RAYLEIGH QUOTIENT ITERATION AND SIMPLIFIED JACOBI-DAVIDSON METHOD WITH PRECONDITIONED ITERATIVE SOLVES

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Abstract. We show that for the non-Hermitian eigenvalue problem simplified Jacobi-Davidson with preconditioned iterative solves is equivalent to inexact Rayleigh quotient iteration where the preconditioner is altered by a simple rank change. This extends existing equivalence results to the case of preconditioned iterative solves. Numerical experiments are shown to agree with the theory.

Key words. Eigenvalue approximation, Iterative methods, Preconditioning.

1. Introduction. Consider the problem of computing a simple, well-separated eigenvalue and corresponding eigenvector of a large, sparse, non-Hermitian matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$, that is,

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}, \quad \mathbf{x}^H\mathbf{x} = 1.$$

Many popular methods involve the inexact solution of a shifted linear system: examples are inexact inverse iteration, [6, 2, 3] inexact Rayleigh quotient iteration [11] and the Jacobi-Davidson method [7, 12]. As a practical tool, the Jacobi-Davidson method builds a subspace from which the approximate eigenvector is chosen. In this note, we shall consider only the simplified version, (also known as the Newton-Grassmann method [11]) where no use is made of previous information.

In [11] it is proved that for Hermitian matrices, simplified Jacobi-Davidson is equivalent to Rayleigh quotient iteration if no preconditioner is used in the inner solve. This equivalence is based on a Lemma from [15] which also holds for the non-Hermitian case, though no use of this fact is made in [11]. In [8] this equivalence is generalised to two-sided Jacobi-Davidson for nonnormal matrices to accelerated two-sided Rayleigh quotient iteration. However, as noted in [8] these results do not hold if a preconditioner is used to speed up the iterative solves.

In this note we extend the result of [11] to preconditioned iterative solves for non-Hermitian eigenvalue problems where we utilise the "tuning" of any standard preconditioner as introduced in [5, 4]. Specifically, we shall show in Section 2 that, assuming a Galerkin-Krylov solver is used and in exact arithmetic, the inexact Rayleigh quotient iteration with the altered preconditioner and the inexact simplified Jacobi-Davidson method with the standard preconditioner produce equivalent approximate eigenvectors. Numerical results that support the theory are presented in Section 3.

The equivalence result proved here is of interest since, in most applications, preconditioned iterative solves will be applied. Additionally, there is the possibility of further equivalence results for subspace based methods.

2. Inexact Rayleigh quotient iteration and inexact Jacobi-Davidson method. In this section we describe the inexact Rayleigh quotient algorithm and the inexact Jacobi-Davidson algorithm to find a simple eigenvalue of a large and sparse non-Hermitian matrix $\mathbf{A}$.

Let $\mathbf{x}$ be an approximate unit eigenvector and let the corresponding approximate eigenvalue be given by $\rho(\mathbf{x}) = \mathbf{x}^H\mathbf{A}\mathbf{x}$. The Rayleigh quotient iteration gives a new approximate eigenvector by normalising the solution $\mathbf{y}$ of the system

$$(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbf{y} = \mathbf{x}. \tag{2.1}$$

Alternatively, the simplified Jacobi-Davidson method produces a correction $\mathbf{s}$ to $\mathbf{x}$, which satisfies $\mathbf{s} \perp \mathbf{x}$, from the correction equation

$$(\mathbf{I} - \mathbf{x}\mathbf{x}^H)(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})(\mathbf{I} - \mathbf{x}\mathbf{x}^H)\mathbf{s} = -\mathbf{r}, \tag{2.2}$$

where

$$\mathbf{r} = (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbf{x} \tag{2.3}$$

is the current eigenvalue residual. The new eigenvector approximation is then given by the normalisation of $\mathbf{x} + \mathbf{s}$. In practice the Jacobi-Davidson approach builds up a subspace, from which an improved eigendirection is obtained, but in this paper we concentrate on the simplified version which ignores previous information. It has been shown that, if both systems (2.1) and (2.2) are solved exactly, then $\mathbf{y}$ and $\mathbf{x} + \mathbf{s}$ have the same direction (see [11, 13]). Hence, in exact arithmetic both methods produce the same sequence of eigenvector approximations. For inexact solves this property need not hold. However, Simoncini and Eldén [11] have shown that if the same Galerkin-Krylov subspace method is applied to solve (2.1) and (2.2), then there exists a constant $c \in \mathbb{C}$, such that

$$\mathbf{y}_{k+1} = c(\mathbf{x} + \mathbf{s}_k),$$

where $\mathbf{y}_{k+1}$ and $\mathbf{s}_k$ denote the approximate solution of (2.1) and (2.2) after $k + 1$ and k steps respectively. (Note that the proof of [11, Proposition 3.2] applies to non-Hermitian matrices, even thought the paper only considers Hermitian positive definite matrices). This means that if $k + 1$ steps of a Galerkin-Krylov method were applied to (2.1) and k steps of the same Galerkin-Krylov method were applied to (2.2) then the resulting approximate eigenvectors are the same. The results in Figure 3.1 in the next section support this equivalence. Hochstenbach and Sleijpen [8] have extended these results to the case of a two-sided Rayleigh quotient iteration and a two-sided Jacobi-Davidson, when BiCG is used as the iterative solver. However, both papers also observe that these results do not hold if preconditioned Krylov methods are used with the inexact iterative solve. In this note, we extend these results to the case of preconditioned solves, where a special "tuned" preconditioner is applied to the Rayleigh quotient iteration.

2.1. Preconditioned Rayleigh-quotient iteration and Jacobi-Davidson. First, we give an account of how both inexact Rayleigh quotient iteration and inexact simplified Jacobi-Davidson are preconditioned. We restrict ourselves to right-preconditioned methods here, although the results extend to left-preconditioned methods. (Note that in order to preserve symmetry for Hermitian eigenproblems a split preconditioner may be used for the inner iteration. However, a split preconditioner may be transformed to either a left- or a right-preconditioner using a different inner product, (see [10]).)

Let $\mathbf{P}$ be any preconditioner for $\mathbf{A} - \rho(\mathbf{x})\mathbf{I}$. Then right-preconditioned (2.1) has the form

$$(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbf{P}^{-1}\tilde{\mathbf{y}} = \mathbf{x}, \quad \text{with} \quad \mathbf{y} = \mathbf{P}^{-1}\tilde{\mathbf{y}}. \tag{2.4}$$

Hence, for a Krylov method applied to (2.4) the solution $\tilde{\mathbf{y}}$ lies in the Krylov subspace

$$\text{span}\{\mathbf{x}, (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbf{P}^{-1}\mathbf{x}, ((\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbf{P}^{-1})^2\mathbf{x}, \ldots\}. \tag{2.5}$$

The preconditioning of an iterative solver for the approximate solution of (2.2) has to be discussed more carefully. The preconditioner $\mathbf{P}$ is restricted to the subspace orthogonal to $\mathbf{x}$, so that,

$$\tilde{\mathbf{P}} := (\mathbf{I} - \mathbf{x}\mathbf{x}^H)\mathbf{P}(\mathbf{I} - \mathbf{x}\mathbf{x}^H), \tag{2.6}$$

is used instead of $\mathbf{P}$. Clearly $\tilde{\mathbf{P}}$ is singular on $\mathbb{C}^n$, but is assumed to be nonsingular on the subspace $\mathbb{C}^n_\perp := \{\mathbf{v} \in \mathbb{C}^n : \mathbf{v} \perp \mathbf{x}\}$. Let $\tilde{\mathbf{P}}^\dagger$ denote the pseudo-inverse of $\tilde{\mathbf{P}}$. Right preconditioned (2.2) then has the form

$$(\mathbf{I} - \mathbf{x}\mathbf{x}^H)(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})(\mathbf{I} - \mathbf{x}\mathbf{x}^H)\tilde{\mathbf{P}}^\dagger\tilde{\mathbf{s}} = -\mathbf{r}, \quad \text{with} \quad \mathbf{s} = \tilde{\mathbf{P}}^\dagger\tilde{\mathbf{s}}. \tag{2.7}$$

The solution of (2.7) using a Krylov solver requires the action of the matrix $(\mathbf{I} - \mathbf{x}\mathbf{x}^H)(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})(\mathbf{I} - \mathbf{x}\mathbf{x}^H)\tilde{\mathbf{P}}^\dagger$. First we need the efficient implementation of $\tilde{\mathbf{P}}^\dagger\tilde{\mathbf{s}}$ for some $\tilde{\mathbf{s}} \in \mathbb{C}^n_\perp$. This is discussed in [1, 14] as we now describe. Consider $\mathbf{v} = \tilde{\mathbf{P}}^\dagger\tilde{\mathbf{s}}$, where $\mathbf{v}$ and $\tilde{\mathbf{s}}$ in $\mathbb{C}^n_\perp$. Then $\tilde{\mathbf{P}}\mathbf{v} = \tilde{\mathbf{s}}$, and using (2.6) we have

$$(\mathbf{I} - \mathbf{x}\mathbf{x}^H)\mathbf{P}\mathbf{v} = \tilde{\mathbf{s}}$$
$$\mathbf{P}\mathbf{v} - \mathbf{x}\mathbf{x}^H\mathbf{P}\mathbf{v} = \tilde{\mathbf{s}}$$
$$\mathbf{v} - \mathbf{P}^{-1}\mathbf{x}\mathbf{x}^H\mathbf{P}\mathbf{v} = \mathbf{P}^{-1}\tilde{\mathbf{s}}.$$

Hence with $\mathbf{v} \perp \mathbf{x}$ we obtain

$$\mathbf{v} = \left(\mathbf{I} - \frac{\mathbf{P}^{-1}\mathbf{x}\mathbf{x}^H}{\mathbf{x}^H\mathbf{P}^{-1}\mathbf{x}}\right)\mathbf{P}^{-1}\tilde{\mathbf{s}}. \tag{2.8}$$

If $\mathbf{t} = (\mathbf{I} - \mathbf{x}\mathbf{x}^H)(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})(\mathbf{I} - \mathbf{x}\mathbf{x}^H)\tilde{\mathbf{P}}^\dagger\tilde{\mathbf{s}}$, that is $\mathbf{t}$ denotes the action of $(\mathbf{I} - \mathbf{x}\mathbf{x}^H)(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})(\mathbf{I} - \mathbf{x}\mathbf{x}^H)\tilde{\mathbf{P}}^\dagger$ on the vector $\tilde{\mathbf{s}}$, we have

$$\mathbf{t} = (\mathbf{I} - \mathbf{x}\mathbf{x}^H)(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbf{v}.$$

So with $\tilde{\mathbf{s}}$ denoting the approximate solution of the preconditioned linear system in (2.7), $\mathbf{s} = \tilde{\mathbf{P}}^\dagger\tilde{\mathbf{s}}$ is recovered using (2.8). If we introduce the projectors

$$\Pi_1 = \mathbf{I} - \mathbf{x}\mathbf{x}^H \quad \text{and} \quad \Pi_2^{\mathbf{P}} = \left(\mathbf{I} - \frac{\mathbf{P}^{-1}\mathbf{x}\mathbf{x}^H}{\mathbf{x}^H\mathbf{P}^{-1}\mathbf{x}}\right), \tag{2.9}$$

a Krylov solver applied to (2.7) generates the subspace

$$\text{span}\{\mathbf{r}, \Pi_1(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_2^{\mathbf{P}}\mathbf{P}^{-1}\mathbf{r}, (\Pi_1(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_2^{\mathbf{P}}\mathbf{P}^{-1})^2\mathbf{r}, \ldots\}. \tag{2.10}$$

Clearly, the subspaces (2.5) and (2.10) are not the same and the numerical results shown in Figure 3.2, where the corresponding residuals are plotted, confirm that there is no equivalence between the eigenvector approximations obtained from (2.4) and (2.7). However, we shall show that if a small modification is made to the standard preconditioner $\mathbf{P}$ in (2.4) then we obtain an equivalence between the inexact versions of Rayleigh quotient iteration and the simplified Jacobi-Davidson method.

2.2. Equivalence between preconditioned Jacobi-Davidson and Rayleigh quotient iteration. In [5] and [4] a "tuned" preconditioner, $\mathbb{P}$, was introduced. $\mathbb{P}$ is merely a rank-one change to $\mathbf{P}$, a standard preconditioner and has the additional property

$$\mathbb{P}\mathbf{x} = \mathbf{A}\mathbf{x}. \tag{2.11}$$

It is shown in [4] that for Hermitian problems the use of $\mathbb{P}$ instead of $\mathbf{P}$ leads to an overall reduction of the number of matrix-vector multiplications within the inner solve, since the right hand side of the system in (2.4) with $\mathbf{P}$ replaced by $\mathbb{P}$ is approximately in the kernel of the system matrix.

In this note we employ a slightly different choice for $\mathbb{P}$. Specifically, we ask that

$$\mathbb{P}\mathbf{x} = \mathbf{x}, \qquad (2.12)$$

and in this paper we will achieve this by making the choice

$$\mathbb{P} = \mathbf{P} + (\mathbf{I} - \mathbf{P})\mathbf{x}\mathbf{x}^H. \qquad (2.13)$$

An immediate consequence of (2.12) is that for the projector $\Pi_2^{\mathbb{P}}$ in (2.9) we have

$$\Pi_2^{\mathbb{P}} = \Pi_1. \qquad (2.14)$$

Using the Sherman-Morrison formula and assuming $\mathbf{x}^H \mathbf{P}^{-1} \mathbf{x} \neq 0$ we obtain

$$\mathbb{P}^{-1} = \mathbf{P}^{-1} - \frac{(\mathbf{P}^{-1}\mathbf{x} - \mathbf{x})\mathbf{x}^H \mathbf{P}^{-1}}{\mathbf{x}^H \mathbf{P}^{-1} \mathbf{x}}. \qquad (2.15)$$

The application of $\mathbb{P}^{-1}$ involves only one extra solve per outer iteration, since $\mathbf{P}^{-1}\mathbf{x}$ has to be computed only once in the iteration process.

The following Lemma is a generalisation of [15, Lemma 4.1] for preconditioned iterative solves.

LEMMA 2.1. *Let* $\mathbf{x}$ *be a unit-norm vector and let* $\rho(\mathbf{x}) = \mathbf{x}^H \mathbf{A}\mathbf{x}$. *Let* $\mathbf{P}$ *be a preconditioner for* $\mathbf{A}$ *and let* Π_1 *be defined as in (2.9). Let the tuned preconditioner* $\mathbb{P}$ *satisfy (2.12) and let* $\mathbf{r} = \mathbf{A}\mathbf{x} - \rho(\mathbf{x})\mathbf{x} = \Pi_1 \mathbf{r}$. *Introduce*

$$\mathcal{K}_k = span\{\mathbf{x}, \mathbf{A}\mathbb{P}^{-1}\mathbf{x}, (\mathbf{A}\mathbb{P}^{-1})^2\mathbf{x}, \ldots, (\mathbf{A}\mathbb{P}^{-1})^k\mathbf{x}\}$$

and

$$\mathcal{L}_k = span\{\mathbf{x}, \mathbf{r}, \Pi_1 \mathbf{A}\Pi_2^{\mathbb{P}}\mathbb{P}^{-1}\mathbf{r}, \ldots, (\Pi_1 \mathbf{A}\Pi_2^{\mathbb{P}}\mathbb{P}^{-1})^{k-1}\mathbf{r}\}.$$

Then, for every $k \geq 1$, *we have* $\mathcal{L}_k = \mathcal{K}_k$.

Proof. As noted in (2.14), $\Pi_2^{\mathbb{P}} = \Pi_1$, and

$$\Pi_2^{\mathbb{P}}\mathbb{P}^{-1} = \Pi_1 \mathbb{P}^{-1} = \mathbb{P}^{-1}(\mathbf{I} - \mathbf{x}\mathbf{x}^H \mathbb{P}^{-1}). \qquad (2.16)$$

In order to prove the equivalence between $\mathcal{L}_k$ and $\mathcal{K}_k$ in the non-Hermitian case we use induction over k. Note that by construction $\mathcal{K}_k$ and $\mathcal{L}_k$ are $k + 1$-dimensional subspaces. Clearly $\mathcal{L}_0 = \mathcal{K}_0$ and since $\mathbf{A}\mathbb{P}^{-1}\mathbf{x} = \mathbf{A}\mathbf{x}$ we also have $\mathcal{L}_1 = \mathcal{K}_1$. Assume that $\mathcal{L}_i = \mathcal{K}_i$ for $i < k$.

For $\mathbf{z} \in \mathcal{L}_k$, there exists a $\mathbf{u}_1 \in \mathcal{L}_{k-1} = \mathcal{K}_{k-1}$ and $\gamma \in \mathbb{C}$ such that

$$\mathbf{z} = \mathbf{u}_1 + \gamma \left(\Pi_1 \mathbf{A}\mathbb{P}^{-1}(\mathbf{I} - \mathbf{x}\mathbf{x}^H \mathbb{P}^{-1})\right)^{k-1}\mathbf{r}$$
$$= \mathbf{u}_1 + \Pi_1 \mathbf{A}\mathbb{P}^{-1}(\mathbf{I} - \mathbf{x}\mathbf{x}^H \mathbb{P}^{-1})\mathbf{u}_2,$$

where $\mathbf{u}_2 = \gamma \left(\Pi_1 \mathbf{A}\mathbb{P}^{-1}(\mathbf{I} - \mathbf{x}\mathbf{x}^H \mathbb{P}^{-1})\right)^{k-2}\mathbf{r} \in \mathcal{L}_{k-1} = \mathcal{K}_{k-1}$. Then we obtain

$$\mathbf{z} = \mathbf{u}_1 + (\mathbf{I} - \mathbf{x}\mathbf{x}^H)\mathbf{A}\mathbb{P}^{-1}\left(\mathbf{u}_2 - \mathbf{x}\mathbf{x}^H \mathbb{P}^{-1}\mathbf{u}_2\right)$$
$$= \mathbf{u}_1 + \mathbf{A}\mathbb{P}^{-1}\mathbf{u}_2 - \mathbf{x}^H \mathbf{A}\mathbb{P}^{-1}\mathbf{u}_2\mathbf{x} - \mathbf{x}^H \mathbb{P}^{-1}\mathbf{u}_2\mathbf{A}\mathbb{P}^{-1}\mathbf{x} + \mathbf{x}^H \mathbf{A}\mathbb{P}^{-1}\mathbf{x}\mathbf{x}^H \mathbb{P}^{-1}\mathbf{u}_2\mathbf{x}.$$

We have $\mathbf{u}_1 \in \mathcal{K}_{k-1}$, $\mathbf{x} \in \mathcal{K}_1$, $\mathbf{A}\mathbb{P}^{-1}\mathbf{x} \in \mathcal{K}_2$ and, by the induction hypothesis $\mathbf{A}\mathbb{P}^{-1}\mathbf{u}_2 \in \mathcal{K}_k$. Thus $\mathbf{z} \in \mathcal{K}_k$ and $\mathcal{L}_k \subseteq \mathcal{K}_k$. Finally, if $\mathcal{L}_k$ is of full rank, then its dimension is $k + 1$, the same as $\mathcal{K}_k$ and hence the two spaces must be equal and the lemma is proved. If $\mathcal{L}_k$ is not of full dimension, then let i be the largest index such that $\mathcal{L}_i$ is full rank, then $\mathcal{L}_{i+1} = \mathcal{L}_i = \mathcal{K}_i$. Now let $\mathbf{u}_3 \in \mathcal{K}_i$, then, we deduce that $\Pi_1 \mathbf{A}\mathbb{P}^{-1} \left(\mathbf{I} - \mathbf{x}\mathbf{x}^H \mathbb{P}^{-1} \right) \mathbf{u}_3 \in \mathcal{K}_i$. Using similar equations to the ones displayed above we obtain that $\mathbf{A}\mathbb{P}^{-1}\mathbf{u}_3 \in \mathcal{K}_i$, so that $\mathcal{K}_{i+1} = \mathcal{K}_i$. By induction we have $\mathcal{L}_k = \mathcal{L}_i = \mathcal{K}_i = \mathcal{K}_k$ for all $k \geq i$, which completes the proof. $\square$

REMARK 2.1. *We note that for a Hermitian preconditioner the Lemma is just a Corollary of [15, Lemma 4.1], since, if the tuned $\mathbb{P}$ satisfies (2.12) and is also constructed to be Hermitian then $\mathbb{P}^{-1}$ commutes with Π_1, and the equivalence of $\mathcal{L}_k$ and $\mathcal{K}_k$ is a corollary of [15, Lemma 4.1] applied to $\mathbf{A}\mathbb{P}^{-1}$.*

However, as we now show, a wider result is possible, in that, there is an equivalence between $\mathcal{L}_k$ and the subspace built by the Jacobi-Davidson method using the standard preconditioner, rather than the tuned preconditioner.

LEMMA 2.2. *Let the assumptions of Lemma 2.1 hold. With $\mathbb{P}$ given by (2.13),*

$$\mathcal{L}_k = span\{\mathbf{x}, \mathbf{r}, \Pi_1 \mathbf{A}\Pi_2^{\mathbb{P}}\mathbb{P}^{-1}\mathbf{r}, \dots, (\Pi_1 \mathbf{A}\Pi_2^{\mathbb{P}}\mathbb{P}^{-1})^{k-1}\mathbf{r}\},$$

and

$$\mathcal{M}_k = span\{\mathbf{x}, \mathbf{r}, \Pi_1 \mathbf{A}\Pi_2^{\mathbf{P}}\mathbf{P}^{-1}\mathbf{r}, \dots, (\Pi_1 \mathbf{A}\Pi_2^{\mathbf{P}}\mathbf{P}^{-1})^{k-1}\mathbf{r}\},$$

we have $\mathcal{L}_k = \mathcal{M}_k$ for every $k > 1$.

Proof. In order to prove this equivalence it is sufficient to show that

$$\Pi_2^{\mathbb{P}}\mathbb{P}^{-1} = \Pi_2^{\mathbf{P}}\mathbf{P}^{-1}.$$

With (2.15) we have

$$\Pi_2^{\mathbb{P}}\mathbb{P}^{-1} = \Pi_1 \mathbb{P}^{-1} = \mathbb{P}^{-1} - \mathbf{x}\mathbf{x}^H \mathbb{P}^{-1}$$

$$= \mathbf{P}^{-1} - \frac{(\mathbf{P}^{-1}\mathbf{x} - \mathbf{x})\mathbf{x}^H \mathbf{P}^{-1}}{\mathbf{x}^H \mathbf{P}^{-1}\mathbf{x}} - \mathbf{x}\mathbf{x}^H \left(\mathbf{P}^{-1} - \frac{(\mathbf{P}^{-1}\mathbf{x} - \mathbf{x})\mathbf{x}^H \mathbf{P}^{-1}}{\mathbf{x}^H \mathbf{P}^{-1}\mathbf{x}} \right)$$

$$= \mathbf{P}^{-1} - \frac{\mathbf{P}^{-1}\mathbf{x}\mathbf{x}^H \mathbf{P}^{-1}}{\mathbf{x}^H \mathbf{P}^{-1}\mathbf{x}}$$

and hence

$$\Pi_2^{\mathbb{P}}\mathbb{P}^{-1} = \left(\mathbf{I} - \frac{\mathbf{P}^{-1}\mathbf{x}\mathbf{x}^H}{\mathbf{x}^H \mathbf{P}^{-1}\mathbf{x}} \right) \mathbf{P}^{-1} = \Pi_2^{\mathbf{P}}\mathbf{P}^{-1}.$$

which gives the required result. $\square$

Combining Lemma 2.1 and Lemma 2.2 we have that $\mathcal{K}_k = \mathcal{L}_k = \mathcal{M}_k$ for every $k > 1$. Note, that the space $\mathcal{K}_k := \mathcal{K}_k(\mathbf{A}\mathbb{P}^{-1}, \mathbf{x})$ is a Krylov subspace. A Galerkin-Krylov method to solve the right preconditioned system $\mathbf{A}\mathbb{P}^{-1}\tilde{\mathbf{y}} = \mathbf{x}$, constructs an approximate solution $\tilde{\mathbf{y}}_k \in \mathcal{K}_k(\mathbf{A}\mathbb{P}^{-1}, \mathbf{x})$ such that the residual $\mathbf{x} - \mathbf{A}\mathbb{P}^{-1}\tilde{\mathbf{y}}_k$ is orthogonal to the Krylov subspace $\mathcal{K}_k(\mathbf{A}\mathbb{P}^{-1}, \mathbf{x})$, assuming the starting guess is zero. An example of such a method is the preconditioned conjugate gradient method (for symmetric systems) or preconditioned FOM (for nonsymmetric linear systems), see [10]. Note that Lemma 2.1 and Lemma 2.2 also hold for shifted systems $\mathbf{A} - \sigma\mathbf{I}$ for any $\sigma \in \mathbb{C}$, by simply replacing $\mathbf{A}$ by $\mathbf{A} - \sigma\mathbf{I}$ in Lemmata 2.1 and 2.2. The next theorem, which

is the main result of this paper, is an extension of [11, Proposition 3.2] and will make use of Lemma 2.1 and Lemma 2.2 applied to shifted systems.

THEOREM 2.3. *Let the unit vector* $\mathbf{x}$ *be an approximate eigenvector of the non-Hermitian matrix* $\mathbf{A}$ *and set* $\rho(\mathbf{x}) = \mathbf{x}^H\mathbf{A}\mathbf{x}$. *Let the assumptions of Lemma 2.1 hold and let* $\mathbf{y}_{k+1}^{RQ}$ *and* $\mathbf{s}_k^{JD}$ *be the approximate solutions to*

$$(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\tilde{\mathbf{y}} = \mathbf{x}, \quad with \quad \mathbf{y} = \mathbb{P}^{-1}\tilde{\mathbf{y}}, \tag{2.17}$$

and

$$(\mathbf{I} - \mathbf{x}\mathbf{x}^H)(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})(\mathbf{I} - \mathbf{x}\mathbf{x}^H)\tilde{\mathbf{P}}^\dagger\tilde{\mathbf{s}} = -\mathbf{r}, \quad with \quad \mathbf{s} = \tilde{\mathbf{P}}^\dagger\tilde{\mathbf{s}}, \tag{2.18}$$

respectively, obtained by $k + 1$ *(k, respectively) steps of the same Galerkin-Krylov method with starting vector zero. Then there exists a constant* $c \in \mathbb{C}$ *such that*

$$\mathbf{y}_{k+1}^{RQ} = c(\mathbf{x} + \mathbf{s}_k^{JD}). \tag{2.19}$$

Proof. The proof consists of two parts. First we compute the solution $\mathbf{s}_k^{JD}$ to (2.18) and then the solution $\mathbf{y}_{k+1}^{RQ}$ to (2.17) and then we compare them.

(a) The solution $\mathbf{s}_k^{JD}$ to (2.18).

Let $\mathbf{r} = (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbf{x}$. The Krylov subspace for the solution $\tilde{\mathbf{s}}_k^{JD}$ of (2.18) is given by

$$\mathrm{span}\{\mathbf{r}, \Pi_1(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_2^{\mathbf{P}}\mathbf{P}^{-1}\mathbf{r}, \ldots, (\Pi_1(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_2^{\mathbf{P}}\mathbf{P}^{-1})^{k-1}\mathbf{r}\}.$$

which, by Lemma 2.2 (with $\mathbf{A}$ replaced by $\mathbf{A} - \rho(\mathbf{x})\mathbf{I}$ and $\Pi_2^{\mathbb{P}} = \Pi_1$ is equal to

$$\mathrm{span}\{\mathbf{r}, \Pi_1(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_1\mathbb{P}^{-1}\mathbf{r}, \ldots, (\Pi_1(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_1\mathbb{P}^{-1})^{k-1}\mathbf{r}\}.$$

Let $\mathbf{V}_k$ be an orthogonal basis of this subspace. Note that $\mathbf{x} \perp \mathbf{V}_k$, so that $\mathbf{V}_k^H\mathbf{x} = 0$ and $\mathbf{V}_k^H\Pi_1 = \mathbf{V}_k^H$. Then the Galerkin-Krylov solution is given by $\tilde{\mathbf{s}}_k^{JD} = \mathbf{V}_k\mathbf{w}^{JD}$, with $\mathbf{w}^{JD} \in \mathbb{C}^k$, and where the Galerkin condition imposes

$$\mathbf{V}_k^H\Pi_1(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_1\mathbb{P}^{-1}\mathbf{V}_k\mathbf{w}^{JD} = -\mathbf{V}_k^H\mathbf{r},$$

or $\mathbf{V}_k^H(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_1\mathbb{P}^{-1}\mathbf{V}_k\mathbf{w}^{JD} = -\mathbf{V}_k^H\mathbf{A}\mathbf{x}$. Thus

$$\mathbf{w}^{JD} = -(\mathbf{V}_k^H(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_1\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x},$$

and hence $\tilde{\mathbf{s}}_k^{JD} = -\mathbf{V}_k(\mathbf{V}_k^H(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_1\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x}$. Using (2.8), with $\mathbb{P}$ replacing $\mathbf{P}$, and $\Pi_2^{\mathbb{P}} = \Pi_1$ we obtain

$$\mathbf{s}_k^{JD} = -\Pi_1\mathbb{P}^{-1}\mathbf{V}_k(\mathbf{V}_k^H(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\Pi_1\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x} \tag{2.20}$$

as an approximate Galerkin solution to (2.18) after k steps of the method. We can rewrite $\mathbf{s}_k^{JD}$ in the following way. Using the definition of Π_1 we have

$$\mathbf{w}^{JD} = -(\mathbf{V}_k^H(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k - \mathbf{V}_k^H\mathbf{A}\mathbf{x}\mathbf{x}^H\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x},$$

and using the Sherman-Morrison formula we have

$$\mathbf{w}^{JD} = -\mathbf{S}_k^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x}\left(1 + \frac{\mathbf{x}^H\mathbb{P}^{-1}\mathbf{V}_k\mathbf{S}_k^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x}}{1 - \mathbf{x}^H\mathbb{P}^{-1}\mathbf{V}_k\mathbf{S}_k^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x}}\right),$$

where $\mathbf{S}_k = \mathbf{V}_k^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k$. Then, with $\mathbf{s}_k^{JD}$ from (2.20) we obtain

$$\mathbf{s}_k^{JD} = -\Pi_1 \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x} \left(1 + \frac{\mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}}{1 - \mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}} \right).$$

Using again the definition of Π_1 we get

$$\mathbf{s}_k^{JD} = -\mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x} \left(1 + \frac{\mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}}{1 - \mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}} \right)$$

$$+ \mathbf{x}\mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x} \left(1 + \frac{\mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}}{1 - \mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}} \right)$$

$$= -\mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x} \left(1 + \frac{\mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}}{1 - \mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}} \right)$$

$$+ \mathbf{x} \left(\mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x} + \frac{(\mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x})^2}{1 - \mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}} \right)$$

$$= -\mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x} - \left(\mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x} - \mathbf{x} \right)\xi,$$

where ξ is a constant given by

$$\xi = \frac{\mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}}{1 - \mathbf{x}^H \mathbb{P}^{-1}\mathbf{V}_k \mathbf{S}_k^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x}}. \tag{2.21}$$

Finally, using 2.12 and the definition of $\mathbf{S}_k$ we obtain

$$\mathbf{s}_k^{JD} = -\mathbb{P}^{-1}\mathbf{V}_k (\mathbf{V}_k^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x} -$$
$$\left(\mathbb{P}^{-1}\mathbf{V}_k (\mathbf{V}_k^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H \mathbf{A}\mathbf{x} - \mathbf{x} \right)\xi. \tag{2.22}$$

(b) The solution $\mathbf{y}_{k+1}^{RQ}$ to (2.17).

Consider now the solution of (2.17). According to Lemma 2.1 (with $\mathbf{A}$ replaced by $\mathbf{A} - \rho(\mathbf{x})\mathbf{I}$), the columns of $[\mathbf{x}, \mathbf{V}_k]$ form an orthogonal basis of

$$\text{span}\{\mathbf{x}, (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{x}, ((\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1})^2\mathbf{x}, \ldots, ((\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1})^k\mathbf{x}\},$$

which is the same space as generated by the Krylov subspace method applied to (2.4). Then the approximate solution to (2.4) is given by $\tilde{\mathbf{y}}_{k+1}^{RQ} = h\mathbf{x} + \mathbf{V}_k \mathbf{h}$, where $h \in \mathbb{C}$ and $\mathbf{h} \in \mathbb{C}^k$. The values of h and $\mathbf{h}$ are determined by imposing the Galerkin condition on (2.4):

$$\begin{bmatrix} \mathbf{x}^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{x} & \mathbf{x}^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k \\ \mathbf{V}_k^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{x} & \mathbf{V}_k^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k \end{bmatrix} \begin{bmatrix} h \\ \mathbf{h} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

Note that $\mathbf{x}^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{x} = \mathbf{x}^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbf{x} = 0$. From the second row we obtain

$$\mathbf{V}_k^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{x}h + \mathbf{V}_k^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k \mathbf{h} = 0,$$

and hence

$$\mathbf{V}_k^H \mathbf{A}\mathbf{x}h + \mathbf{V}_k^H (\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k \mathbf{h} = 0,$$

where we have used $\mathbb{P}\mathbf{x} = \mathbf{x}$ and $\mathbf{V}_k^H \mathbf{x} = 0$. Therefore we have

$$\mathbf{h} = -(\mathbf{V}_k^H(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x}h,$$

and thus from $\tilde{\mathbf{y}}_{k+1}^{RQ} = h\mathbf{x} + \mathbf{V}_k\mathbf{h}$

$$\tilde{\mathbf{y}}_{k+1}^{RQ} = h(\mathbf{x} - \mathbf{V}_k(\mathbf{V}_k^H(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x}).$$

Finally from (2.4) with the tuned preconditioner $\mathbb{P}$ we obtain

$$\mathbf{y}_{k+1}^{RQ} = h(\mathbf{x} - \mathbb{P}^{-1}\mathbf{V}_k(\mathbf{V}_k^H(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x}), \qquad (2.23)$$

where we have used $\mathbb{P}^{-1}\mathbf{x} = \mathbf{x}$.

Combining both the results of (a) and (b), (2.23) and (2.22) and setting

$$\mathbf{t}_k := \mathbb{P}^{-1}\mathbf{V}_k(\mathbf{V}_k^H(\mathbf{A} - \rho(\mathbf{x})\mathbf{I})\mathbb{P}^{-1}\mathbf{V}_k)^{-1}\mathbf{V}_k^H\mathbf{A}\mathbf{x}$$

we obtain $\mathbf{y}_{k+1}^{RQ} = h(\mathbf{x} - \mathbf{t}_k)$ and $\mathbf{s}_k^{JD} = -\mathbf{t}_k - (\mathbf{t}_k - \mathbf{x})\xi$. Rewriting these equations and using $\xi \neq -1$ yields

$$\mathbf{y}_{k+1}^{RQ} = \frac{h}{1+\xi}(\mathbf{x} + \mathbf{s}_k^{JD}).$$

$\xi \neq -1$ follows straight from (2.21). The required result follows with $c = \dfrac{h}{1+\xi}$. $\square$

Note that for a Hermitian tuned preconditioner, the result follows straight from (2.23) using (2.20) and $\mathbb{P}^H = \mathbb{P}$ as well as $\mathbf{V}_k^H\Pi_1 = \mathbf{V}_k^H$ such that $\Pi_1\mathbb{P}^{-1}\mathbf{V}_k = \mathbb{P}\Pi_1\mathbf{V}_k = \mathbb{P}\mathbf{V}_k$.

Theorem 2.3 shows that, in exact arithmetic, solving (2.4) and (2.7) with the same preconditioned Galerkin-Krylov method where in (2.4) the tuned preconditioner and in (2.7) the standard preconditioner is used, are equivalent. Note that Rayleigh quotient iteration uses one step more than Jacobi-Davidson ($k+1$ instead of k) because simplified Jacobi-Davidson already uses a matrix-vector multiplication to compute the residual.

REMARK 2.2. *Theorem 2.3 also holds if a fixed shift σ is used for both methods (2.4) and (2.7) instead of a Rayleigh quotient shift $\rho(\mathbf{x})$.*

3. Numerical examples. In this section we illustrate the equivalence in Theorem 2.3 by two numerical examples; one for a fixed shift and one for Rayleigh quotient shifts. In both examples the iterative solver is the Full Orthogonalisation Method (FOM).

EXAMPLE 3.1 (Problem from the Matrix Market library [9]). *Consider matrix* `sherman5.mtx` *from the Matrix Market library [9]. It is a real nonsymmetric matrix of size 3312×3312 with 20793 nonzero entries. We seek the eigenvector belonging to the smallest eigenvalue $4.692e-02$. We use a fixed shift $\sigma = 0$ and an initial starting guess of all ones and compare inexact inverse iteration with simplified inexact Jacobi-Davidson method and investigate the following approaches to preconditioning:*
(a) no preconditioner is used for the inner iteration.
(b) a standard preconditioner is used for the inner iteration.
(c) a tuned preconditioner with $\mathbb{P}\mathbf{x} = \mathbf{x}$ is used for the inner iteration.

We use FOM as a solver with incomplete LU factorisation with drop tolerance 0.005 as preconditioner where appropriate. Furthermore, we carry out exactly 4 steps of preconditioned FOM for the inner solve in the simplified Jacobi-Davidson method, while precisely 5 steps of preconditioned FOM are taken for each inner solve in the inexact inverse iteration. If no preconditioner is used 124 steps of FOM are carried out in each inner step of simplified Jacobi-Davidson whilst 125 steps of FOM are used in each inner step of inverse iteration. We do this in order to verify (2.19). We also restrict the number of total outer solves to 20.
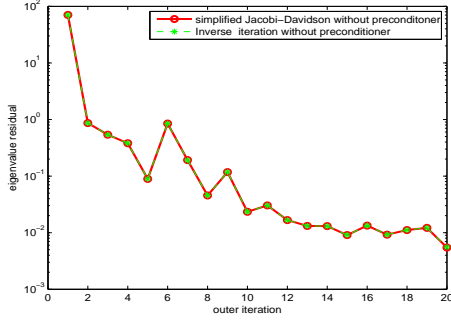

FIG. 3.1.   *Convergence history of the eigenvalue residuals for Example 3.1, case (a); no preconditioner*
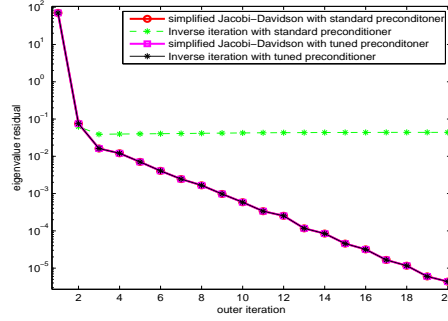
FIG. 3.2.   *Convergence history of the eigenvalue residuals for Example 3.1, cases (b) and (c); standard/tuned preconditioner*

Figures 3.1-3.2 show the results for Example 3.1. For unpreconditioned solves (Figure 3.1) we observe that inexact simplified Jacobi-Davidson exhibits the same convergence behaviour as inexact inverse iteration, which confirms the results in [11]. For preconditioned solves with a standard preconditioner this property is lost, as it can be readily observed in Figure 3.2. For inexact inverse iteration with the standard preconditioner the eigenvalue residual stagnates!

For the tuned preconditioner which satisfies $\mathbb{P}\mathbf{x} = \mathbf{x}$, we see in Figure 3.2 that with inexact inverse iteration we obtain the same convergence behaviour as for the simplified inexact Jacobi-Davidson method, which confirms the results in Theorem 2.3.

EXAMPLE 3.2. *We use the same matrix as in Example 3.1, but a Rayleigh quotient shift is employed to find the eigenvector belonging to the smallest eigenvalue. The initial eigenvector approximation is close enough to the desired eigenvector. Again methods (a), (b) and (c) from Example 3.1 are tested and we used (un)preconditioned FOM as iterative inner solver. We carry out exactly 4 steps of preconditioned FOM for the inner solve in the simplified Jacobi-Davidson method, while precisely 5 steps of preconditioned FOM are taken for each inner solve in the inexact Rayleigh quotient iteration. If no preconditioner is used 124 steps of FOM are carried out in each inner step of simplified Jacobi-Davidson whilst 125 steps of FOM are used in each inner step of Rayleigh quotient iteration. The maximum number of outer iterations is taken to be 20.*

Figures 3.3-3.4 show the results for Example 3.2. Note that outer convergence is much faster than in Example 3.1, reaching about 10^{-6} instead of 10^{-3} for unpreconditioned solves and 10^{-10} instead of 10^{-5} for preconditioned solves as is seen by comparing the size of the eigenvalue residuals on the vertical axes of Figures 3.1-3.4. For unpre-
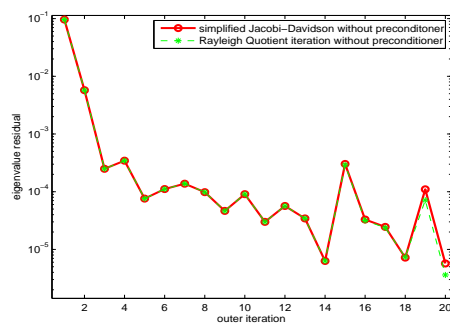
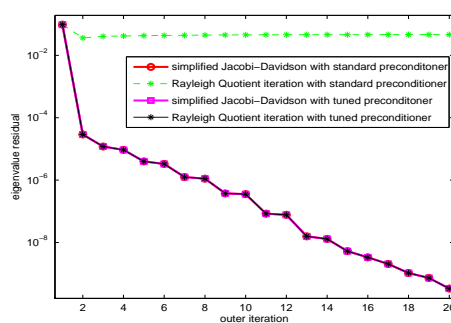FIG. 3.3. *Convergence history of the eigenvalue residuals for Example 3.2, case (a); no preconditioner*

FIG. 3.4. *Convergence history of the eigenvalue residuals for Example 3.2, cases (b) and (c); standard/tuned preconditioner*

conditioned solves (Figure 3.3) we observe that inexact Rayleigh quotient iteration shows the same convergence behaviour as the simplified Jacobi-Davidson method. If a preconditioner is used, this equivalence holds only if a tuned preconditioner is used for the inexact Rayleigh quotient iteration (Figure 3.4). For the standard preconditioner stagnation is observed in this case (Figure 3.4). This again supports the theoretical results in Theorem 2.3.

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