

Citation for published version:
Freitag, MA & Kürschner, P 2015, 'Tuned preconditioners for inexact two-sided inverse and Rayleigh quotient iteration', Numerical Linear Algebra with Applications, vol. 22, no. 1, pp. 175-196. https://doi.org/10.1002/nla.1945

DOI: 10.1002/nla.1945

Publication date: 2015

Document Version Peer reviewed version

Link to publication

This is the peer reviewed version of the following article: Freitag, MA & Kürschner, P 2015, 'Tuned preconditioners for inexact two-sided inverse and Rayleigh quotient iteration' Numerical Linear Algebra with Applications, vol 22, no. 1, pp. 175-196., which has been published in final form at http://dx.doi.org/10.1002/nla.1945. This article may be used for non-commercial purposes in accordance with Wiley Terms and Conditions for Self-Archiving.

## **University of Bath**

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Download date: 13. May. 2019

Numer. Linear Algebra Appl. 0000; 00:1-25

Published online in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/nla

## Tuned preconditioners for inexact two-sided inverse and Rayleigh quotient iteration

Melina A. Freitag<sup>1</sup> and Patrick Kürschner<sup>2\*</sup>

<sup>1</sup>Department of Mathematical Sciences, University of Bath, Claverton Down, BA2 7AY, United Kingdom.

<sup>2</sup>Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, 39106 Magdeburg, Germany.

#### **SUMMARY**

Convergence results are provided for inexact two-sided inverse and Rayleigh quotient iteration, which extend the previously established results to the generalized non-Hermitian eigenproblem and inexact solves with a decreasing solve tolerance. Moreover, the simultaneous solution of the forward and adjoint problem arising in two-sided methods is considered and the successful tuning strategy for preconditioners is extended to two-sided methods, creating a novel way of preconditioning two-sided algorithms. Furthermore, it is shown that inexact two-sided Rayleigh quotient iteration and the inexact two-sided Jacobi-Davidson method (without subspace expansion) applied to the generalized preconditioned eigenvalue problem are equivalent when a certain number of steps of a Petrov-Galerkin-Krylov method is used and when this specific tuning strategy is applied.

Copyright © 0000 John Wiley & Sons, Ltd.

Received ...

KEY WORDS: Two-sided (in)exact Rayleigh quotient iteration, inexact inverse iteration, convergence rate, preconditioning, Krylov subspace methods, Bi-conjugated gradients, two-sided Jacobi-Davidson method

#### 1. MOTIVATION

Our aim is to find solutions to the two-sided generalized non-Hermitian eigenvalue problem

$$Ax = \lambda Mx, \quad A^H y = \overline{\lambda} M^H y, \tag{1}$$

where  $A, M \in \mathbb{C}^{n \times n}$  are assumed to be large and sparse matrices, and the nonzero vectors  $x \in \mathbb{C}^n$  and  $y \in \mathbb{C}^n$  are the right and left eigenvectors corresponding to the eigenvalue  $\lambda \in \mathbb{C}^n$ . We especially focus on the case when at least one of the matrices A, M is non-Hermitian and the right eigenvectors are different from the left ones which is referred to as the non-normal case. The sought eigenvalues of A, M are assumed to be finite and simple, such that  $y^H M x \neq 0$  is satisfied

Copyright © 0000 John Wiley & Sons, Ltd.

<sup>\*</sup>Correspondence to: Patrick Kürschner, Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, 39106 Magdeburg, Germany. E-mail: kuerschner@mpi-magdeburg.mpg.de

for the corresponding eigenvectors. If M = I, the finite condition number of a simple eigenvalue  $\lambda$  is given by  $\kappa(\lambda) = |y^H x|^{-1}$  if ||x|| = ||y|| = 1.

Computing both right *and* left eigenvectors simultaneously is of interest in several important applications, e.g., in eigenvalue based model order reduction [1, 2] or for computing eigenvalue condition numbers. In fact, the algorithms for computing certain eigentriples discussed in [1, 2] are closely related to the methods investigated here.

If only the right (or the left) eigenvectors are sought, (one-sided) inverse or Rayleigh quotient iteration (RQI) provide basic methods for this purpose. In general inverse iteration converges linearly and RQI achieves quadratic, in the normal case (x = y) even cubic, convergence [3, 4]. If inexact solves are used with a fixed solve tolerance, then the order of convergence is reduced by one. If a decreasing tolerance proportional to the eigenvalue residual norm is chosen for the inexact solve, then the same convergence order as for exact solves can be recovered (see, for example [5, 6, 7, 8, 9]). For the standard Hermitian eigenproblem, some relaxed conditions for achieving linear, quadratic, or cubic convergence are given in [10]. It is also known that (one-sided) accelerated RQI (RQI with subspace expansion) is equivalent to the Jacobi-Davidson method [11] if all linear systems are solved either exactly or, for Hermitian problems, by a certain number of steps of the conjugate gradient method [12]. This result has been extended to preconditioned non-Hermitian problems in [9], when a special preconditioner is used.

For this paper we are interested in *two-sided* versions of inverse iteration, RQI and the related two-sided Jacobi-Davidson method [13, 14]. We consider three important aspects of these methods: Firstly, we extend the convergence theory of inverse iteration and RQI when inexact solves are used, that is, we discuss the convergence of the outer iterative method. Secondly, we consider the inner iteration arising within these inexact solves and suggest a new preconditioning strategy for this two-sided iteration called the tuned preconditioner. Thirdly, we show that, under certain conditions, the new preconditioning strategy is equivalent to a form of the two-sided Jacobi-Davidson method.

Convergence of the outer iterative method. Next to the aforementioned need for computing left eigenvectors in applications such as model order reduction, a further important motivation for considering two-sided eigenvalue iterations is that they can achieve a higher convergence rate for non-normal problems. For instance, two-sided RQI achieves (for M=I) cubic convergence [3, 13, 4] if the linear systems are solved exactly. Under inexact solves the convergence is locally quadratic [13]. We extend these results to the generalized eigenvalue problem, and moreover show that for inexact solves we can recover the convergence rate of the exact algorithms if we choose a decreasing solve tolerance.

**Preconditioners for the inner iterative method.** An important consideration independent of the convergence rate of the outer iteration is the choice of the preconditioner for the solution to the linear systems. For standard (one-sided) eigenproblems a "tuned" preconditioner, a rank-1 modification of the standard preconditioner, reduces the number of iterations for the inner solve considerably [7, 8, 15], a result that has been extended to inverse subspace iteration in [16, 17]. As our main novel contribution of this article we extend the result to two-sided inverse iteration and RQI, where, due to the structure and the simultaneous solution of a forward and adjoint linear system, a rank-2 modification of the standard preconditioner is necessary for an efficient tuning strategy. In particular,

Numer. Linear Algebra Appl. (0000)

we observe that the simultaneous solution of the inner linear systems is often advantageous to solving the forward and adjoint linear systems separately.

**Relation to two-sided Jacobi-Davidson method.** For the standard eigenproblem M=I the simplified two-sided Jacobi-Davidson method is equivalent to two-sided RQI, when all pairs of linear equations are solved by a certain number of steps of a Petrov-Galerkin-Krylov method in each outer iteration [13]. We show that our proposed novel tuned preconditioner and the techniques from [15, 9] for the one-sided algorithms allow to establish similar equivalence results to generalized eigenproblems and to preconditioned solves.

**Plan of this article.** We review and extend convergence results for two-sided inverse and Rayleigh quotient iteration both for the exact and inexact methods in Section 2 and provide new preconditioning strategies for the inner iteration of the two-sided methods in Section 3. In Section 4 we show the equivalence of two-sided Rayleigh quotient iteration and the Jacobi-Davidson method, when certain preconditioners are used. Section 5 supports our theory with numerical examples.

**Notation.**  $\mathbb{R}$  and  $\mathbb{C}$  denote the real and complex numbers,  $\mathbb{R}^{n \times m}$ ,  $\mathbb{C}^{n \times m}$  are  $n \times m$  real and complex matrices, respectively. We use  $A^T$  and  $A^H = \overline{A}^T$  for the transpose and complex conjugate transpose of real and complex matrices. If not stated otherwise  $\|\cdot\|$ , is the Euclidean vector, or subordinate matrix norm. The expression  $x^\perp$  stands for the orthogonal complement  $\{z \in \mathbb{C}^n \setminus \{0\} : z \perp x\}$  of  $x \in \mathbb{C}^n$ .

## 2. CONVERGENCE THEORY FOR TWO-SIDED INVERSE ITERATION AND RQI

The two-sided inverse iteration (TII) is illustrated in Algorithm 1 and requires a sufficiently good eigenvalue approximation  $\theta \approx \lambda$  which is used as fixed shift. The two-sided RQI (TRQI) was originally proposed in [18] and is obtained by choosing the current shift  $\theta_k$  in step 5 as the two-sided generalized Rayleigh quotient

$$\rho(u_k, v_k) := \frac{v_k^H A u_k}{v_k^H M u_k} \tag{2}$$

Numer. Linear Algebra Appl. (0000)

DOI: 10.1002/nla

of the previous iterates, where  $u_k$  and  $v_k$  are approximate right and left eigenvectors. Another early occurrence of this two-sided iteration can be found in [19, Section 13]. The main computational effort is done in the steps 6 and 7, where two linear systems with adjoint coefficient matrices have to be solved in each iteration to obtain new right and left eigenvector approximations. Throughout the rest of the paper we refer to the linear system in step 6 for  $u_{k+1}$  as forward linear system, and the one in step 7 for  $v_{k+1}$  as adjoint linear system. Moreover, subscripts k always denote quantities of the kth iteration of Algorithm 1. In this section we review existing convergence results on the exact and inexact methods, adapting the notation used in [13]. Note that we consider the generalized eigenproblem here as opposed to the standard eigenproblem M = I in [13]. A result on inexact TRQI from [13] is then extended to the generalized eigenproblem and to inexact solves with decreasing solve tolerance.

## Algorithm 1: Two-sided inverse iteration (TII) and two-sided RQI (TRQI)

```
Input : Matrices A, M, initial vectors u_1, \ v_1, \ v_1^H M u_1 \neq 0.

Output: Approximate eigentriple (\lambda_{k_{\max}}, \ u_{k_{\max}}, \ v_{k_{\max}}).

1 u_1 = u_1/\|u_1\|, \ v_1 = v_1/\|v_1\|.

2 for k = 1, 2, \ldots do

3 | Set \lambda_k = \rho(u_k, \ v_k).

4 | Test for convergence.

5 | Choose shift \theta_k.

6 | Solve (A - \theta_k M) u_{k+1} = M u_k for u_{k+1} and normalize.

7 | Solve (A - \theta_k M)^H v_{k+1} = M^H v_k for v_{k+1} and normalize.
```

## 2.1. Review of the convergence of the exact methods

For investigating the convergence rate of the methods, we assume that they converge, i.e.,  $u_k \to x$  and  $v_k \to y$  and hence,  $\theta_k \to \lambda$  as  $k \to \infty$ . Then it is possible to write

$$u_k = \alpha_k(x + \delta_k d_k)$$
 and  $v_k = \beta_k(y + \epsilon_k e_k),$  (3)

where  $\delta_k, \epsilon_k \geq 0$ ,  $u_k, v_k, d_k, e_k, x$ , y are unit vectors with  $d_k \perp M^H y$ ,  $e_k \perp M x$  and  $\alpha_k, \beta_k$  are non-zero normalization constants. Moreover, the matrices  $A - \mu M, A^H - \overline{\mu} M^H$  are surjective mappings from  $(M^H y)^\perp$  to  $y^\perp$  and  $(Mx)^\perp$  to  $x^\perp$ , respectively, for all  $\mu \in \mathbb{C}$  in a sufficiently small vicinity of  $\lambda$ . Thus, there exists a  $\psi \geq 0$  such that

$$\|(A - \mu M)s\| > \psi \|s\|$$
 and  $\|(A - \mu M)^H t\| > \psi \|t\|$  (4)

for all  $\mu$  in a neighborhood of  $\lambda$  and  $s \in (M^H y)^{\perp}$ ,  $t \in (Mx)^{\perp}$  (cf. [1]). The following result extends the work from [13] to the generalized eigenproblem.

Theorem 1 (Convergence of exact two-sided II and RQI)

Under the above assumptions, with  $u_k$ ,  $v_k$  be as in (3), the following convergence results hold.

1. For TII, let  $\theta_k \equiv \theta$  be approximation to the simple eigenvalue  $\lambda$  with  $|\theta - \lambda| = \nu$ . Then Algorithm 1 converges linearly, i.e.,

$$\delta_{k+1} \le \gamma^{\text{TII}} \delta_k + \text{h.o.t.}, \quad \epsilon_{k+1} \le \gamma^{\text{TII}} \epsilon_k + \text{h.o.t.},$$
 (5)

where  $\gamma^{\text{TII}} := \nu ||M||/\psi^{\text{TII}}$ .

2. TRQI achieves locally cubic convergence, i.e.,

$$\delta_{k+1} \le \gamma^{\text{TRQI}} \delta_k^2 \epsilon_k + \text{h.o.t.} \quad \text{and,} \quad \epsilon_{k+1} \le \gamma^{\text{TRQI}} \delta_k \epsilon_k^2 + \text{h.o.t.}$$
 (6)

with 
$$\gamma^{\text{TRQI}} := \omega(\lambda) ||M|| ||A - \lambda M|| / \psi^{\text{TRQI}}$$
 and  $\omega(\lambda) := |y^H M x|^{-1}$ .

The constants  $\psi^{\text{TII}}$ ,  $\psi^{\text{TRQI}} \ge 0$  originate from (4) when using a constant or Rayleigh quotient shift and h.o.t. stands for higher-order terms in  $\delta_k$  and  $\epsilon_k$ .

## Proof

As in the proof of [13, Theorem 3.1] for TRQI, which is a slight generalization of the original

convergence proof in [3, p. 689], one can find nonzero  $\alpha_{k+1}$ ,  $\beta_{k+1}$  such that

$$u_{k+1} = \alpha_{k+1} \left( x + \delta_k (\lambda - \theta_k) \hat{d}_k \right), \quad v_{k+1} = \beta_{k+1} \left( y + \epsilon_k (\overline{\lambda - \theta_k}) \hat{e}_k \right)$$
 (7)

with  $\hat{d}_k$ ,  $\hat{e}_k$  solving  $(A - \theta_k M)\hat{d}_k = Md_k$  and  $(A - \theta_k M)^H\hat{e}_k = M^He_k$ . Applying (4) we have

$$\|\hat{d}_k\| \le \frac{\|(A - \mu M)\hat{d}_k\|}{\psi} = \frac{\|Md_k\|}{\psi} \le \frac{\|M\|}{\psi}, \quad \|\hat{e}_k\| \le \frac{\|M\|}{\psi},$$

and the result for exact TII in (5) follows. Basic calculations yield

$$|\lambda - \theta_k| = \left| \frac{\delta_k \epsilon_k e_k^H (A - \lambda M) d_k}{y^H M x + \delta_k \epsilon_k e_k^H M d_k} \right| \le \omega(\lambda) \delta_k \epsilon_k |e_k^H (A - \lambda M) d_k| + \text{h.o.t.}$$
 (8)

revealing that (2) can (like the one-sided Rayleigh quotient) be seen as a quadratically accurate eigenvalue approximation. Replacing  $\nu$  in the TII result with this estimate gives the desired bound (6).

## 2.2. Convergence under inexact solves

Now consider the situation when the linear systems in steps 6 and 7 are solved inexactly, for instance,

$$||(A - \theta_k M)u_{k+1} - Mu_k|| \le \xi_k^{\mathbf{R}} ||Mu_k|| < 1,$$
  
$$||(A - \theta_k M)^H v_{k+1} - M^H v_k|| \le \xi_k^{\mathbf{L}} ||M^H v_k|| < 1,$$
  
(9)

where the scalars  $\xi_k^R$ ,  $\xi_k^L$  define the accuracy to which the linear systems are solved in the kth iteration of Algorithm 1. This inexact solution is usually carried out using Krylov subspace methods for unsymmetric linear systems, e.g., GMRES, BiCG, BiCGstab, BiCGStab( $\ell$ ), QMR [20, 21], IDR(s) [22] to name at least a few. From now on, the method used to solve the linear systems is referred to as inner solver and its iterations are called inner iterations. The iterations of the eigenvalue method TII or TRQI (Algorithm 1) are hence referred to as the outer iterations.

For investigating the convergence of inexact two-sided inverse and Rayleigh quotient iteration, the following statement is helpful which immediately follows from (9):

$$(A - \theta_k M) u_{k+1} = M(u_k + \tilde{\xi}_k^R || M u_k || f_k),$$
  
$$(A - \theta_k M)^H v_{k+1} = M^H(v_k + \tilde{\xi}_k^L || M^H v_k || g_k),$$

where  $0 \le \|Mf_k\|\tilde{\xi}_k^{\rm R} \le \xi_k^{\rm R}$ ,  $0 \le \|M^H g_k\|\tilde{\xi}_k^{\rm L} \le \xi_k^{\rm L}$ , and  $f_k$ ,  $g_k$  are unit vectors. The following Theorem extends [13, Theorem 5.2] to the generalized eigenproblem.

Theorem 2 (Convergence with fixed inner accuracies [13, Theorem 5.2]) Let  $\xi_k^R \equiv \xi^R$ ,  $\xi_k^L \equiv \xi^L \ \forall k \ \text{in (9)}$  with  $\max(\xi^R \|Mu_k\|, \xi^L \|M^H v_k\|) \|\omega(\lambda) < 1$  and define

$$\zeta_k^{\mathrm{R}} := \frac{\xi^{\mathrm{R}}\omega(\lambda)\|Mu_k\|}{1 - \xi^{\mathrm{R}}\omega(\lambda)\|Mu_k\|}, \quad \zeta_k^{\mathrm{L}} := \frac{\xi^{\mathrm{L}}\omega(\lambda)\|M^Hv_k\|}{1 - \xi^{\mathrm{L}}\omega(\lambda)\|M^Hv_k\|}.$$

1. Then we have for one step of inexact two-sided inverse iteration

$$\delta_{k+1} \le \gamma^{\text{TII}} \zeta_k^{\text{R}} + \text{h.o.t.}, \quad \text{and} \quad \epsilon_{k+1} \le \gamma^{\text{TII}} \zeta_k^{\text{L}} + \text{h.o.t.}.$$
 (10)

2. For one step of inexact TRQI it holds

$$\delta_{k+1} \le \delta_k \epsilon_k \gamma^{\text{TRQI}} \zeta_k^{\text{R}} + \text{h.o.t.}, \quad \text{and} \quad \epsilon_{k+1} \le \delta_k \epsilon_k \gamma^{\text{TRQI}} \zeta_k^{\text{L}} + \text{h.o.t.},$$
 (11)

i.e., inexact TRQI with fixed inner tolerances converges locally quadratic.

The constants  $\gamma^{\text{TII}}$ ,  $\gamma^{\text{TRQI}}$  are as in Theorem 1.

## Proof

For instance, for the forward linear system, using (3) and decomposing  $f_k$  as

$$f_k = \frac{xy^H M}{y^H M x} f_k + \left( I - \frac{xy^H M}{y^H M x} \right) f_k,$$

we find

$$\begin{split} u_k + \tilde{\xi}_k^{\mathrm{R}} \| M u_k \| f_k &= \left( \alpha_k + \tilde{\xi}_k^{\mathrm{R}} \| M u_k \| \frac{y^H M f_k}{y^H M x} \right) x + \alpha_k \delta_k d_k + \tilde{\xi}_k^{\mathrm{R}} \| M u_k \| \left( I - \frac{x y^H M}{y^H M x} \right) f_k \\ &= \tilde{\alpha}_k \left( x + \frac{\tilde{\delta}_k}{\tilde{\alpha}_k} \tilde{d}_k \right), \quad \tilde{d}_k \perp M^H y. \end{split}$$

Since  $|\tilde{\alpha}_k| \geq |\alpha_k| - \tilde{\xi}_k^{\mathsf{R}} \|Mf_k\| \|Mu_k\| \omega(\lambda)$ ,  $\tilde{\delta}_k \leq |\alpha_k| \delta_k + \tilde{\xi}_k^{\mathsf{R}} \|Mf_k\| \|Mu_k\| \omega(\lambda)$  and  $|\alpha_k| = 1 + \text{h.o.t.}$ , we obtain

$$\left| \frac{\tilde{\delta}_k}{\tilde{\alpha}_k} \right| = \zeta_k^{\text{R}} + \text{h.o.t.},$$

using  $\|Mf_k\|\tilde{\xi}_k^{\mathrm{R}} \leq \xi_k^{\mathrm{R}} \equiv \xi^{\mathrm{R}}$ . The remainder of the proof is similar to the proof of Theorem 1.

Theorem 2 shows that inexact TII can stagnate if the steps 6, 7 of Algorithm 1 are solved to a fixed accuracy, whereas inexact TRQI achieves quadratic convergence, as we would expect.

For one-sided methods it can be shown that, by using increasing inner accuracies, i.e., decreasing sequences  $\xi_k^R \leq \xi_{k-1}^R$  and  $\xi_k^L \leq \xi_{k-1}^L$ , the convergence rate of the exact methods can be reestablished in the inexact ones [7, 15, 23]. The next theorem shows that this can also be achieved for the two-sided methods by asking that  $\xi_k^R$  and  $\xi_k^L$  are proportional to the eigenvalue residual norms  $\|r_{u_k}\|$  and  $\|r_{v_k}\|$ , respectively. Hence we can achieve the same convergence rates for inexact TII and inexact TRQI as for the exact versions of the algorithms if a decreasing inner solve tolerance is used.

Theorem 3 (Convergence with decreasing inner tolerances)

Let the assumptions of Theorem 2 hold but choose

$$\xi_k^{\rm R} = \eta_k^{\rm R} \| r_{u_k} \| \quad \text{and} \quad \xi_k^{\rm L} = \eta_k^{\rm L} \| r_{v_k} \|,$$
 (12)

for some  $\eta_k^R$ ,  $\eta_k^L > 0$ , where  $r_{u_k} = (A - \theta_k M)u_k$  and  $r_{v_k} = (A - \theta_k M)^H v_k$ . Then there exist  $\eta_k^R$ ,  $\eta_k^L < 1$  such that the following estimates hold.

#### 1. For inexact TII:

$$\delta_{k+1} < \gamma^{\text{TII}} \delta_k + \text{h.o.t.}$$
 and,  $\epsilon_{k+1} \le \gamma^{\text{TII}} \epsilon_k + \text{h.o.t.}$ 

## 2. For inexact TRQI:

$$\delta_{k+1} < \gamma^{\text{TRQI}} \delta_k^2 \epsilon_k + \text{h.o.t.}$$
 and  $\epsilon_{k+1} \le \gamma^{\text{TRQI}} \epsilon_k^2 \delta_k + \text{h.o.t.}$ 

The constants  $\gamma^{\text{TII}}$ ,  $\gamma^{\text{TRQI}}$  are again the ones from Theorem 1.

#### Proof

We proceed through the proof for the linear system for the right eigenvector approximation. The result for  $\epsilon_{k+1}$  in the adjoint linear system for the left eigenvector approximation can be obtained similarly. Using (3), (8), and  $|\alpha_k| = 1 + \text{h.o.t.}$  one finds

$$||r_{u_k}|| = ||Au_k - \theta_k M u_k|| = ||\alpha_k (\lambda - \theta_k) M x - \alpha_k \delta_k (A - \theta_k M) d_k||$$

$$\leq \delta_k ||(A - \theta_k M) d_k|| + \text{h.o.t.},$$
(13)

and, using (12), this can be plugged into the expression for  $\zeta_k^{\rm R}$  to obtain

$$\zeta_k^{\mathbf{R}} \le \frac{\eta_k^{\mathbf{R}} \delta_k \|M u_k\| \|(A - \theta_k M) d_k\| \omega(\lambda)}{1 - \eta_k^{\mathbf{R}} \delta_k \|M u_k\| \|(A - \theta_k M) d_k\| \omega(\lambda)}.$$
(14)

The fraction on the right hand side of the above expression can be bounded from above by  $\delta_k$  if

$$\eta_k^{\rm R} < ((1+\delta_k)||Mu_k||||(A-\theta_k M)d_k||\omega(\lambda))^{-1}$$
.

Assuming that this inequality holds, the result for inexact TII then follows from using (14) in (10). For the left eigenvector approximation one finds in a similar way that

$$\eta_k^{\rm L} < ((1 + \epsilon_k) \| M^H v_k \| \| (A - \theta_k M)^H e_k \| \omega(\lambda))^{-1}.$$

has to hold. The result for inexact TRQI follows as before from (8).

#### Remark 4

Note that due to the large constants in any of the previous theorems, the actual convergence might be slower than stated for highly non-normal problems. Hence, it might be more adequate to rephrase the statement of Theorem 3 in the sense that the convergence of the inexact methods can be improved by using increasing inner accuracies. It is possible that the bound on  $\eta_k$  can be very small, in particular for highly non-normal problems and simple, but not very well separated eigenvalues. Hence, theoretically a full solution might be required using these bounds, however, in practice, numerical experiments show that much larger constants are possible and no full solution is required.

## Remark 5

In order to implement the decreasing solve tolerance in practice one usually chooses  $\xi_k^{\rm R} = \min\{\varphi_0^{\rm R}, \ \|r_{u_k}\|\}$  or  $\xi_k^{\rm R} = \min\{\varphi_1^{\rm R}, \ \varphi_2^{\rm R}\|r_{u_k}\|\}$ , and  $\xi_k^{\rm L} = \min\{\varphi_0^{\rm L}, \ \|r_{v_k}\|\}$  or  $\xi_k^{\rm L} = \min\{\varphi_1^{\rm L}, \ \varphi_2^{\rm L}\|r_{v_k}\|\}$ , where  $\varphi_i^{\rm R} < 1, \ \varphi_i^{\rm L} < 1, \ i = 0, 1, 2$ , are sufficiently small constants.

Inspired by TRQI a two-sided Jacobi-Davidson method with bi-orthogonal basis vectors can be designed [14, 13] (see Section 4). It is well known that a simplified version of the Jacobi-Davidson method (a method without subspace expansion) is equivalent to Rayleigh quotient iteration if the linear systems are solved exactly. Hence, the same convergence rates as stated in Theorem 1 can be expected (see also [13, Theorem 4.1]).

For the inexact versions of both algorithms the equivalence between the methods does not hold and, hence, the convergence theories cannot be carried over. In fact, in [13, Theorem 5.3]) it was shown that two-sided Jacobi-Davidson achieves locally linear convergence whereas TRQI converges locally quadratically (see Theorem 2) for a fixed solve tolerance. However, as also noted in [13], this does not mean that inexact two-sided JD has a worse behavior than inexact TROI.

In Section 4 we show that both methods are in fact still equivalent for inexact solves if a certain preconditioner and type of linear system solver is used, and, hence, the convergence theories for both methods can be carried over.

#### 3. THE INNER ITERATION AND TUNED PRECONDITIONERS

In this section we investigate the behavior of preconditioned Krylov subspace methods for solving the linear systems (9) inexactly. We distinguish between two strategies: Solving those two linear systems separately by two runs of a Krylov subspace method or, since the matrices in both linear systems are adjoint to each other, simultaneously by suitable Krylov subspace methods. Superscripts (i) refer to quantities related to the ith inner iteration.

## 3.1. Separate solution

If the systems in (9) are solved separately, a whole range of Krylov subspace methods are available. For illustration purposes GMRES is considered here. For the solution of the linear system  $Cu_{k+1} = Mu_k$  or  $C^Hv_{k+1} = M^Hv_k$ , where  $C = (A - \theta_k M)$ , consider, for instance, Cx = b. If the right hand side b is an eigenvector of C and we start GMRES (or in fact any Krylov method) with zero initial guess, then the method converges within one step. For inexact inverse iteration or Rayleigh quotient iteration without a preconditioner and M = I, the right hand side b turns out to be an approximation to the eigenvector of C which becomes increasingly better as the outer iteration proceeds (see [12]) and, thus, an improved performance of the inner iteration is observed even if the system becomes more and more singular. If (left or right) preconditioners are applied, this property gets lost and the right hand side b is generally far from a good approximation to the eigenvector of C. For the standard, one-sided methods tuned preconditioners have been proposed, which are rank-one updates of the standard preconditioners and force the right hand side of the linear system to be an approximation to the eigenvector of the system matrix, in fact, in the limit, i.e., if the outer iteration has converged, they are exact eigenvectors of the system matrix [9, 7, 24, 15, 25].

For the analysis we concentrate on a fixed shift and the forward linear system, the motivation for the adjoint linear system and variable shifts is similar. Moreover, we choose decreasing inner tolerances  $\xi_k^R = \eta^R ||r_{u_k}||$  in order to obtain convergence, see Theorem 3. We explain our strategy using a right preconditioner, but the theory extends to the case of left preconditioners (see [15]).

Numer. Linear Algebra Appl. (0000)

Let the smallest eigenvalue  $c_1$  of C be separated from the other n-1 eigenvalues. We block-diagonalise C as

$$C = [v_{c_1} V_{C_2}] \begin{bmatrix} c_1 & 0 \\ 0 & C_2 \end{bmatrix} [v_{c_1} V_{C_2}]^{-1},$$
(15)

where  $||v_{c_1}|| = 1$  and  $V_{C_2}$  has orthonormal columns. The following Lemma explains the role the right hand side plays in the solution of the linear system Cx = b when Krylov subspace methods are used. It follows directly from [16, Theorem 3.7],[17, Lemma 3.1].

## *Lemma 6* ([17, Lemma 3.1])

Suppose the field of values  $W(C_2)=\{\frac{z^*C_2z}{z^*z}:z\in\mathbb{C}^{n-1},z\neq 0\}$  or the  $\varepsilon$ -pseudospectrum  $\Lambda_{\varepsilon}=\{z\in\mathbb{C}^{n-1}:\|(zI-C_2)^{-1}\|>\varepsilon\}$  is contained in a convex closed bounded set E in the convex plane with  $0\not\in E$ . Assume GMRES is used to solve Cx=b, where  $b\in\mathbb{C}^n$  can be decomposed as  $b=v_{c_1}b_1+V_{C_2}b_2$ , where  $v_{c_1}$  and  $V_{C_2}$  are given in (15) and  $b_2\in\mathbb{C}^{n-1}$ ,  $b_1\neq 0$ . Let  $x^{(i)}$  be the approximate solution to Cx=b obtained after the ith GMRES iteration with  $x^{(0)}=0$ . If

$$i \ge 1 + D_a \left( D_b + \log \frac{\|b_2\|}{\xi \|b\|} \right),$$
 (16)

then  $||b - Cx^{(i)}||/||b|| < \xi$ . The constants  $D_a$  and  $D_b$  depend on the spectrum of C.

For details about  $D_a$  and  $D_b$  we refer the reader to [16, 15], for our analysis these constants have very little significance. We have the following Theorem for the number of inner iterations of the unpreconditioned algorithm (see [17, Theorem 3.2]) applied to the forward linear system.

## Theorem 7

Assume that (un)preconditioned GMRES is used to solve the linear system  $Cu_{k+1} = Mu_k$ , where  $C = A - \theta M$  to the prescribed tolerance in (9), and  $\xi_k^R = \eta^R ||r_{u_k}||$  from (12). Then under assumptions in Theorem 3 we have  $u_k \to x$  linearly, and the lower bound on the GMRES iterations from Lemma 6 increases as the outer iteration proceeds.

## Proof

From (16) the lower bound on the GMRES iterations is

$$i_k \ge 1 + D_a \left( D_b + \log \frac{\|(b_2)_k\|}{\eta^R \|r_{u_k}\| \|Mu_k\|} \right).$$
 (17)

Using (13) we have

$$\eta^R \|r_{u_k}\| \|Mu_k\| \le \delta_k \|(A - \theta_k M) d_k \|\eta^R \|M\| + \text{h.o.t.},$$

and clearly the denominator in the second term of (17) converges to zero as  $u_k \to x$  since  $\delta_k \to 0$ . The nominator  $(b_2)_k$  is the component of  $Mu_k = v_{c_1}(b_1)_k + V_{C_2}(b_2)_k$  which is not in the direction of the eigenvector  $v_{c_1}$  of C. As  $Mu_k \to Mx$  which is not an eigenvector of  $C = A - \theta M$  we have  $\|(b_2)_k\| \to \|b_2\| \neq 0$ , where  $Mx = v_{c_1}b_1 + V_{C_2}b_2$ . Hence, the expression on the right of (17) increases as the outer iteration k increases.

#### Remark 8

An equivalent result to Theorem 7 holds for the adjoint linear system in step 7 of Algorithm 1. Note that Theorem 7 only shows that a lower bound on  $i_k$  increases, there is no result on the behaviour of the actual iteration count. However, numerical results in [15] endorse that our theoretical findings on the iteration bound are indicative of the actual performance of the iterations.

Now consider the (right) preconditioned systems

$$CP^{-1}\tilde{u}_{k+1} = Mu_k, \quad P^{-1}\tilde{u}_{k+1} = u_{k+1},$$
 (18)

where P is a preconditioner for  $C = A - \theta M$ . Theorem 7 also holds for (18), as, in general, the right hand side  $Mu_k$  is not an approximate eigenvector of  $CP^{-1}$ . (In the limit, Mx is not an eigenvector of  $CP^{-1}$ .) A new type of preconditioner was considered in [7, 15]. Consider preconditioners  $\mathbb{P}_k$  such that

$$\mathbb{P}_k u_k = M u_k \quad \text{or} \quad \mathbb{P}_k u_k = A u_k.$$
 (19)

In both cases the right hand side  $Mu_k$  is an approximate eigenvector of  $\mathbb{CP}_k^{-1}$ , since, using (3),

$$(A - \theta M)\mathbb{P}_k^{-1}Mu_k - (\lambda - \theta)Mu_k = (A - \lambda M)u_k = \alpha_k \delta_k (A - \lambda M)d_k,$$

or, assuming  $\lambda \neq 0$ , after basic calculations

$$(A - \theta M) \mathbb{P}_k^{-1} M u_k - \frac{\lambda - \theta}{\lambda} M u_k = \alpha_k \delta_k \left( \frac{I - (A - \theta M) \mathbb{P}_k^{-1}}{\lambda} \right) (A - \lambda M) d_k,$$

and, as  $u_k \to x$  we have  $\delta_k \to 0$  and  $Mu_k$  is an approximate eigenvector of  $(A - \theta M)\mathbb{P}_k^{-1}$ . For the choices of  $\mathbb{P}_k$  in (19) we then have  $\|(b_2)_k\| = D_c \delta_k$  in Theorem 7 and the lower bound on the iteration number does not increase. We observe this in the numerical examples in [15].

In order to satisfy the first condition in (19) we may choose

$$\mathbb{P}_k = I + (Mu_k - u_k)u_k^H \quad \text{or} \quad \mathbb{P}_k = P + (Mu_k - Pu_k)u_k^H, \tag{20}$$

depending on the availability of a preconditioner. We refer to this as M-variant of  $\mathbb{P}_k$ . Similar we may choose the A-variant,

$$\mathbb{P}_k = I + (Au_k - u_k)u_k^H \quad \text{or} \quad \mathbb{P}_k = P + (Au_k - Pu_k)u_k^H, \tag{21}$$

in order to satisfy the second condition in (19). Note that these choices are just rank-one updates of the identity or the preconditioner and can be efficiently implemented using the Sherman-Morrison-Woodbury formula [26].

## Remark 9

For the adjoint linear system we use M- and A-variants of a tuned preconditioner  $\mathbb{Q}_k$  such that

$$\mathbb{Q}_k v_k = M^H v_k \quad \text{or} \quad \mathbb{Q}_k v_k = A^H v_k, \tag{22}$$

instead of (19) in order to satisfy the property that the right hand side of the linear system is an approximation for the eigenvector of the system matrix. This can be achieved by

$$\mathbb{Q}_k = P^H + (M^H v_k - P^H v_k) v_k^H, \tag{23}$$

or 
$$\mathbb{Q}_k = P^H + (A^H v_k - P^H v_k) v_k^H$$
. (24)

Note that the strategy of tuning can in fact be applied to any Krylov method (that is, if the right hand side of the system is an approximation for the eigenvector of the system we obtain convergence in few steps), however, explicit bounds are only available for certain Krylov methods such as GMRES.

For steps 6 and 7 of Algorithm 1 it can be more efficient to solve both the forward and adjoint systems simultaneously, which we will consider in the next section. The concept of tuning for simultaneous solution is examined in Section 3.3.

#### 3.2. Simultaneous solution

Since the coefficient matrices in both linear systems are adjoint to each other, they can be solved simultaneously to the desired accuracy in one run of Krylov subspace methods which are based on the two-sided (non-symmetric) Lanczos process. There, for the solution of a linear system Cx = b, biorthogonal bases for the Krylov subspaces

$$\mathcal{K}_{\mathbf{R}}^{(i)}(C,s) = \operatorname{span}\left\{s,Cs,\ldots,C^{i-1}s\right\} \quad \text{and} \quad \mathcal{K}_{\mathbf{L}}^{(i)}(C^H,t) = \operatorname{span}\left\{t,C^Ht,\ldots,(C^H)^{i-1}t\right\}$$

are built for some generating Krylov vectors s and t. Probably the most prominent methods belonging to this class are the bi-conjugate gradient (BiCG) [27] and Quasi Minimal Residual method (QMR) [28], which can also implicitly solve an adjoint system  $C^H y = c$  if the generating vectors are chosen suitably, e.g.,  $s = b - Cx^{(0)}$ ,  $t = c - C^H y^{(0)}$  for some initial guesses  $x^{(0)}$ ,  $y^{(0)}$ . This is, however, only rarely exploited in practice [29, 30], but here we make explicit use of this property.

The two-sided Lanczos process is the generalization of standard Lanczos process for nonsymmetric matrices. Let the columns of  $W^{(i)}$  and  $Z^{(i)}$  span biorthonormal bases for  $\mathcal{K}_{R}^{(i)}$  and  $\mathcal{K}_{L}^{(i)}$ , and assume for simplicity that zero initial vectors  $x^{(0)}$ ,  $y^{(0)}$  are used. Then the approximate solutions after i steps of the two-sided Lanczos for linear systems [21, Algorithm 7.2] are given by

$$x^{(i)} = W^{(i)}(T^{(i)})^{-1}(Z^{(i)})^H b \quad \text{and} \quad y^{(i)} = Z^{(i)}(T^{(i)})^{-H}(W^{(i)})^H c,$$

where  $T^{(i)} := (Z^{(i)})^H CW^{(i)}$  is tridiagonal. In other words, the approximate solutions are constructed according to a Petrov-Galerkin projection of the linear system, and hence we call methods following this approach *Petrov-Galerkin methods* for solving the linear systems when not referring to a particular implementation.

Recursively updating an LU decomposition of  $T^{(i)}$  for solving the small  $i \times i$  linear systems leads to the short-recurrence formulation of BiCG [27] which is more economical in terms of the amount of work since only a small and constant number of vectors needs to be stored in each step to get  $x^{(i)}$ ,  $y^{(i)}$ . In Algorithm 2 the basic preconditioned BiCG algorithm is illustrated. It is possible that Algorithm 2 breaks down. On the one hand when the underlying two-sided Lanczos process

## Algorithm 2: Preconditioned BiCG [20]

```
Input: C, b, c, initial guesses x^{(0)}, y^{(0)}, preconditioner P \approx C.
     Output: \tilde{x}, \tilde{y} approximately solving Cx = b, C^H y = c.
 1 \gamma^{(-1)} = 1, p^{(0)} = q^{(0)} = 0.
 2 f^{(0)} = b - Cx^{(0)}, q^{(0)} = c - C^H y^{(0)}.
 3 for i = 1, 2, ..., do
          Solve Ps^{(i-1)} = f^{(i-1)}, P^Ht^{(i-1)} = q^{(i-1)} for s^{(i-1)}, t^{(i-1)}.
          \gamma^{(i-1)} = (g^{(i-1)})^H s^{(i-1)}, \, \beta^{(i-1)} = \frac{\gamma^{(i-1)}}{\gamma^{(i-2)}}.
 5
          p^{(i)} = s^{(i-1)} + \beta^{(i-1)} p^{(i-1)}, \ a^{(i)} = t^{(i-1)} + \overline{\beta^{(i-1)}} a^{(i-1)}.
 6
          v^{(i)} = Cp^{(i)}, w^{(i)} = C^H q^{(i)}.
          \alpha^{(i)} = \frac{\gamma^{(i-1)}}{(q^{(i)})^H v^{(i)}}.
 8
          x^{(i)} = x^{(i-1)} + \alpha^{(i)} p^{(i)}, y^{(i)} = y^{(i-1)} + \overline{\alpha^{(i)}} q^{(i)}.
       f^{(i)} = f^{(i-1)} - \alpha^{(i)}v^{(i)}, q^{(i)} = q^{(i-1)} - \overline{\alpha^{(i)}}w^{(i)}.
10
```

breaks down, i.e.,  $\gamma^{(i)}=0$  but  $s^{(i)},\ g^{(i)}$  are nonzero vectors, which is referred to as *breakdown* of the first kind or Lanczos breakdown. On the other hand, it is possible that a pivotless LU decomposition of  $T^{(i)}$  does exist which is called breakdown of the second kind or pivot breakdown. This happens in Algorithm 2 when  $(q^{(i)})^H v^{(i)}=0$  in step 8. Lanczos breakdowns can be handled by sophisticated look-ahead strategies (see, e.g., [31] and the references therein) which leads to rather complicated expressions where the short-recurrence property of BiCG is also lost to some extend. In the remainder we assume that these breakdowns do not occur. Breakdowns of the second kind appear to be a special issue in the context of solving the adjoint linear systems of TRQI and are investigated in more depth in the next subsection.

Other less prominent methods which are also capable of a simultaneous solution of forward and adjoint linear system are GLSQR [30, 32, 33] as well as unsymmetric variants of MINRES and SYMMLQ [33], where other Krylov-like subspaces which are not related to the two-sided Lanczos process are used.

3.2.1. Breakdowns of BiCG with two-sided RQI Before discussing tuned preconditioners for the simultaneous solution, we shall have a look at the issue of breakdowns of BiCG within two-sided Rayleigh quotient iteration. Apply the above BiCG to the linear systems occurring in, say iteration k of TRQI, i.e.,  $C = A - \theta_k M$ ,  $b = M u_k$ ,  $c = M^H v_k$ , where  $u_k$ ,  $v_k$  are approximations to right and left eigenvectors of A, M, respectively.

Theorem 10 (Breakdown of BiCG within TROI)

If Algorithm 2 is applied within TRQI with  $x^{(0)} = y^{(0)} = 0$  then BiCG suffers from breakdown of the second kind in the first iteration if  $M = P = I_n$  or  $Pu_k = Mu_k$ ,  $P^Hv_k = M^Hv_k$  holds.

## Proof

For  $M=P=I_n$ , the first BiCG iteration gives  $p^{(1)}=s^{(0)}=f^{(0)}=u_k, \quad q^{(1)}=t^{(0)}=g^{(0)}=v_k.$  With  $v^{(1)}=(A-\theta_kI_n)p^{(1)}$  and  $\theta_k$  being the two-sided Rayleigh quotient this yields

$$(q^{(1)})^H v^{(1)} = v_k^H (A - \theta_k I_n) u_k = v_k^H \left( A - \frac{v_k^H A u_k}{v_k^H u_k} I_n \right) v_k = 0,$$

such that  $\alpha^{(1)}$  in step 8 is not defined and the iteration cannot continue. According to [34] this is exactly a breakdown of the second kind (pivot breakdown). The case  $Pu_k = Mu_k$ ,  $P^Hv_k = M^Hv_k$  can be dealt with similarly.

Note that QMR also encounters a breakdown due to  $(q^{(1)})^H v^{(1)} = 0$  (cf. [20, Figure 2.8]) although this is not referred to as pivot breakdown.

Of course, since in most situations applying a preconditioner  $P \neq I$  might be feasible or even necessary, and  $Pu_k \neq Mu_k$ ,  $P^Hv_k \neq M^Hv_k$  will most likely generically hold, this kind of breakdown appears to be no intrinsic issue. It will, however, play a role for the preconditioners proposed in the next subsection and thus we shall discuss some strategies to circumvent this issue.

Although in inner-outer eigenvalue iterations it is common to start the inner solver with zero initial vectors since they are not biased towards any eigenvector directions, one could also use nontrivial starting vectors, e.g., random ones. A more appealing idea might be to set the starting vectors equal to the approximate eigenvectors of the previous TII / TRQI iteration as  $x^{(0)} = u_k$ ,  $y^{(0)} = v_k$  since  $u_k$ ,  $v_k$  may already be close to the sought solutions of the current step.

Another approach is to use the composite step BiCG (CSBCG) algorithm [34] which is intrinsically designed to deal with those pivot breakdowns. The CSBCG/LAL implementation [35] of this method appears to be the most stable choice for our purpose and will therefore be used in our numerical examples.

#### 3.3. Tuned preconditioners for the simultaneous solution

Now we discuss the application of tuned preconditioners for a Petrov-Galerkin method to solve both systems in Algorithm 1 in one run. If  $\mathbb{S}_k$  is a tuned preconditioner for the forward linear system, then  $\mathbb{S}_k^H$  should be a tuned preconditioner for the adjoint one. Additionally, by incorporating the concept of tuning, the M- and A-variant of  $\mathbb{S}_k$  should satisfy

$$S_k u_k = M u_k \text{ and } S_k^H v_k = M^H v_k, \tag{25}$$

or 
$$\mathbb{S}_k u_k = A u_k$$
 and  $\mathbb{S}_k^H v_k = A^H v_k$ , (26)

respectively. It is easy to see that this cannot be achieved with an rank-one modification of a standard preconditioner as in the one-sided case or when both systems are solved one by one. Instead, we propose a rank-two modification of the form

$$\mathbb{S}_k = P + a_k b_k^H + c_k d_k^H,$$

where  $P \in \mathbb{C}^{n \times n}$  is the standard preconditioner, and  $a_k, b_k, c_k, d_k \in \mathbb{C}^n$  are vectors yet to be determined. For the case (25) we assume w.l.o.g. that  $v_k^H M u_k = 1$ . Choosing  $b_k := M^H v_k$ ,  $c_k := M u_k$  leads to

$$Pu_k + a_k + Mu(d_k^H u_k) = Mu_k, (27)$$

$$P^{H}v_{k} + (M^{H}v_{k}a_{k}^{H})v_{k} + d_{k} = M^{H}v_{k}.$$
(28)

Rearranging (27) for  $a_k$ , and inserting it into (28) gives

$$(P-M)^{H}v_{k} = u_{k}^{H}[(P-M)^{H}v_{k} + d_{k}]M^{H}v_{k} - d_{k},$$

such that we may choose  $d_k := -(P-M)^H v_k$ , which yields  $a_k := -(P-M)u_k + \tau_k u_k$  with  $\tau_k := v_k^H (P+M)u_k$ . The complete tuned preconditioner is then

$$\mathbb{S}_k = P + [Mu_k, Pu_k] \begin{bmatrix} \tau_k & -1 \\ -1 & 0 \end{bmatrix} [M^H v_k, P^H v_k]^H.$$
 (29)

It is checked easily that  $\mathbb{S}_k$  and  $\mathbb{S}_k^H$  satisfy (25). With the Sherman-Morrison-Woodbury formula [26] and  $f_k := P^{-1}Mu_k$ ,  $g_k := P^{-H}M^Hv_k$ ,  $\alpha_k := v_k^HMP^{-1}Mu_k$ , the applications of  $\mathbb{S}_k$ ,  $\mathbb{S}_k^H$  are

$$\mathbb{S}_{k}^{-1} = P^{-1} + [f_{k}, u_{k}] \begin{bmatrix} -\alpha_{k} & 0 \\ 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} g_{k}^{H} \\ v_{k}^{H} \end{bmatrix} = P^{-1} + u_{k} v_{k}^{H} - \frac{f_{k} g_{k}^{H}}{\alpha_{k}}, \tag{30a}$$

$$\mathbb{S}_k^{-H} = P^{-H} + v_k u_k^H - \frac{g_k f_k^H}{\overline{\alpha_k}}.$$
 (30b)

For each outer iteration two extra applications of P are required to compute the vectors  $f_k, g_k$  and apply  $\mathbb{S}_k$ , in particular we need one solve with P and  $P^H$ . This amounts to the same extra costs as for the tuned preconditioner for the separate solution (see Section 3.1). Note that  $f_k, g_k$  as well as the scalar  $\alpha_k$  can be constructed and stored before the inner solver is started. For a tuned preconditioner satisfying (26) the vectors defining  $\mathbb{S}_k$  become  $f_k := P^{-1}Au_k, g_k := P^{-H}A^Hv_k, \alpha_k = v_k^HAf_k$  and using the scaling  $v_k^HAu_k = 1$ . When A is singular this variant of  $\mathbb{S}_k$  should only be used if a nonzero eigenvalue is sought.

# 4. EQUIVALENCE BETWEEN TWO-SIDED RAYLEIGH QUOTIENT ITERATION AND TWO-SIDED SIMPLIFIED JACOBI-DAVIDSON METHOD WITH PRECONDITIONED ITERATIVE SOLVES

The two-sided Jacobi-Davidson [14, 13] (TJD) is an extension of the (one-sided) Jacobi-Davidson [36, 37] to compute eigentriples of nonnormal eigenvalue problems. A first idea of such a method was already briefly mentioned in [36]. Here we discuss the simplified TJD given in Algorithm 3 which does work with one-dimensional subspaces for the right and left eigenvector approximations. In [13, Proposition 5.5.] it was shown (using a result for one-sided methods from [12]) that for the standard eigenvalue problem simplified TJD is equivalent to TRQI when all pairs of linear systems are solved by a certain number of steps of a Petrov-Galerkin-Krylov method<sup>§</sup> in each outer iteration. This result, however, does not extend to the GEP and to preconditioned solves. In this section we show that the result can be extended for the GEP and to preconditioned TRQI and TJD if the preconditioner for TRQI is chosen in a specific way. Note that by Petrov-Galerkin method

<sup>§</sup>The authors of [13] used BiCG in the theorem, which should be understood as any Petrov-Galerkin type method that produces the required bases without suffering from breakdowns (personal communication with M. E. Hochstenbach).

**Algorithm 3**: Simplified two-sided Jacobi-Davidson method (TJD) (biorthogonal version) [14, 13]

```
Input : Matrix A, initial vectors u_1, \ v_1, v_1^H M u_1 \neq 0.

Output: Approximate eigentriple (\theta_{k_{\max}}, \ u_{k_{\max}}, \ v_{k_{\max}}).

1 for k = 1, 2, \dots do

2 | Set \theta_k = \rho(u_k, \ v_k).

3 | Compute residuals r_{u_k} = Au_k - \theta_k M u_k, r_{v_k} = A^H v_k - \overline{\theta_k} M^H v_k.

4 | Test for convergence.

5 | Solve (approximately) s_k \perp M^H v_k, \ t_k \perp M u_k from

\Pi_1(A - \theta_k M)\Pi_2 s_k = -r_{u_k}, \qquad (31a)
\Pi_2^H (A - \theta_k M)^H \Pi_1^H t_k = -r_{v_k}, \qquad (31b)

where \Pi_1 = I - \frac{M u_k v_k^H}{v_k^H M u_k} and \Pi_2 = I - \frac{u_k v_k^H M}{v_k^H M u_k}.

Set u_{k+1} = (u_k + s_k)/\|u_k + s_k\|_2, v_{k+1} = (v_k + t_k)/\|v_k + t_k\|_2.
```

we explicitly refer to any Krylov subspace method that uses biorthonormal bases for dual Krylov subspaces and performs a Petrov-Galerkin type projection for obtaining approximate solutions for dual linear systems in the considered eigenvalue methods. Therefore, we assume that no breakdown occurs or that those are dealt with appropriately (cf. the discussion in Section 3.2.1).

In the following we neglect the index k for the outer iteration as we are only interested in the inner solves. The approximate solutions  $u_{k+1}$ ,  $v_{k+1}$  of the linear systems in Algorithm 1 are denoted by  $u_+$ ,  $v_+$ . Furthermore we assume w.l.o.g. that u and v satisfy the normalisation  $v^H M u = 1$ . Then the projections in Algorithm 3 become  $\Pi_1 = I - M u v^H$  and  $\Pi_2 = I - u v^H M$ .

Since the operators in (31a) and (31b) are adjoint to each other, the above version of TJD allows the application of Petrov-Galerkin-Krylov methods for solving both systems simultaneously. If the application of a preconditioner P is desired, it has to be projected accordingly, i.e. one has to use the projected preconditioners

$$\tilde{P} := \Pi_1 P \Pi_2 \quad \text{and} \quad \tilde{P}^H := \Pi_2^H P^H \Pi_1^H$$
 (32)

Numer. Linear Algebra Appl. (0000)

DOI: 10.1002/nla

for (31a) and (31b), respectively. Note that  $\tilde{P}$ ,  $\tilde{P}^H$  are mappings from  $(M^H v)^{\perp}$  to  $v^{\perp}$  and  $(Mu)^{\perp}$  to  $u^{\perp}$ . Exploiting the inherent biorthogonality relations leads to applications of both projected preconditioners (see [2],[36])

$$\tilde{P}^{\dagger} = \Pi^P P^{-1}, \quad (\tilde{P}^H)^{\dagger} = P^{-H} (\Pi^P)^H,$$

where

$$\Pi^P = \left(I - \frac{P^{-1}Muv^HM}{v^HMP^{-1}Mu}\right).$$

Note that  $\Pi_2\Pi^P=\Pi^P$ . In order to ensure applicability of a Petrov-Galerkin type methods one has to use, e.g., right preconditioning for one correction equation and left preconditioning for the other

one, such that the pair of preconditioned correction equations become

$$\Pi_1(A - \theta M)\Pi^P P^{-1}\tilde{s} = -r_u, \ \Pi^P P^{-1}\tilde{s} = s,$$
$$P^{-H}(\Pi^P)^H (A - \theta M)^H \Pi_1^H t = -P^{-H}(\Pi^P)^H r_v.$$

The preconditioned equations for TRQI are

$$(A - \theta M)P^{-1}\tilde{u} = Mu, \ P^{-1}\tilde{u} = u_+,$$
  
 $P^{-H}(A - \theta M)^H v_+ = P^{-H}M^H v.$ 

Note that the other way around, i.e., using left and right preconditioning in the forward and adjoint linear system, respectively, is of course also possible as well as using both left and right preconditioning for each linear system (cf. [14] for this strategy in TJD). In the following we consider the tuned preconditioner  $\mathbb{S}$  with a rank-two modification which satisfies (25) ( $\mathbb{S}u = Mu$ ,  $\mathbb{S}^Hv = M^Hv$ ) and is given by (29) with its inverse (30). In order to show the equivalence of TRQI with a tuned preconditioner and simplified TJD with a standard preconditioner we require the following Lemma. The proofs of Lemma 11 and Theorem 12 mimic the ones of [12, 38, 9, 13, 15].

Lemma 11 (Generalization of [13, Lemma 5.4], [9, Lemma 1 and Lemma 3] and [15, Lemma 5.1]) Let  $\Pi_1 := I - Muv^H$ ,  $\Pi_2 := I - uv^HM$ ,  $C := A - \theta M$ ,  $r_u = Cu$  and  $r_v = C^Hv$  and  $v^HMu = 1$ . Let P be a standard preconditioner and let the tuned preconditioner  $\mathbb S$  satisfy (25). Introduce the subspaces

$$\mathcal{K}_{\mathbf{R}}^{(i)} = \operatorname{span}\{Mu, C\mathbb{S}^{-1}Mu, (C\mathbb{S}^{-1})^{2}Mu, \dots, (C\mathbb{S}^{-1})^{i}Mu\},$$

$$\mathcal{L}_{\mathbf{R}}^{(i)} = \operatorname{span}\{Mu, r_{u}, (\Pi_{1}C\Pi^{\mathbb{S}}\mathbb{S}^{-1})r_{u}, \dots, (\Pi_{1}C\Pi^{\mathbb{S}}\mathbb{S}^{-1})^{i-1}r_{u}\},$$

$$\mathcal{M}_{\mathbf{R}}^{(i)} = \operatorname{span}\{Mu, r_{u}, (\Pi_{1}C\Pi^{P}P^{-1})r_{u}, \dots, (\Pi_{1}C\Pi^{P}P^{-1})^{i-1}r_{u}\},$$

as well as the subspaces

$$\mathcal{K}_{\mathbf{L}}^{(i)} = \operatorname{span}\{\mathbb{S}^{-H}M^{H}v, \mathbb{S}^{-H}C^{H}\mathbb{S}^{-H}M^{H}v, (\mathbb{S}^{-H}C^{H})^{2}\mathbb{S}^{-H}M^{H}v, \dots \\ \dots, (\mathbb{S}^{-H}C^{H})^{i}\mathbb{S}^{-H}M^{H}v\}, \\ \mathcal{L}_{\mathbf{L}}^{(i)} = \operatorname{span}\{v, \mathbb{S}^{-H}(\Pi^{\mathbb{S}})^{H}r_{v}, (\mathbb{S}^{-H}(\Pi^{\mathbb{S}})^{H}C^{H}\Pi_{1}^{H})\mathbb{S}^{-H}(\Pi^{\mathbb{S}})^{H}r_{v}, \dots \\ \dots, (\mathbb{S}^{-H}(\Pi^{\mathbb{S}})^{H}C^{H}\Pi_{1}^{H})^{i-1}\mathbb{S}^{-H}(\Pi^{\mathbb{S}})^{H}r_{v}\}, \\ \mathcal{M}_{\mathbf{L}}^{(i)} = \operatorname{span}\{v, P^{-H}(\Pi^{P})^{H}r_{v}, (P^{-H}(\Pi^{P})^{H}C^{H}\Pi_{1}^{H})P^{-H}(\Pi^{P})^{H}r_{v}, \dots \\ \dots, (P^{-H}(\Pi^{P})^{H}C^{H}\Pi_{1}^{H})^{i-1}P^{-H}(\Pi^{P})^{H}r_{v}\}.$$

For every  $i \geq 1$  we have  $\mathcal{K}_{\mathbf{R}}^{(i)} = \mathcal{L}_{\mathbf{R}}^{(i)} = \mathcal{M}_{\mathbf{R}}^{(i)}$  and  $\mathcal{K}_{\mathbf{L}}^{(i)} = \mathcal{L}_{\mathbf{L}}^{(i)} = \mathcal{M}_{\mathbf{L}}^{(i)}$ .

Proof

Using (30a) and  $v^H M u = 1$  we have that  $\Pi^{\mathbb{S}} \mathbb{S}^{-1} = \Pi_2 \mathbb{S}^{-1} = \mathbb{S}^{-1} \Pi_1$ . Then  $\mathcal{K}_{\mathbf{R}}^{(i)} = \mathcal{L}_{\mathbf{R}}^{(i)}$  and  $\mathcal{K}_{\mathbf{L}}^{(i)} = \mathcal{L}_{\mathbf{L}}^{(i)}$  follow directly from [13, Lemma 5.4],[15, Lemma 5.1] (applied to  $C\mathbb{S}^{-1}$  and  $\mathbb{S}^{-H} C^H$ ). Furthermore

$$\Pi^{\mathbb{S}}\mathbb{S}^{-1} = \mathbb{S}^{-1} - uv^{H} = P^{-1} - \frac{P^{-1}Muv^{H}MP^{-1}}{v^{H}MP^{-1}Mu} = \Pi^{P}P^{-1},$$

as well as  $\mathbb{S}^{-H}(\Pi^{\mathbb{S}})^H = P^{-H}(\Pi^P)^H$  using (30a), (30b) and both  $\mathcal{L}_{R}^{(i)} = \mathcal{M}_{R}^{(i)}$  and  $\mathcal{L}_{L}^{(i)} = \mathcal{M}_{L}^{(i)}$  follow immediately.

Theorem 12 (Generalization of [13, Proposition 5.5],[15, Theorem 5.2] and [9, Theorem 4]) Let u, v be approximate right and left eigenvectors of A, M, normalized such that  $v^H M u = 1$ . Moreover,  $s^{(i)}, t^{(i)}$  denote the approximate solutions to the correction equations of simplified TJD obtained with a Petrov-Galerkin method using standard preconditioners  $P, P^H$ . Then for the approximate solutions  $u^{(i+1)}, v^{(i+1)}$  to the TRQI equations obtained after i+1 steps of the same Petrov-Galerkin method applying the tuned preconditioner  $\mathbb S$  with  $\mathbb Su = Mu$  and  $\mathbb S^H v = M^H v$  it holds

$$u^{(i+1)} = \mu_1(s^{(i)} + u)$$
 and  $v^{(i+1)} = \mu_2(t^{(i)} + v)$ ,

for some constants  $\mu_1$ ,  $\mu_2$ .

#### Proof

The spaces spanned by i steps of a preconditioned Petrov-Galerkin method applied to the JD correction equations are

$$\operatorname{span} \left\{ r_{u}, (\Pi_{1}C\Pi^{P}P^{-1})r_{u}, \dots, (\Pi_{1}C\Pi^{P}P^{-1})^{i-1}r_{u} \right\},$$

$$\operatorname{span} \left\{ P^{-H}(\Pi^{P})^{H}r_{v}, (P^{-H}(\Pi^{P})^{H}C^{H}\Pi_{1}^{H})P^{-H}(\Pi^{P})^{H}r_{v}, \dots \right\},$$

$$\dots, (P^{-H}(\Pi^{P})^{H}C^{H}\Pi_{1}^{H})^{i-1}P^{-H}(\Pi^{P})^{H}r_{v} \right\},$$

which, according to Lemma 11 and with  $\Pi^{\mathbb{S}} = \Pi_2$ , are equal to

$$\operatorname{span} \left\{ r_{u}, \; (\Pi_{1}C\Pi_{2}\mathbb{S}^{-1})r_{u}, \ldots, (\Pi_{1}C\Pi_{2}\mathbb{S}^{-1})^{i-1}r_{u} \right\},$$

$$\operatorname{span} \left\{ \mathbb{S}^{-H}\Pi_{2}^{H}r_{v}, \; (\mathbb{S}^{-H}\Pi_{2}^{H}C^{H}\Pi_{1}^{H})\mathbb{S}^{-H}\Pi_{2}^{H}r_{v}, \ldots \right.$$

$$\ldots, (\mathbb{S}^{-H}\Pi_{2}^{H}C^{H}\Pi_{1}^{H})^{i-1}\mathbb{S}^{-H}\Pi_{2}^{H}r_{v} \right\},$$

respectively. Let the columns of  $W^{(i)}$  and  $Z^{(i)}$  span the biorthonormal bases for these two spaces generated by the Petrov-Galerkin method. It holds  $Mu \perp Z^{(i)}$  and  $v \perp W^{(i)}$  such that

$$u^H M^H Z^{(i)} = v^H W^{(i)} = 0, \quad \Pi_1 W^{(i)} = W^{(i)}, \ \Pi_1^H Z^{(i)} = Z^{(i)}.$$

The approximate solutions  $s^{(i)}$ ,  $t^{(i)}$  are then given by  $s^{(i)} = \Pi_2 \mathbb{S}^{-1} \tilde{s}^{(i)} = \mathbb{S}^{-1} \Pi_1 \tilde{s}^{(i)}$ ,  $\tilde{s}^{(i)} = W^{(i)} w$ ,  $t^{(i)} = Z^{(i)} z$ , where

$$\begin{split} w &= -(T^{(i)})^{-1}(Z^{(i)})^H r_u = -(T^{(i)})^{-1}(Z^{(i)})^H A u, \\ z &= -(T^{(i)})^{-H}(W^{(i)})^H \mathbb{S}^{-H} \Pi_2^H r_v = -(T^{(i)})^{-H}(W^{(i)})^H \mathbb{S}^{-H} A^H v, \end{split}$$

with  $T^{(i)}:=(Z^{(i)})^HC\mathbb{S}^{-1}W^{(i)}$ . There we have used that  $\mathbb{S}^{-H}\Pi_2^Hr_v=\Pi_1^H(\mathbb{S}^{-H}A^Hv-\overline{\theta}\mathbb{S}^{-H}M^Hv)=\Pi_1^H(\mathbb{S}^{-H}A^Hv-\overline{\theta}v)$  and  $\Pi_1^Hv=0$ . Consequently,

$$\begin{split} s^{(i)} &= -\mathbb{S}^{-1} W^{(i)} (T^{(i)})^{-1} (Z^{(i)})^H A u, \\ t^{(i)} &= -Z^{(i)} (T^{(i)})^{-H} (W^{(i)})^H \mathbb{S}^{-H} A^H v. \end{split}$$

For the linear systems of TRQI we know by Lemma 11 that the columns of  $[Mu, W^{(i)}]$  and  $[v, Z^{(i)}]$  are biorthonormal bases of

$$\operatorname{span}\left\{Mu, C\mathbb{S}^{-1}Mu, \dots, (C\mathbb{S}^{-1})^{i}Mu\right\},$$
$$\operatorname{span}\left\{\mathbb{S}^{-H}M^{H}v, \mathbb{S}^{-H}C^{H}\mathbb{S}^{-H}M^{H}v, \dots, (\mathbb{S}^{-H}C^{H})^{i}\mathbb{S}^{-H}M^{H}v\right\}.$$

The approximate solutions are then given by  $u^{(i+1)} = \mathbb{S}^{-1}\tilde{u}^{(i+1)}$ ,  $\tilde{u}^{(i+1)} = \mu_1 M u + W^{(i)} p$  and  $v^{(i+1)} = \mu_2 v + Z^{(i)} q$ , where  $\mu_1, \mu_2 \in \mathbb{C}$  and  $p, q \in \mathbb{C}^i$  are determined by

$$\hat{T}^{(i)} \begin{bmatrix} \mu_1 \\ p \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad (\hat{T}^{(i)})^H \begin{bmatrix} \mu_2 \\ q \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

with

$$\hat{T}^{(i)} = \begin{bmatrix} v^H C \mathbb{S}^{-1} M u & v^H C \mathbb{S}^{-1} W^{(i)} \\ (Z^{(i)})^H C \mathbb{S}^{-1} M u & T^{(i)} \end{bmatrix}.$$

The (1,1)-entry in  $\hat{T}^{(i)}$  is zero and p,q are hence obtained from

$$p = -\mu_1(T^{(i)})^{-1}(Z^{(i)})^H A u, \quad q = -\mu_2(T^{(i)})^{-H}(W^{(i)})^H \mathbb{S}^{-H} A^H v,$$

and hence  $u^{(i+1)} = \mu_1(s^{(i)} + \mathbb{S}^{-1}Mu)$  and  $v^{(i+1)} = \mu_2(t^{(i)} + v)$ , from which the desired result follows.

## Remark 13

Lemma 11 and Theorem 12 also reveal an equivalence of TRQI and TJD in the unpreconditioned case (P = I) for the GEP when the tuning operator

$$\mathbb{T} = I + [Mu, u] \begin{bmatrix} v^H u + 1 & -1 \\ -1 & 0 \end{bmatrix} [M^H v, v]^H, \tag{33}$$

which satisfies  $\mathbb{T}u = Mu$  and  $\mathbb{T}^Hv = M^Hv$  is used in TRQI and TJD is necessarily preconditioned by  $\Pi_1\Pi_2$  (cf. (32)). If M = I these actions are not required which immediately gives [13, Proposition 5.5.].

## Remark 14

The above theorems also hold when a fixed shift is used, i.e.,  $\theta_k \equiv \theta \ \forall k \geq 1$ , leading to an equivalence result of TII and simplified TJD.

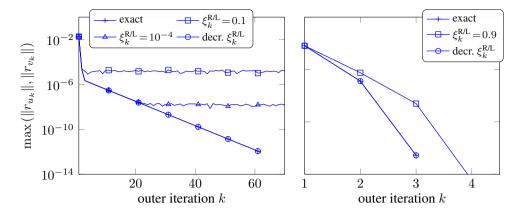


Figure 1. Convergence history of exact and inexact TII (left), TRQI (right) for the reactor example using fixed and decreasing inner tolerances. The decreasing tolerances for TII and TRQI where set via  $\xi_k^{\text{R/L}} = \min\left(0.1, 0.1 \|r_{u_k/v_k}\|\right)$  and  $\xi_k^{\text{R/L}} = \min\left(0.5, \|r_{u_k/v_k}\|\right)$ , respectively.

#### 5. NUMERICAL EXAMPLES

We run numerical experiments regarding the discussed convergence properties of TII / TRQI in Section 2, the preconditioning and tuning strategies in Section 3, and the equivalence of TRQI and simplified TJD in Section 4. All experiments were carried out using MATLAB® 7.11.0 on a compute server using 4 Intel® Xeon® @2.67 GHz CPUs with 8 cores per CPU and 1 TB RAM.

## 5.1. Convergence of inexact methods

At first we verify the convergence results of Section 2 using the nuclear reactor example from [15, Example 5.1]. The dimension of this generalized eigenvalue problem is n = 2048 such that the occurring linear systems can be solved cheaply using the MATLAB® backslash. For the inexact solves the CSBSG/LAL [35] method was employed and no preconditioning was required. We look for the eigenvalue  $\lambda = 8.0097$  and and its associated right and left eigenvectors. The shift for TII was set to  $\theta = 8$ . The initial vectors  $u_1$ ,  $v_1$  are the perturbed eigenvectors corresponding to  $\lambda$  which were generated using the eigs (A, M, 1, 8) and eigs (A', M', 1, 8) commands. The perturbation was chosen small enough such that TRQI, whose convergence strongly depends on the given initial vectors, converged to the sought eigentriple. In Figure 1 max  $(||r_{u_k}||, ||r_{v_k}||)$  is plotted versus the outer iteration number k for both methods. As predicted by Theorem 2 inexact TII stagnates for two different fixed inner accuracies ( $\xi^{R/L} = 0.1$ ,  $10^{-4}$ ). It achieves the same convergence speed as with exact solves when decreasing inner tolerances  $(\xi_k^{R/L} = \min(0.1, 0.1 ||r_{u_k/v_k}||))$  are used as proposed by Theorem 3. A similar observation can be made for inexact TRQI in the right plot, although there the difference between fixed ( $\xi^{R/L} = 0.9$ ) and decreasing inner tolerances  $(\xi_k^{\text{R/L}} = \min(0.5, ||r_{u_k/v_k}||))$  is only marginal due to the fast speed of convergence and the mild nature of the problem.

#### 5.2. Preconditioned inner solves and tuning

For investigating the performance of the inexact solves using the proposed tuned preconditioners, we use three examples which are summarized, together with the settings for TII and TRQI, in Table I.

Numer. Linear Algebra Appl. (0000)

Table I. Matrix dimension n, sought eigenvalue  $\lambda$ , shift  $\theta$ , wanted outer accuracy  $\epsilon_{\rm eig}$ , ilu drop tolerance  $\chi$ , and inner accuracies  $\xi_k^{\rm R/L}$  in inexact TII, TRQI for the examples IFISS, anemo, FDM for testing the standard and tuned preconditioners.

Ex.	n	λ	$\theta$	$\epsilon_{ m eig}$	χ	$\xi_k^{ ext{R/L}}$ TII	$\xi_k^{ ext{R/L}}$ TRQI
	l	2450.8				$0.1\min\left(1,\ r_{u_k/v_k}\ \right)$	$0.5\min\left(1,\ r_{u_k/v_k}\ \right)$
		-305.35				$0.1\min\left(1,\ r_{u_k/v_k}\ \right)$	0.01
FDM	78400	-1011.28	-1000	$10^{-9}$	0.0005	$0.5 \min \left( \xi_{k-1}^{\text{R/L}}, \ r_{u_k/v_k}\  \right)$	0.001

The IFISS example was obtained with the IFISS 3.2 package [39] by discretizing a convection-diffusion equation on  $(-1,1)^2$  by Q1 finite elements on a uniform  $256\times256$  grid. The matrices A, M are provided by the test example T-CD2. The matrices of the anemo example  $^{\ddagger}$  are obtained from a finite element discretization of the temperature flow around an anemometer (flow sensing device) [40]. In the last example, FDM, M = I and A represents a five-point stencil centered finite difference discretization on a uniform  $280 \times 280$  grid of

$$\Delta h - 10\xi_1 \frac{\partial h}{\partial \xi_1} - 1000\xi_2 \frac{\partial h}{\partial \xi_2} = 0$$
 on  $\Omega = (0, 1)^2$  for  $h = h(\xi_1, \xi_2)$ 

with homogeneous Dirichlet boundary conditions.

For all three examples the starting vectors for TRQI were constructed as in the previous example and the outer iteration was terminated when  $\max(\|r_{u_k}\|, \|r_{v_k}\|) < \epsilon_{\text{eig}}$ . The linear systems are solved separately with GMRES and also simultaneously with CSBCG. Without preconditioning the inner solvers did not converge at all or within a reasonable amount of time. The standard preconditioners P are incomplete LU decompositions of  $A - \theta M$  with a drop tolerances of  $\chi$ and  $P^H$  was chosen for the adjoint linear system. The tuned preconditioners are  $\mathbb{P}_k$ ,  $\mathbb{Q}_k$  within GMRES, and  $S_k$  within CSBCG, and are given as in Section 3. We used the M-variants which satisfy (20),(23),(29) as well as the A-variants which satisfies (21),(24). Table II gives the required outer iterations k, the total inner iterations i (i.e., matrix vector products with  $A - \theta_k M$ ) and their average number over all outer iterations, the total number of applications with P and  $P^H$ , and the consumed CPU time for these experiments. Using the tuned preconditioners leads to a decreased number of inner iterations compared to the application of the standard preconditioners in the majority of cases. This reduction is more significant for TII than for TRQI because of the significantly higher number of outer iterations such that savings regarding the runtime are more obvious for TII. With GMRES the outer iterations seemed to have problems converging for some of the used preconditioners in the anemo and FDM example. These happened especially for the M-variant of  $\mathbb{P}_k$ ,  $\mathbb{Q}_k$ . In most cases, these issues could be cured if the inner accuracies or the drop tolerances for the incomplete LU factorization were lowered a bit further. Moreover, similar numerical issues with the tuned preconditioner as reported in [23, Section 6] were observed in some of these problematic cases. For most situations where the outer iterations converged, CSBCG required more inner iterations then GMRES, but thanks to its short recurrence formulation, does so in less time. The storing and orthogonalization of the basis vectors of GMRES is more expensive than the additional iterations, and inherent matrix vector products, of the longer runs of CSBCG.

Numer. Linear Algebra Appl. (0000)

<sup>&</sup>lt;sup>‡</sup>Available at modelreduction.org.

Table II. Results for inexact TII and TRQI using standard and tuned preconditioners for the IFISS, anemo, and FDM examples. There, k and i are the required outer and total inner iterations.

Ex.	Methods	Prec.	k	i	aver.	# precs	time		
IFISS		standard	38	936	25	936	30.6		
	TII - GMRES	tuned, M	39	325	9	401	16.4		
		tuned, A	38	679	18	753	24.2		
		standard	38	1436	39	1436	29.1		
	TII - CSBCG	tuned, $M$	38	856	23	930	19.9		
		tuned, A	38	650	18	724	15.7		
		standard	4	174	58	174	5.9		
	TRQI - GMRES	tuned, $M$	4	110	37	116	3.8		
		tuned, A	4	190	63	196	5.8		
	TRQI - CSBCG	standard	4	258	86	258	5.2		
		tuned, $M$	4	228	76	234	4.6		
		tuned, A	4	194	65	200	4.0		
		standard	8	1685	241	1685	55.6		
	TII - GMRES	tuned, M	stagnation at $\max (\ r_{u_k}\ , \ r_{v_k}\ ) \approx 7.6$						
		tuned, A	10	1398	155	1416	42.3		
		standard	6	1530	306	1530	15.8		
anemo	TII - CSBCG	tuned, $M$	6	1116	223	1126	9.9		
		tuned, A	7	1120	187	1132	10.4		
	TRQI - GMRES	standard	no convergence						
		tuned, M	stagnation at max $(  r_{u_k}  ,   r_{v_k}  ) \approx 7.6$						
		tuned, A		stagnation at a	$\max\left(\ r_{u_k}\ ,\ \right)$	$r_{v_k} \ ) \approx 10^{-4}$			
	TRQI - CSBCG	standard	3	484	242	484	4.6		
		tuned, M	3	466	233	470	4.8		
		tuned, A	3	430	215	434	3.9		
FDM	TII - GMRES	standard	36	1110	32	1110	89.1		
		tuned, M	stagnation at $\max (\ r_{u_k}\ , \ r_{v_k}\ ) \approx 10^{-8}$						
		tuned, A	34	153	5	219	48.7		
	TII - CSBCG	standard	28	1060	39	1060	35.5		
		tuned, M	31	200	7	260	9.9		
		tuned, A	30	116	4	174	7.5		
		standard	3	76	38	76	5.7		
	TRQI - GMRES	tuned, $M$	no convergence						
	_	tuned, A	3	60	30	64	4.7		
		standard	3	168	84	168	5.3		
	TRQI - CSBCG	tuned, $M$	3	142	71	146	4.6		
1		tuned, A	3	152	76	156	5.1		

From this one should by no means conclude that the simultaneous solution via methods such as CSBCG is in general the most efficient way. Good results for the separate solution can also be acquired by other short recurrence methods, e.g., restarted GMRES,  $BiCGstab(\ell)$  [21] or IDR(s) [22]. In Figure 2 the inner iterations are plotted against the outer iterations for the IFISS example. The two plots on the left for inexact TII show that, as predicted by Theorem 7, the number inner iterations increases along the outer iteration when a standard preconditioners is employed. Using tuned preconditioners not only reduces the number of required inner iterations for GMRES (top left plot), but also keeps this number approximately constant after a start up time in the beginning. The effect is similar for CSBCG, although there the number of inner iterations shows a more oscillating behavior.

Although for TRQI (right plots) the reduction of the number of inner iterations is also given, this number does still increase as the outer iteration proceeds. This increase seems to be, however, smaller than for the standard preconditioner which is particularly visible in the CSBCG experiment.

Numer. Linear Algebra Appl. (0000)

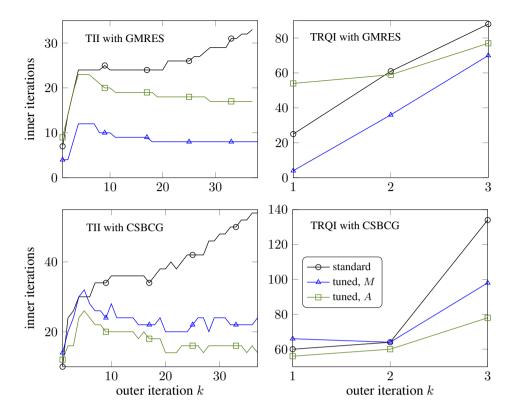


Figure 2. Progress of the required inner iterations against the outer iterations for inexact TII and TRQI using different solvers and preconditioners for the IFISS example.

Similar observation were made for the other two examples. To conclude, the inexact two-sided methods with preconditioned inner solves show a similar behavior as the one-sided methods as it was, e.g., investigated in [15, Theorem 3.5] using GMRES as inner solver.

Comparing the M-and A-variants of the tuned preconditioners in Table II and Figure 2, there is no clear hint which one of these variants performs best. For the IFISS example the M-variant yields the best results when GMRES is used but CSBCG seems to benefit more from the A-variant. In the other two examples, taking the convergence problems with GMRES into account, it appears that the A-variant should be chosen for GMRES, but there is no clear winner for both variants of  $\mathbb S$  in CSBCG. Moreover, different choices regarding the initial vectors, inner accuracies and drop tolerances could lead to different behaviors w.r.t. the M- and A-variants of the tuned preconditioners.

## 5.3. Equivalence of preconditioned RQI and BiJD

We use the IFISS example to investigate the equivalence of TRQI and simplified TJD as proposed in Section 4. The maximum number of inner iterations was restricted to 8 (7) for TRQI (TJD) and we do not stop when a certain inner accuracy is met. To compensate for rounding errors and a possible loss of (bi)orthogonality due to the short recurrence formulation of CSBCG which could spoil the results, we employ the basic two-sided Lanczos method [21, Algorithm 7.2] with rebiorthogonalization of the generated dual Krylov bases. In line with Theorem 12 and Remark 13 we

Numer. Linear Algebra Appl. (0000)

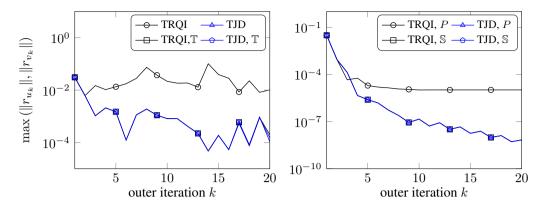


Figure 3. Convergence history of inexact TRQI and simplified TJD with 8, respectively 7, iterations of two-sided Lanczos using no preconditioner and tuning operator (left), standard and tuned preconditioner (right).

use the standard  $(P, P^H)$  and the M-variant of the tuned  $(\mathbb{S}_k)$  preconditioners, as well as the tuning operator  $\mathbb{T}_k$  from (33) and no preconditioner at all for the inner solves.

The convergence history for 20 outer iterations of TRQI, TJD is illustrated in Figure 3. In the left plot the results for P = I are shown. As predicted by Remark 13, TJD and TRQI are equivalent when the tuning operator  $\mathbb{T}_k$  is applied to the linear systems. Not surprisingly, this operator has no effect for TJD. TRQI without the application of  $\mathbb{T}_k$  shows a different behavior which would be identical to the other ones if M = I. We also see that rounding errors induce minor differences between TRQI and TJD using  $\mathbb{T}_k$  in the final outer iterations. In other similar experiments (not reported here) these differences can be larger if more inner or outer iterations are employed.

Similar observations can be made for the preconditioned case in the right plot. As proposed by Theorem 12, TJD using the standard and tuned preconditioner as well as TRQI using the tuned preconditioner give the same results. Again, only TRQI with a standard preconditioner shows a different residual history which would also be the case when M = I.

## 6. CONCLUSIONS

We have discussed, reviewed and extended the convergence analysis on exact and inexact two-sided inverse iteration and Rayleigh quotient iteration established in [13] to the generalized non-Hermitian eigenvalue problem. We showed that, if inexact solves are used with a prescribed decreasing solve tolerance then the inexact two-sided methods recover the convergence rates of the exact two-sided methods, that is linear convergence for inexact two-sided inverse iteration and locally cubic convergence for inexact two-sided Rayleigh quotient iteration.

Moreover, we extended the results on the tuned preconditioner for one-sided inverse iteration and Rayleigh quotient iteration [7, 8, 15] to the two-sided methods, where the forward and adjoint linear systems are solved simultaneously and therefore a rank-two modification of the standard preconditioner has to be used for the tuning strategy.

Finally, we showed that the equivalence of inexact two-sided Rayleigh quotient iteration and inexact two-sided Jacobi-Davidson method (without subspace expansion), which was established in [13] for the standard eigenproblem without a preconditioner (when a certain number of steps

Numer. Linear Algebra Appl. (0000)

of a Petrov-Galerkin-Krylov method is used), also holds for the generalized preconditioned eigenproblem (when a specific preconditioning strategy is applied).

Future work should validate the tuning strategies when subspace acceleration is used in TRQI and TJD as one would use in practice. Moreover, inexact, two-sided, shift-invert Arnoldi [41] can be considered and we expect to be able to use similar tuning ideas as in the one-sided case [42, 43].

#### ACKNOWLEDGEMENTS

The authors would like to thank EPSRC Network Grant EP/G01387X/1 which enabled the second author to visit the first author at the University of Bath. Moreover, we are grateful to M.E. Hochstenbach (TU Eindhoven) for various fruitful discussions.

#### REFERENCES

- Rommes J, Sleijpen GLG. Convergence of the dominant pole algorithm and Rayleigh quotient iteration. SIAM Journal on Matrix Analysis and Applications 2008; 30(1):346–363, doi:10.1137/0726037.
- Rommes J. Methods for eigenvalue problems with applications in model order reduction. PhD Thesis, Universiteit Utrecht 2007.
- 3. Parlett BN. The Rayleigh quotient iteration and some generalizations for nonnormal matrices. *Mathematics of Computation* 1974; **28**(127):679–693, doi:10.1090/S0025-5718-1974-0405823-3.
- Amiraslani A, Lancaster P. Rayleigh quotient algorithms for nonsymmetric matrix pencils. *Numerical Algorithms* 2009; 51:5–22, doi:10.1007/s11075-009-9286-z.
- 5. Smit P, Paardekooper MHC. The effects of inexact solvers in algorithms for symmetric eigenvalue problems. *Linear Algebra and its Applications* 1999; **287**:337–357, doi:10.1016/S0024-3795(98)10201-X.
- Berns-Müller J, Graham IG, Spence A. Inexact inverse iteration for symmetric matrices. *Linear Algebra and its Applications* 2006; 416(2):389–413, doi:10.1016/j.laa.2005.11.019.
- 7. Freitag MA, Spence A. Convergence of inexact inverse iteration with application to preconditioned iterative solves. *BIT Numerical Mathematics* 2007; **47**:27–44, doi:10.1007/s10543-006-0100-1.
- Freitag MA, Spence A. A tuned preconditioner for inexact inverse iteration applied to Hermitian eigenvalue problems. IMA Journal of Numerical Analysis 2008; 28(3):522–551, doi:10.1093/imanum/drm036.
- 9. Freitag MA, Spence A. Rayleigh quotient iteration and simplified Jacobi–Davidson method with preconditioned iterative solves. *Linear Algebra and its Applications* 2008; **428**(8–9):2049–2060, doi:10.1016/j.laa.2007.11.013.
- Jia Z. On convergence of the inexact Rayleigh quotient iteration with MINRES. Journal of Computational and Applied Mathematics 2012; 236(17):4276–4295, doi:10.1016/j.cam.2012.05.016.
- 11. Sleijpen GLG, Van der Vorst HA. A Jacobi-Davidson iteration method for linear eigenvalue problems. *SIAM Journal on Matrix Analysis and Applications* 1996; **17**(2):401–425, doi:10.1137/S0895479894270427.
- Simoncini V, Eldén L. Inexact Rayleigh quotient-type methods for eigenvalue computations. BIT Numerical Mathematics 2002; 42(1):159–182, doi:10.1023/A:1021930421106.
- Hochstenbach ME, Sleijpen GLG. Two-sided and alternating Jacobi–Davidson. Linear Algebra and its Applications 2003; 358(1-3):145–172, doi:10.1016/S0024-3795(01)00494-3.
- Stathopoulos A. A case for a biorthogonal Jacobi–Davidson method: Restarting and correction equation. SIAM Journal on Matrix Analysis and Applications 2002; 24(1):238–259, doi:10.1137/S0895479800373371.
- Freitag MA, Spence A, Vainikko E. Rayleigh quotient iteration and simplified Jacobi-Davidson with preconditioned iterative solves for generalised eigenvalue problems. *Technical report*, Dept. of Mathematical Sciences, University of Bath 2008.
- Robbé M, Sadkane M, Spence A. Inexact inverse subspace iteration with preconditioning applied to non-hermitian eigenvalue problems. SIAM Journal on Matrix Analysis and Applications Feb 2009; 31(1):92–113, doi: 10.1137/060673795.
- 17. Xue F, Elman HC. Fast inexact subspace iteration for generalized eigenvalue problems with spectral transformation. *Linear Algebra and its Applications* 2011; **435**(3):601–622, doi:10.1016/j.laa.2010.06.021.
- 18. Ostrowski AM. On the convergence of the Rayleigh quotient iteration for the computation of the characteristic roots and vectors. III (generalized Rayleigh quotient and characteristic roots with linear elementary divisors). Archive for Rational Mechanics and Analysis 1959; 3:325–240, doi:10.1007/BF00284184.

Copyright © 0000 John Wiley & Sons, Ltd. Prepared using nlaauth.cls Numer. Linear Algebra Appl. (0000)

- 19. Hestenes MR. Inversion of matrices by biorthogonalization and related results. *Journal of the Society for Industrial and Applied Mathematics* 1958; **6**(1):pp. 51–90, doi:10.1137/0106005.
- Barrett R, Berry M, Chan TF, Demmel J, Donato J, Dongarra J, Eijkhout V, Pozo R, Romine C, van der Vorst HA. Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods, 2nd Edition. SIAM: Philadelphia, PA, 1994.
- 21. Saad Y. Iterative Methods for Sparse Linear Systems. SIAM: Philadelphia, PA, USA, 2003.
- 22. Van Gijzen MB, Sonneveld P. Algorithm 913: An elegant IDR(s) variant that efficiently exploits biorthogonality properties. *ACM Trans. Math. Softw.* Dec 2011; **38**(1):5:1–5:19, doi:10.1145/2049662.2049667.
- Szyld D, Xue F. Efficient Preconditioned Inner Solves For Inexact Rayleigh Quotient Iteration and their Connections to the Single-Vector Jacobi–Davidson Method. SIAM Journal on Matrix Analysis and Applications 2011; 32(3):993–1018, doi:10.1137/100807922.
- 24. Freitag MA, Spence A. Convergence theory for inexact inverse iteration applied to the generalised nonsymmetric eigenproblem. *Electronic Transactions on Numerical Analysis* 2007; **28**:40–64.
- Xue F, Elman HC. Convergence analysis of iterative solvers in inexact Rayleigh quotient iteration. SIAM Journal on Matrix Analysis and Applications 2009; 31(3):877–899, doi:10.1137/080712908.
- Golub GH, Van Loan CF. Matrix Computations (3rd ed.). Johns Hopkins University Press: Baltimore, MD, USA, 1996.
- Fletcher R. Conjugate gradient methods for indefinite systems. *Numerical Analysis, Lecture Notes in Mathematics*, vol. 506, Watson G (ed.). Springer Berlin / Heidelberg, 1976; 73–89, doi:10.1007/BFb0080116.
- 28. Freund RW, Nachtigal NM. QMR: a quasi-minimal residual method for non-Hermitian linear systems. *Numerische Mathematik* 1991; **60**:315–339, doi:10.1007/BF01385726.
- Lu J, Darmofal DL. A quasi-minimal residual method for simultaneous primal-dual solutions and superconvergent functional estimates. SIAM Journal on Scientific Computing May 2002; 24(5):1693–1709, doi:10.1137/ S1064827501390625
- Golub GH, Stoll M, Wathen A. Approximation of the scattering amplitude and linear systems. *Electronic Transactions on Numerical Analysis* 2008; 31:178–203.
- 31. Freund R, Gutknecht M, Nachtigal N. An Implementation of the Look-Ahead Lanczos Algorithm for Non-Hermitian matrices. SIAM Journal on Scientific Computing 1993; 14(1):137–158, doi:10.1137/0914009.
- 32. Reichel L, Ye Q. A generalized LSQR algorithm. *Numerical Linear Algebra with Applications* 2008; **15**(7):643–660, doi:10.1002/nla.611.
- Saunders MA, Simon HD, Yip EL. Two conjugate-gradient-type methods for unsymmetric linear equations. SIAM Journal on Numerical Analysis 1988; 25(4):pp. 927–940, doi:10.1137/0725052.
- 34. Bank RE, Chan TF. A composite step bi-conjugate gradient algorithm for nonsymmetric linear systems. *Numerical Algorithms* 1994; **7**:1–16, doi:10.1007/BF02141258.
- 35. Bank RE, Chan TF. An analysis of the composite step biconjugate gradient method. *Numerische Mathematik* 1993; **66**:295–319, doi:10.1007/BF01385699.
- 36. Sleijpen GLG, Booten AGL, Fokkema DR, van der Vorst HA. Jacobi-Davidson type methods for generalized eigenproblems and polynomial eigenproblems. *BIT Numerical Mathematics* 1996; **36**(3):595–633, doi:10.1007/BF01731936.
- 37. Sleijpen GLG, Van der Vorst HA. The Jacobi–Davidson method for eigenvalue problems and its relation with accelerated inexact Newton scheme. *BIT Numerical Mathematics* 1996; **36**(3):595–633.
- Stathopoulos A, Saad Y. Restarting techniques for the (Jacobi-)Davidson symmetric eigenvalue methods. *Electronic Transactions on Numerical Analysis* 1998; 7:163–181.
- 39. Silvester D, Elman H, Ramage A. Incompressible Flow and Iterative Solver Software (IFISS) version 3.2 May 2012. http://www.manchester.ac.uk/ifiss/.
- 40. Benner P, Mehrmann V, Sorensen D. Dimension Reduction of Large-Scale Systems, Lecture Notes in Computational Science and Engineering, vol. 45. Springer-Verlag, Berlin/Heidelberg, Germany, 2005.
- 41. Ruhe A. The two-sided Arnoldi algorithm for nonsymmetric eigenvalue problems. *Matrix Pencils*, vol. 973, Kågström B, Ruhe A (eds.), Springer Berlin / Heidelberg, 1983; 104–120.
- 42. Freitag MA, Spence A. Shift-invert Arnoldi's method with preconditioned iterative solves. SIAM Journal on Matrix Analysis and Applications 2009; 31(3):942–969, doi:10.1137/080716281.
- Xue F, Elman HC. Fast inexact implicitly restarted Arnoldi method for generalized eigenvalue problems with spectral transformation. SIAM Journal on Matrix Analysis and Applications 2012; 33(2):433–459, doi:10.1137/ 100786599.

Numer. Linear Algebra Appl. (0000)