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EFFICIENT PRECONDITIONED INNER SOLVES FOR INEXACT RAYLEIGH QUOTIENT ITERATION AND THEIR CONNECTIONS TO THE SINGLE-VECTOR JACOBI–DAVIDSON METHOD*

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Abstract. We study inexact Rayleigh quotient iteration (IRQI) for computing a simple interior eigenpair of the generalized eigenvalue problem $Av = \lambda Bv$, providing new insights into a special type of preconditioners with "tuning" for the efficient iterative solution of the shifted linear systems that arise in this algorithm. We first give a new convergence analysis of IRQI, showing that locally cubic and quadratic convergence can be achieved for Hermitian and non-Hermitian problems, respectively, if the shifted linear systems are solved by a generic Krylov subspace method with a tuned preconditioner to a reasonably small *fixed* tolerance. We then refine the study by Freitag and Spence [*Linear Algebra Appl.*, 428 (2008), pp. 2049–2060] on the equivalence of the inner solves of IRQI and single-vector Jacobi–Davidson method where a full orthogonalization method with a tuned preconditioner is used as the inner solver. We also provide some new perspectives on the tuning strategy, showing that tuning is essentially needed only in the first inner iteration in the non-Hermitian case. Based on this observation, we propose a flexible GMRES algorithm with a special configuration in the first inner step, and show that this method is as efficient as GMRES with the tuned preconditioner.

Key words. generalized eigenvalue problems, Rayleigh quotient iteration, single-vector Jacobi–Davidson method, Krylov subspace method, tuned preconditioner, FGMRES, GCRO-DR

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1. Introduction.

Rayleigh quotient iteration (RQI) is a classical algorithm for computing a simple eigenpair of a matrix A or a matrix pencil (A, B). This algorithm has been extensively studied for more than fifty years, and is shown to exhibit locally cubic and quadratic convergence rates, respectively, for Hermitian and non-Hermitian problems; see [21], [29], and the references therein. In recent years, there has been considerable interest in inexact eigenvalue algorithms, including inexact Rayleigh quotient iteration (IRQI), with inner-outer iterations for computing eigenvalues of matrices around some specified shift, especially those lying in the interior of the spectrum to which regular Krylov subspace methods fail to provide rapid approximations. In each outer iteration, a shift-invert matrix-vector product is computed inexactly through the iterative solution (inner iteration) of the corresponding linear system. Inexact eigenvalue algorithms are of significant use if the matrices are too large for exact shift-invert matrix-vector products to be affordable, or if the matrices cannot be formed explicitly. In this paper, we provide some new insights into a special type of preconditioners with "tuning" for the efficient iterative solution (inner solves) of the shifted linear system of equations that arises in IRQI for computing a simple interior eigenpair of the generalized eigenvalue problem $Av = \lambda Bv$.

The original motivation of tuning the preconditioner is to resolve the difficulties arising in the preconditioned inner solves for inexact inverse iteration and IRQI. Specifically, a good preconditioner in the usual setting of solving linear systems generally

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does not yield rapid improvement of eigenvector approximation as the inner iteration proceeds. This problem is discussed by Simoncini and Eldén [24], where it is shown that faster improvement of eigenvector approximation in initial inner iterations of IRQI can be achieved by properly tuning the right-hand side of the shifted linear system. This idea is extended in [2], [4] and then improved in [9], [10] by Spence and his collaborators, where tuning the preconditioner is shown to be more effective than tuning the right-hand side, since the former approach does not change the linear systems to be solved and thus will not compromise the best possible convergence rate of outer iterations. The superior performance of the tuned preconditioner over the regular (untuned) counterpart has been established in these references, based on the convergence theory of Krylov subspace minimal residual methods and the fact that the right-hand side of the preconditioned system with tuning is an approximate eigenvector associated with the smallest (in magnitude) eigenvalue of the preconditioned coefficient matrix. In addition, the advantage of using a tuned preconditioner for the inner solves becomes more pronounced as the outer iteration proceeds and converges toward the desired eigenpair.

This paper is a continuation of the investigation of tuning the preconditioner, in the context of IRQI, for efficient Krylov subspace inner solves. We provide insights into tuning in three aspects. First, we give a new local convergence analysis of IRQI, showing under appropriate assumptions that this algorithm demonstrates cubic and quadratic asymptotic convergence rates, respectively, for Hermitian and non-Hermitian problems, if the shifted linear systems are solved by a generic Krylov subspace method with a tuned preconditioner to a reasonably small *fixed* tolerance. This result is an improvement of existing local convergence analyses of IRQI [2], [4], [8], [9], [10], [18], [24], [27], [30], obtained independently of the inner solver, where it is shown that these asymptotic convergence rates can be achieved if a proper *decreasing* sequence of tolerances is used for the inner solves. Second, we provide a refined equivalence result of the inner solves of the single-vector Jacobi–Davidson (JD) method [1] and IRQI. We show that given the same outer iterate x, the two methods deliver the same sequence of inner iterates (up to a constant scaling factor) if the two inner solves are done by the full orthogonalization method (FOM) with a tuned preconditioner $\mathcal{Q}$ satisfying $\mathcal{Q}x = Bx$, independent of the specific construction of $\mathcal{Q}$. Finally, we give some new perspectives on the success of tuning the preconditioner and propose an approach to simplify the use of tuning. We show by both analysis and experiments that tuning is necessary only in the first inner iteration, and that a flexible GMRES algorithm with a special configuration in the first step is as competitive in efficiency as GMRES with a tuned preconditioner; for details on GMRES and flexible GMRES (FGMRES) as well as MINRES, which is mentioned later, see, e.g., [22] or [25].

Since tuning the preconditioner for the inner solves of IRQI bears some close connections to the single-vector JD method, this paper in fact also provides a justification of the use of JD. In practice, to enhance the robustness of the convergence of JD with random initial outer iterates, and to speed up the actual convergence speed in the presence of large errors of inner solves, the regular JD method with subspace acceleration needs to be used. The investigation of tuning in this paper forms a preliminary step toward complete understanding of JD, especially during its asymptotic convergence phase. The nonlocal convergence behavior and the inner solves of JD with subspace acceleration prior to the asymptotic convergence phase are out of the scope of this paper.

The paper is organized as follows. In section 2, we describe IRQI and outline preliminary results needed to study this algorithm. In section 3, we show that locally cubic and quadratic convergence of IRQI can be achieved for Hermitian and non-Hermitian problems, respectively, if the shifted linear systems are solved by a generic Krylov

subspace method with a tuned preconditioner to a moderately small *fixed* tolerance. We refine the equivalence results of the inner solves of IRQI and single-vector JD in section 4. In section 5, we give some new perspectives on tuning, propose an FGMRES algorithm to simplify the use of tuning, and show how this FGMRES solve is connected to a modified correction equation of single-vector JD. Numerical experiments are given in section 6 to validate the new convergence analysis and the equivalence results—to show that IRQI with tuning for the inner solve is superior to the inexact Arnoldi method for the eigenvalue problem under discussion, and to demonstrate the effectiveness of the alternative inner solver.

2. Preliminaries. We are interested in computing a simple eigenpair of a regular matrix pencil (A, B) by IRQI. Consider the generalized eigenvalue problem

$$Av = \lambda Bv, \tag{2.1}$$

where A, $B \in \mathbb{C}^{n\times n}$, $v \in \mathbb{C}^n$, and $\lambda \in \mathbb{C}$. To simplify the analysis, we assume that B is nonsingular and there exist an invertible matrix of eigenvectors $V = [v_1, v_2, \ldots, v_n]$ and a diagonal matrix of eigenvalues $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ so that $AV = BV\Lambda$. This decomposition can also be written as $U^*A = \Lambda U^*B$, where

$$U^* = V^{-1}B^{-1} = [u_1, u_2, \ldots, u_n]^*$$

is the matrix of left eigenvectors. The left and right eigenvectors are connected by the relation $U^*BV = I$.

The classification of (2.1) is as follows [1]: if A and B are Hermitian, and if A, B, or $\alpha A + \beta B$ is positive definite for some scalars α and β, (2.1) is known as the generalized Hermitian eigenvalue problem (GHEP); otherwise it is a generalized non-Hermitian eigenvalue problem (GNHEP). By redefining matrices, all GHEPs can be cast into the standard form (2.1) with Hermitian positive definite B. In this case, it is well known that $U = V$ and hence the eigenvectors are orthogonal with respect to the B inner product; in addition, all eigenvalues λ_j are real. We assume in this paper that GHEPs are of this standard form. In the following, we simply refer to GHEPs and GNHEPs as Hermitian and non-Hermitian problems, respectively.

Algorithm 2.1 describes a typical version of (one-sided) IRQI to find a simple right eigenpair of a matrix pencil (A, B).

Algorithm 2.1. Inexact Rayleigh quotient iteration (IRQI).
Given $x^{(0)}$ with $x^{(0)}$ normalized with respect to the B (Hermitian case)
or B^*B (non-Hermitian case) inner product.
For $i = 0, 1, 2, \ldots$, until convergence

1. Compute the Rayleigh quotient

$$\sigma^{(i)} = \frac{w^{(i)*}Ax^{(i)}}{w^{(i)*}Bx^{(i)}},$$

where $w^{(i)} = x^{(i)}$ (Hermitian case), or $w^{(i)} = Bx^{(i)}$ (non-Hermitian case).

2. Choose $\tau^{(i)}$ and solve $(A - \sigma^{(i)}B)y^{(i)} = Bx^{(i)}$ inexactly such that

$$\frac{\|Bx^{(i)} - (A - \sigma^{(i)}B)y^{(i)}\|}{\|Bx^{(i)}\|} \le \tau^{(i)}.$$

3. Update $x^{(i+1)} = h^{(i)} y^{(i)}$ with some scalar $h^{(i)}$ such that $x^{(i+1)}$ is normalized with respect to the B (Hermitian case) or B^*B (non-Hermitian case) inner product.
4. Test for convergence.

End For

Suppose that (λ_1, v_1) is the desired (right) eigenpair of (A, B). To analyze IRQI, we decompose the outer iterate $x^{(i)}$ as

$$x^{(i)} = \gamma^{(i)}(c^{(i)} v_1 + s^{(i)} z^{(i)}), \tag{2.2}$$

where $\gamma^{(i)} = \| U^*Bx^{(i)}\|$, $z^{(i)} = V e_z^{(i)} \in \text{span}\{v_2, v_3, \ldots, v_n\}$ with $e_z^{(i)} \perp e_1$ and $\| e_z^{(i)}\| = 1$. Therefore $U^*Bx^{(i)} = \gamma^{(i)}(c^{(i)} e_1 + s^{(i)} e_z^{(i)})$,

$$\sqrt{|c^{(i)}|^2 + |s^{(i)}|^2} = \| c^{(i)} e_1 + s^{(i)} e_z^{(i)}\| = \| U^*Bx^{(i)}\| / \gamma^{(i)} = 1.$$

Here $s^{(i)}$ and $c^{(i)}$ are generalizations of the sine and cosine of $\angle(x^{(i)}, v_1)$. Let $F = (I - e_1 e_1^T) U^*B$ such that $Fv_1 = 0$ and $Fv_j = e_j$, for $j = 2, 3, \ldots, n$. The generalized tangent of $\angle(x^{(i)}, v_1)$ can be defined as

$$\text{gtan} \angle (x^{(i)}, v_1) \equiv t^{(i)} = \frac{|s^{(i)}|}{|c^{(i)}|} = \frac{\|\gamma^{(i)} s^{(i)} U^*Bz^{(i)}\|}{\|\gamma^{(i)} c^{(i)} e_1\|} = \frac{\|Fx^{(i)}\|}{\|(U^*B - F)x^{(i)}\|}, \tag{2.3}$$

which measures the approximation of $x^{(i)}$ to the desired eigenvector v_1. For standard Hermitian problems where $B = I$, $t^{(i)} = \text{gtan} \angle (x^{(i)}, v_1) = \tan \angle(x^{(i)}, v_1)$. For small $\angle(x^{(i)}, v_1)$, we have $O(t^{(i)}) = O(s^{(i)})$ as $c^{(i)} \approx 1$ and $t^{(i)} \approx s^{(i)}$.

In our analysis, we will use the fact shown below that the Rayleigh quotient approaches the corresponding eigenvalue as $O(|s^{(i)}|^2)$ in the Hermitian case, and as $O(|s^{(i)}|)$ in the non-Hermitian case. In fact, for Hermitian problems with positive definite B, the Rayleigh quotient

$$\sigma^{(i)} = \frac{x^{(i)*} A x^{(i)}}{x^{(i)*} B x^{(i)}}$$

satisfies

$$\begin{aligned}
\sigma^{(i)} - \lambda_1 &= \frac{x^{(i)*}(A - \lambda_1 B)x^{(i)}}{x^{(i)*} B x^{(i)}} \\
&= \frac{(\bar{c}^{(i)} v_1^* + \bar{s}^{(i)} z^{(i)*})(A - \lambda_1 B)(c^{(i)} v_1 + s^{(i)} z^{(i)})}{(\bar{c}^{(i)} v_1^* + \bar{s}^{(i)} z^{(i)*}) B (c^{(i)} v_1 + s^{(i)} z^{(i)})} \\
&= \frac{|s^{(i)}|^2 z^{(i)*}(A - \lambda_1 B) z^{(i)}}{|c^{(i)}|^2 + |s^{(i)}|^2} = (e_z^{(i)*} \Lambda e_z^{(i)} - \lambda_1)|s^{(i)}|^2.
\end{aligned} \tag{2.4}$$

For non-Hermitian problems, the generalized Rayleigh quotient is

$$\sigma^{(i)} = \frac{w^{(i)*} A x^{(i)}}{w^{(i)*} B x^{(i)}}$$

with some vector $w^{(i)}$; see, e.g., [16]. For one-sided RQI for computing only the right eigenpair, a common choice is $w^{(i)} = Bx^{(i)}$ (see [13], [14]), and therefore

$$\begin{aligned}\sigma^{(i)} - \lambda_1 &= \frac{x^{(i)*}B^*(A-\lambda_1 B)x^{(i)}}{x^{(i)*}B^*Bx^{(i)}} \\ &= \frac{s^{(i)}(\bar{c}^{(i)}v_1^* + \bar{s}^{(i)}z^{(i)*})B^*(A-\lambda_1 B)z^{(i)}}{(\bar{c}^{(i)}v_1^* + \bar{s}^{(i)}z^{(i)*})B^*B(c^{(i)}v_1 + s^{(i)}z^{(i)})} \\ &= \frac{\langle (\Lambda-\lambda_1 I)e_z^{(i)},\, c^{(i)}e_1 + s^{(i)}e_z^{(i)}\rangle_{V^*B^*BV}}{\|c^{(i)}e_1 + s^{(i)}e_z^{(i)}\|_{V^*B^*BV}}\, s^{(i)}, \end{aligned} \tag{2.5}$$

where for positive definite M, $\langle u, v\rangle_M = v^*Mu$ is an inner product on $\mathbb{C}^n$.

The corresponding eigenvalue residual is

$$\begin{aligned} r^{(i)} &= Ax^{(i)} - \sigma^{(i)}Bx^{(i)} \\ &= \gamma^{(i)}(A-\lambda_1 B)(c^{(i)}v_1 + s^{(i)}z^{(i)}) - (\sigma^{(i)} - \lambda_1)Bx^{(i)} \\ &= \gamma^{(i)}s^{(i)}BV(\Lambda - \lambda_1 I)e_z^{(i)} - (\sigma^{(i)} - \lambda_1)Bx^{(i)}. \end{aligned} \tag{2.6}$$

As the norm of $\gamma^{(i)}s^{(i)}BV(\Lambda-\lambda_1 I)e_z^{(i)}$ is proportional to $s^{(i)}$, it follows from (2.4) and (2.5) that $\|r^{(i)}\| = O(|s^{(i)}|)$ for both Hermitian and non-Hermitian problems. In addition, it follows from the definition of the Rayleigh quotient that $r^{(i)} \perp x^{(i)}$ in the Hermitian case and $r^{(i)} \perp Bx^{(i)}$ in the non-Hermitian case.

From here through the end of the paper, we focus on the behavior of the inner solve —i.e., the solution of step 2 of Algorithm 2.1—in a given outer iteration, and we drop the superscript (i) denoting the number of outer iterations, unless otherwise stated.

3. Some local convergence analysis of IRQI. In this section, we present some local convergence analysis of IRQI where Krylov subspace methods are used for approximately solving the linear system arising in the outer iteration (step 2 of Algorithm 2.1). Specifically, we first show that if an unpreconditioned Krylov subspace method is used in IRQI for *standard* Hermitian and non-Hermitian problems, locally cubic or quadratic convergence of the outer iteration can be achieved if a *fixed constant* moderately smaller than 1 is used as the relative tolerance of the inner solve. We then show that this result also holds for IRQI for *generalized* eigenvalue problems if the inner solve is done by a *preconditioned* Krylov subspace method with a special type of preconditioner with "tuning."

From now on, for simplicity, we omit the word "local" for the description of convergence whenever there is no ambiguity. We begin with the following theorem on Krylov subspace iterative solution of a linear system $My = b$, showing how the approximate solution y_m behaves if the right-hand side b is an approximate eigenvector corresponding to the smallest (in magnitude) eigenvalue of the coefficient matrix M. We will show how this theorem is used to study the shifted linear systems with a tuned preconditioner arising in IRQI and how it helps establish the new convergence analysis.

THEOREM 3.1. *Suppose that an unpreconditioned Krylov subspace method with zero starting vector $y_0 = 0$ is used to solve $My = b$. Let (λ_i^M, w_i) be the eigenpairs of $M = W\Lambda_M W^{-1}$ with eigenvalues ordered as $0 < |\lambda_1^M| < |\lambda_2^M| \le \cdots \le |\lambda_n^M|$. Let $b = \gamma(cw_1 + sz)$ with $|s| < |c|$, where $\gamma = \|W^{-1}b\|$ and $z \in \operatorname{span}\{w_2, w_3, \ldots, w_n\}$ such that $e_z = W^{-1}z$ is a unit vector orthogonal to e_1. Let y_m be an approximate solution in the Krylov subspace $\mathcal{K}_m(M, b)$, $r_m = b - My_m = p_m(M)b$ be the associated linear residual, where $p_m(\chi) = 1 - \chi\, q_{m-1}(\chi)$ (with $p_m(0) = 1$) is the corresponding residual polynomial of degree no larger than m (note in particular that $p_0(\chi) \equiv 1$), $t_0 = |s|/|c| = \operatorname{gtan} \angle(b, w_1)$, and $t_m = \operatorname{gtan} \angle(y_m, w_1)$. Let*

$$\alpha_m = \|\Lambda_M^{-1}(I - p_m(\Lambda_M))e_z\|, \tag{3.1}$$

$C_0 \in (0,1)$, and $\kappa(W)$ be the condition number of W (note in particular that $\kappa(W) = 1$ for Hermitian M). If the relative residual norm $\|r_m\|/\|b\| \le |c|(1-C_0)/\kappa(W)$, then

$$t_m \le \frac{|\lambda_1^M|}{C_0}\alpha_m t_0. \tag{3.2}$$

Proof. The proof follows the lines of that of Theorem 4.1 in [24]. Note that $y_1 \in \mathcal{K}_1(M,b) = \mathrm{span}\{b\}$ is a multiple of b if a zero starting vector $y_0 = 0$ is used for this linear solve. It follows that

$$y_m = q_{m-1}(M)b = \gamma W(cq_{m-1}(\lambda_1^M)e_1 + sq_{m-1}(\Lambda_M)e_z),$$

and therefore $\mathrm{gtan}\,\angle(y_m, w_1)$ is

$$t_m = \frac{\|sq_{m-1}(\Lambda_M)e_z\|}{\|cq_{m-1}(\lambda_1^M)e_1\|} = \frac{\|\Lambda_M^{-1}(I - p_m(\Lambda_M))e_z\|}{|(\lambda_1^M)^{-1}(1-p_m(\lambda_1^M))|}\frac{|s|}{|c|} = \frac{|\lambda_1^M|}{|1-p_m(\lambda_1^M)|}\alpha_m t_0, \tag{3.3}$$

where $\alpha_m = \|\Lambda_M^{-1}(I - p_m(\Lambda_M))e_z\|$ satisfies

$$\min_{2\le i\le n}\frac{|1-p_m(\lambda_i^M)|}{|\lambda_i^M|} \le \alpha_m \le \max_{2\le i\le n}\frac{|1-p_m(\lambda_i^M)|}{|\lambda_i^M|}. \tag{3.4}$$

Formula (3.3) shows that the behavior of t_m is determined by $|\lambda_1^M|/|1-p_m(\lambda_1^M)|$ and α_m, both of which involve the residual polynomial $p_m(\chi)$.

To analyze $|\lambda_1^M|/|1-p_m(\lambda_1^M)|$, note that the residual vector

$$r_m = p_m(M)b = \gamma p_m(M)\,W(ce_1 + se_z) = \gamma\, W(cp_m(\lambda_1^M)e_1 + sp_m(\Lambda_M)e_z). \tag{3.5}$$

It follows that the relative residual norm

$$\begin{aligned}\frac{\|p_m(M)b\|}{\|b\|} &= \frac{\|\,W(cp_m(\lambda_1^M)e_1 + sp_m(\Lambda_M)e_z)\|}{\|\,W(ce_1+se_z)\|}\\ &\ge \frac{\sigma_{\min}(\,W)(|c|^2|p_m(\lambda_1^M)|^2 + |s|^2\|p_m(\Lambda_M)e_z\|^2)^{\frac12}}{\|\,W\|} > \frac{|c||p_m(\lambda_1^M)|}{\kappa(\,W)}.\end{aligned} \tag{3.6}$$

Thus, if $\|r_m\|/\|b\| \le |c|(1-C_0)/\kappa(W)$ with $C_0 \in (0,1)$, then $|p_m(\lambda_1^M)| < 1 - C_0$, and

$$t_m = \frac{|\lambda_1^M|}{|1-p_m(\lambda_1^M)|}\alpha_m t_0 \le \frac{|\lambda_1^M|}{|1-|p_m(\lambda_1^M)||}\alpha_m t_0 \le \frac{|\lambda_1^M|}{C_0}\alpha_m t_0, \tag{3.7}$$

which completes the proof. ∎

Theorem 3.1 shows that t_m/t_0 is effectively bounded by $\alpha_m|\lambda_1^M|$ if a constant moderately smaller than $1/\kappa(W)$ is used as the relative tolerance for the Krylov subspace linear solve. For instance, if $\|r_m\|/\|b\| \le |c|(1-C_0)/\kappa(W) = 0.01/\kappa(W)$, then $C_0 \approx 0.99$, and $t_m/t_0 \lessapprox \alpha_m|\lambda_1^M|$.

To analyze α_m, consider from (3.5) the components of r_m in $\mathrm{span}\{w_2, \ldots, w_n\}$, namely, $\gamma s\,W p_m(\Lambda_M)e_z$, and the corresponding components $\gamma s\,W p_0(\Lambda_M)e_z$ of $r_0 = b$. If the former is not considerably larger than the latter (i.e., if $\|p_m(\Lambda_M)e_z\|$ is not much larger than $\|p_0(\Lambda_M)e_z\| = \|e_z\| = 1$), then

$$\alpha_m = \|\Lambda_M^{-1}(I - p_m(\Lambda_M))e_z\| \le \|\Lambda_M^{-1}e_z\| + \|\Lambda_M^{-1}p_m(\Lambda_M)e_z\|$$

is a moderate multiple of $\|\Lambda_M^{-1}e_z\|$. Therefore, $\text{gtan}\angle(y_m, w_1) = t_m$ is a moderate multiple of $\text{gtan}\angle(y^*, w_1) = |\lambda_1^M|\|\Lambda_M^{-1}e_z\|t_0$, where $y^* = M^{-1}b$ is the exact solution of $My = b$. In practice, we may assume that $\|r_m\| = \|p_m(M)b\| \to 0$ as $m \to n$, and therefore $\|p_m(\Lambda_M)e_z\| \to 0$. It is thus reasonable to expect that $\|p_m(\Lambda_M)e_z\|$ is not much larger than $\|e_z\| = 1$, and of course it will eventually be smaller than 1. It then follows that $\text{gtan}\angle(y_m, w_1)$ is a moderate multiple of $\text{gtan}\angle(y^*, w_1)$ if the relative residual norm $\|r_m\|/\|b\|$ is moderately small (assuming that the eigenvector matrix of M is not ill-conditioned).

Theorem 3.1 can be used to study the convergence of IRQI. We will first apply this theorem to study IRQI for standard eigenvalue problems in Corollary 3.3 below by letting $M = (A - \sigma I)$, $b = x$. In Propositions 3.6 and 3.7 and Theorem 3.8, in particular, M and b correspond to the *preconditioned* coefficient matrix and right-hand side, respectively, of the linear systems arising in IRQI. In preparation for Corollary 3.3 and for use later on in the paper, we first recall that for a very small angle θ, $\sin\theta$, θ, and $\tan\theta$ are very close to each other.

PROPOSITION 3.2. *For any $\theta \ll 1$, there exist constants C_2 and C_3 slightly smaller and larger than 1, respectively, such that $C_2\theta \le \sin\theta \le \theta \le \tan\theta \le C_3\theta$.*

COROLLARY 3.3. *Suppose that Algorithm 2.1 is used to compute a simple eigenpair of a diagonalizable matrix $A = W\Lambda_A W^{-1}$, and an unpreconditioned Krylov subspace method with a zero starting vector is used to solve $(A - \sigma I)y = x$. Let y_m be the approximate solution in the mth inner iteration, $r_m = x - (A - \sigma I)y_m$ be the residual vector, C_1 be a moderate constant, and τ be a constant moderately smaller than $1/\kappa(W)$. If $\alpha_m \le C_1$, and τ is used as the relative tolerance for the inner solve (e.g., $\|r_m\|/\|x\| \le \tau = 0.01/\kappa(W)$ needs to be satisfied), then the convergence of Algorithm 2.1 is cubic and quadratic for Hermitian and non-Hermitian A, respectively.*

Proof. For $M = A - \sigma I$, note from (2.4) and (2.5) that the eigenvalue of smallest magnitude $\lambda_1^M = \lambda_1^A - \sigma$ is of the order $O(|s|^2)$ for Hermitian A and $O(s)$ for non-Hermitian A. If $\|r_m\|/\|x\| \le \tau$, then $t_m \lessapprox \alpha_m|\lambda_1^M|t_0 \le C_1|\lambda_1^M||s|/|c| = C_1|(\lambda_1 - \sigma)t|$, which is on the order of $O(t^3)$ or $O(t^2)$ (see (2.4) and (2.5)). The cubic and quadratic convergence of IRQI is thus established. ∎

Assuming that α_m (defined in (3.1)) is bounded by a modest constant, Corollary 3.3 shows that the convergence of IRQI is not obviously compromised as long as the shifted linear system is solved to a tolerance moderately smaller than the reciprocal of the condition number of the eigenvector matrix of A. In particular, if $\|p_m(\Lambda_M)e_z\|$ is not considerably larger than 1, and hence α_m is a small multiple of $\|\Lambda_M^{-1}e_z\|$, then the convergence of IRQI is almost the same as exact RQI. This observation explains why, to achieve full convergence of IRQI, it is generally enough to solve the shifted linear systems by Krylov subspace solvers to a moderate accuracy. Although we have no proof of this fact, we observed in practice that this assumption of the uniform boundedness seems valid. Specifically, in the ith outer iteration, let $\alpha_{m^*}^{(i)}$ be the value of α_m in the inner iteration step, where the tolerance of the inner iteration solve is satisfied for the first time. We found from all numerical tests that $\alpha_{m^*}^{(i)}$ is almost a constant as the outer iteration proceeds, if the fixed tolerance for inner solves is small, and it tends to increase mildly (much less rapidly than $O(1/s^{(i)})$) and is thus practically uniformly bounded by a moderate constant if the fixed tolerance is relatively large.[1] In the latter case,

[1] How small is small and how large is relatively large depends on the given problem.

the local convergence of IRQI is in fact "subcubical" (or superquadratical) and "subquadratical" (or superlinear) in the Hermitian and non-Hermitian cases, respectively.

The above convergence result of IRQI may not hold, however, if the linear systems are solved by a *preconditioned* Krylov subspace method. For example, consider Algorithm 2.1 for the generalized eigenvalue problem, and suppose a preconditioner Q is used for the inner solve of the following linear systems:

$$\begin{aligned} &L^{-1}(A-\sigma B)L^{-*}\tilde{y} = L^{-1}Bx \quad \text{with} \quad y = L^{-*}\tilde{y},\ Q = LL^*, && \text{(Hermitian problems)}\\ &(A-\sigma B)Q^{-1}\tilde{y} = Bx \quad \text{with} \quad y = Q^{-1}\tilde{y}. && \text{(non-Hermitian problems)} \end{aligned} \tag{3.8}$$

For standard Hermitian problems, Simoncini and Eldén [24] and Xue and Elman [31] provide evidence that $t_m = \operatorname{gtan}\angle(y_m, v_1)$ can be much larger than $t_0 = \operatorname{gtan}\angle(x, v_1)$ for a large number of inner iterations, in which $\angle(y_m, v_1)$ decreases very slowly with m, until m becomes large enough. This undesirable behavior, in fact, can also be observed for standard non-Hermitian and generalized problems. The reason is that for the preconditioned Krylov subspace linear solve, the initial inner iterate $y_1 = Q^{-1}Bx$ (up to a scaling factor) is generally far from a good approximation to the desired eigenvector v_1, even if the current outer iterate $x \approx v_1$. To resolve this difficulty, Freitag and Spence [9], [10] propose a special type of preconditioner with "tuning." Given some preconditioner Q appropriate for $A - \sigma B$, a tuned preconditioner $\mathcal{Q}$ is a low-rank update of Q, which satisfies $\mathcal{Q}x = Bx$, or, equivalently, $\mathcal{Q}^{-1}Bx = x$. Examples of such preconditioners $\mathcal{Q}$ used in literature include the following:

$$\mathcal{Q} = Q + \frac{(Bx - Qx)(Bx - Qx)^*}{(Bx - Qx)^* x}, \tag{3.9a}$$

$$\mathcal{Q} = Q - \frac{(Qx)(Qx)^*}{(Qx)^* x} + \frac{(Bx)(Bx)^*}{(Bx)^* x}, \text{or} \tag{3.9b}$$

$$\mathcal{Q} = Q + \frac{(Bx - Qx)p^*}{p^* x} \text{ with some vector } p \text{ such that } p^* x \neq 0. \tag{3.9c}$$

Note that $\mathcal{Q}$ constructed in (3.9a) and (3.9b) is Hermitian if Q and B are both Hermitian; in addition, it is shown in [31] that $\mathcal{Q}$ defined in (3.9b) is positive definite if B and Q are positive definite. Therefore it is advisable to construct a tuned preconditioner by (3.9b) for the inner solves for Hermitian problems. On the other hand, (3.9c) is usually used in this setting for non-Hermitian problems. At each step of the inner solve, the matrix-vector product involving $\mathcal{Q}^{-1}$ is computed by the Sherman–Morrison–Woodbury formula; for example,

$$\mathcal{Q}^{-1}v = Q^{-1}v - \frac{(Q^{-1}Bx - x)p^* Q^{-1}v}{p^* Q^{-1}Bx}, \tag{3.10}$$

where $\mathcal{Q}$ is defined in (3.9c). The additional cost for the use of the tuned preconditioner is minimal, as both $(Q^{-1}Bx - x)$ and $p^*Q^{-1}Bx$ need to be computed only once in each outer iteration for the inner solve.

Intuitively, with the tuned preconditioner, if $x \approx v_1$, then the initial inner iterate $y_1 = \mathcal{Q}^{-1}Bx = x$ is a good approximate eigenvector. The eigenvector approximation continues to improve as the inner iteration proceeds, and the difficulty arising in the

solution of (3.8) with (untuned) Q is thus resolved (see [31] for a detailed discussion of the virtue of the tuned preconditioner).

We now show that Corollary 3.3 holds for Algorithm 2.1 if the inner solve is done by a tuned preconditioner $\mathcal{Q}$ satisfying $\mathcal{Q}x = Bx$. To this end, we begin with some preliminary propositions.

PROPOSITION 3.4. *Let p, $q \in \mathbb{C}^n$ be nonzero vectors and $K \in \mathbb{C}^{n\times n}$. Then* $\sin\angle(Kp, Kq) \le \kappa(K)\tan\angle(p, q)$.

Proof. Suppose without loss of generality that p and q are both unit vectors. Let $p = cq + sr$, where $r \in \mathbb{C}^n$ is a unit vector orthogonal to q and $\tan\angle(p, q) = |s|/|c|$. It follows that $Kp = cKq + sKr$, and thus using elementary geometry

$$\sin\angle(Kp, Kq) \le \frac{\|sKr\|}{\|cKq\|} \le \kappa(K)\tan\angle(p, q).$$

Note that the first inequality is sharp if $Kp \perp Kr$. ∎

PROPOSITION 3.5 (Theorem 9.1 in [3]). *Suppose that (λ_1, v_1) is an algebraically simple right eigenpair of (A, B) with corresponding left eigenvector u_1^*. Let Q_l and Q_r be nonsingular matrices, and suppose that $u_1^* Q_l Q_r v_1 \neq 0$. If σ is an approximation to λ_1 such that $\lambda_1 - \sigma$ is sufficiently small, then the matrix $Q_l^{-1}(A - \sigma B)Q_r^{-1}$ has an algebraically simple eigenvalue μ_1, and there exist constants c_4 and C_4 such that*

$$c_4|\lambda_1 - \sigma| \le |\mu_1| \le C_4|\lambda_1 - \sigma|. \tag{3.11}$$

PROPOSITION 3.6. *Consider $M_H\tilde{y} \equiv \mathcal{L}^{-1}(A - \sigma B)\mathcal{L}^{-*}\tilde{y} = \mathcal{L}^{-1}Bx$ with $\mathcal{L}\mathcal{L}^* = \mathcal{Q}$ and $M_{nH}\tilde{y} \equiv (A - \sigma B)\mathcal{Q}^{-1}\tilde{y} = Bx$ arising in IRQI for Hermitian and non-Hermitian problems, respectively. Let w_1^H and w_1^{nH} be the eigenvector of M_H and M_{nH}, respectively, corresponding to the eigenvalue of smallest magnitude. Suppose that $x = \gamma(cv_1 + su)$ is a good approximation to v_1 such that $t = |s|/|c|$ is small enough; then there exists a constant C_5 such that*

$$\tan\angle(w_1^H, \mathcal{L}^{-1}Bx) \le C_5 t, \tag{3.12}$$

and so is $\operatorname{gtan}\angle(w_1^{nH}, Bx)$.

Proof. The proof is very similar to that of Theorem 3.6 in [10]. ∎

Remark. Proposition 3.6 shows that the preconditioned linear systems with tuning are similar to the unpreconditioned linear system $(A - \sigma I)y = x$, in the sense that the preconditioned right-hand side is an approximate eigenvector of the preconditioned system matrix M_H or M_{nH} corresponding to the eigenvalue of smallest magnitude λ_1^M. Therefore Theorem 3.1 can be applied to study the preconditioned inner solve, with $\tan\angle(w_1^H, \mathcal{L}^{-1}Bx)$ and $\operatorname{gtan}\angle(w_1^{nH}, Bx)$ denoted as t_0 in that theorem.

PROPOSITION 3.7 (Proposition 2.1 in [13]). *Suppose that $M \in \mathbb{C}^{n\times n}$ has a simple eigenpair (λ_1^M, w_1) well separated from the rest of the spectrum. The Schur decomposition of M is*

$$M = [w_1, W_2]\begin{bmatrix} \lambda_1^M & n_{12}^* \\ 0 & N_{22} \end{bmatrix}[w_1, W_2]^*,$$

where $[w_1, W_2]$ is unitary. Let $M\hat{w} = \xi\hat{w} + f$ with $\|\hat{w}\| = 1$. That is, $(\xi, \hat{w})$ is an approximate eigenpair of M with eigenvalue residual f. If $\|f\|$ is small enough such that

$$\|f\| < \frac{1}{2}\operatorname{sep}(\lambda_1^M, N_{22}) \quad \text{and} \quad \frac{\|f\|(\|f\| + \|n_{12}\|)}{(\operatorname{sep}(\lambda_1^M, N_{22}) - 2\|f\|)^2} < \frac{1}{4}, \tag{3.13}$$

where $\mathrm{sep}(\lambda_1^M, N_{22}) = \|(\lambda_1^M I - N_{22})^{-1}\|^{-1}$, *then*

$$\hat{w} = \frac{w_1 + W_2 p}{\sqrt{1 + p^* p}},$$

where p *is a unique vector satisfying*

$$\|p\| = \tan \angle(w_1, \hat{w}) \le \frac{2\|f\|}{\mathrm{sep}(\lambda_1^M, N_{22}) - 2\|f\|}. \tag{3.14}$$

We are ready now to present the major theorem on the convergence of IRQI.

THEOREM 3.8. *Let* $x = \gamma(cv_1 + su)$ *be an approximation to the desired eigenvector* v_1, $t = |s|/|c|$, $\mathcal{Q}$ *be a tuned preconditioner satisfying* $\mathcal{Q}x = Bx$,

$$M_H = \mathcal{L}^{-1}(A - \sigma B)\mathcal{L}^{-*} \quad with \quad \mathcal{L}\mathcal{L}^* = \mathcal{Q}$$

and $M_{nH} = (A - \sigma B)\mathcal{Q}^{-1}$, $f_H = (\lambda_1 - \sigma)t(\mathcal{L}^* u - \mathcal{L}^{-1}Bu)/\|\mathcal{L}^* v_1\|$, *and*

$$f_{nH} = (\lambda_1 - \quad \sigma)t(\mathcal{Q}u - Bu)/\|\mathcal{Q}v_1\|.$$

Suppose that t *is small enough, and therefore* $\|f_H\|$ *and* $\|f_{nH}\|$ *are small enough such that the assumption* (3.13) *is satisfied for* M_H *and* M_{nH}. *Suppose that the shifted linear system in step* 2 *of Algorithm* 2.1 *is solved by a preconditioned Krylov subspace solver with* $\mathcal{Q}$ *as preconditioner and a zero starting vector. Then cubic and quadratic convergence of IRQI can be achieved if a constant moderately smaller than* $1/\kappa(W)$ *is used as the relative tolerance for the preconditioned inner solve, where* W *is the matrix of eigenvectors of* M_H *and* M_{nH} *for Hermitian and non-Hermitian problems, respectively. (Note in particular that* $\kappa(W) = 1$ *for* M_H.)

Proof. We first show that the desired eigenvector v_1 of (A, B) is closely related to an approximate eigenvector of the preconditioned matrix $M_H = \mathcal{L}^{-1}(A - \sigma B)\mathcal{L}^{-*}$ or $M_{nH} = (A - \sigma B)\mathcal{Q}^{-1}$ corresponding to eigenvalue $\lambda_1 - \sigma$. In fact, for Hermitian problems, we have

$$\begin{aligned}
&Av_1 = \lambda_1 Bv_1 \Leftrightarrow (A - \sigma B)v_1 = (\lambda_1 - \sigma)Bv_1 \\
&\Leftrightarrow \mathcal{L}^{-1}(A - \sigma B)v_1 = (\lambda_1 - \sigma)\mathcal{L}^{-1}Bv_1 \\
&\Leftrightarrow \mathcal{L}^{-1}(A - \sigma B)\mathcal{L}^{-*}(\mathcal{L}^* v_1) = (\lambda_1 - \sigma)(\mathcal{L}^* v_1) + (\lambda_1 - \sigma)(\mathcal{L}^{-1}B - \mathcal{L}^*)v_1 \\
&\qquad = (\lambda_1 - \sigma)(\mathcal{L}^* v_1) + (\lambda_1 - \sigma)(\mathcal{L}^{-1}B - \mathcal{L}^*)\frac{x/\gamma - su}{c} \\
&\qquad = (\lambda_1 - \sigma)(\mathcal{L}^* v_1) + (\lambda_1 - \sigma)t(\mathcal{L}^* u - \mathcal{L}^{-1}Bu) \quad (\text{as } \mathcal{L}^{-1}Bx = \mathcal{L}^* x) \\
&\Leftrightarrow M_H \hat{w}_H = \xi \hat{w}_H + f_H, \qquad (3.15)
\end{aligned}$$

where $\hat{w}_H = \mathcal{L}^* v_1/\|\mathcal{L}^* v_1\|$, $\xi = \lambda_1 - \sigma$, and $f_H = (\lambda_1 - \sigma)t(\mathcal{L}^* u - \mathcal{L}^{-1}Bu)/\|\mathcal{L}^* v_1\|$. For non-Hermitian problems, similarly,

$$\begin{aligned}
&(A - \sigma B)\mathcal{Q}^{-1}(\mathcal{Q}v_1) = (\lambda_1 - \sigma)(\mathcal{Q}v_1) + (\lambda_1 - \sigma)t(\mathcal{Q}u - Bu) \\
&\qquad \Leftrightarrow M_{nH}\hat{w}_{nH} = \xi \hat{w}_{nH} + f_{nH}, \qquad (3.16)
\end{aligned}$$

where $\hat{w}_{nH} = \mathcal{Q}v_1/\|\mathcal{Q}v_1\|$, $\xi = \lambda_1 - \sigma$, and $f_{nH} = (\lambda_1 - \sigma)t(\mathcal{Q}u - Bu)/\|\mathcal{Q}v_1\|$. Let w_1^H and w_1^{nH} be the eigenvectors of M_H and M_{nH}, respectively, corresponding to the eigenvalue of smallest magnitude λ_1^M. We know from (3.14) that for small enough t,

$$\left.\begin{matrix}\tan\angle(w_1^H, \mathcal{L}^* v_1)\\ \tan\angle(w_1^{nH}, \mathcal{Q} v_1)\end{matrix}\right\} \le \frac{2|(\lambda_1-\sigma)t|\|g\|}{\mathrm{sep}(\lambda_1^M, N_{22}) - 2|(\lambda_1-\sigma)t|\|g\|} \le C_6|(\lambda_1-\sigma)t|, \tag{3.17}$$

where $g = (\mathcal{L}^* u - \mathcal{L}^{-1}Bu)/\|\mathcal{L}^* v_1\|$ and $g = (\mathcal{Q}u - Bu)/\|\mathcal{Q}v_1\|$ for Hermitian and non-Hermitian problems, respectively.

Suppose that a Krylov subspace method with a zero starting vector is applied to solve $M_H \tilde{y} = \mathcal{L}^{-1}Bx$ with $y = \mathcal{L}^{-*}\tilde{y}$ or $M_{nH}\tilde{y} = Bx$ with $y = \mathcal{Q}^{-1}\tilde{y}$. To make the proof concise, we only study Hermitian problems, as the derivation for non-Hermitian problems is quite similar. To begin the analysis, suppose at the mth inner step, the relative residual norm of the linear system $\mathcal{L}^{-1}(A-\sigma B)L^{-*}\tilde{y} = \mathcal{L}^{-1}Bx$ is moderately smaller than $1/\kappa(W)$, and that $\alpha_m \le C_1$ (as assumed in Corollary 3.3). From Theorem 3.1 and Propositions 3.2, 3.4, 3.5, and 3.6, we have

$$\begin{aligned}
&\tan\angle(v_1, y_m) = \tan\angle(v_1, \mathcal{L}^{-*}\tilde{y}_m) \le C_3 \angle(v_1, \mathcal{L}^{-*}\tilde{y}_m) && \text{(Proposition 3.2)}\\
&\le C_3(\angle(v_1, \mathcal{L}^{-*}w_1^H) + \angle(\mathcal{L}^{-*}w_1^H, \mathcal{L}^{-*}\tilde{y}_m))\\
&\le \frac{C_3}{C_2}(\sin\angle(v_1, \mathcal{L}^{-*}w_1^H) + \sin\angle(\mathcal{L}^{-*}w_1^H, \mathcal{L}^{-*}\tilde{y}_m)) && \text{(Proposition 3.2)}\\
&\le \frac{\kappa(\mathcal{L}^{-*})C_3}{C_2}(\tan\angle(\mathcal{L}^* v_1, w_1^H) + \tan\angle(w_1^H, \tilde{y}_m)) && \text{(Proposition 3.4)}\\
&\le \frac{\kappa(\mathcal{L}^{-*})C_3}{C_2}\left(C_6|(\lambda_1-\sigma)t| + \frac{|\lambda_1^M|}{C_0}\alpha_m \tan\angle(w_1^H, \mathcal{L}^{-1}Bx)\right) && \text{((3.17) and (3.2))}\\
&\le \frac{\kappa(\mathcal{L}^{-*})C_3}{C_2}\left(C_6 + \frac{C_1 C_4 C_5}{C_0}\right)|(\lambda_1-\sigma)t| = O(t^3) && \text{((3.12) and (3.11))}
\end{aligned} \tag{3.18}$$

for Hermitian problems. Similarly, we can show for non-Hermitian problems that $\mathrm{gtan}\angle(y_m, v_1)$ can be bounded above by $O((\lambda_1-\sigma)t) = O(t^2)$. The cubic and quadratic convergence of IRQI is thus established where the inner solve is done by a preconditioned Krylov subspace solver with tuning. ∎

We now make some remarks on the results in this section. First, Corollary 3.3 and Theorem 3.8 provide some important improvements of existing general convergence results of IRQI in literature. Specifically, it is shown by different approaches in [2], [4], [8], [9], [10], [30] that IRQI converges quadratically and linearly for Hermitian and non-Hermitian problems, respectively, if the relative residual norm of the shifted linear system is bounded by a small *constant*, and it converges cubically and quadratically for the two types of problems if the relative residual norm is bounded by $O(|s|)$ (indicating a sequence of *decreasing* tolerances for the inner solves as the outer iteration proceeds). Our results, assuming $\alpha_{m^*}^{(i)}$ uniformly bounded by a moderate constant C_1 in all outer iterations, show that a moderate small *fixed* relative tolerance for a properly preconditioned Krylov subspace inner solve is sufficient to guarantee full convergence rates of IRQI. In addition, our conclusion indicates that a slower convergence rate—for example, quadratic and linear convergence for Hermitian and non-Hermitian problems—might be achieved even if the inner solve is done with very low accuracy.

In addition, Theorem 3.1 and Corollary 3.3 indicate that an ideal Krylov subspace solver used in IRQI is supposed to decrease both the residual norm $\|p_m(M)b\|$ and $\alpha_m = \|\Lambda_M^{-1}(I - p_m(\Lambda_M))e_z\|$ as quickly as possible. Therefore, MINRES and GMRES may have some advantage over other Krylov subspace methods as they minimize the residual norm at any given step m. The behavior of α_m for different solvers is less

clear, but our numerical results indicate that the minimal residual methods still tend to decrease α_m more quickly than other methods.

4. Equivalence of the inner solves of IRQI and single-vector JD. In this section, we refine the equivalence results of inner solves of IRQI and the single-vector JD method shown in [11], [13].

It is suggested in [26] that the shifted linear system $(A-\sigma B)y = Bx$ arising in RQI can be equivalently reformulated as a single-vector JD correction equation

$$\left(I - \frac{Bxw^*}{w^*Bx}\right)(A-\sigma B)\left(I - \frac{xu^*}{u^*x}\right)s = -r := -(A-\sigma B)x \quad \text{with} \quad s \perp u, \tag{4.1}$$

where the generalized Rayleigh quotient

$$\sigma = \frac{w^*Ax}{w^*Bx},$$

and s is the correction vector to x such that $x+s$ is supposed to be an improved eigenvector approximation. For simplicity of notation, let

$$\Pi_1 = I - \frac{Bxw^*}{w^*Bx} \quad \text{and} \quad \Pi_2 = I - \frac{xu^*}{u^*x}, \tag{4.2}$$

where a most common choice is $w = x$ and $u = Bx$ for Hermitian problems, and $w = Bx$ for non-Hermitian problems; see [26] for other possible choices of w and u. In this section, we consider the non-Hermitian case and thus have $w = Bx$.

It can be shown that $(A-\sigma B)y = Bx$ and (4.1) are equivalent in the sense that $y = \eta(x+s)$ for some $\eta \in \mathbb{C}$. In terms of inexact solutions to these equations, [24] gives an equivalence result for standard Hermitian problems: if the same *unpreconditioned* Krylov suspace method satisfying the Galerkin condition

$$\text{(residual of the linear system is orthogonal to the Krylov subspace)} \tag{4.3}$$

is applied to solve both equations, then $y_{k+1} = \eta_k(x+s_k)$, where $\eta_k \in \mathbb{C}$, y_{k+1}, and s_k are the approximate solutions of the two equations obtained in the $(k+1)$th and kth iteration, respectively. This result is extended in [15] to a two-sided RQI and a two-sided JD for non-Hermitian problems, where the shifted linear system is solved iteratively by unpreconditioned BiCG method. The equivalence result is further extended in [11], [13] to *preconditioned* solves for both standard and generalized non-Hermitian problems. Assuming that the tuned preconditioner $\mathcal{Q}_{RQ}$ is defined as in (3.9c), Freitag and Spence [11] and Freitag, Spence, and Vainikko [13] show that $y_{k+1} = \eta_k(x+s_k)$ if the same Krylov subspace method satisfying the Galerkin condition (4.3) is applied to the preconditioned systems

$$(A-\sigma B)\mathcal{Q}_{RQ}^{-1}\tilde{y} = Bx \quad \text{with} \quad y = \mathcal{Q}_{RQ}^{-1}\tilde{y}, \quad \text{and} \tag{4.4a}$$

$$\Pi_1(A-\sigma B)\Pi_2 Q_{JD}^{\dagger}\tilde{s} = -r := -(A-\sigma B)x \quad \text{with} \quad s = Q_{JD}^{\dagger}\tilde{s}, \tag{4.4b}$$

where $Q_{JD}^{\dagger}$ is the pseudoinverse of $Q_{JD} = \Pi_1 Q \Pi_2$, where Q is as in (3.9).

In this section, we refine the equivalence results given in [11], [13]. We show that $y_{k+1} = \eta_k(x+s_k)$ always holds if the same Krylov subspace method satisying the Galerkin condition (4.3) is applied to (4.4a) and

$$\Pi_1(A-\sigma B)\Pi_2\mathcal{Q}_{JD}^{\dagger}\tilde{s}=-r \quad \text{with} \quad s=\mathcal{Q}_{JD}^{\dagger}\tilde{s}, \tag{4.4c}$$

where $\mathcal{Q}_{JD}^{\dagger}$ is the pseudoinverse of $\mathcal{Q}_{JD}=\Pi_1\mathcal{Q}_{RQ}\Pi_2$, and $\mathcal{Q}_{RQ}$ is *any* preconditioner satisfying $\mathcal{Q}_{RQ}x=Bx$ used in (4.4a). Moreover, whether the equivalence result holds for (4.4a) and (4.4b) depends on the specific construction of $\mathcal{Q}_{RQ}$.

LEMMA 4.1 (Proposition 7.2 in [26]). *Let Π_1 and Π_2 be the two projectors defined in* (4.2)*, and define $P_{JD}=\Pi_1 P\Pi_2$, where P is* any *given nonsingular matrix of the same order as B. If $u^*P^{-1}Bx\neq 0$, then*

$$P_{JD}^{\dagger}=\Pi_2^P P^{-1}\equiv\left(I-\frac{P^{-1}Bxu^*}{u^*P^{-1}Bx}\right)P^{-1}. \tag{4.5}$$

LEMMA 4.2. *Introduce two subspaces as follows:*

$$\begin{aligned}\mathcal{K}_k&=\operatorname{span}\{Bx, K\mathcal{Q}_{RQ}^{-1}Bx, (K\mathcal{Q}_{RQ}^{-1})^2Bx, \ldots, (K\mathcal{Q}_{RQ}^{-1})^kBx\}, \quad \textit{and}\\ \mathcal{L}_k&=\operatorname{span}\{Bx, Kx, \Pi_1K\Pi_2\mathcal{Q}_{JD}^{\dagger}Kx, \ldots, (\Pi_1K\Pi_2\mathcal{Q}_{JD}^{\dagger})^{k-1}Kx\},\end{aligned} \tag{4.6}$$

where K is any given matrix of the same order as B, and $\mathcal{Q}_{RQ}$ is any preconditioner satisfying $\mathcal{Q}_{RQ}x=Bx$. Then $\mathcal{K}_k=\mathcal{L}_k$.

Proof. The proof is similar to that of Lemma 1 in [11] (for standard non-Hermitian problems), which is done for two subspaces generated by $A\mathcal{Q}_{RQ}^{-1}$ and $\Pi_1A\Pi_2\mathcal{Q}_{JD}^{\dagger}$, respectively. For the purpose of completeness and clarity, we study $\mathcal{K}_k$ and $\mathcal{L}_k$ involving the operators $K\mathcal{Q}_{RQ}^{-1}$ and $\Pi_1K\Pi_2\mathcal{Q}_{JD}^{\dagger}$ for generalized non-Hermitian problems, and outline the proof as follows.

First of all, from Lemma 4.1, we have

$$\mathcal{Q}_{JD}^{\dagger}=\left(I-\frac{\mathcal{Q}_{RQ}^{-1}Bxu^*}{u^*\mathcal{Q}_{RQ}^{-1}Bx}\right)\mathcal{Q}_{RQ}^{-1}=\left(I-\frac{xu^*}{u^*x}\right)\mathcal{Q}_{RQ}^{-1}=\Pi_2\mathcal{Q}_{RQ}^{-1}. \tag{4.7}$$

The proof is based on induction. First, it is obvious that $\mathcal{K}_0=\mathcal{L}_0=\operatorname{span}\{Bx\}$ and $\mathcal{K}_1=\mathcal{L}_1$, since $K\mathcal{Q}_{RQ}^{-1}Bx=Kx$. Then, suppose $\mathcal{K}_i=\mathcal{L}_i$ for all $i\le k-1$, let $p=(\Pi_1K\Pi_2\mathcal{Q}_{JD}^{\dagger})^{k-2}Kx\in\mathcal{L}_{k-1}$, and consider $(\Pi_1K\Pi_2\mathcal{Q}_{JD}^{\dagger})^{k-1}Kx$:

$$\begin{aligned}&(\Pi_1K\Pi_2\mathcal{Q}_{JD}^{\dagger})^{k-1}Kx=\Pi_1K\Pi_2\mathcal{Q}_{RQ}^{-1}(\Pi_1K\Pi_2\mathcal{Q}_{JD}^{\dagger})^{k-2}Kx \qquad (\text{by (4.7)})\\ &=\Pi_1K\Pi_2\mathcal{Q}_{RQ}^{-1}p=K\Pi_2\mathcal{Q}_{RQ}^{-1}p-Bx\frac{w^*K\Pi_2\mathcal{Q}_{RQ}^{-1}p}{w^*Bx} \qquad (\text{by (4.2)})\\ &=K\mathcal{Q}_{RQ}^{-1}p-Kx\frac{u^*\mathcal{Q}_{RQ}^{-1}p}{u^*x}-\frac{w^*K\Pi_2\mathcal{Q}_{RQ}^{-1}p}{w^*Bx}Bx \qquad (\text{by (4.2)})\\ &=K\mathcal{Q}_{RQ}^{-1}p-\frac{u^*\mathcal{Q}_{RQ}^{-1}p}{u^*x}Kx-\frac{w^*K\Pi_2\mathcal{Q}_{RQ}^{-1}p}{w^*Bx}Bx.\end{aligned} \tag{4.8}$$

In other words, given $p\in\mathcal{L}_{k-1}=\mathcal{K}_{k-1}$, $(\Pi_1K\Pi_2\mathcal{Q}_{JD}^{\dagger})p\in\mathcal{L}_k$ is in $\mathcal{K}_k$, and therefore $\mathcal{L}_k\subseteq\mathcal{K}_k$. If $\mathcal{L}_k$ is of dimension $k+1$, so is $\mathcal{K}_k$, and thus $\mathcal{K}_k=\mathcal{L}_k$.

Otherwise let $i<k$ be the largest index such that $\mathcal{L}_i$ is of dimension $i+1$. That is, $\mathcal{L}_{i+1}=\mathcal{L}_i=\mathcal{K}_i$. Let q be any vector in $\mathcal{K}_i$; then $\Pi_1K\Pi_2\mathcal{Q}_{JD}^{\dagger}q\in\mathcal{L}_{i+1}=\mathcal{K}_i$. Using derivations similar to (4.8), we can show easily that $K\mathcal{Q}_{RQ}^{-1}q$, a vector in $\mathcal{K}_{i+1}$, is also in $\mathcal{K}_i$. Therefore $\mathcal{K}_{i+1}=\mathcal{K}_i=\mathcal{L}_i=\mathcal{L}_{i+1}$, and by induction we have $\mathcal{K}_j=\mathcal{L}_j$ for all $j>i$. This completes the proof. ∎

Let $K = A - \sigma B$ in Lemma 4.2. Then $\mathcal{K}_k$ and $\mathcal{L}_k \setminus \{Bx\}$ are generated in the process of applying a Krylov subspace solver with a zero starting vector to (4.4a) and (4.4c), respectively. By the assumption that $w = Bx$ in Π_1, it is obvious that $\text{span}\{Bx\}$ and $\mathcal{L}_k \setminus \{Bx\}$ are orthogonal complements of each other. Let U_k be a matrix whose columns form a set of orthonormal basis vectors of $\mathcal{L}_k \setminus \{Bx\}$; then the columns of

$$\begin{bmatrix} \frac{Bx}{\|Bx\|} & U_k \end{bmatrix}$$

form a set of orthonormal basis vectors of $\mathcal{K}_k$. This fact is used in the proof of Theorem 4 (the major equivalence result) in [11].

THEOREM 4.3. *Suppose the same Krylov subspace method satisfying the Galerkin condition* (4.3) *with a zero starting vector is applied to* (4.4a) *and* (4.4c). *Let* y_{k+1} *and* s_k *be the approximate solution obtained in the* $(k+1)$*th and* k*th iterations, respectively. Then there exists a constant* $\eta_k \in \mathbb{C}$ *such that* $y_{k+1} = \eta_k(x + s_k)$.

Proof. The proof is similar to the proof of Theorem 4 in [11]. ∎

We emphasize that $y_{k+1} = \eta_k(x + s_k)$ holds for (4.4a) and (4.4c) as long as the preconditioner $\mathcal{Q}_{RQ}$ used for (4.4a) satisfies $\mathcal{Q}_{RQ}x = Bx$ and the preconditioner $\mathcal{Q}_{JD} = \Pi_1 \mathcal{Q}_{RQ} \Pi_2$ is used for (4.4c). However, whether the equivalence of (4.4a) and (4.4c) can be extended to (4.4b) depends on the *specific construction* of $\mathcal{Q}_{RQ}$. To see this point, suppose that $\mathcal{Q}_{RQ}$ is constructed in some manner from a preconditioner Q, and let $Q_{JD} = \Pi_1 Q \Pi_2$. If somehow $\mathcal{Q}_{JD} = Q_{JD}$, the equivalence result can be extended to (4.4b), because it is trivially equivalent to (4.4c). For example, for the tuned preconditioner $\mathcal{Q}_{RQ}$ defined in (3.9c), if we choose $p = u$, then

$$\begin{aligned} \mathcal{Q}_{JD} = \Pi_1 \mathcal{Q}_{RQ} \Pi_2 &= \Pi_1 \left(Q + \frac{(B - Q)xu^*}{u^*x} \right) \left(I - \frac{xu^*}{u^*x} \right) \\ &= \Pi_1 Q \left(I - \frac{xu^*}{u^*x} \right) = Q_{JD}. \qquad (u^* \Pi_2 = 0) \end{aligned}$$

Since $\mathcal{Q}_{JD} = Q_{JD}$ for this specific $\mathcal{Q}_{JD}$, Theorem 4.3 automatically leads to the equivalence result shown in [11], [13] for (4.4a) and (4.4b) ((4.4c) is not discussed therein). For $\mathcal{Q}_{RQ}$ defined in (3.9a) and (3.9b), it is easy to show that $\mathcal{Q}_{JD} \neq Q_{JD}$, and thus the equivalence of (4.4a) and (4.4c) cannot be extended to (4.4b).

5. Alternative strategies for solving $(A - \sigma B)y = Bx$. To evaluate the efficiency of *inner solves* of IRQI, one is most concerned about how quickly significant improvement of eigenvector approximation can be achieved as the inner iteration proceeds. In terms of preconditioners for the inner solve, it is shown in [9], [10], [13], [31] that a regular preconditioner Q used in the usual setting of solving linear systems is less competitive than a tuned variant $\mathcal{Q}$ that satisfies $\mathcal{Q}x = Ax$ or $\mathcal{Q}x = Bx$. The major reason is that the initial iterate of the preconditioned inner solve with tuning is $y_1 = \mathcal{Q}^{-1}Bx = x$ up to a scaling factor (assuming that $\mathcal{Q}x = Bx$), i.e., the best eigenvector approximation currently available; in addition, x is kept in the subspace of approximate solutions throughout the inner iteration process. This is not the case if the untuned Q is used, and, in particular, $y_1 = Q^{-1}Bx$ is generally a poor eigenvector approximation.

The motivation of tuning is that an appropriate eigenvector approximation is generated in the first inner iteration; this approximation is further refined in subsequent inner iterations, in which tuning is in fact no longer needed. This motivation can also

be achieved by two alternative inner solvers, both of which keep x in the subspace of candidate solutions and do not require the use of a tuned preconditioner.

The first alternative strategy is to solve $(A-\sigma B)y = Bx$ by GCRO-DR [20] with a special recycled vector. GCRO-DR is a typical iterative solver with "subspace recycling" originally developed for solving a sequence of slowly changing linear systems. Usually, a small set of vectors from the subspace of candidate approximate solutions for one linear system is carefully selected and "recycled," i.e., used for the solution of the next linear system. The cost of solving subsequent linear systems may be reduced, as the subspace of candidate solutions need not be built from scratch. In our setting, we select a special single recycled vector such that x is kept in the subspace for approximate solutions.

The framework of GCRO-DR is as follows. Suppose that a zero starting vector is used to solve the linear system $My = b$ with a set of recycled vectors $\{\tilde{p}_1, \tilde{p}_2, \ldots, \tilde{p}_k\}$. Using a QR factorization, it is easy to generate a block of vectors $P_k = [p_1, p_2, \ldots, p_k]$ such that $D_k = MP_k$ has orthonormal columns and $\text{range}(P_k) = \text{span}\{\tilde{p}_1, \tilde{p}_2, \ldots, \tilde{p}_k\}$. As the algorithm starts, we first generate an intermediate solution $y_{\text{tmp}} = P_k D_k^* b$ (the minimal residual solution over $\text{range}(P_k)$), compute $b_{\text{tmp}} = b - D_k D_k^* b$, and let $u_1 = b_{\text{tmp}}/\|b_{\text{tmp}}\|$. Then, the subspace $\mathcal{K}_{m-k+1}((I - D_k D_k^*)M, u_1)$ with orthonormal basis vectors U_{m-k+1} is generated through the Arnoldi process, which produces the decomposition $(I - D_k D_k^*)M U_{m-k} = U_{m-k+1}\bar{H}_{m-k}$. Since $U_{m-k+1} \perp D_k$, we have

$$M\hat{U}_m = \hat{W}_{m+1}\bar{G}_m, \quad \text{where}$$

$$\hat{U}_m = [\,P_k \quad U_{m-k}\,], \quad \hat{W}_{m+1} = [\,D_k \quad U_{m-k+1}\,], \quad \text{and} \quad \bar{G}_m = \begin{bmatrix} I_k & D_k^* M U_{m-k} \\ 0 & \bar{H}_{m-k} \end{bmatrix}. \tag{5.1}$$

Finally, we construct the approximate solution $y_{m-k} = y_{\text{tmp}} + \hat{U}_m t$, where t minimizes $\|\|b_{\text{tmp}}\| e_{k+1} - \bar{G}_m t\|$, and evaluate the corresponding residual of the linear system $res = b_{\text{tmp}} - M\hat{U}_m t = b_{\text{tmp}} - \hat{W}_{m+1}\bar{G}_m t$. See the appendix of [20] for details.

In the setting of IRQI, consider solving the preconditioned linear system $M\tilde{y} \equiv (A-\sigma B)Q^{-1}\tilde{y} = Bx \equiv b$ with $y = Q^{-1}\tilde{y}$ by GCRO-DR. We can choose a single recycled vector p_1 such that $y_{m-1} = Q^{-1}\tilde{y}_{m-1}$ belongs to a subspace of which x is a basis vector. Given the GCRO-DR factorization (5.1), with $k = 1$, we have

$$\begin{aligned} P_1 = p_1 &= Qx/\|r\| \quad \text{with} \quad r = (A-\sigma B)x \perp Bx, \\ D_1 &= r/\|r\|, \\ y_{\text{tmp}} &= P_1 D_1^* Bx = 0, \\ b_{\text{tmp}} &= (I - D_1 D_1^*)Bx = Bx, \quad \text{and} \\ u_1 &= Bx/\|Bx\|. \end{aligned} \tag{5.2}$$

Therefore, $y_{m-1} = Q^{-1}\tilde{y}_{m-1} \in Q^{-1}\text{range}(\hat{U}_m) = Q^{-1}\text{range}(P_1) + Q^{-1}\text{range}(U_{m-1})$, or equivalently, since $(I - (rr^*)/\|r\|^2)Bx = Bx$,

$$y_{m-1} \in \text{span}\{x\} + Q^{-1}\mathcal{K}_{m-1}\left(\left(I - \frac{rr^*}{\|r\|^2}\right)(A-\sigma B)Q^{-1}\left(I - \frac{rr^*}{\|r\|^2}\right), Bx\right). \tag{5.3}$$

Thus, improvement of the eigenvector approximation x comes from a correction vector in $Q^{-1}\mathcal{K}_{m-1}((I - (rr^*)/\|r\|^2)(A-\sigma B)Q^{-1}(I - (rr^*)/\|r\|^2), Bx)$.

The second alternative approach to keep x in the subspace of candidate solutions is to use the FGMRES [22] algorithm with a special configuration for the first inner

iteration. FMGRES is a flexible variant of the right-preconditioned GMRES algorithm, where the preconditioner is not a fixed operator. Compared to the regular GMRES algorithm, at the jth step, an additional intermediate vector $z_j = Q_j^{-1} v_j$ must be saved, where Q_j and v_j, respectively, are the current preconditioning operator and the Arnoldi vector. Assuming that FGMRES with a zero starting vector is used to solve $My = b$, we see easily that $MZ_m = V_{m+1}\bar{H}_m$ holds with $v_1 = b/\|b\|$. The approximate solution obtained at the mth step is $y_m = Z_m t$, where t minimizes $\|\|b\|e_1 - \bar{H}_m t\|$, and y_m minimizes the residual norm $\|b - Mx_m\|$ over range(Z_m).

Consider solving $(A - \sigma B)y = Bx$ by FGMRES with a zero starting vector. The first Arnoldi vector is $v_1 = Bx/\|Bx\|$. To keep x in the subspace for candidate solutions, we choose Q_1 such that

$$z_1 = Q_1^{-1} v_1 = Q_1^{-1}(Bx/\|Bx\|) = x \tag{5.4}$$

up to a scaling factor. Obviously, a tuned preconditioner $\mathcal{Q}$ with $\mathcal{Q}x = Bx$ precisely satisfies this condition, and $z_1 = x/\|Bx\|$ can be generated directly without actually using $\mathcal{Q}$. It then follows that

$$v_2 = (A - \sigma B)Q_1^{-1} v_1 - \langle (A - \sigma B)Q_1^{-1} v_1, v_1\rangle v_1 = r - \langle r, Bx/\|Bx\|\rangle v_1 = r \tag{5.5}$$

up to a scaling factor. In all subsequent FGMRES steps, we use a *fixed* untuned preconditioner Q such that $\{z_2, \ldots, z_m\}$ need not be saved for constructing y_m. In fact, $y_m = Z_m t = \sum_{i=1}^m z_i t(i) = z_1 t(1) + Q^{-1}(\sum_{i=2}^m v_i t(i))$ can be computed without using any z_j for $2 \le j \le m$. With the fixed preconditioner Q, we can see without difficulty that the subspace spanned by $\{v_2, \ldots, v_m\}$ is in fact a Krylov subspace generated with the operator $(I - v_1 v_1^*)(A - \sigma B)Q^{-1}$ and the vector v_2. Therefore, we have

$$\begin{aligned} y_m &\in \text{range}(Z_m) = \text{span}(z_1) + Q^{-1}\text{range}([v_2, \ldots, v_m]) \\ &= \text{span}\{x\} + Q^{-1}\mathcal{K}_{m-1}\left(\left(I - \frac{Bx(Bx)^*}{\|Bx\|^2}\right)(A - \sigma B)Q^{-1}\left(I - \frac{Bx(Bx)^*}{\|Bx\|^2}\right), r\right). \end{aligned} \tag{5.6}$$

Similarly, refinement of the eigenvector approximation x comes from some correction in $Q^{-1}\mathcal{K}_{m-1}((I - (Bx)(Bx)^*/\|Bx\|^2)(A - \sigma B)Q^{-1}, r)$. Interestingly, there exists a duality between the Krylov subspace in (5.6) and that in (5.3).

Both the above GCRO-DR and FGMRES algorithms include x in the subspace of candidate solutions, but numerical experiments in section 6 show that FGMRES is considerably more efficient than GCRO-DR in this setting, in the sense that it provides much better eigenvector approximation than GCRO-DR as the inner iteration proceeds, until the linear residual norms of both solves become sufficiently small. Some insight can be obtained from a connection between the Krylov subspace in (5.6) generated by FGMRES and that generated from the iterative solution of a modified correction equation of single-vector JD. In fact, consider the correction equation (4.1), and note that the projector $\Pi_2 = (I - xu^*/(u^*x))$ may be replaced by some alternative projectors, for example, Π_1; see [26], [34] for other variants of the correction equation. Considering the typical choice of $w = Bx$ for Π_1 in the non-Hermitian case, we have the modified correction equation

$$\left(I - \frac{Bx(Bx)^*}{\|Bx\|^2}\right)(A - \sigma B)\left(I - \frac{Bx(Bx)^*}{\|Bx\|^2}\right)s = -r, \qquad s \perp Bx. \tag{5.7}$$

The exact solution of (5.7) is

$$s = \frac{(Bx)^* x}{(Bx)^*(A-\sigma B)^{-1}Bx}(A-\sigma B)^{-1}Bx - x$$

(assuming that $(Bx)^*(A-\sigma B)^{-1}Bx \neq 0$); that is, if $(Bx)^* x \neq 0$, then $x + s = (A-\sigma B)^{-1}Bx$—the exact solution of $(Ax-\sigma B)y = Bx$ arising in RQI, up to a scaling factor. The preconditioned system $\Pi_1(A-\sigma B)\,Q_{JD}^{\dagger}\Pi_1 \tilde{s} = -r$ can be solved by any proper Krylov subspace methods, where $Q_{JD}^{\dagger}$ is the pseudoinverse of $Q_{JD} = \Pi_1 Q \Pi_1$. Therefore, the approximate correction $s_{m-1} = Q_{JD}^{\dagger}\tilde{s}_{m-1}$ is extracted from the subspace

$$Q_{JD}^{\dagger}\mathcal{K}_{m-1}\left(\left(I - \frac{Bx(Bx)^*}{\|Bx\|^2}\right)(A-\sigma B)\,Q_{JD}^{\dagger}\left(I - \frac{Bx(Bx)^*}{\|Bx\|^2}\right), r\right).$$

The close similarity between this subspace and that in (5.6) for the correction vector provides some insight into the advantage of FGMRES over GCRO-DR in this setting.

6. Numerical experiments. In this section, we first illustrate the convergence analysis of IRQI given in section 3, showing that IRQI converges almost as quickly as exact RQI if the inner linear systems are solved by Krylov subspace methods with a tuned preconditioner to some reasonably small fixed tolerances. We also show that IRQI outperforms inexact Arnoldi method in efficiency for computing a single interior eigenpair of GNHEP, if a good initial eigenvector approximation is available. We then demonstrate the refined equivalence results discussed in section 4 for the inner solves of IRQI and single-vector JD. We also show that one of the alternative strategies—namely, the FGMRES algorithm discussed in section 5—performs as efficiently as the GMRES algorithm with a tuned preconditioner.

We use six Hermitian and six non-Hermitian test problems. Basic information of these problems and corresponding incomplete factorization preconditioners used for the inner solve is given in Table 6.1. For example, the first Hermitian problem $bcsstk(m)13$ stands for $Av = \lambda Bv$ with $A = bcsstk13.mtx$ and $B = bcsstm13.mtx$ from the Matrix Market [17] (abbreviated as MM). A and B are of order $n = 2003$, and the sum of nonzero entries of the two matrices is $nnz = 105064$. The desired eigenvalue is $\lambda_1 = 1.4753 \times 10^3$. An incomplete Cholesky preconditioner is generated by the MATLAB function `cholinc` for $A - \sigma B$ (where $\sigma = 10^3$) with drop tolerance

TABLE 6.1

Information about test problems and corresponding preconditioners. Top 6*: Hermitian problems. Bottom* 6*: non-Hermitian problems.*

Problems	*src*	n	nnz	λ_1	σ	*droptol*
$bcsstk(m)13$	MM	2003	105064	$1.4753e+3$	$1e+3$	$1e-4$
$K(M)uu$	UFL	7102	510334	$9.7834e+0$	$9e+0$	$1.25e-2$
$bcsstk(m)36$	UFL	23052	1463746	$6.4097e+2$	$6e+2$	$1.25e-7$
$bcsstk(m)39$	UFL	46772	2107434	$-2.5897e+1$	$-3e+1$	$1e-4$
$therm\_tk(c)$	UFL	102158	1423116	$7.2421e-15$	$-1e-1$	$1e-4$
$LT1024$	—	1044484	8351782	$4.7036e-1$	0	$2e-3$
$utm1700a(b)$	MM	1700	42822	$3.2428e-2$	$3e-2$	$1e-3$
$mhd4800a(b)$	MM	4800	129772	$-8.1617e+2$	$-8e+2$	$6.5e-7$
$k(m)3plates$	UFL	11107	385566	$1.0376e+5$	$1e+5$	$2.5e-5$
$therm\_dk(m)$	UFL	204316	4269344	$2.3485e+8$	$2e+8$	$5e-4$
IFISS1	IFISS	72867	3699934	$-2.5955e-2$	—	—
IFISS2	IFISS	474499	24631664	$-6.3100e-3$	—	—

$droptol = 10^{-4}$. The shifts σ are manually chosen according to the desired eigenvalue λ_1 computed by MATLAB function `eigs` in the "shift-invert" mode, which is based on the sparse LU decomposition of $(A - \sigma B)$. Similarly, the third non-Hermitian problem $k(m)3plates$ comes from the University of Florida sparse matrix collection (UFL), and the corresponding incomplete LU preconditioner is generated by `ilu` for $A - \sigma B$ with drop tolerance 2.5×10^{-5}. The last Hermitian problem $LT1024$ is constructed directly by MATLAB commands, where `A=1e+5*delsq(numgrid('S',1024))` is a five-point finite difference Laplacian on a two-dimensional "S" shaped domain with 1024 grid points in both x and y directions, and B is a tridiagonal matrix with 2.01 on the main diagonal and 1 on the subdiagonal and superdiagonal. The last two non-Hermitian problems, IFISS1 and IFISS2, arise from the linear stability analysis of a model of two-dimensional incompressible fluid flow over a backward facing step, constructed using the IFISS software package [5], [6]. The domain is $[-1, L] \times [-1, 1]$ with $[-1, 0] \times [-1, 0]$ cut out, where $L = 15$ in IFISS1 and $L = 25$ in IFISS2; the Reynolds numbers are 500 and 1200, respectively. Let $u = u(x, y)$ and $v = v(x, y)$ be the horizontal and vertical components of the velocity, $p = p(x, y)$ be the pressure, and ν be the viscosity. The boundary conditions are

$$
\begin{aligned}
& u = 4y(1-y), v = 0 \quad \text{(parabolic inflow)} && \text{on } x = -1, y \in [0, 1]; \\
& \nu \frac{\partial u}{\partial x} - p = 0, \frac{\partial v}{\partial y} = 0 \quad \text{(natural outflow)} && \text{on } x = L, y \in [-1, 1]; \\
& u = v = 0 \quad \text{(no-slip)} && \text{on all other boundaries.}
\end{aligned} \tag{6.1}
$$

We use a biquadratic/bilinear $(Q_2 - Q_1)$ finite element discretization with element width $1/16$ and $1/32$, respectively (grid parameter 6 and 7 in the IFISS code) for IFISS1 and IFISS2. Inner linear solves are done using the least squares commutator preconditioner [7]. The desired eigenvalue λ_1 is the right-most critical eigenvalue that determines the linear stability of the steady-state solution of the fluid flow model. All numerical experiments are performed using MATLAB R2009b on a 64-bit Red Hat Enterprise Linux Server Release 5.3 system with a quad-core 2.2 GHz AMD Operon processor and 8GB memory.

We first give numerical results to illustrate the convergence analysis in section 3. For all test problems, we compute an accurate approximation to the desired eigenpair (λ_1, v_1) by `eigs` in the shift-invert mode (suppose that v_1 is normalized with respect to the B or B^*B inner product for Hermitian and non-Hermitian problems, respectively), and let the initial eigenvector approximation $x^{(0)}$ be some random perturbation of the accurate eigenvector approximation generated by the "seed" numbers given in Tables 6.2 and 6.3. For example, for $bcsstk(m)13$, $x^{(0)}$ is generated by the following code:

```
randstr=RandStream('mt19937ar','seed',421010018);
x_0=v_1+5e-6*randn(randstr,length(v1),1);
```

These initial outer iterates are not very close to the desired eigenvector, in the sense that an initial iterate with slightly larger perturbation leads to a Rayleigh quotient closer to an undesired eigenvalue and hence failure of convergence toward the desired eigenpair [19]. We then run IRQI (Algorithm 2.1) until the error angle of $x^{(i)}$ in some outer iteration is reasonably close to machine precision and cannot be further significantly reduced due to the conditioning of the linear system. The inner solves are performed by preconditioned MINRES, GMRES, or IDR(4) [28] with the tuned preconditioners

TABLE 6.2
Seeds for $x^{(0)}$ and eigenvalue residual norms of outer iterates for Hermitian problems.

prob & seed	*relative tol*	*initial error*	*iter* 1 *error*	*iter* 2 *error*	*iter* 3 *error*	*total inner*
$bcsstk(m)13$	$5e-4$	$1.403e-4$	$2.368e-2$	$1.690e-5$	$3.274e-12$	71
421010018	$1e-6$		$2.993e-4$	$6.818e-11$	—	109
$5e-6$	exact		$2.400e-4$	$1.005e-11$	—	—
$K(M)uu$	$1e-3$	$1.1216e-2$	$1.0939e-3$	$3.6466e-8$	—	49
263398171	$1e-4$		$5.0859e-4$	$3.2243e-10$	—	70
$7e-3$	exact		$1.2761e-4$	$3.4369e-12$	—	—
$bcsstk(m)36$	$2e-4$	$2.0874e-3$	$4.1501e-1$	$3.6537e-5$	—	51
165906907	$2e-5$		$6.5398e-2$	$1.3726e-7$	—	85
$1.25e-4$	exact		$3.8270e-3$	$8.4592e-8$	—	—
$bcsstk(m)39$	$1e-3$	$1.1626e-3$	$2.0426e-2$	$1.5086e-5$	$4.2022e-12$	92
400466919	$2.5e-6$		$1.3547e-3$	$2.0753e-9$	—	126
$8e-6$	exact		$1.8604e-4$	$8.8151e-12$	—	—
$thermo\_tk(c)$	$1.25e-2$	$8.8808e-3$	$1.3759e-2$	$3.7919e-5$	$4.5113e-12$	92
39850235	$1.25e-4$		$2.6774e-3$	$1.8239e-8$	—	97
$2.6e-4$	exact		$4.4756e-4$	$1.2356e-10$	—	—
$LT1024$	$1e-4$	$1.0241e-2$	$1.8136e-3$	$2.1864e-8$	—	134
326568604	$7.5e-6$		$4.0308e-4$	$2.8484e-10$	—	176
$5e-6$	exact		$3.4887e-4$	$6.2949e-11$	—	—

TABLE 6.3
Seeds for $x^{(0)}$ and eigenvalue residual norms of outer iterates for non-Hermitian problems.

prob & seed	*relative tol*	*initial error*	*iter* 1 *error*	*iter* 2 *error*	*iter* 3 *error*	*iter* 4 *error*	*total inner*
$utm1700a(b)$	$5e-5$	$2.012e-3$	$1.777e-3$	$1.056e-5$	$9.033e-9$	—	167
823128701	$5e-6$		$1.755e-3$	$2.649e-6$	$5.357e-10$	—	177
$5e-4$	exact		$1.753e-3$	$2.474e-6$	$1.130e-11$	—	—
$mhd4800a(b)$	$7.5e-4$	$1.718e-7$	$2.709e-3$	$3.261e-5$	$9.749e-9$	—	198
552557946	$5e-5$		$1.092e-4$	$1.407e-5$	$5.086e-11$	—	237
$1e-2$	exact		$1.071e-4$	$7.689e-9$	$4.224e-14$	—	—
$k(m)3plates$	$7.5e-2$	$2.553e-3$	$1.840e-1$	$3.437e-3$	$1.265e-5$	$8.149e-9$	202
110831261	$5e-3$		$3.560e-2$	$1.913e-5$	$7.035e-10$	—	175
$2e-3$	exact		$6.845e-2$	$6.523e-5$	$1.659e-10$	—	—
$thermo\_dk(m)$	$2.5e-2$	$1.165e-2$	$9.874e-3$	$3.782e-3$	$8.426e-6$	$1.632e-10$	332
626185418	$1e-3$		$3.008e-3$	$1.272e-6$	$1.825e-11$	—	342
$1e-0$	exact		$1.443e-3$	$3.336e-6$	$2.037e-11$	—	—
IFISS1	$1e-1$	$5.837e-2$	$1.211e-1$	$1.346e-2$	$1.307e-4$	$2.292e-7$	149
759497213	$1e-3$		$6.148e-3$	$2.851e-5$	$7.633e-10$	—	174
$2e-1$	exact		$6.698e-3$	$3.353e-5$	$7.290e-10$	—	—
IFISS2	$1e-1$	$4.662e-2$	$3.179e-1$	$3.501e-2$	$2.010e-4$	$9.055e-8$	402
462537766	$1e-3$		$3.116e-2$	$2.045e-5$	$3.570e-11$	—	419
$2.5e-1$	exact		$3.270e-2$	$2.048e-5$	$2.912e-11$	—	—

defined in (3.9b) for Hermitian problems and in (3.9c) with $p = Q^{-1}Bx$ for non-Hermitian problems. A reasonably small *fixed* tolerance is chosen for each problem.

Tables 6.2 and 6.3 give the error angles $\angle(v_1, x^{(i)})$ of outer iterates generated by exact and inexact RQI; the relative tolerances of inner solves and total inner iterations are also listed. We can see from these tables that the local convergence rates of IRQI are not obviously compromised if the shifted linear systems are solved by minimal residual methods with tuned preconditioners to a moderately small fixed tolerance; in particular, full convergence rates can be achieved without using a decreasing sequence of tolerances for the inner solves.

In practice, as Tables 6.2 and 6.3 show, the relative tolerances for inner solves used to guarantee the full convergence rate of IRQI for non-Hermitian problems do not seem to be significantly smaller than those needed for Hermitian problems. This indicates that the bound of the tolerances given in Theorem 3.8 (constants moderately smaller than $1/\kappa(W)$) might be pessimistic for non-Hermitian problems. It seems from these 12 problems that relative tolerances between 10^{-3} and 10^{-6} for the inner solve may be enough to guarantee full convergence rates of IRQI for both Hermitian and non-Hermitian problems.

In addition, we found that our IRQI algorithm is superior to the inexact Arnoldi method in efficiency for computing a single interior eigenpair for GNHEP. Both eigenvalue algorithms start with the same outer iterate $x^{(0)}$ or $x^{(1)}$ (obtained from *exact* RQI). The shift of the shift-invert operator used for the inexact Arnoldi method is chosen to be the Rayleigh quotient generated from the initial outer iterate; that is, the same linear system $(A - \sigma^{(i)}B)y = Bx^{(i)}$ $(i = 0 \text{ or } 1)$ is solved in the first outer iteration of both algorithms. The inner solves for the inexact Arnoldi method are performed with the *untuned* preconditioner, and the tolerance is chosen such that the eigenvalue residual norm of the computed eigenvector approximation is comparable to that computed by IRQI. For each problem, we compare these two algorithms using both long-term recurrence minimum residual methods (GCRO-DR or GMRES without restarting) and the short-term recurrence solver IDR(4) as the inner solver. For GCRO-DR, we recycle Ritz vectors corresponding to the largest Ritz values obtained in the GMRES iterations for the first inner solve of the inexact Arnoldi method; 40 Ritz vectors are used for the problems $thermo\_dk(m)$ and IFISS1, and 20 Ritz vectors are used for other problems. The use of subspace recycling helps reduce the inner iteration counts. Table 6.4 shows the tolerances for the inner solves, eigenvalue residual norms of the final eigenvector approximation computed by these methods, and total number of outer and inner iteration steps. One can see clearly from the table that our IRQI (abbreviated as RQ) consistently outperforms the inexact Arnoldi method (abbreviated as AR) in terms of the total number of inner iterations (and thus total computational time), for both types of inner solvers. The only exception is problem $thermo\_dk(m)$, for which IDR(4) fails to converge to the relative tolerance 10^{-1} in 1200 steps for the inner solve of IRQI. We speculate that the problem is due to the severe floating point errors associated with the tuned preconditioner (see Figure 6.2, middle right), and the way to work around this problem is to use FGMRES. Note that IDR(4) also fails to converge to the tolerance 10^{-6} for the inner solves of the inexact Arnoldi method.

The efficiency of the inexact Arnoldi method can be improved by the use of a variable tolerance for the inner solves. In fact, it is shown in [12], [23], [33] that a relaxed tolerance inversely proportional to the eigenvalue residual norm of the desired eigenpair can be used. Numerical experiences show that the use of variable tolerance usually leads to reduction of total inner iteration counts by a factor up to 2. Using this observation as

TABLE 6.4
Comparison of inexact Arnoldi with inexact RQI for computing a single interior eigenpair.

problem	$utm1700a(b)$		$mhd4800a(b)$		$k(m)3plates$	
init iter	$x^{(0)}$		$x^{(0)}$		$x^{(1)}$	
method	AR/GCRO	RQ/GMRES	AR/GCRO	RQ/GMRES	AR/GCRO	RQ/GMRES
inner tol	$1e-6$	$5e-6$	$2.5e-9$	$5e-5$	$2.5e-7$	$2e-3$
eigres	$1.567e-10$	$5.357e-10$	$5.115e-11$	$6.024e-12$	$3.285e-8$	$2.109e-8$
outer	5	3	8	3	7	2
inner	296	177	765	237	425	143
method	AR/IDR	RQ/IDR	AR/IDR	RQ/IDR	AR/IDR	RQ/IDR
inner tol	$1e-6$	$5e-6$	$2.5e-9$	$5e-5$	$2.5e-7$	$2e-2$
eigres	$1.735e-10$	$1.111e-10$	$3.085e-11$	$2.155e-12$	$8.913e-8$	$2.536e-7$
outer	5	3	8	9	6	3
inner	552	320	1474	639	1047	569
problem	$thermo\_dk(m)$		IFISS1		IFISS2	
init iter	$x^{(1)}$		$x^{(0)}$		$x^{(0)}$	
method	AR/GCRO	RQ/GMRES	AR/GCRO	RQ/GMRES	AR/GCRO	RQ/GMRES
inner	$5e-9$	$1e-3$	$5e-8$	$1e-3$	$1e-8$	$1e-3$
eigres	$1.251e-8$	$7.839e-9$	$7.859e-10$	$7.945e-10$	$1.182e-09$	$1.845e-10$
outer	6	2	12	3	19	3
inner	992	251	965	174	3164	409
method	AR/IDR	RQ/IDR	AR/IDR	RQ/IDR	AR/IDR	RQ/IDR
inner tol	$5e-9$	$1e-1$	$5e-8$	$1e-3$	$1e-8$	$1e-3$
eigres	$3.148e-5$	—	$7.699e-10$	$7.659e-10$	$1.669e-09$	$1.511e-10$
outer	4	—	12	3	19	3
inner	943	—	1705	253	8820	954

a rough estimate, we can predict with some certainty that our IRQI would still be at least as competitive as the inexact Arnoldi method for computing a single interior eigenpair, if a reasonable initial eigenvector approximation is available. The superior efficiency of IRQI can be explained by two facts: first, IRQI converges quadratically or cubically toward the desired eigenpair, whereas the convergence of the Arnoldi method is linear or superlinear; second, the inner solves for IRQI can be done with moderate accuracy, as we have shown, but the inner solves usually need to be performed with high accuracy, at least in the initial outer steps, for inexact Arnoldi. In addition, IRQI can also be used with subspace acceleration, which may further relax the tolerances for the inner solves without penalty of the convergence; see, e.g., [34].

To demonstrate the refined equivalence results for the inner solves of IRQI and single-vector JD, it is enough to use one test problem, e.g., $utm1700a(b)$. Given some initial eigenvector approximation $x^{(0)}$, we use FOM [22], a Krylov subspace method satisfying the Galerkin condition (4.3), to solve the linear system in IRQI (see (4.4a)), and the correction equation of single-vector JD (see (4.4b) and (4.4c)). In Figure 6.1, eigenvalue residual norms of inner iterates are plotted against inner iteration steps. The curves with different markers are as follows:

1. "RQI—tuning" ($\diamond$ with solid line)—eigenvalue residual norms of y_{k+1}—the approximate solution of (4.4a) in the $(k+1)$th inner iteration.
2. "JD—tuning" ($\triangledown$ with dashed line)—eigenvalue residual norms of $x+s_k$, where s_k is the approximate solution of (4.4b) in the kth inner iteration.
3. "JD—no tuning" ($\bigcirc$ with dash-dot line)—eigenvalue residual norms of $x+s_k$, where s_k is the approximate solution of (4.4c) in the kth inner iteration.

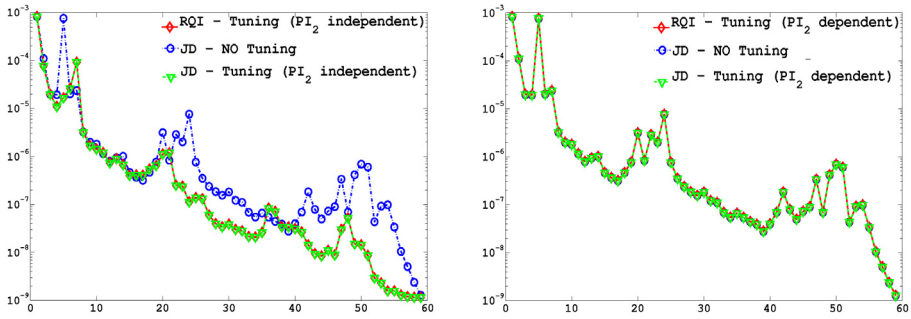

FIG. 6.1. *Eigenvalue residual norms of eigenvector approximation obtained from the iterative solution of* (4.4a), (4.4b), *and* (4.4c). *Left:* $\mathcal{Q}_{RQ}$ *is defined with* $p \neq u$, *where* p *is defined in* (3.9c) *and* u *is defined in* (4.1). *Right:* $\mathcal{Q}_{RQ}$ *is defined with* $p = u$.

For all the inner solves shown above, let Q be the fixed incomplete LU preconditioner for $utm1700a(b)$ described in Table 6.1 and u be the fixed random vector used for the projector

$$\Pi_2 = I - \frac{xu^*}{u^*x}.$$

In Figure 6.1(left), the solution of $(A - \sigma B)y = Bx$ is obtained by FOM with a tuned preconditioner $\mathcal{Q}_{RQ}$ defined in (3.9c) with $p \neq u$ (see "$\diamond$ RQI—tuning (Π_2 independent)"), and $\Pi_1(A - \sigma B)\Pi_2 s = -r$ is solved by FOM with the preconditioner $\mathcal{Q}_{JD} = \Pi_1 \mathcal{Q}_{RQ} \Pi_2$ (see "$\triangledown$ JD—tuning (Π_2 independent)") and the untuned preconditioner Q (see "$\bigcirc$ JD—no tuning"), respectively. Clearly, the curves with $\diamond$ and $\triangledown$ are identical, showing that $y_{k+1} = \eta_k(x + s_k)$ holds for (4.4a) and (4.4c). The curve with $\bigcirc$ is not identical to the above two curves, because $\mathcal{Q}_{JD} \equiv \Pi_1 \mathcal{Q}_{RQ} \Pi_2 \neq \Pi_1 Q \Pi_2 \equiv Q_{JD}$. In Figure 6.1(right), the tuned preconditioner $\mathcal{Q}_{RQ}$ is defined by (3.9c) with $p = u$ (Π_2 dependent) such that $\mathcal{Q}_{JD} = Q_{JD}$; as a result, all the three curves are identical, which means the equivalence result holds for (4.4a), (4.4b), and (4.4c) with this specific $\mathcal{Q}_{RQ}$.

Finally, we compare the efficiency of four different strategies as inner solvers for IRQI. We first generate an initial eigenvector approximation x using the "seed" numbers and size of perturbation given in Table 6.5, and apply these strategies to solve $(A - \sigma B)y = Bx$. In Figure 6.2, eigenvalue residual norms of inner iterates are plotted against inner iteration steps as follows:

1. "$\triangle$ GMRES – no tuning"—the GMRES algorithm with an untuned preconditioner Q.

TABLE 6.5

Seeds and size of perturbation used to generate initial eigenvector approximation for non-Hermitian problems in Figure 6.2.

seed	*perturbation*	
$utm1700a(b)$	688261033	$1e-5$
$mhd4800a(b)$	131645203	$1e-4$
$k(m)3plates$	509223938	$1e-6$
$thermo\_dk(m)$	484521866	$1e-3$
IFISS1	422815323	$2e-5$
IFISS2	714804650	$2.5e-4$

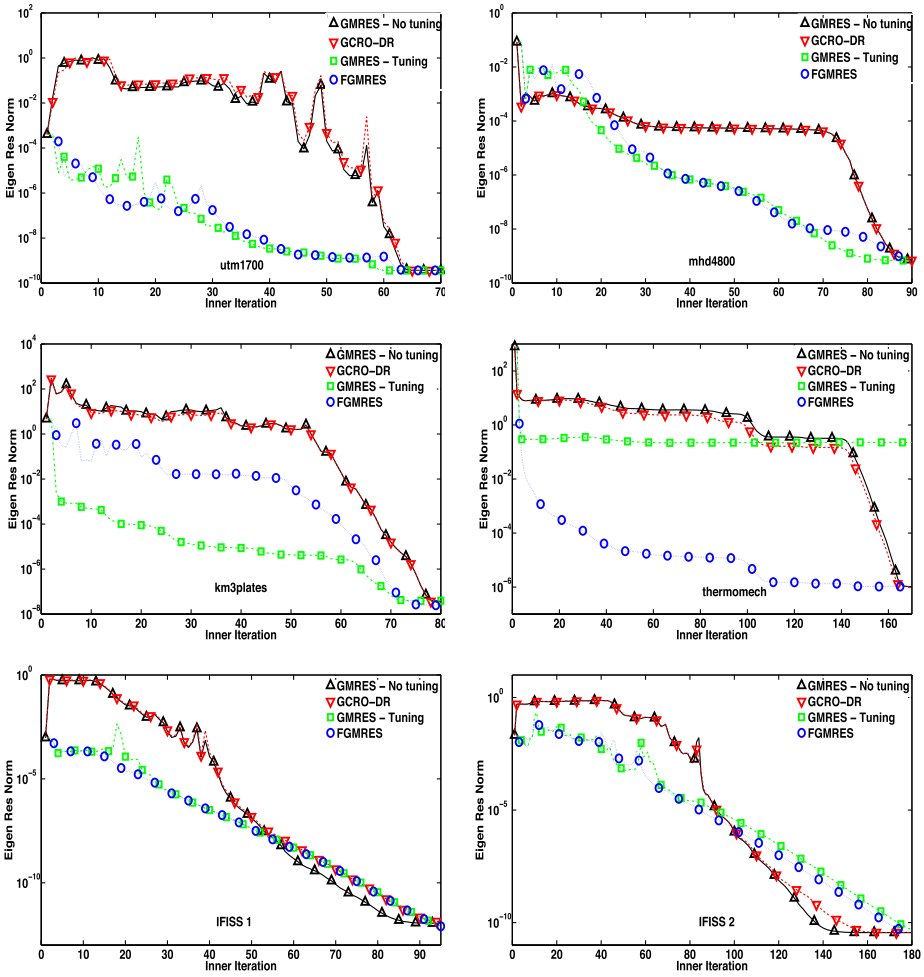

FIG. 6.2. *Eigenvalue residual norms of inner iterates obtained from four strategies for solving* $(A - \sigma B)y = Bx$.

2. "▽ GCRO-DR"—the GCRO-DR algorithm discussed in section 5, where Q is used in all inner iterations.
3. "□ FGMRES"—the FGMRES algorithm discussed in section 5, where in the first inner iteartion $z_1 = x$ up to a scaling factor, and a tuned preconditioner need not be used; Q is used in all subsequent inner iterations.
4. "○ GMRES – tuning"—the GMRES algorithm with the tuned preconditioner defined in (3.9c) with $p = Q^{-1}Bx$.

Obviously, the efficiency of a solution strategy can be evaluated by the rate at which the eigenvalue residual norm of inner iterates decreases. We can see from Figure 6.2 that both GMRES with an untuned preconditioner and the GCRO-DR algorithm discussed in section 5 perform poorly in general, though GCRO-DR keeps x in the subspace of candidate solutions. The FGMRES algorithm, on the other hand, is almost as efficient as the GMRES algorithm with a tuned preconditioner for $utm1700a(b)$, $mhd4800a(b)$, and the two IFISS problems. For $k(m)3plates$, FGMRES is less competitive than

GMRES with a tuned preconditioner, but is still considerably more efficient than the other two strategies. For $thermo\_dk(m)$, however, the performance of GMRES with a tuned preconditioner is much worse than expected. The reason for this abnormal behavior is that the matrix-vector product involving $\mathcal{Q}^{-1}$ requires the evaluation of $Q^{-1}Bx - x$, but $\|x\|$ is about 10^{13} times as large as $\|Q^{-1}Bx\|$ for this problem; therefore $\mathcal{Q}^{-1}$ cannot be computed accurately, and thus GMRES with this tuned preconditioner cannot work properly. Fortunately, FGMRES does not use the tuned preconditioner and therefore performs much better.

For the IFISS problems, especially IFISS2 with Reynolds number $Re = 1200$, it is worth noting that the GMRES algorithm with the *untuned* preconditioner outperforms the other three solvers in the last dozens of inner iterations. Some insight into the phenomenon can be obtained by the following observation. As the Reynolds number increases, the right-most critical eigenvalue λ_1 arising from the linear stability analysis approaches zero from the left (see Table 6.1), and therefore the shifted matrix $A - \sigma B$ arising in IRQI becomes closer to A (suppose that the Rayleigh quotient $\sigma \approx \lambda_1$). In this case, our experience is that the *untuned* least squares commutator preconditioner Q [7] seems more efficient than the tuned variant $\mathcal{Q}$ for $A - \sigma B$ in the sense of clustering eigenvalue distribution of the preconditioned coefficient matrix; see [32] for this observation in the setting of inexact subspace iteration. As a result, the linear residual norm decreases more quickly in the asymptotic convergence phase for the untuned preconditioned solve. On the other hand, it is suggested in [31] that for IRQI for standard Hermitian problems, the asymptotic convergence rate of solving $(A - \sigma I) = x$ by MINRES with a tuned preconditioner may be a reasonable indication of the rate at which the eigenvalue residual norm of inner iterates decreases. The correlation of the two rates may also hold for non-Hermitian problems, and thus it provides some explanation into the advantage of GMRES with untuned preconditioner in the later stage of inner iterations.

In light of the performance of the four solution strategies shown in Figure 6.2, we conclude that GMRES with a tuned preconditioner is in general the best inner solver for IRQI. However, if numerical difficulties associated with tuning arise, the FGMRES algorithm as described in section 5 can be used without significant performance penalty. In addition, if tuning is considerably counterproductive in clustering the eigenvalues of the preconditioned matrix, and if one needs to achieve the full convergence rate of IRQI, then GMRES with the untuned preconditioner might also be considered.

7. Conclusions. We have studied IRQI for solving generalized Hermitian and non-Hermitian eigenvalue problems. We show that the full convergence rates of IRQI can be achieved if the shifted linear system is solved by a Krylov subspace method with a special preconditioner with tuning to a reasonably small fixed tolerance. A refined equivalence result is given for the inner solves of IRQI and single-vector JD. We then provide new understanding of the motivation of tuning: an appropriate eigenvector approximation is generated in the first inner iteration, and is refined in subsequent iterations where tuning is no longer needed. We show that this motivation can be realized by alternative strategies without the use of tuning. One of the alternatives, an FGMRES algorithm with a special configuration in the first inner step, performs as efficiently as GMRES with a tuned preconditioner. For the eigenvalue problem under discussion, our IRQI consistently outperforms the inexact Arnoldi method in efficiency.

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