
\varepsilon &= \frac{\|(I - P_V)\hat{u} - (I - P_V)u\|}{\|u\|\|f_\perp\|} \\
&= \frac{\|(I - P_V)\hat{u} - (I - P_V)u\|}{\|u\|\|f_\perp\|} \frac{\|(I - P_V)f\|}{\|u\| \sin \angle(V, f)} \\
&= \frac{\|(I - P_V)\hat{u} - (I - P_V)u\|}{\|u\|\|f_\perp\|} \hat{\varepsilon} = \frac{\|(I - P_V)u\|}{\|u\| \sin \angle(V, f)} \hat{\varepsilon}.
\end{align*}
\]
By (13), we substitute $u = \alpha_1 By + \alpha_2 y$ into the above, giving

$$
\varepsilon = \frac{\|(I - P_V)(\alpha_1 By + \alpha_2 y)\|}{\alpha_1 By + \alpha_2 y} \sin \angle (V, f) \tilde{\varepsilon} = \frac{\|\alpha_1 (I - P_V)By\|}{\alpha_1 By + \alpha_2 y} \sin \angle (V, f) \tilde{\varepsilon} = \frac{\|(I - P_V)By\|}{\|By + \alpha_2 y\|} \sin \angle (V, f) \tilde{\varepsilon}.
$$

(22)

Decompose $y$ into the orthogonal direct sum

$$
y = \cos \angle (y, x)x + \sin \angle (y, x)g
$$

with $g \perp x$ and $\|g\| = 1$. Then we get

$$(I - P_V)By = (I - P_V)(\cos \angle (y, x)Bx + \sin \angle (y, x)Bg) = (I - P_V)\left(\frac{\cos \angle (y, x)}{\lambda - \sigma}x + \sin \angle (y, x)Bg\right) = \frac{\cos \angle (y, x)}{\lambda - \sigma}x_\perp + \sin \angle (y, x)(I - P_V)Bg,$$

where $x_\perp = (I - P_V)x$. Making use of $\|x_\perp\| = \sin \angle (V, x) \leq \sin \angle (y, x)$ and $\frac{1}{|\lambda - \sigma|} \leq \|B\|$, we obtain

$$
\|(I - P_V)By\| = \left\|\frac{\cos \angle (y, x)}{\lambda - \sigma}x_\perp + \sin \angle (y, x)(I - P_V)Bg\right\| \leq \left\|\frac{\cos \angle (y, x)}{\lambda - \sigma}\right\|\|x_\perp\| + \|(I - P_V)Bg\| \sin \angle (y, x) \leq \left(\frac{\cos \angle (y, x)}{|\lambda - \sigma|} + \|(I - P_V)Bg\|\right) \sin \angle (y, x) \leq \left(\frac{1}{|\lambda - \sigma|} + \|B\|\right) \sin \angle (y, x) \leq 2\|B\| \sin \angle (y, x).
$$

(24)

Therefore, combining the last relation with (22) establishes (21).

Observe that the linear system $(A - \sigma I)u = y$, which is also the one in the inverse power method at each step, falls into the form of (12) by taking $\alpha_1 = 1$ and $\alpha_2 = 0$. For this case, from (21) we have

$$
\varepsilon \leq \frac{2\|B\| \sin \angle (y, x)}{\|By\| \sin \angle (V, f)} \tilde{\varepsilon}.
$$

(25)

We comment that (i) $\sin \angle (V, f)$ is moderate as $f$ is a general vector and (ii) $\|B\|/\|By\| = O(1)$ if $y$ is a reasonably good approximation to $x$ and in the worst case $\|B\|/\|By\| \leq \kappa(B)$. In case that $\sin \angle (V, f)$ is small, $\varepsilon$ becomes big for a fixed small $\tilde{\varepsilon}$, that is, linear system (12) is allowed to be solved with less accuracy. So a small $\sin \angle (V, f)$ is a lucky event.

We can use this theorem to further illustrate why it is bad to solve $(A - \sigma I)u = y$ iteratively. For a fixed small $\tilde{\varepsilon}$, (25) tells us that $\varepsilon$ should become smaller as $\sin \angle (y, x) \to 0$ as the algorithms converge. As a result, we have to solve inner linear systems with higher accuracy as $y$ becomes more accurate. More generally, this is the case when $\|By - \alpha y\|$ is not small and typically of $O(\|B\|)$. Therefore, for $\alpha = 0$ and more general $\alpha$, the resulting
method and SIA type methods are similar and no winner in theory. They are common in that they all require to solve inner linear systems accurately for some steps and they are different in that the former solves inner linear systems with poor accuracy initially and then with increasing accuracy as the algorithm converges, while the latter ones solve inner linear systems with high accuracy in some initial outer iterations and then with decreasing accuracy as the algorithms converge.

Based on (21), it is natural for us to maximize its upper bound with respect to $\alpha$ for a fixed $\tilde{\varepsilon}$. This will make $\varepsilon$ as small as possible, so that we pay least computational efforts to solve (12). This amounts to minimizing $\|By - \alpha y\|$. As is well known, the optimal $\alpha$ is

$$\arg\min_{\alpha\in\mathbb{C}} \|By - \alpha y\| = y^H By,$$  \hfill (26)

Such $\alpha = -\frac{\alpha_2}{\alpha_1}$ corresponds to the choice $\alpha_1 = -\frac{1}{y^H By}$ and $\alpha_2 = 1$ in (12), exactly leading to linear system (11) in the JD method. Therefore, in the sense of minimizing $\|By - \alpha y\|$, the JD method is the best. If we take $\alpha = \frac{1}{\lambda - \sigma}$, which is the approximation to $\frac{1}{\lambda - \sigma}$ in SIRA, by letting $\alpha_1 = \sigma - \nu$ and $\alpha_2 = 1$, then (12) becomes

$$(A - \sigma I)u = (A - \sigma I)y + (\sigma - \nu)y = r_S,$$

which is exactly the linear system in the SIRA method. In each of JD and SIRA, $\|By - \alpha y\|$ is the residual norm of an approximate eigenpair $(\alpha, y)$ of $B$.

In what follows, we denote $\varepsilon$ by $\varepsilon_S$ and $\varepsilon_J$ in the SIRA and JD methods, respectively. To derive our final and key relationships between $\sin \angle(y, x)$ and the residual norm $\|By - \alpha y\|$, we need the following lemma, which is direct from Theorem 6.1 of [9] and establishes a close and compact relationship between $\sin \angle(y, x)$ and the residual norm $\|By - \alpha y\|$.\hfill

**Lemma 2.** Suppose $\left(\frac{1}{\lambda - \sigma}, x\right)$ is a simple desired eigenpair of $B \in \mathbb{C}^{n \times n}$ and let $(x, X_\perp)$ be unitary. Then

$$\begin{bmatrix} x^H \\ X_\perp^H \end{bmatrix} B \begin{bmatrix} x \\ X_\perp \end{bmatrix} = \begin{bmatrix} \frac{1}{\lambda - \sigma} & c^H \\ 0 & \mathbb{I} \end{bmatrix},$$  \hfill (27)

where $c^H = x^H B X_\perp$ and $L = X_\perp^H B X_\perp$. Let $(\alpha, y)$ be an approximation to $\left(\frac{1}{\lambda - \sigma}, x\right)$, assume that $\alpha$ is not an eigenvalue of $L$ and define

$$\text{sep} (\alpha, L) = \| (L - \alpha I)^{-1} \|^{-1} > 0.$$  \hfill (28)

Then

$$\sin \angle(y, x) \leq \frac{\|By - \alpha y\|}{\text{sep} (\alpha, L)}.$$  \hfill (29)

Combining (29) with Theorem 2 we obtain one of our main results.\hfill

**Theorem 3.** Assume that $\alpha$ is an approximation to $\frac{1}{\lambda - \sigma}$ and is not an eigenvalue of $L$. Then

$$\varepsilon \leq \frac{2\|B\|}{\text{sep} (\alpha, L) \sin \angle(V, f)} \tilde{\varepsilon}.$$  \hfill (30)

In particular, for $\alpha = \frac{1}{\nu - \sigma}$ and $\alpha = y^H B y$, which correspond to the SIRA and JD methods, respectively, assume that each of them is not an eigenvalue of $L$. Then it holds that

$$\varepsilon_S \leq \frac{2\|B\|}{\text{sep} \left(\frac{1}{\nu - \sigma}, L\right) \sin \angle(V, f)} \tilde{\varepsilon},$$  \hfill (31)

and

$$\varepsilon_J \leq \frac{2\|B\|}{\text{sep} (y^H B y, L) \sin \angle(V, f)} \tilde{\varepsilon}. \hfill (32)$$
This theorem shows that once \( \bar{\epsilon} \) is known we can a-priori determine the accuracy requirements \( \epsilon_S \) and \( \epsilon_J \) on approximate solutions of inner linear systems \( (5) \) and \( (6) \).

It is important to observe from (30) that

\[
\epsilon \leq \frac{2\|B\|}{\text{sep}(\alpha, L) \sin \angle(V', f)} \bar{\epsilon} = \frac{2\|B\|}{O(\|B\|)} \bar{\epsilon} = O(\bar{\epsilon})
\]

if \( \alpha \) is well separated from the eigenvalues of \( B \) other than \( \frac{1}{\lambda_0} \) and \( B \) is normal or mildly non-normal and \( \sin \angle(V', f) \) is not small. For \( \sin \angle(V', f) \) small, noting that bound (30) is compact, we are lucky to have a bigger \( \epsilon \), i.e., to solve the inner linear system with less accuracy. If \( \text{sep}(\alpha, L) \) is considerably smaller than \( \|B\| \), then \( \epsilon \) may be bigger than \( \bar{\epsilon} \) considerably and we are likely lucky to solve the inner linear system with less accuracy.

For the \( \alpha \)'s in the SIRA and JD methods, by continuity the corresponding two \( \text{sep}(\alpha, L) \)'s are close. Therefore, for a given \( \bar{\epsilon} \), we have essentially the same upper bounds for \( \epsilon_S \) and \( \epsilon_J \). This means that we need to solve the corresponding inner linear systems \( (5) \) and \( (6) \) in the SIRA and JD methods with essentially the same accuracy \( \epsilon \). In other words, the SIRA and JD methods behave very similar when \( (5) \) and \( (6) \) are solved with the same accuracy.

4 Subspace improvement and selection of \( \bar{\epsilon} \) and \( \epsilon \)

In this section, we first focus on the fundamental problem of how to select \( \bar{\epsilon} \) to make the inexact SIRA and JD mimic the exact SIRA very well from the current step to the next one. Then we show how to achieve our ultimate goal: the determination of \( \epsilon \).

Recall that the subspace expansion vectors are \( v \) and \( \tilde{v} \) for the exact SIRA and the inexact SIRA or JD; see (17). Define \( V_+ = [ V \ v ] \), \( V_+ = \text{span}\{V_+\} \) and \( \tilde{V}_+ = [ V \ \tilde{v} ] \), \( \tilde{V}_+ = \text{span}\{\tilde{V}_+\} \). In order to make the inexact SIRA method mimic the exact SIRA method very well, we must require that the two expanded subspaces \( V_+ \) and \( \tilde{V}_+ \) have almost the same quality, namely, \( \sin \angle(V_+, x) \approx \sin \angle(\tilde{V}_+, x) \), whose quantitative meaning will be clear later.

**Theorem 4.** With the notations above, assume \( \sin \angle(v, x_{\perp}) \neq 0 \) with \( x_{\perp} = (I - P_V)x \). Then we have

\[
\sin \angle(V_+, x) = \sin \angle(V_+, x_{\perp}) \sin \angle(v, x_{\perp}) \tag{33}
\]

\[
\sin \angle(\tilde{V}_+, x) = \sin \angle(\tilde{V}_+, x_{\perp}) \sin \angle(\tilde{v}, x_{\perp}) \tag{34}
\]

Suppose \( \angle(\tilde{v}, v) \) is acute. If \( \tau = \frac{2\bar{\epsilon}}{\sin \angle(\tilde{V}_+, x_{\perp})} < 1 \), we have

\[
1 - \tau \leq \frac{\sin \angle(\tilde{V}_+, x)}{\sin \angle(V_+, x)} \leq 1 + \tau. \tag{35}
\]

**Proof.** Since

\[
\sin^2 \angle(V, x) - \sin^2 \angle(V_+, x) = \| (I - P_V)x \|^2 - \| (I - P_{V_+})x \|^2 = |v^Hx|^2,
\]

by \( \|x_{\perp}\| = \sin \angle(V, x) \) we obtain

\[
\frac{\sin \angle(V_+, x)}{\sin \angle(V, x)} = \sqrt{1 - \left( \frac{|v^Hx|}{\sin \angle(V, x)} \right)^2}.
\]

\[\text{If it fails to hold, it is seen from (33) that } \sin \angle(V_+, x) = 0 \text{ and the exact SIRA, SIA and JD methods terminate prematurely if } \dim(V_+) < n. \text{ In this case, } V_+ \text{ is an invariant subspace of } A \text{ and we stop subspace expansion. We will exclude this rare case.} \]
\[
\sqrt{1 - \left( \frac{|v^H x_\perp|}{\sin \angle(V, x)} \right)^2} = \sqrt{1 - \left( \frac{\|x_\perp\| \cos \angle(v, x_\perp)}{\sin \angle(V, x)} \right)^2} = \sqrt{1 - \cos^2 \angle(v, x_\perp)} = \sin \angle(v, x_\perp),
\]
which proves \((33)\). Similarly, we have
\[
\frac{\sin \angle(\tilde{\mathcal{V}}_+, x)}{\sin \angle(\tilde{\mathcal{V}}, x)} = \sin \angle(\tilde{v}, x_\perp). \tag{36}
\]
Hence, from \((33)\) and \((36)\), we get \((34)\).

Exploiting the trigonometric identity
\[
\sin \angle(\tilde{v}, x_\perp) - \sin \angle(v, x_\perp) = 2 \cos \frac{\angle(\tilde{v}, x_\perp) + \angle(v, x_\perp)}{2} \sin \frac{\angle(\tilde{v}, x_\perp) - \angle(v, x_\perp)}{2},
\]
the angle triangle inequality
\[
|\angle(\tilde{v}, x_\perp) - \angle(v, x_\perp)| \leq \angle(\tilde{v}, v).
\]
and the monotonic increasing property of the \(\sin\) function in the first quadrant, we get
\[
|\sin \angle(\tilde{v}, x_\perp) - \sin \angle(v, x_\perp)| \leq 2 \sin \frac{\angle(\tilde{v}, x_\perp) - \angle(v, x_\perp)}{2} \leq 2 \sin \frac{\angle(\tilde{v}, v)}{2} \leq 2 \sin \angle(\tilde{v}, v). \tag{37}
\]
From \((33)\), \((37)\) and \((14)\), we obtain
\[
\left| \frac{\sin \angle(\tilde{\mathcal{V}}_+, x)}{\sin \angle(\tilde{\mathcal{V}}_+, x)} - 1 \right| = \left| \frac{\sin \angle(\tilde{v}, x_\perp)}{\sin \angle(v, x_\perp)} - 1 \right| = \left| \frac{\sin \angle(\tilde{v}, x_\perp) - \sin \angle(v, x_\perp)}{\sin \angle(v, x_\perp)} \right| \leq \frac{2 \sin \angle(\tilde{v}, v)}{\sin \angle(v, x_\perp)} \leq \frac{2 \varepsilon}{\sin \angle(v, x_\perp)} = \tau,
\]
from which it follows that \((35)\) holds.

From \((33)\), we see that \(\sin \angle(v, x_\perp)\) is exactly one step subspace improvement when \(\mathcal{V}\) is expanded to \(\mathcal{V}_+\).

\((35)\) shows that, to make \(\sin \angle(\tilde{\mathcal{V}}_+, x) \approx \sin \angle(\mathcal{V}_+, x)\), \(\tau\) should be small. Meanwhile, \((35)\) also indicates that a very small \(\tau\) cannot improve the bounds essentially. Actually, for our purpose, a fairly small \(\tau\), e.g., \(\tau = 0.01\), is enough since we have
\[
0.99 \leq \frac{\sin \angle(\tilde{\mathcal{V}}_+, x)}{\sin \angle(\mathcal{V}_+, x)} \leq 1.01
\]
and the lower and upper bounds are very near and differ marginally. Therefore, \( \hat{V}_+ \) and \( V_+ \) are of almost the same quality for approximating \( x \). As a result, it is expected that the inexact SIRA or JD computes new approximation over \( \hat{V}_+ \) to the desired \((\lambda, x)\) that has almost the same accuracy as that obtained by the exact SIRA over \( V_+ \). More precisely, the accuracy of the approximate eigenpair by the exact SIRA and that by the inexact SIRA or JD are generally the same within roughly a multiple \( c \in [1 - \tau, 1 + \tau] \) (this assertion can be justified from the results in [39]). So how near the constant \( c \) is to one is insignificant, the inexact SIRA and JD generally mimic the exact SIRA very well when \( \tau \) is fairly small. Concisely, we may well draw the conclusion that \( \tau = 0.01 \) makes the inexact SIRA mimic the exact SIRA very well, that is, the exact and inexact SIRA methods use almost the same outer iterations to achieve the convergence.

Next we discuss the selection of \( \hat{\epsilon} \). Once \( \hat{\epsilon} \) is available, in principle we can exploit compact bounds (61) and (62) to determine the accuracy requirements \( \epsilon_S \) and \( \epsilon_J \) on inner iterations in the SIRA and JD.

From the definition of \( \tau \), we have

\[
\hat{\epsilon} = \frac{\tau}{2} \sin \angle(v, x_\perp). \quad (38)
\]

As Theorem 4 requires \( \tau < 1 \), we must have \( \hat{\epsilon} < \frac{1}{2} \sin \angle(v, x_\perp) \). But \( x_\perp \) is not available and a-priori, so we can only use a reasonable estimate on \( \sin \angle(v, x_\perp) \) in (38). In the following, we will look into \( \sin \angle(v, x_\perp) \) and show that it is actually independent of the quality of the approximate eigenvector \( y \), i.e., \( \sin \angle(y, x) \), and the subspace quality, i.e., \( \sin \angle(V, x) \). This means that \( \sin \angle(v, x_\perp) \) stays around some constant during outer iterations. Then we analyze its size, which is shown to be problem dependent and stay around some certain constant during outer iterations. Based on these results, we can propose a general practical selection of \( \hat{\epsilon} \). Obviously, in order to achieve a given \( \tau \), the smaller \( \sin \angle(v, x_\perp) \) is, the smaller \( \hat{\epsilon} \) must be and the more accurately we need to solve the inner linear system.

We now investigate \( |\cos \angle(v, x_\perp)| \) and show that it is bounded independently of \( \sin \angle(y, x) \) and \( \sin \angle(V, x) \), so is \( \sin \angle(v, x_\perp) \). From (10) and (17), it is known that \( v \) and \( (I - P_V)By \) are in the same direction. Therefore, from decomposition (23) of \( y \), we have

\[
|\cos \angle(v, x_\perp)| = \frac{|x^H_+(I - P_V)By|}{\|x_\perp\|(I - P_V)By} = \frac{|x^H_+(I - P_V)B(\cos \angle(y, x)x + \sin \angle(y, x)g)|}{\|x_\perp\|(I - P_V)By} = \frac{|x^H_+(I - P_V)\left(\frac{\cos \angle(y, x)}{\lambda - \sigma}x + \sin \angle(y, x)Bg\right)|}{\|x_\perp\|(I - P_V)By} \leq \frac{|\cos \angle(y, x)||x_\perp||^2 + (\lambda - \sigma)\sin \angle(y, x)x^H_+Bg|}{|\lambda - \sigma||x_\perp||(I - P_V)By|} \sin \angle(y, x)x^H_+Bg|}{\|x_\perp\||(I - P_V)By||}.
\]

Note that \( |x^H_+Bg| \leq \|x_\perp\||Bg| \leq \|x_\perp\||B| \) and \( \|x_\perp\| = \sin \angle(V, x) \leq \sin \angle(y, x) \). So

\[
|\cos \angle(v, x_\perp)| \leq \frac{|\cos \angle(y, x)||x_\perp| + \sin \angle(y, x)||Bg|}{|\lambda - \sigma||x_\perp||(I - P_V)By|} \leq \frac{\left(\frac{|\cos \angle(y, x)|}{|\lambda - \sigma|} + |B|\right)\sin \angle(y, x)}{|(I - P_V)By|} \leq 2||B||\sin \angle(y, x)}}{|(I - P_V)By|}. \quad (39)
\]
Combining (39) and (24), we have
\[
|\cos \angle(v, x_\perp)| \leq \frac{O(\|B\|) \sin \angle(y, x)}{O(\|B\|) \sin \angle(y, x)} = O(1),
\]
a seemingly trivial bound. However, the proof clearly shows that our derivation is general and does not miss anything essential. We are not able to make the bound essentially sharper and more elegant as the inequalities used in the proof cannot be sharpened generally. Nevertheless, this is enough for our purpose. A key implication is that the bound is independent of \(\sin \angle(y, x)\) and \(\sin \angle(V, x)\), so \(|\cos \angle(v, x_\perp)|\) is expected to be around some constant during outer iterations, so is \(\sin \angle(v, x_\perp)\).

It is possible to estimate \(\sin \angle(v, x_\perp)\) in some important cases. For the starting vector \(v_1\), it is known that the exact SIRA, SIA and JD methods work on the standard Krylov subspaces \(V = V_m = K_m(B, v_1)\) and \(V_+ = V_{m+1} = K_{m+1}(B, v_1)\). Here we have temporarily added iteration subscripts and assume that the current iteration step is \(m\). It is direct from (41) to get
\[
\sin \angle(V_{m+1}, x) = \sin \angle(v_1, x) \prod_{i=2}^{m+1} \sin \angle(v_i, x_{i,\perp}),
\]
where the \(v_i\) are exact subspace expansion vectors and \(x_{i,\perp} = (I - P_{V_i})x\) at steps \(i = 2, 3, \ldots, m+1\).

For the Krylov subspaces \(V_m\) and \(V_{m+1}\), there have been some estimates on \(\sin \angle(V_{m+1}, x)\) in [5,7,15]. For \(B\) is diagonalizable, suppose all the \(\lambda_i, i = 1, 2, \ldots, n\) and \(\sigma\) are real and \(\frac{\lambda - \sigma}{\lambda} is also the algebraically largest eigenvalue of \(B\), and define
\[
\eta = 1 + 2\left(\frac{\lambda - \sigma}{\lambda} - \frac{\lambda_2 - \sigma}{\lambda_2}\right) = 1 + 2\left(\frac{(\lambda_2 - \lambda)(\lambda_n - \sigma)}{(\lambda_n - \lambda)(\lambda - \sigma)}\right) > 1.
\]
Then it is shown in [7,15] that
\[
\sin \angle(V_{m+1}, x) = \sin \angle(v_1, x) \prod_{i=2}^{m+1} \sin \angle(v_i, x_{i,\perp}) \leq C_{V_1} \sin \angle(v_1, x) \left(\frac{1}{\eta + \sqrt{\eta^2 - 1}}\right)^m,
\]
where \(C_{V_1}\) is a certain constant only depending on \(v_1\) and the conditioning of the eigensystem of \(B\). So, ignoring the constant factor \(C_{V_1}\), we see the product \(\prod_{i=2}^{m+1} \sin \angle(v_i, x_{i,\perp})\) converges to zero at least as rapidly as
\[
\left(\frac{1}{\eta + \sqrt{\eta^2 - 1}}\right)^m.
\]
As we have argued, all the \(\sin \angle(v_i, x_{i,\perp}), i = 2, 3, \ldots, m+1\), stay around a certain constant. So basically, each step subspace improvement \(\sin \angle(v_i, x_{i,\perp}), i = 2, 3, \ldots, m+1\), behaves like and is no more than the factor
\[
\frac{1}{\eta + \sqrt{\eta^2 - 1}},
\]
the average convergence factor for one step. Returning to our notation, we see the size of \(\sin \angle(v, x_\perp)\) crucially depends on the eigenvalue distribution. The better \(\frac{1}{\lambda - \sigma}\) is separated from the other eigenvalues of \(B\), the smaller \(\sin \angle(v, x_\perp)\) is. Conversely, if \(\frac{1}{\lambda - \sigma}\) is poorly separated from the others, \(\sin \angle(v, x_\perp)\) may be near to one. For more complicated complex eigenvalues and/or \(\sigma\), quantitative results are obtained for \(\sin \angle(V_{m+1}, x)\) and similar conclusions are drawn in [5,7]. However, we should point that these estimates may be conservative
and also only predict linear convergence. In practice, a slightly superlinear convergence may occur sometimes, as has been observed in [11].

For $\tau = 0.01$, if $\sin \angle (v, x_{\perp}) \in [0.02, 0.2]$, then by (38) we have $\bar{\varepsilon} \in [10^{-4}, 10^{-3}]$. Such $\sin \angle (v, x_{\perp})$ means that $\frac{1}{\lambda - \sigma}$ is well separated from the other eigenvalues of $B$ and the exact SIRA generally converges fast. In practice, however, for a given $\bar{\varepsilon}$ we do not know the value of $\tau$ produced by $\bar{\varepsilon}$ as $\sin \angle (v, x_{\perp})$ and its bound are not known. For a given $\bar{\varepsilon}$, if we are unlucky to get a $\tau$ not small like 0.01, the inexact SIRA may use more outer iterations than the exact SIRA. Suppose we select $\bar{\varepsilon} = \frac{10^{-3}}{2}$. Then if each $\sin \angle (v, x_{\perp}) = 0.1$, we get $\tau = 0.01$. For this case, we have a very good subspace $V_m$ for $m = 10$ since $\sin(|v_{10}^T x|) \leq 10^{-9}$, so the exact SIRA generally converges very fast! For a real-world problem, however, one should not expect that $\frac{1}{\lambda - \sigma}$ is generally so well separated from the other eigenvalues that the convergence can be so rapid. Therefore, we generally expect that $\bar{\varepsilon} \in [10^{-4}, 10^{-3}]$ makes $\tau \leq 0.01$, so that the inexact SIRA and JD mimic the exact SIRA very well.

Summarizing the above, we propose taking

$$\bar{\varepsilon} \in [10^{-4}, 10^{-3}]. \quad (42)$$

Our ultimate goal is to determine $\varepsilon_S$ and $\varepsilon_J$ for the inexact SIRA and JD. Compact bounds (31) and (32) show that they are generally of $O(\bar{\varepsilon})$. However, it is impossible to compute the bounds cheaply and accurately. We will consider their practical estimates on $\varepsilon_S$ and $\varepsilon_J$ in Section 5 where we demonstrate that these estimates are cheaply obtainable.

5 Restarted algorithms and practical stopping criteria for inner iterations

Due to the storage requirement and computational cost, Algorithms 1–2 will be impractical for large steps of outer iterations. To be practical, it is necessary to restart them for difficult problems. Let $M_{\max}$ be the maximum of outer iterations allowed. If the basic SIRA and JD algorithms do not converge, then we simply update $v_1$ and restart them. We call the resulting restarted algorithms Algorithms 3–4, respectively.

In implementations, we adopt the following strategy to update $v_1$. For outer iteration steps $i = 1, 2, \ldots, M_{\max}$ during the current cycle, suppose $((\nu_1^{(i)}, y_1^{(i)}))$ is the candidate for approximating the desired eigenpair $(\lambda, x)$ of $A$ at the $i$-th outer iteration. Then we take

$$v_1 = y = \arg \min_{i=1,2,\ldots,M_{\max}} \| (A - \nu_1^{(i)} I) y_1^{(i)} \| \quad (43)$$

as the updated starting vector in the next cycle. Such a restarting strategy guarantees that we use the best candidate Ritz vector in the sense of (43) to restart the algorithms.

In what follows we consider some practical issues and design practical stopping criteria for inner iterations in the (non-restarted and restarted) inexact SIRA and JD algorithms.

Given $\varepsilon$, since $L$ is not available, it is impossible to compute $\text{sep}(\frac{1}{\nu_{i-\sigma}}, L)$ and $\text{sep}(y_{H}^T B y_{L}, L)$ in (31) and (32). Also, we cannot compute $\sin \angle (V, f)$ in (31) and (32). In practice, we simply replace the insignificant factor $\sin \angle (V, f)$ by one, which makes $\varepsilon_S$ and $\varepsilon_J$ as small as possible, so that the inexact SIRA and JD algorithms are the safest to mimic the exact SIRA. We replace $\|B\|$ by $\frac{1}{\nu_{i-\sigma}}$ in the inexact SIRA and JD, respectively. For $\text{sep}(\frac{1}{\nu_{i-\sigma}}, L)$, we can exploit the spectrum information of $H$ to estimate it. Let $\nu_i, i = 2, 3, \ldots, m$ be the other eigenvalues (Ritz values) of $H$ other than $\nu$. Then we use the estimate

$$\text{sep} \left( \frac{1}{\nu_{i-\sigma}}, L \right) \approx \min_{i=2,3,\ldots,m} \left| \frac{1}{\nu_{i-\sigma}} - \frac{1}{\nu_i - \sigma} \right|. \quad (44)$$
Note that it is very expensive to compute $y^H By$ but $y^H By \approx \frac{1}{\nu - \sigma}$. So we simply use $\frac{1}{\nu - \sigma}$ to estimate $\text{sep}(y^H By, L)$. With these estimates and taking the equalities in compact bounds (31) and (32), we get

$$\varepsilon_S = \varepsilon_J = \varepsilon = 2\tilde{\varepsilon} \max_{i=2,3,\ldots,m} \left| \nu_i - \sigma \right|.$$  \hfill (45)

It might be possible to have $\varepsilon \geq 1$ for a given $\tilde{\varepsilon}$. This would make $\tilde{u}$ no accuracy as an approximation to $u$. As a remedy, from now on we set

$$\varepsilon = \min\{\varepsilon, 0.1\}.$$  \hfill (46)

For $m = 1$, we simply set $\varepsilon = \tilde{\varepsilon}$.

Note that $\frac{\|\tilde{u} - u\|}{\|u\|}$ is a-priori and uncomputable. We are not able to determine whether it is below $\varepsilon$ or not. However, it is easy to verify that

$$\frac{1}{\kappa(B)} \frac{\|\tilde{u} - u\|}{\|u\|} \leq \frac{\|r_S - (A - \sigma I)\tilde{u}\|}{\|r_S\|} \leq \kappa(B) \frac{\|\tilde{u} - u\|}{\|u\|}$$  \hfill (47)

and

$$\frac{1}{\kappa(B')} \frac{\|\tilde{u} - u\|}{\|u\|} \leq \frac{\|r_J - (I - yy^H)(A - \sigma I)(I - yy^H)\tilde{u}\|}{\|r_J\|} \leq \kappa(B') \frac{\|\tilde{u} - u\|}{\|u\|},$$  \hfill (48)

where $\tilde{u} \perp y$ and $B' = B|_{y^\perp} = (A - \sigma I)^{-1}|_{y^\perp}$, the restriction of $B$ to the orthogonal complement of $\text{span}\{y\}$. Alternatively, based on the above two relations, in practice we require that inner solves stop when the a-posteriori computable relative residual norms

$$\frac{\|r_S - (A - \sigma I)\tilde{u}\|}{\|r_S\|} \leq \varepsilon$$  \hfill (49)

and

$$\frac{\|r_J - (I - yy^H)(A - \sigma I)(I - yy^H)\tilde{u}\|}{\|r_J\|} \leq \varepsilon$$  \hfill (50)

for the inexact SIRA and JD, respectively.

Remark. In [3, 16, 17], a-priori accuracy requirements have been determined for inner iterations in SIA type methods. In computation, a-posteriori residuals are intuitive, and are probably the only practical way to approximate the a-priori residuals. Here, by the above lower and upper bounds (47) and (48) that relate the a-posteriori relative residuals to the a-priori errors of approximate solutions, we have simply demonstrated that (49) and (50) are reasonable stopping criteria for inner solves. We see that the a-priori errors and the a-posteriori errors are definitely comparable once the linear systems are not ill conditioned.

6 Numerical experiments

We report numerical experiments to confirm our theory. Our aims are mainly three-fold: (i) Regarding outer iterations, for fairly small $\tilde{\varepsilon} = 10^{-3}$ and $10^{-4}$, the (non-restarted and restarted) inexact SIRA and JD behave very like the (non-restarted and restarted) exact SIRA. Even a bigger $\tilde{\varepsilon} = 10^{-2}$ often works very well. (ii) Regarding inner iterations and overall efficiency, the inexact SIRA and JD algorithms are considerably more efficient than the inexact SIA. (iii) SIRA and JD are similarly effective.

All the 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 $\epsilon_{\text{mach}} = 2.22 \times 10^{-16}$ under the Microsoft Windows XP operating system.
At the $m$th step of the inexact SIRA or JD method, we have $H_m = V_m^H A V_m$. Let $(\nu^{(m)}_i, z^{(m)}_i), \ i = 1, 2, \ldots, m$ be the eigenpairs of $H_m$, which are ordered as

$$|\nu^{(m)}_1 - \sigma| < |\nu^{(m)}_2 - \sigma| \leq \cdots \leq |\nu^{(m)}_m - \sigma|.$$  

We use the Ritz pair $(\nu_m, y_m) := (\nu^{(m)}_1, V_m z^{(m)}_1)$ to approximate the desired eigenpair $(\lambda, x)$ of $A$, and the associated residual is $r_m = Ay_m - \nu_m y_m$.

We stop the algorithms if

$$\|r_m\| \leq tol = \max \{\|A\|, 1\} \times 10^{-10}.$$  

In the inexact SIRA and JD, we stop inner solves when (49) and (50) are satisfied, respectively, and denote by SIRA($\bar{\varepsilon}$) and JD($\bar{\varepsilon}$) the inexact SIRA and JD algorithms with the given parameter $\bar{\varepsilon}$. We use the following stopping criteria for inner iterations in the exact SIRA and SIA algorithms and the inexact SIA algorithm.

- For the “exact” SIRA algorithm, we require the approximate solution $\tilde{u}_{m+1}$ to satisfy

$$\frac{\|r_m - (A - \sigma I)\tilde{u}_{m+1}\|}{\|r_m\|} \leq 10^{-14}.$$  

- For the inexact SIA algorithm, we take the same outer iteration tolerance $tol = \max \{\|A\|, 1\} \times 10^{-10}$, and use the stopping criterion (3.14) in [3] for inner solve, where $\varepsilon = tol$ and the steps $m$ suitably bigger than the number of outer iterations used by the exact SIRA so as to ensure the convergence of the inexact SIA with the same accuracy. For the restarted inexact SIA, we take $m$ the maximum outer iterations $M_{\text{max}}$ allowed for each cycle.

In the numerical experiments, we always take the zero vector as an initial approximate solution to each inner linear system and solve it by the right-preconditioned GMRES(30) method. Outer iterations start with the normalized vector $\frac{1}{\sqrt{m}}(1, 1, \ldots, 1)^H$. For the correction equation in the JD method, we use

$$M_m = (I - y_m y_m^H)M(I - y_m y_m^H)$$

the restriction of $M$ to the orthogonal complement of $\text{span}\{y_m\}$, as a preconditioner, which is suggested in [21]. $M_m^{-1}|_{y_m}$ means the inverse of $M_m$ restricted to the orthogonal complement of $\text{span}\{y_m\}$. Here $M \approx A - \sigma I$ is some preconditioner used for all the inner linear systems involved in the algorithms tested except JD. We use the Matlab function $[L, U] = ilu(A - \sigma I)$ to compute the sparse incomplete LU factorization of $A - \sigma I$ with a given dropping tolerance $setup.droptol$. We then take $M = LU$. van der Vorst [21] shows how to use $M_m$ as a left preconditioner for (6). It can also be used a right preconditioner for (6) in the same spirit. Adapted from [21] p. 137-8], we briefly describe how to do so.

Suppose that a Krylov solver for (6) with right-preconditioning starts with zero vector as an initial guess to the solution. Then the starting vector for the Krylov solver is $r_m$, which is in the subspace orthogonal to $y_m$, and all iteration vectors for the Krylov solver are in that subspace. We compute $M_m^{-1}|_{y_m} w$ for a vector $w$ supplied by the Krylov solver at each inner iteration. Let $z = M_m^{-1}|_{y_m} w$ and note that $z \perp y_m$. Then it follows that

$$w = M_m z = (I - y_m y_m^H)Mz = Mz - \beta y_m,$$
where $\beta = y_m^H M z$. Equivalently, $z = M^{-1} w + \beta M^{-1} y_m$. Again, using $z \perp y_m$, we have $y_m^H M^{-1} w + \beta y_m^H M^{-1} y_m = 0$, i.e., $\beta = -\frac{y_m^H M^{-1} w}{y_m^H M^{-1} y_m}$. Therefore, we can compute $\tilde{M}_m^{-1} y_m w$ by

$$\tilde{M}_m^{-1} w = M^{-1} w - \left( \frac{y_m^H M^{-1} w}{y_m^H M^{-1} y_m} \right) M^{-1} y_m.$$  

In all the tables below, we denote by $I_{\text{out}}$ the number of outer iterations to achieve the convergence, by $I_{\text{inn}}$ the total number of inner iterations, i.e., the products of the matrix $A$ by vectors used by the Krylov solver, by $I_{0.1}$ the times of $\varepsilon = 0.1$, by $T_1$ the total CPU time of solving the small eigenproblems, by $T_2$ the total CPU time of generating the orthonormal basis $V$ and forming the projection matrix $H$, by $T_3$ the time of constructing the preconditioner and by $T_4$ the total CPU time of the Krylov solver for solving right-preconditioned inner linear systems. We point out that the (inexact and exact) SIRA and JD methods must form the projection matrices explicitly while SIA does not and it gives its projection matrix as a byproduct when generating the orthonormal basis of $V$. As a result, for the same dimension of subspace, $T_2$ for SIA is smaller than that for SIRA and JD. This will be confirmed clearly in later numerical experiments, and we will not mention this observation later. For Examples 1–3 we test Algorithms 1–2 the inexact SIA and exact SIRA; for Example 4 we test these algorithms and the restarted Algorithms 3–4 as well as the restarted inexact SIA.

**Example 1.** This problem is a large nonsymmetric standard eigenvalue problem of cry10000 of $n = 10000$ that arises from the stability analysis of a crystal growth problem from [1]. We are interested in the eigenvalue nearest to $\sigma = 7$. The computed eigenvalue is $\lambda \approx 6.7741$. The preconditioner $M$ is obtained by the sparse incomplete LU factorization of $A - \sigma I$ with setup.droptol = 0.001. Table I reports the results obtained, and the left and right parts of Figure 1 depict the convergence curve of $\|r_m\|_{A_m}$ versus $I_{\text{out}}$ and the curve of $I_{\text{inn}}$ versus $I_{\text{out}}$ for the algorithms, respectively.

![Figure 1](image1.png)

*Figure 1: Example 1. cry10000 with $\sigma = 7$. Left: relative outer residual norms versus outer iterations. Right: the numbers of inner iterations versus outer iterations.*

We see from Table I and Figure 1 that for both $\varepsilon = 10^{-2}, 10^{-3}$ the inexact SIRA and JD behaved like the exact SIRA very much and used almost the same outer iterations, while the inexact SIA had a small convergence delay. Clearly, smaller $\varepsilon$ is not necessary as it cannot reduce outer iterations anymore.

Regarding the overall efficiency, the exact SIRA was obviously the most expensive, as $I_{\text{inn}}$ and the dominant CPU time $T_3$, $T_4$ indicated. It used $27 \sim 29$ inner iterations per outer iteration. The inexact SIA was the second most expensive, in terms of the same measures. For it, the numbers of inner iterations were comparable and between $11 \sim 14$ at each of
the first 7 outer iterations where the accuracy of approximate eigenpairs was poor and the inner linear systems must be solved with high accuracy. As the approximate eigenpairs started converging, the relaxation strategy came into picture and the inner linear systems were solved with decreasing accuracy, leading to fewer inner iterations at subsequent outer iterations. Inner iterations used by the inexact SIA were only comparable to and finally below those used by the inexact SIRA and JD in the last very few iterations. In contrast, the figure indicates that, for the same \( \tilde{\varepsilon} \), the inexact SIRA and JD solved the linear systems with almost the same inner iterations per outer iteration. Because of this, the inexact SIRA and JD were much more efficient than the inexact SIA and used much fewer inner iterations and computing time than the latter. Both the \( I_{inn} \) and the total computing time in Table 1 show that they were roughly one and a half to three times as fast as the inexact SIA, and SIRA and JD with \( \tilde{\varepsilon} = 10^{-2} \) were considerably more efficient than that with \( \tilde{\varepsilon} = 10^{-3}, 10^{-4} \). Finally, we observe that the inexact SIRA and JD were equally effective, as indicated by the \( I_{inn} \) and the computing time used for each \( \tilde{\varepsilon} \).

In addition, we see from Table 1 that \( T_3 \) is comparable to and can be more than \( T_4 \) when inner linear systems are solved with low accuracy, and it is less important for the inexact SIA, where the accuracy of inner iterations increases as outer iterations proceed, and especially for the exact SIRA, where inner linear systems are required to be solved exactly in finite precision arithmetic.

**Example 2.** We consider the unsymmetric sparse matrix sherman5 of \( n = 3312 \) that has been used in [3, 16] for testing the relaxation theory with \( \sigma = 0 \). The computed eigenvalues is \( \lambda \approx 4.6925 \times 10^{-2} \). The preconditioner \( M \) is obtained by the sparse incomplete LU factorization of \( A - \sigma I \) with setup.droptol = 0.001. Table 1 and Figure 1 describe the results and convergence processes.

We see from the left part of Figure 2 that the inexact SIRA, JD and SIA behaved like the exact SIRA very much and used very comparable outer iterations. They mimic the exact SIRA better for \( \tilde{\varepsilon} = 10^{-3}, 10^{-4} \) than for \( \tilde{\varepsilon} = 10^{-2} \). The table also tells us that a smaller \( \tilde{\varepsilon} < 10^{-3} \) is definitely not necessary as it could not reduce the number of outer iterations and meanwhile consumed more inner iterations. The results confirm our theory and indicate that our selection of \( \tilde{\varepsilon} \) and \( \varepsilon \) worked very well. It is obvious that, as far as outer iterations are concerned, all the algorithms converged quickly and smoothly.

For the overall efficiency, the situation is very different. As is expected, we see from Table 2 and Figure 2 that the exact SIRA was the most expensive and the inexact SIA with was the second most expensive, as the \( I_{inn} \) and the total computing time indicated. The exact SIRA used 28 \~ 29 inner iterations per outer iteration, and the inexact SIA used 17 inner iterations at each of the first 3 outer iterations where the accuracy of approximate eigenpairs was poor and the inner linear systems must be solved with high accuracy. As the approximate eigenpairs started converging, the relaxation strategy came into picture and the inner linear systems were solved with decreasing accuracy, leading to fewer inner iterations at subsequent outer iterations. Inner iterations used by the inexact SIA were only comparable to and finally below those used by the inexact SIRA and JD in the last very few iterations. In contrast, the figure indicates that, for the same \( \tilde{\varepsilon} \), the inexact SIRA and JD solved the linear systems with almost the same inner iterations per outer iteration. Because of this, the inexact SIRA and JD were much more efficient than the inexact SIA and used much fewer inner iterations and computing time than the latter. Both the \( I_{inn} \) and the total computing time in Table 1 show that they were roughly one and a half to three times as fast as the inexact SIA, and SIRA and JD with \( \tilde{\varepsilon} = 10^{-2} \) were considerably more efficient than that with \( \tilde{\varepsilon} = 10^{-3}, 10^{-4} \). Finally, we observe that the inexact SIRA and JD were equally effective, as indicated by the \( I_{inn} \) and the computing time used for each \( \tilde{\varepsilon} \).

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We see from the left part of Figure 2 that the inexact SIRA, JD and SIA behaved like the exact SIRA very much and used very comparable outer iterations. They mimic the exact SIRA better for \( \tilde{\varepsilon} = 10^{-3}, 10^{-4} \) than for \( \tilde{\varepsilon} = 10^{-2} \). The table also tells us that a smaller \( \tilde{\varepsilon} < 10^{-3} \) is definitely not necessary as it could not reduce the number of outer iterations and meanwhile consumed more inner iterations. The results confirm our theory and indicate that our selection of \( \tilde{\varepsilon} \) and \( \varepsilon \) worked very well. It is obvious that, as far as outer iterations are concerned, all the algorithms converged quickly and smoothly.

For the overall efficiency, the situation is very different. As is expected, we see from Table 2 and Figure 2 that the exact SIRA was the most expensive and the inexact SIA with was the second most expensive, as the \( I_{inn} \) and the total computing time indicated. The exact SIRA used 28 \~ 29 inner iterations per outer iteration, and the inexact SIA used 17 inner iterations at each of the first 3 outer iterations where the accuracy of approximate

### Table 1: Example 1. cry10000 with \( \sigma = 7 \) (The unit of \( T_1 \sim T_4 \) is 0.001 second).

| Algorithm    | \( I_{inn} \) | \( I_{out} \) | \( I_{0,1} \) | \( T_1 \) | \( T_2 \) | \( T_3 \) | \( T_4 \) |
|--------------|---------------|---------------|---------------|----------|----------|----------|----------|
| SIRA(10^{-2})| 36            | 11            | 0             | 1        | 18       | 121      | 81       |
| JD(10^{-2})  | 38            | 12            | 0             | 2        | 21       | 121      | 103      |
| SIRA(10^{-3})| 57            | 12            | 0             | 2        | 21       | 121      | 120      |
| JD(10^{-3})  | 57            | 12            | 0             | 2        | 21       | 121      | 136      |
| SIRA(10^{-4})| 88            | 13            | 0             | 2        | 24       | 121      | 184      |
| JD(10^{-4})  | 78            | 12            | 0             | 2        | 21       | 121      | 176      |
| Inexact SIA  | 131           | 14            | –             | 2        | 13       | 121      | 340      |
| “Exact” SIRA | 277           | 11            | –             | 1        | 18       | 121      | 1386     |
eigenpairs was poor and the inner linear systems must be solved with high accuracy. As the approximate eigenpairs started converging, the relaxation strategy took effect and the inner linear systems were solved with decreasing accuracy, so that the numbers of inner iterations became increasingly smaller as outer iterations proceeded. In contrast, the inexact SIRA and JD were much more efficient than the inexact SIA, they used much fewer inner iterations and computing time than the latter and were roughly one and a half to two times as fast as the inexact SIA. Furthermore, we observe that the inexact JD and SIRA used quite few and almost constant inner iterations per outer iteration for each ˜ε, respectively, but the former was more effective than the latter. This may be due to the better conditioning of the coefficient matrix in the correction equation of JD.

Also, we observe from Table 2 that the time $T_4$ of solving preconditioned inner linear systems dominates the total CPU time and on the other hand the construction of preconditioners is the second most expensive. So solving inner linear systems overwhelms is much more than the others, and both $I_{inn}$ and the sum of $T_4$ and $T_3$ reflect the overall efficiency of each algorithm very well.

**Example 3.** This problem arises from computational fluid dynamics and the test matrix af23560 of $n = 23560$ is from transient stability analysis of Navier-Stokes solvers [1]. We want to find the eigenvalue nearest to $\sigma = 0$. The computed eigenvalue is $\lambda \approx -0.2731$. The preconditioner $M$ is obtained by the sparse incomplete LU factorization of $A - \sigma I$ with setup.droptol = 0.01; see Table 3 and Figure 3 for the results.

Compared with Examples 1–2, we see from both Table 3 and Figure 3 that for this problem

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**Table 2: Example 2. sherman5 with $\sigma = 0$ (The unit of $T_1 \sim T_4$ is 0.0001 second).**

| Algorithm    | $I_{inn}$ | $I_{out}$ | $I_{0.1}$ | $T_1$ | $T_2$ | $T_3$ | $T_4$ |
|--------------|-----------|-----------|-----------|-------|-------|-------|-------|
| SIRA($10^{-2}$) | 58        | 8         | 0         | 7     | 32    | 483   | 1713  |
| JD($10^{-2}$)  | 38        | 10        | 0         | 8     | 44    | 483   | 1425  |
| SIRA($10^{-3}$) | 62        | 7         | 0         | 5     | 25    | 483   | 1820  |
| JD($10^{-3}$)  | 37        | 7         | 0         | 5     | 24    | 483   | 1259  |
| SIRA($10^{-4}$) | 74        | 7         | 0         | 5     | 26    | 483   | 2174  |
| JD($10^{-4}$)  | 48        | 7         | 0         | 5     | 26    | 483   | 1567  |
| Inexact SIA   | 94        | 7         | –         | 4     | 12    | 483   | 2821  |
| “Exact” SIRA  | 172       | 7         | –         | 6     | 29    | 484   | 6583  |

**Figure 2: Example 2. sherman5 with $\sigma = 0$. Left: relative outer residual norms versus outer iterations. Right: the numbers of inner iterations versus outer iterations.**
all the algorithms used considerably more outer iterations $I_{out}$ but $I_{inn}$ increases more rapidly than $I_{out}$ does. So this problem was considerably more difficult than the previous two ones. The difficulty is two-fold: the eigenvalue problem itself and the inner linear systems involved in the algorithms. The second difficulty means that $T_4$ is more dominant than it for Examples 1–2. Moreover, we see that $T_4$ is much more than the corresponding $T_3$, the setup time of the preconditioner. As as whole, $I_{inn}$ and the time of solving inner linear systems reflect the overall efficiency of an algorithm more accurately.

In this example, the case that $\varepsilon = 0.1$ occurred at about 60% and 75% of outer iterations in SIRA($10^{-2}$) and JD($10^{-2}$), respectively. Regarding outer iterations, we observe from Figure 3 that for $\tilde{\varepsilon} = 10^{-3}$ the inexact SIRA, JD and SIA behaved like the exact SIRA very much. For the bigger $\tilde{\varepsilon} = 10^{-2}$, the inexact SIRA and SIA used more outer iterations and did not mimic the exact SIRA well. It is amazing that SIRA($10^{-4}$) and JD($10^{-4}$) used one less outer iteration than the exact SIRA. Again, the results confirmed our theory and showed that a low or modest accuracy $\tilde{\varepsilon} = 10^{-3}$ is enough, a looser $\tilde{\varepsilon} = 10^{-2}$ worked quite well and only a little bit more outer iterations were needed for it.

For the overall efficiency, the inexact SIA was better than the exact SIRA but much inferior to the inexact SIRA and JD. Actually, as $I_{inn}$ and $T_1$ show, the inexact SIRA and JD with $\tilde{\varepsilon} = 10^{-2}, 10^{-3}$ were twice to almost four times as fast as the inexact SIA. Although SIRA($10^{-2}$) and JD($10^{-2}$) used more outer iterations than the others, they were the most efficient in terms of both $I_{inn}$ and $T_4$. The exact SIRA used roughly 85 inner iterations per outer iteration. The inexact SIA used many inner iterations and needed to solve inner
linear systems with high accuracy for most of the outer iterations. Even after the relaxation strategy played a role, it still used much more inner iterations than the inexact SIRA and JD with $\tilde{\varepsilon} = 10^{-2}, 10^{-3}$ at each outer iteration. Although SIRA($10^{-4}$) and JD($10^{-4}$) behaved like the exact SIRA best and won all the others in terms of $I_{out}$, the overall efficiency of them was not as good as that of the the inexact methods with bigger $\tilde{\varepsilon}$. We find that, for the same accuracy $\tilde{\varepsilon}$, the inexact SIRA and JD solved the linear systems with slowly varying inner iterations at each outer iteration. This is expected as the accuracy requirements of inner iterations were almost the same. In terms of $I_{inn}$ and $T_4$, we also observe from Table 3 that the inexact SIRA and JD were equally effective and had very similar efficiency.

Still, similar to Examples 1–2, we see from $T_1 \sim T_4$ that solving preconditioned inner linear systems is the most expensive and dominates the overall efficiency of each algorithm, while the construction of preconditioners overwhelms the solutions of small eigensystems as well as the generations of orthonormal basis and projected matrices.

**Example 4.** This unsymmetric eigenvalue problem dw8192 of $n = 8192$ arises from dielectric channel waveguide problems [1]. We are interested in the eigenvalue nearest to the complex target $\sigma = 0.01i$. The computed eigenvalue is $\lambda \approx 3.3552 \times 10^{-3} + 1.1082 \times 10^{-3}i$. The preconditioner $M$ is obtained by the sparse incomplete LU factorization of $A - \sigma I$ with setup.droptol = 0.001. Table 4 displays the results.

| Algorithm         | $I_{inn}$ | $I_{out}$ | $I_{0.1}$ | $T_1$ | $T_2$ | $T_3$ | $T_4$ |
|-------------------|-----------|-----------|-----------|-------|-------|-------|-------|
| SIRA($10^{-2}$)   | 312       | 99        | 82        | 12    | 53    | 3     | 129   |
| JD($10^{-2}$)     | 276       | 93        | 81        | 11    | 47    | 3     | 144   |
| SIRA($10^{-3}$)   | 386       | 87        | 0         | 8     | 41    | 3     | 144   |
| JD($10^{-3}$)     | 428       | 94        | 1         | 11    | 47    | 3     | 192   |
| SIRA($10^{-4}$)   | 466       | 71        | 0         | 4     | 26    | 3     | 171   |
| JD($10^{-4}$)     | 451       | 70        | 0         | 4     | 25    | 3     | 183   |
| Inexact SIA       | 1663      | 86        | –         | 7     | 8     | 3     | 616   |
| “Exact” SIRA      | 1940      | 66        | –         | 3     | 21    | 3     | 741   |

Table 4: Example 4. dw8192 with $\sigma = 0.01i$ (The unit of $T_1 \sim T_4$ is 0.1 second).

As far as the eigenvalue problem is concerned, Table 4 clearly indicates that this problem is much more difficult than Examples 1–3 since all the algorithms used much more outer iterations to achieve the convergence than those needed for Examples 1–3. But our inexact SIRA and JD algorithms still worked very well. The inexact SIRA and JD with $\tilde{\varepsilon} = 10^{-4}$ behaved more like the exact SIRA than with $\tilde{\varepsilon} = 10^{-3}$ and $\tilde{\varepsilon} = 10^{-2}$. Therefore, we can infer that a smaller $\tilde{\varepsilon} < 10^{-4}$ is not necessary and cannot improve the behavior of the inexact SIRA and JD; it will make the inexact methods use almost the same outer iterations as the exact SIRA but consume more inner iterations. Furthermore, we have observed the inexact SIA did not mimic the exact SIRA very well as it used considerably more outer iterations than the exact SIRA.

For the overall efficiency, Table 4 exhibited similar features to those in all the previous tables for Examples 1–3. The inexact SIRA and JD were similarly effective. Both of them were much more efficient than the inexact SIA and actually three to five times as fast as the latter, in terms of both $I_{inn}$ and the total computing time.

Since this problem is difficult, we turn to use restarted SIRA and JD algorithms, Algorithms 3–4, to solve it with the maximum $M_{max} = 30$ outer iterations allowed during each cycle. We also test the implicitly restarted inexact SIA method [3,23] with the same $M_{max} = 30$ and make a comparison of all the restarted algorithms. Table 5 lists the results.
obtained by the restarted inexact SIRA, JD and SIA as well as the restarted exact SIRA, where \( I_{\text{restart}} \) denotes the number of restarts used, i.e., the number of the cycles of Algorithms 1–2 for the given \( M_{\text{max}} \). Figure 4 depicts the convergence curve of all the restarted algorithms and the curve of \( I_{\text{inn}} \) versus \( I_{\text{restart}} \), in which the zeroth restart in abscissa denotes the first cycle of Algorithms 3–4 and corresponds to the first restart in the left figure.

![Graphs showing convergence curves](image)

**Figure 4: Example 4.** Restarted algorithms with \( M_{\text{max}} = 30 \). Left: outer residual norms versus outer iterations. Right: the numbers of inner iterations versus restarts.

| Algorithm         | \( I_{\text{inn}} \) | \( I_{\text{restart}} \) | \( I_{\text{out}} \) | \( I_{0.1} \) | \( T_1 \) | \( T_2 \) | \( T_3 \) | \( T_4 \) |
|-------------------|----------------------|--------------------------|----------------------|----------------|--------|--------|--------|--------|
| SIRA(\( 10^{-2} \)) | 876                  | 8                        | 250                  | 142            | 2      | 32     | 3      | 346    |
| JD(\( 10^{-2} \))    | 578                  | 5                        | 175                  | 98             | 2      | 23     | 3      | 284    |
| SIRA(\( 10^{-3} \)) | 518                  | 3                        | 115                  | 0              | 1      | 15     | 3      | 203    |
| JD(\( 10^{-3} \))    | 532                  | 3                        | 117                  | 1              | 1      | 15     | 3      | 234    |
| SIRA(\( 10^{-4} \)) | 601                  | 3                        | 100                  | 0              | 1      | 12     | 3      | 222    |
| JD(\( 10^{-4} \))    | 624                  | 3                        | 98                   | 0              | 1      | 12     | 3      | 262    |
| Inexact SIA         | 1710                 | 3                        | 95                   | –              | 1      | 3      | 3      | 602    |
| “Exact” SIRA       | 2521                 | 2                        | 89                   | –              | 1      | 11     | 3      | 971    |

*Table 5: Example 4. Restarted algorithms with \( M_{\text{max}} = 30 \) (The unit of \( T_1 \sim T_4 \) is 0.1 second).*

It is seen from Table 5 and the left part of Figure 4 that all the algorithms other than SIRA(\( 10^{-2} \)) and JD(\( 10^{-2} \)) solved the problem very successfully with no more than three restarts used and the convergence processes were very smooth. The restarted inexact SIA behaved like the restarted exact SIRA well but not so well as the restarted SIRA and JD with \( \tilde{\varepsilon} = 10^{-4} \), which behaved very like the restarted exact SIRA in the first two restarts and almost converged to our prescribed convergence accuracy at the second restart.

We also find that, compared with Table 5, the restarted SIRA(\( 10^{-4} \)), JD(\( 10^{-4} \)) and exact SIRA performed excellently since \( I_{\text{out}} \)’s used by them were very near to the ones used by their corresponding non-restarted versions, respectively. For the restarted SIRA(\( 10^{-2} \)) and JD(\( 10^{-2} \)), the case that \( \varepsilon = 0.1 \) occurred at 50% of outer iterations. They did not mimic the exact SIRA well and used considerably more outer iterations than the inexact SIRA and JD with \( \tilde{\varepsilon} = 10^{-3} \) and \( \tilde{\varepsilon} = 10^{-4} \). So \( \tilde{\varepsilon} = 10^{-2} \) is not a good choice for the restarted inexact SIRA and JD for this example, though \( I_{\text{inn}} \) and the total computing time are not so considerably more than those used by the algorithms with \( \tilde{\varepsilon} = 10^{-3} \), \( 10^{-4} \).
Regarding the overall performance, for given $\tilde{\epsilon} = 10^{-3}$ and $\tilde{\epsilon} = 10^{-4}$, the restarted SIRA and JD algorithms performed very similarly and were about more than twice as fast as the restarted inexact SIA, in terms of both $I_{inn}$ and the total computing time (actually $T_4$ now). During the last cycle, the restarted inexact SIRA($10^{-4}$) and JD($10^{-4}$) had already achieved the convergence at the tenth and eighth outer iteration, respectively. So we stopped the algorithm at that step and actually solved only about a third of twenty-nine inner linear systems needed to solve in each of the previous cycles. As a result, the number of inner iterations needed in the last circle was also about a third of that needed in each of the first three cycles. This is the reason why, in the right part of Figure 4, the curves for the restarted SIRA($10^{-4}$) and JD($10^{-4}$) had a drastic decrease at last restart. As is expected, the restarted inexact SIRA and JD algorithms used almost constant inner iterations for the same $\tilde{\epsilon}$ per restart, while the inexact SIA used fewer and fewer inner iterations as outer iterations converged. The figure clearly shows that the restarted inexact SIA used much more inner iterations than the restarted SIRA($10^{-4}$) and JD($10^{-4}$) at each of the first three cycles.

We see from Tables 4–5 that for this example the dominant cost is still paid to the solutions of preconditioned inner linear systems but unlike Examples 1–3 the construction of preconditioners is very cheap and negligible, compared with $T_4$.

In summary, it is seen from all the numerical experiments that both $I_{inn}$ and $T_4$ are reasonable measures of overall performance of SIRA, JD and SIA algorithms.

We have tested some other problems. We have also tested the algorithms when tuning is applied to our preconditioner $M$. All of them have shown that the inexact SIRA and JD mimic the inexact SIA and the exact SIRA very well for $\tilde{\epsilon} = 10^{-3}, 10^{-4}$ and use much fewer inner iterations than the inexact SIA. As far as the overall efficiency is concerned, SIRA($10^{-2}$) and JD($10^{-2}$) may work well and often use comparably inner iterations than SIRA($10^{-3}$) and JD($10^{-3}$), but they are likely to need considerably more outer iterations and cannot mimic the exact SIRA well. Therefore, for the robust and general purpose, we propose using $\tilde{\epsilon} \in [10^{-4}, 10^{-3}]$ in practice. We have found that the tuned preconditioning has no advantage over the usual preconditioning and is often inferior to the latter for the linear systems involved in the inexact SIRA, JD and SIA algorithms. For example, we have found that for Example 3 the tuned preconditioning used about three times more inner iterations than the usual preconditioning.

7 Conclusions and future work

We have quantitatively analyzed the convergence of the SIRA and and JD methods over one step and proved that one only needs to solve all the inner linear systems involved in them with low or modest accuracy. Based on the theory established, we have designed practical stopping criteria for inner iterations of the inexact SIRA and JD. Numerical experiments have illustrated that our theory works very well and the non-restarted and restarted inexact SIRA and JD algorithms behave very like the non-restarted and restarted exact SIRA algorithms. Meanwhile, we have confirmed that the inexact SIRA and JD algorithms are similarly effective and both of them are much more efficient than the inexact SIA algorithms.

It is known that the (inexact) JD method with variable shifts is used more commonly. The analysis approach proposed in this paper may be extended to analyze the accuracy requirements of inner iterations in the JD method with variable shifts and a rigorous general theory may be expected. This work is in progress.

Since the harmonic projection may be more suitable to solve the interior eigenvalue problem, it is very significant to consider the harmonic version of SIRA. Moreover, it is known that the standard projection, i.e., the Rayleigh–Ritz method, and its harmonic version may
have convergence problem when computing eigenvectors. So it is worthwhile and appealing to use the refined Rayleigh–Ritz procedure and the refined harmonic version for solving the large eigenproblem considered in this paper. These constitute our future work.

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