Inexact Inverse Iteration for Symmetric Matrices

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Abstract

In this paper we analyse inexact inverse iteration for the real symmetric eigenvalue problem $\mathbf{Av} = \lambda\mathbf{v}$. Our analysis is designed to apply to the case when $\mathbf{A}$ is large and sparse and where iterative methods are used to solve the shifted linear systems $(\mathbf{A} - \sigma\mathbf{I})\mathbf{y} = \mathbf{x}$ which arise. We present a convergence theory that is independent of the nature of the inexact solver used, and though the use of the Rayleigh quotient is emphasised our analysis also extends to quite general choices for shift and inexact solver strategies. Additionally, the convergence framework allows us to treat both standard preconditioning and to present a new analysis of the variation introduced by Simoncini and Eldén (BIT, Vol 42, pp.159-182, 2002). In addition, we provide an analysis of the performance of inner iteration solves when preconditioned MINRES is used as the inexact solver. This analysis provides descriptive bounds which are shown to predict well the actual behaviour observed in practice. Also, it explains the improvement in performance of the modification introduced by Simoncini and Eldén over the standard preconditioned form. Importantly, our analysis shows that letting the shift tend to the eigenvalue, as is the case if the Rayleigh quotient is used, does not harm significantly the performance of the iterative method. An empirical study comparing the standard residual stopping condition with the stopping condition proposed by Simoncini and Eldén is also given. Throughout the paper numerical results are given to illustrate the theory.

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1 Introduction

In this paper we discuss the effect of inexact (iterative) solves on inverse iteration for the eigenvalue problem

$$\mathbf{Av} = \lambda\mathbf{v}, \tag{1}$$

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where $\mathbf{A}$ is a large, sparse, symmetric real matrix. Inverse iteration requires the solution of shifted linear systems of the form

$$(\mathbf{A} - \sigma\mathbf{I})\mathbf{y} \;\; = \;\; \mathbf{x}, \tag{2}$$

where σ is the shift. If $\mathbf{A}$ is large and sparse, say arising from a discretised partial differential equation in 3D, direct methods become impractical and iterative methods with preconditioning become necessary to solve (2). In this setting we arrive at an inner-outer iterative method for (1): the outer iteration is the basic iterative inverse iteration algorithm requiring the solve of (2) at each step, with the inner iteration being the inexact iterative solution of (2).

Here we are thinking of inverse iteration as a technique in its own right for finding an eigenvalue and eigenvector (and which can be interpreted as Newton's method, see, for example, [4]) rather than the standard technique of finding an eigenvector given a very accurate estimate for the eigenvalue. Of course nowadays one would almost certainly use a Lanczos-type algorithm, perhaps in the shift-invert mode, to solve (1), but we believe that an in-depth understanding of the basic inexact inverse iteration algorithm for a simple eigenvalue is required before we can hope to understand properly the performance of more sophisticated algorithms if inexact solves are used for shifted systems.

A very early paper on the use of iterative methods to solve (2) is [19]. Inexact inverse iteration for symmetric matrices was discussed in [22] where a general theory, independent of the details of the solver was presented along with some new eigenvalue bounds. An important recent paper on inexact inverse iteration is [20] where a version of inexact Rayleigh quotient iteration is discussed. Several new ideas are introduced especially with regard to the appropriate linear system to be solved when Cholesky preconditioning is applied to (2), and with regard to the stopping condition in the inner iteration. We shall discuss these ideas in detail in this paper. Also [20] contains a theoretical discussion on the equivalence of inexact inverse iteration and Jacobi-Davidson (or projected Newton's Method). For nonsymmetric matrices a fixed shift inexact inverse iteration algorithm is discussed in [6]. A convergence theory is given along with an analysis of the choice of tolerance used in the inner solves. Convergence results for non-symmetric matrices are also given in [13]. Other related work on the use of inexact Rayleigh quotient iteration to compute the smallest eigenvalue of generalised Hermitian eigenvalue problems is discussed in [10], [12] and [14]. Particularly successful for extreme eigenvalues is the LOBPCG method discussed in [11]

There are several new features in the present paper. In Section 2 we present a convergence theory, independent of the details of the inexact iterative solver. This allows us to recover and extend existing results of [22] on inexact Rayleigh quotient iteration, and also to obtain a quite general convergence result. Next we extend the theory to include the alteration in the right hand side of (2) introduced in [20], but note that our analysis is valid for any preconditioner and is not restricted to Cholesky preconditioners as in [20]. In Section 3 we use some standard results for MINRES (see, for example, [16, 8]) to provide new bounds on the number of inner iterations at each step of the outer iteration. These bounds are seen in our numerical examples to provide qualitatively correct information about the performance of both unpreconditioned and preconditioned inner solves. We also present analysis that confirms the superiority of the system introduced by [20] for preconditioned Rayleigh quotient iteration over the standard preconditioned system. Our analysis also shows that we need not be concerned that the Krylov solver is applied to a matrix which is becoming more and more singular. The explanation lies in the interplay between the shift tending towards the eigenvalue and the right hand side tending to the corresponding eigenvector, together with the fact that Krylov solvers handle very well nearly singular systems with only a small number of critical eigenvalues. Similar ideas were explored in [19]. In Section 4 we present an empirical study of two stopping conditions when using the Krylov solver MINRES to implement the inexact solves. Specifically, we compare the performance of a standard residual stopping condition with the one proposed in [20].

A key feature of this paper is that we use a residual stopping condition in the convergence theory of §2, in our numerical experiments using MINRES, and in the analysis of the performance of the inner solve in §3. This allows a unified account of both the theory and practice.

We mention that a more detailed account of the material in this paper, including more extensive numerical tests, is contained in Chapters 2 and 3 of [1].

2 Inexact Inverse Iteration

2.1 Preliminaries

Consider the solution of the eigenvalue problem

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}, \quad \| \mathbf{v} \| = 1, \tag{3}$$

where $\mathbf{A}$ is a real symmetric $n \times n$ matrix, with eigenvalues λ_j, $j = 1, \dots, n$ and corresponding orthonormalised eigenvectors $\mathbf{v}_j$, $j = 1, \dots, n$. Inverse iteration for (3) requires the solution of shifted systems of the form $(\mathbf{A} - \sigma\mathbf{I})\mathbf{y} = \mathbf{x}$ for some chosen real shift σ. Let $(\lambda_1, \mathbf{v}_1)$ denote a simple eigenpair of (3) which we wish to compute. Throughout this paper we will be interested in shifts σ which are close enough to λ_1 in the sense that

$$0 < |\lambda_1 - \sigma| < \frac{1}{2} \min_{j=2,\dots,n} |\lambda_1 - \lambda_j| \, . \tag{4}$$

Then we have an induced ordering on the eigenvalues

$$0 < |\lambda_1 - \sigma| < |\lambda_2 - \sigma| \leq \dots \leq |\lambda_n - \sigma| \, .$$

This ordering depends on σ but for convenience we ignore this in the notation.

We are interested in the case when $\mathbf{A}$ is large and sparse and so the shifted systems will be solved (inexactly) by some iterative algorithm. In Section 3 we will consider in detail the case when the iterative solver is MINRES (see, for example,

[8]), which is appropriate since $\mathbf{A} - \sigma\mathbf{I}$ is symmetric but is likely to be indefinite. However, in this section we will present a convergence theory that is independent of the solver.

The inexact inverse iteration algorithm is given in Algorithm 1.

Algorithm 1: Inexact Inverse Iteration $\boxed{\text{alg1}}$

Given $\mathbf{x}^{(0)}$ with $\| \mathbf{x}^{(0)} \| = 1$. For $i = 0, 1, 2, \ldots$

(1) Choose $\sigma^{(i)}$ and $\tau^{(i)}$

(2) Solve $(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} = \mathbf{x}^{(i)}$ inexactly, that is,
$\| (\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} - \mathbf{x}^{(i)} \| \leq \tau^{(i)}$

(3) Update $\mathbf{x}^{(i+1)} = \mathbf{y}^{(i)} / \| \mathbf{y}^{(i)} \|$

(4) Test for convergence

We refer to the iteration in Algorithm 1 as the *outer* iteration and the iteration implicit in the inexact solve as the *inner* iteration, and so inexact inverse iteration is an example of an inner-outer iterative algorithm (see, for example, [2, 3, 21, 5]).

Before we analyse the convergence of Algorithm 1 we recall some definitions and notation. A key concept is the orthogonal splitting used in [17, p. 63]. If $\mathbf{x}^{(i)}$ is any unit vector approximating $\mathbf{v}_1$, we introduce the splitting

$$\mathbf{x}^{(i)} = \cos\theta^{(i)}\, \mathbf{v}_1 + \sin\theta^{(i)}\, \mathbf{u}^{(i)}, \quad \mathbf{u}^{(i)} \perp \mathbf{v}_1, \tag{5}$$

with $\| \mathbf{v}_1 \| = \| \mathbf{u}^{(i)} \| = 1$ and $\theta^{(i)} = \angle(\mathbf{x}^{(i)}, \mathbf{v}_1)$, the error angle. For convenience we usually write

$$c^{(i)} = \cos\theta^{(i)}, \quad s^{(i)} = \sin\theta^{(i)}, \quad \text{and} \quad t^{(i)} = |s^{(i)}|/|c^{(i)}| = |\tan\theta^{(i)}|. \tag{6}$$

From (5), $\|\mathbf{x}^{(i)} - c^{(i)}\mathbf{v}_1\| = |s^{(i)}| \leq t^{(i)}$ and normally we use $|s^{(i)}|$ or $t^{(i)}$ as a measure of the convergence of $\mathbf{x}^{(i)}$ to span $\{\mathbf{v}_1\}$. However, we note that convergence occurs if we can prove one of $|\theta^{(i)}| \to 0, |s^{(i)}| \to 0, t^{(i)} \to 0$, or $|c^{(i)}| \to 1$. Also, recall that, for $\mathbf{x}^{(i)}$ given by (5), the Rayleigh quotient, $\varrho(\mathbf{x}^{(i)}) = \mathbf{x}^{(i)^T}\mathbf{A}\mathbf{x}^{(i)}$, satisfies

$$\lambda_1 - \varrho(\mathbf{x}^{(i)}) = (s^{(i)})^2[\lambda_1 - \varrho(\mathbf{u}^{(i)})], \tag{7}$$

and the eigenvalue residual, $\mathbf{r}^{(i)}$, defined by

$$\mathbf{r}^{(i)} := (\mathbf{A} - \varrho(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i)} \tag{8}$$

satisfies ([17], Theorem 11.7.1)

$$|s^{(i)}|\, |\lambda_2 - \varrho(\mathbf{x}^{(i)})| \leq \| \mathbf{r}^{(i)} \| \leq |s^{(i)}|\, |\lambda_n - \lambda_1|. \tag{9}$$

2.2 Convergence Theory

We now present a convergence theory for inexact inverse iteration. Various choices for $\sigma^{(i)}$ and $\tau^{(i)}$ in Algorithm 1 are possible and our analysis allows us to obtain a full understanding of the effects of the different options. However, the most important choice for $\sigma^{(i)}$ is the Rayleigh quotient, and we shall emphasise this case throughout. For example, it is a classical result, proved in [15], that inverse iteration with Rayleigh quotient shifts and exact linear solves converges cubically when applied to symmetric matrices (see [17] for an elegant treatment). It is natural to ask how the tolerance $\tau^{(i)}$ should be chosen so that inexact inverse iteration with Rayleigh quotient shifts can recover cubic convergence. We shall see in Theorem 2.1 how to do this.

We start with a bound for the error after one step of Algorithm 1. Similar results are to be found in [22] and, for nonsymmetric matrices with fixed shift, [6]. First we provide some notation. Because of step (2) of Algorithm 1 we have a residual

$$\mathbf{res}^{(i)} \quad := \quad \mathbf{x}^{(i)} - (\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} \tag{10}$$

which satisfies

$$\| \mathbf{res}^{(i)} \|_2 \quad \leq \quad \tau^{(i)}. \tag{11}$$

Note that the "inner linear solve" residual $\mathbf{res}^{(i)}$ should not be confused with the outer eigenvalue residual $\mathbf{r}^{(i)}$ which was defined in (8). Now we can state the following Lemma.

Lemma 2.1 *If $\mathbf{x}^{(i)}$ is such that*

$$|c^{(i)}| > \tau^{(i)}, \tag{12}$$

then one step of Algorithm 1 yields $\mathbf{x}^{(i+1)}$ with

$$\frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_n - \sigma^{(i)}|} \, \frac{\big|\, |s^{(i)}| - \|\Pi\, \mathbf{res}^{(i)}\| \,\big|}{|c^{(i)}| + \tau^{(i)}} \leq t^{(i+1)} \leq \frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_2 - \sigma^{(i)}|} \, \frac{|s^{(i)}| + \tau^{(i)}}{|c^{(i)}| - \tau^{(i)}}. \tag{13}$$

where $\mathbf{res}^{(i)}$ satisfies (10) and (11), and $\Pi := \mathbf{I} - \mathbf{v}_1\mathbf{v}_1^T$.

Proof: First use step (3) in Algorithm 1 and (5) to rewrite (10) as

$$\|\mathbf{y}^{(i)}\| \, (\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{x}^{(i+1)} \quad = \quad \cos\theta^{(i)}\, \mathbf{v}_1 + \sin\theta^{(i)}\, \mathbf{u}^{(i)} - \mathbf{res}^{(i)},$$

and using (5) again gives

$$\begin{aligned} \|\mathbf{y}^{(i)}\| \, \{c^{(i+1)}(\lambda_1 - \sigma^{(i)})\mathbf{v}_1 + s^{(i+1)}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{u}^{(i+1)}\} & \\ = c^{(i)}\mathbf{v}_1 + s^{(i)}\mathbf{u}^{(i)} - \mathbf{res}^{(i)}. & \end{aligned} \tag{14}$$

Because $\mathbf{v}_1$ is orthogonal to both $\mathbf{u}^{(i)}$ and $\mathbf{u}^{(i+1)}$ we can resolve (14) into two equations in span$\{\mathbf{v}_1\}$ and $\{\mathbf{v}_1\}^\perp$, respectively. Along $\mathbf{v}_1$ we have

$$\|\mathbf{y}^{(i)}\| \, c^{(i+1)}(\lambda_1 - \sigma^{(i)}) \quad = \quad c^{(i)} - \mathbf{v}_1^T\mathbf{res}^{(i)}, \tag{15}$$

and in $\{\mathbf{v}_1\}^\perp$ we have

$$\|\mathbf{y}^{(i)}\| \; s^{(i+1)}(\mathbf{A}-\sigma^{(i)}\mathbf{I})\mathbf{u}^{(i+1)} \;\; = \;\; s^{(i)}\mathbf{u}^{(i)} - \Pi\, \mathbf{res}^{(i)}. \tag{16}$$

Now let $(\mathbf{A}-\sigma^{(i)}\mathbf{I})_\perp$ denote the restriction of $(\mathbf{A}-\sigma^{(i)}\mathbf{I})$ to $\{\mathbf{v}_1\}^\perp$. This linear operator is invertible on $\{\mathbf{v}_1\}^\perp$ and satisfies $\| (\mathbf{A}-\sigma^{(i)}\mathbf{I})_\perp^{-1} \| = | \lambda_2 - \sigma^{(i)} |^{-1}$, and $\|(\mathbf{A}-\sigma^{(i)}\mathbf{I})_\perp\| = |\lambda_n - \sigma^{(i)}|$. Thus from (16) we obtain

$$\|\mathbf{y}^{(i)}\| \; |s^{(i+1)}| \;\; \leq \;\; |\lambda_2 - \sigma^{(i)}|^{-1} \, \{|s^{(i)}| + \|\Pi\, \mathbf{res}^{(i)}\|\}. \tag{17}$$

Combining this with a trivial lower bound on $\|\mathbf{y}^{(i)}\| \; c^{(i+1)}$ from (15) we obtain

$$t^{(i+1)} = \frac{\|\mathbf{y}^{(i)}\| \; |s^{(i+1)}|}{\|\mathbf{y}^{(i)}\| \; |c^{(i+1)}|} \;\; \leq \;\; \left|\frac{\lambda_1 - \sigma^{(i)}}{\lambda_2 - \sigma^{(i)}}\right| \;\; \frac{|s^{(i)}| + \|\Pi\, \mathbf{res}^{(i)}\|}{|c^{(i)}| - |\mathbf{v}_1^T \mathbf{res}^{(i)}|}, \tag{18}$$

from which the right hand side of (13) follows on applying (11).

A similar approach is used to obtain the left hand side of (13). First observe

$$\begin{aligned}
\|\mathbf{y}^{(i)}\| \; |s^{(i+1)}| \;\; &= \;\; \|(\mathbf{A}-\sigma^{(i)}\mathbf{I})_\perp^{-1}(s^{(i)}\mathbf{u}^{(i)} + \Pi\, \mathbf{res}^{(i)})\| && (19)\\
&\geq \;\; \frac{1}{|\lambda_n - \sigma^{(i)}|} \; \|s^{(i)}\mathbf{u}^{(i)} + \Pi\, \mathbf{res}^{(i)})\| && (20)\\
&\geq \;\; \frac{1}{|\lambda_n - \sigma^{(i)}|} \; \big||s^{(i)}| - \|\Pi\, \mathbf{res}^{(i)}\|\big|. && (21)
\end{aligned}$$

Then combine this with a trivial upper bound on $\|\mathbf{y}^{(i)}\| \; c^{(i+1)}$ from (15), to obtain

$$\left|\frac{\lambda_1 - \sigma^{(i)}}{\lambda_n - \sigma^{(i)}}\right| \;\; \frac{\big||s^{(i)}| - \|\Pi\, \mathbf{res}^{(i)}\|\big|}{|c^{(i)}| + |\mathbf{v}_1^T \mathbf{res}^{(i)}|} \leq t^{(i+1)}, \tag{22}$$

from which the left-hand side of (13) follows. $\square$

Note that if $\tau^{(i)} = 0$, as is the case for exact solves, then we recover the standard results for exact solves (see, for example, [17]).

Since we restrict attention to symmetric matrices there are two main choices for $\sigma^{(i)}$, namely the natural Rayleigh quotient shift (popular because of its ease of computation and its quadratic approximation property when the approximate eigenvector is accurate enough), and a fixed shift (employed in cases where the approximate eigenvector may be poor). We restrict to the Rayleigh quotient case here but return to the fixed shift case in §2.3. Then with $\sigma^{(i)} = \varrho(\mathbf{x}^{(i)})$ we have from (7)

$$|\lambda_1 - \sigma^{(i)}| = |\lambda_1 - \varrho(\mathbf{u}^{(i)})||s^{(i)}|^2. \tag{23}$$

There are also two practical options for the choice of tolerance $\tau^{(i)}$. Either we can choose to decrease $\tau^{(i)}$ as the outer iteration proceeds, or $\tau^{(i)}$ can be held fixed. Let us first consider the case of a decreasing tolerance, so assume in addition to (12) that there is a constant C_2, independent of i, such that

$$\tau^{(i)} \leq C_2|s^{(i)}| < |c^{(i)}| \tag{24}$$

as would be the case if $\tau^{(i)}$ were chosen bounded by a multiple of the eigenvalue residual $\|\mathbf{r}^{(i)}\|$, see (8) and (9). Then the right hand inequality in (13) combined with (23) and (24) gives

$$\frac{t^{(i+1)}}{(t^{(i)})^3} \leq \frac{|\lambda_1 - \varrho(\mathbf{u}^{(i)})|(c^{(i)})^2}{|\lambda_2 - \varrho(\mathbf{x}^{(i)})|} \frac{1 + C_2}{1 - C_2 t^{(i)}}, \tag{25}$$

(cf. [17] eqn(4.22)). Equation (25) shows that in the asymptotic regime we achieve cubic convergence, just as would be attained if exact solves were used. This result is implicit in [22].

The more interesting and practical case is when the tolerances $\tau^{(i)}$ are not required to decrease as the outer iteration proceeds so that the inner solves are implemented with a fixed tolerance and hence are potentially cheaper. So, in contrast to (24), let us assume that

$$\tau^{(i)} = \tau^{(0)}, \quad \forall i; \quad \tau^{(0)} \leq C_3 |c^{(i)}|, \quad C_3 < 1. \tag{26}$$

With this choice for $\tau^{(i)}$, (13) with (23) gives

$$\frac{t^{(i+1)}}{(t^{(i)})^2} \leq \frac{|\varrho(\mathbf{u}^{(i)}) - \lambda_1|(c^{(i)})^2}{|\lambda_2 - \varrho(\mathbf{x}^{(i)})|} \quad \frac{t^{(i)} + C_3}{1 - C_3}. \tag{27}$$

Thus with a fixed tolerance cubic convergence is lost but quadratic convergence is maintained because of the quadratic convergence of the Rayleigh quotient. We gather together these results in the following Theorem.

Theorem 2.1 *Let* $\mathbf{A}$ *be a real* $n \times n$ *symmetric matrix and consider the application of Algorithm 1 with* $\sigma^{(i)}$ *chosen to be the Rayleigh quotient* $\varrho(\mathbf{x}^{(i)})$*. Assume* $c^{(i)}$ *and* $s^{(i)}$ *are given by* $\mathbf{x}^{(i)} = c^{(i)}\mathbf{v}_1 + s^{(i)}\mathbf{u}^{(i)}$ *and (11) is satisfied.*

(a) (Decreasing tolerance) If $\tau^{(i)}$ *in (11) satisfies (24) then Algorithm 1 converges cubically.*

(b) (Fixed tolerance) If $\tau^{(i)}$ *in (11) is chosen to satisfy (26) then Algorithm 1 converges quadratically.*

This theorem follows from bounds (25) and (27) above. It is also a corollary of Theorem 2.2 that allows more general choices for $\sigma^{(i)}$ and $\tau^{(i)}$, and which is proved in the next subsection.

Now we look at some numerical results from a simple model problem to illustrate Theorem 2.1.

Example 2.1 *Consider the eigenvalue problem for the 2-D Laplacian,* $-\nabla^2 u = \lambda u$*, with homogenous Dirichlet boundary conditions on the rectangle* $0 \leq x \leq 1$*,* $0 \leq y \leq 1.3$*, which is discretised using finite differences with the 5-point Laplacian approximation on a* 12×12 *regular grid. In Table 1 we present numerical results obtained when calculating* λ_1 *(*$\simeq 15.6$*) the smallest (simple) eigenvalue of the discretised matrix. Using unpreconditioned MINRES as the inexact solver we apply the two versions of inexact inverse iteration discussed in Theorem 2.1, namely*

	RQId $\tau^{(0)} = 0.1$, $C_2 =$ 0.1		RQIf $\tau^{(0)} = 0.1$	
i	$\log_{10} s^{(i)}$	$k^{(i-1)}$	$\log_{10} s^{(i)}$	$k^{(i-1)}$
0	-0.14		-0.12	
1	-1.62	15	-1.41	19
2	-4.33	24	-3.85	19
3	-12.90	45	-9.03	33
4	-36.19	78	-19.46	50
5	-82.66	113	-40.72	76
6			-82.96	108
$\sum k^{(i)}$		275		305

Table 1: Numerical results for unpreconditioned MINRES applied to Example 2.1 using the methods in Theorem 2.1. Here $s^{(i)}$ denotes $\sin\theta^{(i)}$ defined by (5), $k^{(i)}$ denotes the number of inner iterations at the ith step, and C_2 is the constant in (24).

RQId: *Rayleigh quotient shift, decreasing tolerance,*

RQIf: *Rayleigh quotient shift, fixed tolerance,*

(cases a) and b) in Theorem 2.1 respectively). Each row in Table 1 provides the outer iteration number, $\log_{10} s^{(i)}$ *(calculated using the exact* $\mathbf{v}_1$*) and* $k^{(i-1)}$ *the number of inner iterations needed to satisfy the residual condition in step (2) of the Algorithm. To illustrate accurately the convergence rates attained, the experiment was carried out using MATLAB with variable precision arithmetic using 128 decimal digit arithmetic. In both experiments we used* $\|(\mathbf{A} - \varrho(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i)}\| \leq 10^{-80}|\varrho(\mathbf{x}^{(i)})|$ *as the test for convergence in step (4) of Algorithm 1.*

As predicted in Theorem 2.1, we observe in Table 1 quadratic convergence for **RQIf** and cubic convergence for **RQId**. At a practical level (that is, to double precision on most of the current computers) our experiments have shown that there is little difference between the two methods with both needing roughly speaking about the same number of inner iterations in total.

2.3 Theory for a General Method

In this subsection we provide the details of the convergence theory for Algorithm 1 for general choices for $\sigma^{(i)}$and $\tau^{(i)}$. We shall use the right hand bound in (13)

$$t^{(i+1)} \leq \frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_2 - \sigma^{(i)}|} \frac{|s^{(i)}| + \tau^{(i)}}{|c^{(i)}| - \tau^{(i)}}, \tag{28}$$

though a more refined analysis would be possible using the right-hand side of (18), namely,

$$t^{(i+1)} \quad \leq \quad \frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_2 - \sigma^{(i)}|} \, \frac{|s^{(i)}| + \|\Pi \, \mathbf{res}^{(i)}\|}{|c^{(i)}| - |\mathbf{v}_1^T \mathbf{res}^{(i)}|}, \tag{29}$$

if more were known about the size of certain components of $\mathbf{res}^{(i)}$ (see [1]). Similar expressions are found in [22] and [20], where a bound is derived directly using the properties of a Krylov solver. In the latter paper the observation is made that for a Krylov solver the term $\mathbf{v}_1^T \mathbf{res}^{(i)}$ is likely to reduce significantly in the first few iterations since $\mathbf{x}^{(i)}$ is rich in the direction $\mathbf{v}_1$. Hence, since $|c^{(i)}|$ tends to 1, the factor $|c^{(i)}| - |\mathbf{v}_1^T \mathbf{res}^{(i)}|$ is unlikely to cause any problems in practice.

Equation (28) is used in the proof of the following general convergence result.

Theorem 2.2 *Let $\mathbf{A}$ be a real $n \times n$ symmetric matrix and consider the application of Algorithm 1 to find a simple eigenpair $(\lambda_1, \mathbf{v}_1)$. Assume $\mathbf{x}^{(i)}$ is given by (5) and that $\sigma^{(i)}$ satisfy (4). Additionally, assume $\sigma^{(i)}$ and $\tau^{(i)}$ are chosen to satisfy*

$$\begin{aligned} |\lambda_1 - \sigma^{(i)}| \quad &\leq \quad C_1 |s^{(i)}|^{\alpha} \\ \tau^{(i)} \quad &\leq \quad \min\{C_2 |s^{(i)}|^{\beta}, C_3 |c^{(i)}|\} \end{aligned}$$

for some constants $\alpha, \beta, C_1, C_2, C_3$ independent of i with $0 \leq \beta \leq 1$, $0 \leq C_3 < 1$ and $\alpha + \beta \geq 1$. If $c^{(0)} \neq 0$, and the initial approximation $\mathbf{x}^{(0)}$ is such that

$$C_4 := |s^{(0)}|^{\alpha+\beta-1} \, \frac{2C_1(1+C_2)}{|\lambda_2 - \lambda_1|(1 - C_3)} < 1$$

then

$$t^{(i+1)} \leq C_4 t^{(i)},$$

with C_4 independent of i, and the method converges. In this case,

$$t^{(i+1)} \leq C (t^{(i)})^{\alpha+\beta}$$

with $C = C_4 / \, |s^{(0)}|^{\alpha+\beta-1}$, and so convergence is of order $(\alpha + \beta)$.

Proof: From (28) and the above hypothesis we have

$$t^{(i+1)} \leq \frac{2C_1 |s^{(i)}|^{\alpha}}{|\lambda_2 - \lambda_1|} \, \frac{|s^{(i)}| + C_2 |s^{(i)}|^{\beta}}{|c^{(i)}| - C_3 |c^{(i)}|} \leq C_4 t^{(i)} \frac{|s^{(i)}|^{\alpha+\beta-1}}{|s^0|^{\alpha+\beta-1}}.$$

Convergence follows by induction on i. Finally

$$t^{(i+1)} \leq \frac{C_4}{|s^{(0)}|^{\alpha+\beta-1}} (t^{(i)})^{\alpha+\beta}. \tag{30}$$

□

As a consequence of Theorem 2.2 we obtain the convergence of $\mathbf{x}^{(i)}$ to $\pm\mathbf{v}_1$ and $\varrho(\mathbf{x}^{(i)})$ to λ_1 as $i \to \infty$. Note that the condition $c^{(0)} \neq 0$ ensures that the starting vector is not orthogonal to the required direction $\mathbf{v}_1$.

Theorem 2.1 is a special case of Theorem 2.2. For Rayleigh quotient shifts we have $\alpha = 2$, and cases (a) and (b) in Theorem 2.1 correspond to $\beta = 1$ and $\beta = 0$ respectively.

In addition to the two strategies examined in Theorem 2.1 a third strategy could be based on keeping $\sigma^{(i)}$ fixed and choosing $\tau^{(i)} \leq C_2|s^{(i)}|$ as would be the case if $\tau^{(i)} = O(\|\mathbf{r}^{(i)}\|)$ (see (9)). Theorem 2.2 shows that this approach would attain at least linear convergence for accurate enough $\sigma^{(0)}$ and $\mathbf{x}^{(0)}$. Also the theory indicates that there is likely to be little gain in ever choosing $\tau^{(i)} = o(|s^{(i)}|)$.

Finally we see that a strategy based on a fixed shift $\sigma^{(0)}$ and a fixed tolerance $\tau^{(0)} \neq 0$ is unlikely to converge as can be verified by the following simple example.

Example 2.2 *Suppose that* $\mathbf{x}^{(i)} = c^{(i)}\mathbf{v}_1 + s^{(i)}\mathbf{v}_2$*. If we construct a particular* $\mathbf{y}^{(i)}$ *via the formula,* $\mathbf{y}^{(i)} = \frac{c^{(i)}}{\lambda_1-\sigma^{(0)}}\mathbf{v}_1 + \frac{s^{(i)}+\tau^{(0)}}{\lambda_2-\sigma^{(0)}}\mathbf{v}_2$ *then* $\mathbf{x}^{(i)}$ *and* $\mathbf{y}^{(i)}$ *satisfy* $\|\mathbf{x}^{(i)} - (\mathbf{A} - \sigma^{(0)}\mathbf{I})\mathbf{y}^{(i)}\| = \tau^{(0)}$*. Then computing* $\mathbf{x}^{(i+1)}$ *and representing it in the form (5) we obtain* $\tan\theta^{(i+1)} = \frac{\lambda_1-\sigma^{(0)}}{\lambda_2-\sigma^{(0)}}\frac{\sin\theta^{(i)}+\tau^{(0)}}{\cos\theta^{(i)}}$*. Repeating this formula for each* i *we obtain a fixed point iteration for* $\theta^{(i)}$*. If* $\theta^{(i)} \to \theta$ *as* $i \to \infty$ *then* θ *satisfies* $\sin\theta = \frac{\lambda_1-\sigma^{(0)}}{\lambda_2-\lambda_1}\tau^{(0)}$*, which is nonzero unless* $\sigma^{(0)} = \lambda_1$ *or* $\tau^{(0)} = 0$*. Such non-convergence is often refered to as stagnation, see, for example, [18].*

2.4 Convergence Theory for Preconditioned Solves

In this subsection we first discuss briefly the convergence theory for standard inverse iteration with preconditioned inner solves. Then we shall use this to derive a new convergence analysis of the variant of preconditioned inverse iteration introduced by [20].

Whatever iterative algorithm is used to solve

$$(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} = \mathbf{x}^{(i)} \tag{31}$$

in Algorithm 1 it will almost certainly be applied to a preconditioned system, and since $\mathbf{A}$ is symmetric it is common to use a symmetric positive definite preconditioner. If $\mathbf{P}$ is a positive definite symmetric matrix that approximates $(\mathbf{A} - \sigma^{(i)}\mathbf{I})$ in some way, then, at least for the theory, we may introduce a factorisation $\mathbf{P} = \mathbf{P}_1\mathbf{P}_1^T$, and to preserve the symmetry in the system we may consider the symmetrically preconditioned system

$$\mathbf{P}_1^{-1}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T}\widetilde{\mathbf{y}}^{(i)} \ = \ \mathbf{P}_1^{-1}\mathbf{x}^{(i)}; \qquad \mathbf{y}^{(i)} \ = \ \mathbf{P}_1^{-T}\widetilde{\mathbf{y}}^{(i)}. \tag{32}$$

Of course the preconditioner $\mathbf{P}$ or the factorisation $\mathbf{P} = \mathbf{P}_1\mathbf{P}_1^T$ is often not needed in practice and implementation of iterative methods for (32) may only require the action of $\mathbf{P}^{-1}$.

We shall assume that the stopping condition for (32) is based on the residual of the original system, that is, although $(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} = \mathbf{x}^{(i)}$ is solved using (32) the iteration stops when $\|\mathbf{res}^{(i)}\| \leq \tau^{(i)}$ where $\mathbf{res}^{(i)}$ is defined by (10). Hence the convergence theory for the outer iteration given in the previous subsections applies, and is not repeated here.

An alternative to (32) is discussed in [20]. As we shall see in Section 3, this alternative is beneficial for the performance of the preconditioned iterative solver. The idea is to replace (32) by

$$\mathbf{P}_1^{-1}(\mathbf{A}-\sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T}\widetilde{\mathbf{y}}^{(i)} \;=\; \mathbf{P}_1^{T}\mathbf{x}^{(i)}; \qquad \mathbf{y}^{(i)} \;=\; \mathbf{P}_1^{-T}\widetilde{\mathbf{y}}^{(i)}. \tag{33}$$

Here the right hand side in the shifted linear system differs from that of (32). Multiplying by $\mathbf{P}_1$ shows that (33) is equivalent to

$$(\mathbf{A}-\sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} \;=\; \mathbf{P}\mathbf{x}^{(i)}, \tag{34}$$

so that the basic step in inverse iteration is changed by replacing $\mathbf{x}^{(i)}$ by $\mathbf{P}\mathbf{x}^{(i)}$ on the right hand side. Not surprisingly, our analysis will show that this alteration removes the possibility of attaining cubic convergence (except in a very special case, see Example 2.4). If we assume that the iterative solution of (33) is stopped by a relative residual test on (34), namely,

$$\|(\mathbf{A}-\sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} - \mathbf{P}\mathbf{x}^{(i)}\| \leq \tau^{(i)}\, \|\mathbf{P}\mathbf{x}^{(i)}\|, \tag{35}$$

then we obtain Algorithm 2. Note that putting $\mathbf{P} = \mathbf{I}$ in Algorithm 2 recovers Algorithm 1.

Algorithm 2: Preconditioned Inexact Rayleigh Quotient Iteration $\boxed{\text{alg2}}$

Choose $\mathbf{P}$. Given $\mathbf{x}^{(0)}$ with $\| \mathbf{x}^{(0)} \| = 1$.
For $i = 0, 1, 2, \ldots$

(1) Choose $\sigma^{(i)}$ as the Rayleigh quotient

(2) Choose $\tau^{(i)}$

(3) Solve $(\mathbf{A}-\sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} = \mathbf{P}\mathbf{x}^{(i)}$ inexactly using the preconditioner $\mathbf{P}$, such that
$\| (\mathbf{A}-\sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} - \mathbf{P}\mathbf{x}^{(i)} \| \leq \tau^{(i)}\, \|\mathbf{P}\mathbf{x}^{(i)}\|$

(4) Update $\mathbf{x}^{(i+1)} = \mathbf{y}^{(i)} / \|\mathbf{y}^{(i)}\|$

(5) Test for convergence

To analyse Algorithm 2 let us introduce

$$\mathbf{res}^{(i)} := \mathbf{P}\mathbf{x}^{(i)} - (\mathbf{A}-\sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)}, \tag{36}$$

where, as indicated by step (3) of Algorithm 2,

$$\|\mathbf{res}^{(i)}\| \leq \tau^{(i)} \ \|\mathbf{P}\mathbf{x}^{(i)}\| \ . \tag{37}$$

If we assume (cf. (12))

$$|\mathbf{v}_1^T \mathbf{P}\mathbf{x}^{(i)}| > |\mathbf{v}_1^T \mathbf{res}^{(i)}|, \tag{38}$$

then by carrying out an analysis similar to the proof of Lemma 2.1 we obtain the one step bound

$$t^{(i+1)} \ \leq \ \frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_2 - \sigma^{(i)}|} \, \frac{\|\top \mathbf{P}\mathbf{x}^{(i)}\| + \|\top \mathbf{res}^{(i)}\|}{|\mathbf{v}_1^T \mathbf{P}\mathbf{x}^{(i)}| - |\mathbf{v}_1^T \mathbf{res}^{(i)}|}, \tag{39}$$

which reduces to (18) if $\mathbf{P} = \mathbf{I}$.

Now it is likely that little will be known about the quantity $\|\top \mathbf{P}\mathbf{x}^{(i)}\|$ on the numerator of the right hand side of (39) except that (for general choices of $\mathbf{P}$) it is unlikely to tend to zero, and so there will be little point in choosing decreasing tolerances $\tau^{(i)}$. Hence Algorithm 2 will typically be used with a fixed tolerance. Now, if we assume that there exists a C_3, independent of i, such that

$$\tau^{(i)} = \tau^{(0)}, \quad \forall i; \quad \tau^{(0)} \ \|\mathbf{P}\mathbf{x}^{(i)}\| \leq C_3 \ |\mathbf{v}_1^T \mathbf{P}\mathbf{x}^{(i)}|, \quad C_3 < 1, \tag{40}$$

(which if $\mathbf{P} = \mathbf{I}$ reduces to (26)) then recalling $\sigma^{(i)}$ is the Rayleigh quotient

$$\frac{t^{(i+1)}}{(t^{(i)})^2} \ \leq \ \frac{|\lambda_1 - \varrho(\mathbf{u}^{(i)})| |c^{(i)}|^2}{|\lambda_2 - \sigma^{(i)}|} \ \frac{\|\mathbf{P}\mathbf{x}^{(i)}\| \ (1 + \tau^{(0)})}{|\mathbf{v}_1^T \mathbf{P}\mathbf{x}^{(i)}| \ (1 - C_3)}. \tag{41}$$

Hence we have the following Theorem:

Theorem 2.3 *Let $\mathbf{A}$ be a real $n \times n$ matrix and consider the application of Algorithm 2 to find a simple eigenpair $(\lambda_1, \mathbf{v}_1)$. Assume $c^{(0)} \neq 0$, $\tau^{(i)} = \tau^{(0)}$ for all i, and that (38) and (40) hold. Then the method is quadratically convergent for a sufficiently close starting guess.*

For a general preconditioner we will be required to have available a subroutine for computing the action of $\mathbf{P}^{-1}$, but little may be known about the action of $\mathbf{P}$. Thus in general one may not be able to say much about the second quotient on the right hand side of (41). However, we can interprete condition (40) as describing the quality of $\mathbf{P}$ as a preconditioner for the eigenvalue problem. In particular, if $\mathbf{x}^{(i)} \to \mathbf{v}_1$,

$$\frac{\|\mathbf{P}\mathbf{x}^{(i)}\|}{|\mathbf{v}_1^T \mathbf{P}\mathbf{x}^{(i)}|} \to \frac{\|\mathbf{P}\mathbf{v}_1\|}{|\mathbf{v}_1^T \mathbf{P}\mathbf{v}_1|}, \tag{42}$$

then (40) requires that $\mathbf{P}\mathbf{v}_1$ should be rich in the direction $\mathbf{v}_1$. In Example 2.3 for the calculation of the 20^{th} eigenvalue of a certain matrix, direct evaluation found that $\|\mathbf{P}\mathbf{x}^{(i)}\| < 1.5 \ |\mathbf{v}_1^T \mathbf{P}\mathbf{x}^{(i)}|$ for all i, which is consistent with assumption (40). In

	RQIf $\tau = 0.9$			SEf $\tau = 0.1$		
	$\Vert r^{(i)} \Vert / \vert\rho^{(i)}\vert$	$tan\theta^{(i)}$	$k^{(i-1)}$	$\Vert r^{(i)} \Vert / \vert\rho^{(i)}\vert$	$tan\theta^{(i)}$	$k^{(i-1)}$
0	6.6e-02	1.0e-03		6.6e-02	1.0e-03	
1	3.4e-05	6.4e-05	52	3.9e-05	6.1e-05	36
2	1.1e-09	1.0e-09	74	3.0e-10	5.1e-10	65
3	5.5e-11	9.4e-11	87	7.4e-11	4.3e-10	8
$\sum k^{(i-1)}$			213			109

Table 2: Numerical results for Algorithm 2 using preconditioned MINRES applied to Example 2.3 using the methods in Theorem 2.1 and Theorem 2.3. The second and fifth columns give the respective relative eigenvalue residual.

these same experiments $|\mathbf{v}_1^T\mathbf{res}^{(i)}| \leq 2 \times 10^{-3}$ for all i, and (38) is satisfied. The fact that $\mathbf{v}_1^T\mathbf{res}^{(i)}$ is likely to be small when a Krylov method is used as inexact solver was noted by [20].

Comparing (41) with (27), the corresponding bound for unpreconditioned solves with fixed tolerance, we see that quadratic convergence of the outer iteration is again attained, but the asymptotic constant may be larger than in the standard preconditioned case with consequently more outer iterations required for convergence.

Bound (39) also shows that choosing $\mathbf{res}^{(i)}$ to decrease like $|s^{(i)}|$ will normally not produce cubic convergence because of the presence of the $\|\Pi\ \mathbf{P}\mathbf{x}^{(i)}\|$ term in the numerator of the right hand side.

Numerical results illustrating this theory are given in the following Example.

Example 2.3 To show the advantage of (34) over (31) *Consider the matrix market example 'bcsstk09', a symmetric matrix of dimension* 1083. *In Tables 2 we present computations of* $\lambda_{20} = 4.06 \times 10^5$ *the 20th smallest eigenvalue. The inner solve was carried out by preconditioned MINRES, with preconditioner taken to be an incomplete Cholesky decomposition of* $\mathbf{A}$ *using the matlab routine 'cholinc' with droptol=1e-2. We compare two methods both with Rayleigh quotient shift and with a fixed tolerance, so that both have quadratic convergence.*

(a) **RQIf***: Solve (32) using preconditioned MINRES with stopping condition* $\|\mathbf{res}^{(i)}\| \leq \tau^{(0)} = 0.1$ *where* $\mathbf{res}^{(i)} = \mathbf{x}^{(i)} - (\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)}$*, so Theorem 2.1 applies.*

(b) **SEf***: Solve (34) using preconditioned MINRES with stopping condition* $\|\mathbf{res}^{(i)}\| \leq \tau^{(0)}\ \|\mathbf{P}\mathbf{x}^{(i)}\|$ *with* $\tau^{(0)} = 0.1$*, so Theorem 2.3 applies.*

In all runs we stopped when the relative eigenvalue residual satisfied $\| (\mathbf{A} - \varrho(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i)} \| \ / \ | \varrho(\mathbf{x}^{(i)}) | \leq 10^{-10}$*. Table 2 presents the numerical results. Here, as in following examples, we take the starting vector* $\mathbf{x}^{(0)} = c^{(0)}\mathbf{v}_1 + s^{(0)}\mathbf{u}^{(0)}$ *where* $t^{(0)} = s^{(0)}/c^{(0)} = 0.02$*. Other starting guesses were taken but no qualitative differences in the results were observed.*

In Table 2 we observe that both methods exhibit quadratic convergence as predicted by the theory. Both took the same number of outer iterations, but **SEf** was more efficient in terms of the total number of inner iterations required. In fact, this is the key motivation for the modification (34), namely that it is better suited for the application of the Krylov solver since it leads to reduced inner iteration counts. We return to this point in §3.

For theoretical interest only, we note that if $\mathbf{P} = \mathbf{A}$ in Algorithm 2 then (37) and (39) imply

$$t^{(i+1)} \quad \leq \quad \frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_2 - \sigma^{(i)}|} \, \frac{|s^{(i)}||\lambda_n| + \tau^{(i)}}{|c^{(i)}||\lambda_1| - \tau^{(i)}}. \tag{43}$$

Hence it is possible to recover a cubically convergent method if $\tau^{(i)}$ is choosen proportional to $|s^{(i)}|$ and this is obtained by preconditioning the shifted system (31) by $\mathbf{A}$.

The results in Table 2 show a dramatic reduction in the number of inner iterations taken by **SEf** compared to **RQIf**. The reason for this improvement is analysed in §3. However before doing this analysis we also note that the domain of convergence of the outer iteration may be reduced significantly when we decide to solve $(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} = \mathbf{P}\mathbf{x}^{(i)}$ rather than $(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} = \mathbf{x}^{(i)}$ as the following simple example shows.

Example 2.4 (Reduced domain of convergence using (33)) *Assume* $\mathbf{A}$ *is symmetric positive definite and let* $\mathbf{P} = \mathbf{A}$. *Take the factorisation* $\mathbf{P}_1 = \mathbf{A}^{\frac{1}{2}}$. *Then* $\mathbf{P}_1^{-1}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-1}\tilde{\mathbf{y}}^{(i)} = \mathbf{P}_1^T\mathbf{x}^{(i)}$, *which is the preconditioned system (33), reduces to* $(\mathbf{I} - \sigma^{(i)}\mathbf{A}^{-1})\mathbf{y}^{(i)} = \mathbf{x}^{(i)}$. *Assume now* $\mathbf{x}^{(i)} = c^{(i)}\mathbf{v}_1 + s^{(i)}\mathbf{v}_2$ *and that exact solves are used to obtain* $\mathbf{y}^{(i)}$. *We readily obtain the one step bound*

$$\frac{t^{(i+1)}}{t^{(i)}} \quad \leq \quad \frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_2 - \sigma^{(i)}|} \, \frac{|\lambda_2|}{|\lambda_1|}.$$

Now the factor $|\lambda_2/\lambda_1|$ *may be large enough to significantly reduce the domain of convergence of the outer iteration. The domain of convergence would be reduced further if one added the effects of an inexact solver and a less good preconditioner.*

With such a possible drawback there must be some gain in considering this option. As we prove in Section 3.3 the benefit comes when one considers the number of inner iterations needed to solve the linear system when using a Krylov method.

3 The Iterative Solver

Our aim in this section is to understand the performance of the inner iteration part of the inexact inverse iteration algorithm, and since $(\mathbf{A} - \sigma^{(i)}\mathbf{I})$ is symmetric but probably indefinite the natural Krylov method to solve $(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} = \mathbf{x}^{(i)}$ is MINRES (see, for example, [7]).

First, we summarise some known results on MINRES in a form convenient for our use. In §3.1 we provide bounds on ratios of eigenvalues for two common preconditioners that are needed for §3.3. Then in §3.2 and §3.3 we provide an analysis of the number of iterations needed for unpreconditioned and preconditioned inner solves. Section 3.4 contains a discussion on 'a posteriori' bounds.

As discussed in the previous section the linear system will normally be solved iteratively using a preconditioner, $\mathbf{P}$ say, where $\mathbf{P}$ is positive definite and approximates $(\mathbf{A} - \sigma^{(i)}\mathbf{I})$ in some way. If $\mathbf{A}$ arises from a discretised partial differential equation $\mathbf{P}^{-1}$ may be constructed for example using a domain decomposition or multigrid technique. Alternatively $\mathbf{P}$ may be obtained using a Cholesky factorisation of $\mathbf{A}$ (or of a shifted $\mathbf{A}$). In this section we describe the theory for MINRES that is used to understand the inner iteration behaviour for both unpreconditioned and preconditioned solves in Algorithms 1 and 2. Specifically we derive a particular bound on the residual which will be used to provide bounds on the number of iterations needed for the inner solves.

Let us first review some standard results on MINRES applied to a linear system

$$\mathbf{B}\mathbf{z} = \mathbf{b}, \tag{44}$$

where $\mathbf{B}$ is a real symmetric $n \times n$ matrix. Define the Krylov space $\mathcal{K}_k(\mathbf{B}, \mathbf{b})$ by

$$\mathcal{K}_k(\mathbf{B}, \mathbf{b}) \quad = \quad \operatorname{span}\{\mathbf{b}, \mathbf{B}\mathbf{b}, \ldots, \mathbf{B}^{k-1}\mathbf{b}\}.$$

Throughout this paper we take an initial guess $\mathbf{z}_0 = \mathbf{0}$, though other choices are possible. MINRES seeks a solution $\mathbf{z}_k \in \mathcal{K}_k(\mathbf{B}, \mathbf{b})$ characterised by the property $\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\|_2 = \min_{\mathbf{z} \in \mathcal{K}_k} \|\mathbf{b} - \mathbf{B}\mathbf{z}\|_2$.

Assume $\mathbf{B}$ has an eigenvalue decomposition of the form $\mathbf{B} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^T$, where $\mathbf{W}$ is orthogonal and $\mathbf{\Lambda} = \operatorname{diag}(\mu_1, \ldots, \mu_n)$. Then

$$\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\|_2 \quad = \quad \min_{q \in P_k} \|q(\mathbf{B})\mathbf{b}\|_2$$

where P_k denotes the space of polynomials of degree k with $q(0) = 1$, and

$$\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\|_2 \quad = \quad \min_{q \in P_k} \|q(\mathbf{\Lambda})\mathbf{W}^T\mathbf{b}\|_2, \tag{45}$$

from which a straightforward analysis (see, for example, p.54 of [7]) shows that

$$\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\|_2 \quad \leq \quad 2\left(\sqrt{\frac{\kappa - 1}{\kappa + 1}}\right)^{k-1} \|\mathbf{b}\|_2 \tag{46}$$

where $\kappa = \frac{\max_i |\mu_i|}{\min_i |\mu_i|}$. However, this bound may not reflect the performance of MINRES in our application, where because of the particular distribution of the spectrum, MINRES performs significantly better than indicated by (46).

Assume that the spectrum of $\mathbf{B}$ contains a small number of successive eigenvalues which are in some way distinguished from the remaining eigenvalues of $\mathbf{B}$. If $J \subset \mathbb{N}_n := \{1, 2, \ldots n\}$ then $\{\mu_j\}_{j \in J}$ is the distinguished set and $|J|$ denotes the number of elements in it. Set $J^c := N_n - J$ and $\mathbf{Q}_J := \operatorname{diag}\{\delta_1, \ldots, \delta_n\}$ where $\delta_j = 0$ if $j \in J$ and $\delta_j = 1$ otherwise. Further, as in [7, §3.1] or [9, §7.3.6], introduce the polynomial

$$p_J(t) \quad := \quad \prod_{j \in J} \frac{\mu_j - t}{\mu_j} \tag{47}$$

which vanishes for $t \in \{\mu_j\}_{j\in J}$. Clearly $q\,p_J \in \mathcal{P}_k$ for any $q \in \mathcal{P}_{k-|J|}$ and so (45) implies

$$
\begin{aligned}
\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\|_2 &\leq \min_{q\in\mathcal{P}_{k-|J|}} \|q(\mathbf{\Lambda})p_J(\mathbf{\Lambda})\mathbf{W}^T\mathbf{b}\|_2 \\
&\leq \min_{q\in\mathcal{P}_{k-|J|}} \|q(\mathbf{\Lambda})p_J(\mathbf{\Lambda})\mathbf{Q}_J\mathbf{W}^T\mathbf{b}\|_2 \\
&\leq \min_{q\in\mathcal{P}_{k-|J|}} \|q(\mathbf{\Lambda})p_J(\mathbf{\Lambda})\mathbf{Q}_J\|\ \|\mathbf{Q}_J\mathbf{W}^T\mathbf{b}\|_2 \\
&\leq \min_{q\in\mathcal{P}_{k-|J|}} \max_{j\in J^c} |q(\mu_j)p_J(\mu_j)|\|\mathbf{Q}_J\mathbf{W}^T\mathbf{b}\|_2 \\
&\leq \left\{\min_{q\in\mathcal{P}_{k-|J|}} \max_{j\in J^c} |q(\mu_j)|\right\} \max_{j\in J^c} |p_J(\mu_j)|\ \|\mathbf{Q}_J\mathbf{W}^T\mathbf{b}\|_2\,. \qquad (48)
\end{aligned}
$$

Using (48) and standard results on Chebyshev polynomials (see, for example, [8, §3.1] or [9, §7.3.4]) we have the following theorem.

Theorem 3.1 *Suppose that the symmetric matrix* $\mathbf{B}$ *has eigenvalues* $\mu_1, \ldots, \mu_n$ *with corresponding eigenvectors* $\mathbf{w}_1, \ldots, \mathbf{w}_n$. *Let* $\{\mu_j\}_{j\in J}$ *be* $|J|$ *successive eigenvalues of* $\mathbf{B}$ *and introduce the reduced condition number*
$\kappa_J(\mathbf{B}) := \max_{j\in J^c} |\mu_j|/\min_{j\in J^c}|\mu_j|$. *With* $p_J(t)$ *and* $\mathbf{Q}_J$ *defined as above then*

$$
\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\|_2 \leq 2(\max_{j\in J^c}|p_J(\mu_j)|)\left\{\frac{\sqrt{\kappa_J(\mathbf{B})}-1}{\sqrt{\kappa_J(\mathbf{B})}+1}\right\}^{k-|J|} \|\mathbf{Q}_J\mathbf{W}^T\mathbf{b}\|_2
$$

when $\{\mu_j\}_{j\in J^C}$ *contains only elements of the same sign, and*

$$
\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\|_2 \leq 2(\max_{j\in J^c}|p_J(\mu_j)|)\left(\sqrt{\frac{\kappa_J(\mathbf{B})-1}{\kappa_J(\mathbf{B})+1}}\right)^{k-|J|-1} \|\mathbf{Q}_J\mathbf{W}^T\mathbf{b}\|_2
$$

otherwise.

Note that the use of the matrix $\mathbf{Q}_J$ is nonstandard. It will play an important role in the analysis of the inner solves in Algorithm 2 later.

From now on we shall assume that the distinguished set of eigenvalues of $\mathbf{B}$ consists of a simple eigenvalue μ_1 so that $J = 1$. This is the simplest case but is all that we need in the remainder of this paper. In this case we write $\mathbf{Q}_J = \mathbf{Q}_1$, $\kappa_J(\mathbf{B}) = \kappa_1(\mathbf{B}) = \max_{j=2,\ldots,n}|\mu_j|\,/\min_{j=2,\ldots,n}|\mu_j|$, and $p_1(t) = (\mu_1 - t)/\mu_1$. Also we define the two quantities

$$
q_e := \frac{\sqrt{\kappa_1(\mathbf{B})}-1}{\sqrt{\kappa_1(\mathbf{B})}+1}, \qquad (49)
$$

$$
\text{and} \qquad q_i := \sqrt{\frac{\kappa_1(\mathbf{B})-1}{\kappa_1(\mathbf{B})+1}}, \qquad (50)
$$

where q_e refers to the case where μ_1 is an extreme eigenvalue and $\mu_2, \ldots, \mu_n$ are of the same sign, and q_i covers all other situations. For this case we have the following key result.

Corollary 3.1 *Let the assumptions of Theorem 3.1 hold with $J = \{1\}$. Then*

$$\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\|_2 \;\leq\; 2\left(\max_{j=2,\ldots,n} \frac{|\mu_1 - \mu_j|}{|\mu_1|}\right)(q)^{k-\delta}\, \|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\|_2, \tag{51}$$

where $q = q_e, \delta = 1$ if μ_1 is an extreme eigenvalue and $\mu_2, \ldots, \mu_n$ have all the same sign, and $q = q_i, \delta = 2$ otherwise. In addition, if

$$k \geq \delta + \left(\log 2(\max_{j=2,\ldots,n} |\mu_1 - \mu_j|) + \log \frac{\|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\|}{|\mu_1|\tau}\right) / \log q^{-1} \tag{52}$$

then $\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\| \leq \tau$.

Proof: From (51) $\|\mathbf{b} - \mathbf{B}\mathbf{z}_k\| \leq \tau$ will be satisfied provided k is such that

$$2\left(\max_{j=2,\ldots,n} |\mu_1 - \mu_j|\right)\frac{\|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\|}{|\mu_1|\;\tau}(q)^{k-\delta} \leq 1,$$

and the last result follows by taking logs. □

Note that if $q = q_e$ then the residual reduction indicated by (51) is the same as that achieved by the Conjugate Gradient method applied to a positive definite symmetric matrix.

We shall use bound (52) in the following subsections to help understand the behaviour of MINRES inner iterations in inexact inverse iteration. To do this we require bounds on $\|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\|$ for the three main choices for $\mathbf{B}$ and $\mathbf{b}$. This is done in the following Lemma.

Lemma 3.1 *Let $\mathbf{W}$ be the orthogonal matrix of eigenvectors of $\mathbf{B}$ and let $\mathbf{x}^{(i)}$ be as in (5).*

(a) (No Preconditioning) With $\mathbf{B} = (\mathbf{A} - \sigma^{(i)}\mathbf{I}),\ \mathbf{b} = \mathbf{x}^{(i)}$ then

$$\|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\| = \|\mathbf{Q}_1\mathbf{W}^T\mathbf{x}^{(i)}\| \leq |s^{(i)}|. \tag{53}$$

(b) (Standard Preconditioning) With $\mathbf{B} = \mathbf{P}_1^{-1}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T},\ \mathbf{b} = \mathbf{P}_1^{-1}\mathbf{x}^{(i)}$ then

$$\|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\| = \|\mathbf{Q}_1\mathbf{W}^T\mathbf{P}_1^{-1}\mathbf{x}^{(i)}\| \leq \|\mathbf{P}_1^{-1}\|\ . \tag{54}$$

(c) (Simoncini-Elden Preconditioning) With $\mathbf{B} = \mathbf{P}_1^{-1}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T},\ \mathbf{b} = \mathbf{P}_1^{T}\mathbf{x}^{(i)}$ and $\sigma^{(i)}$ chosen to be the Rayleigh quotient then

$$\|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\| = \|\mathbf{Q}_1\mathbf{W}^T\mathbf{P}_1^{T}\mathbf{x}^{(i)}\| \leq\ C'|s^{(i)}| \tag{55}$$

where C' is a positive constant independent of i.

Proof: Parts (a) and (b) are straightforward. To prove (c) write $\mathbf{B}$ in the form

$$\mathbf{B} = \mathbf{P}_1^{-1}(\mathbf{A} - \lambda_1\mathbf{I})\mathbf{P}_1^{-T} + (\lambda_1 - \sigma^{(i)})\mathbf{P}_1^{-1}\mathbf{P}_1^{-T}$$

where we note that $\mathbf{P}_1^{-1}(\mathbf{A}-\lambda_1\mathbf{I})\mathbf{P}_1^{-T}(\mathbf{P}_1^T\mathbf{v}_1)=\mathbf{0}$. Standard perturbation theory for simple eigenvalues of symmetric matrices shows that $\mathbf{B}$ has a simple eigenvalue μ_1 say near 0 with corresponding eigenvector $\mathbf{w}_1$ near $\mathbf{P}_1^T\mathbf{v}_1$. In fact

$$\|\mathbf{P}_1^T\mathbf{v}_1-\mathbf{w}_1\|\leq C|\lambda_1-\sigma^{(i)}|, \tag{56}$$

for some C independent of i. Thus,

$$\begin{aligned}\mathbf{Q}_1\mathbf{W}^T\mathbf{b} &= \mathbf{Q}_1\mathbf{W}^T\mathbf{P}_1^T\mathbf{x}^{(i)} = c^{(i)}\mathbf{Q}_1\mathbf{W}^T\mathbf{P}_1^T\mathbf{v}_1+s^{(i)}\mathbf{Q}_1\mathbf{W}^T\mathbf{P}_1\mathbf{u}^{(i)}\\ &= c^{(i)}\mathbf{Q}_1\mathbf{W}^T(\mathbf{w}_1+(\mathbf{P}_1^T\mathbf{v}_1-\mathbf{w}_1))+s^{(i)}\mathbf{Q}_1\mathbf{W}^T\mathbf{P}_1\mathbf{u}^{(i)}.\end{aligned}$$

Now we see the importance of the $\mathbf{Q}_1$ matrix, which in this case is $\mathrm{diag}\{0,1,\ldots,1\}$. Since $\mathbf{W}^T\mathbf{w}_1=\mathbf{e}_1$ we have that $\mathbf{Q}_1\mathbf{W}^T\mathbf{w}_1=\mathbf{0}$, and so we immediately obtain

$$\|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\| \leq |\lambda_1-\sigma^{(i)}|C+s^{(i)}\,\|\mathbf{P}_1\|\leq C's^{(i)}, \tag{57}$$

for some positive constants C and C' independent of i, since $\sigma^{(i)}$ is the Rayleigh quotient. $\square$

3.1 Eigenvalue bounds

In the analysis of §3.3 we shall assume bounds for $|\lambda_1-\sigma^{(i)}|\,/\,|\mu_1|$, where μ_1 is the smallest eigenvalue (in modulus) of $\mathbf{B}=\mathbf{P}_1^{-1}(\mathbf{A}-\sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T}$. In many practical applications it may be hard to obtain rigorous bounds, but here we examine two cases where bounds are possible.

Example 3.1 (Domain Decomposition Preconditioners) *If $\mathbf{A}$ is a symmetric positive definite matrix arising from discretization of an elliptic PDE and a symmetric positive definite preconditioner $\mathbf{P}^{-1}$ is constructed using domain decomposition methods then one typically has a bound on the condition number of $\mathbf{P}^{-1}\mathbf{A}$. Thus if we denote the eigenvalues of any matrix $\mathbf{M}$ by $\lambda_j(\mathbf{M})$ we assume*

$$\gamma_L \leq \lambda_j(\mathbf{P}^{-1}\mathbf{A}) \leq \gamma_U$$

for some positive constants γ_L,γ_U. Now with $\mathbf{B}=\mathbf{P}_1^{-1}(\mathbf{A}-\sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T}$ we have

$$\lambda_j(\mathbf{B}) = \lambda_j(\mathbf{P}_1^{-1}\mathbf{A}^{\frac{1}{2}}(\mathbf{I}-\sigma^{(i)}\mathbf{A}^{-1})\mathbf{A}^{\frac{1}{2}}\mathbf{P}_1^{-T})$$

and Sylvester's Inertia Theorem can be used to provide bounds on $\lambda_j(\mathbf{B})$. For example, if $\lambda_1<\sigma^{(i)}<\lambda_2$ then with $\mu_1=\lambda_1(\mathbf{B})$ we have $\mu_1<0$ and

$$(1-\frac{\sigma^{(i)}}{\lambda_1})\lambda_n(\mathbf{P}^{-1}\mathbf{A}) \leq \mu_1 \leq (1-\frac{\sigma^{(i)}}{\lambda_1})\lambda_1(\mathbf{P}^{-1}\mathbf{A}),$$

using Sylvester's Inertia Theorem, so that

$$\frac{\lambda_1}{\gamma_U} \leq \frac{\lambda_1}{\lambda_n(\mathbf{P}^{-1}\mathbf{A})} \leq \frac{|\lambda_1-\sigma^{(i)}|}{|\mu_1|} \leq \frac{\lambda_1}{\lambda_1(\mathbf{P}^{-1}\mathbf{A})} \leq \frac{\lambda_1}{\gamma_L}. \tag{58}$$

Example 3.2 (Cholesky Preconditioners) *If* $\mathbf{A}$ *is symmetric positive definite, and an incomplete Cholesky factorisation of* $\mathbf{A}$ *is used to find* $\mathbf{P}$*, i.e.* $\mathbf{A} = \mathbf{P}_1\mathbf{P}_1^T + \mathbf{E}$ *with* $\mathbf{E}$ *'small', say* $\|\mathbf{E}\| < \lambda_1$*. Then using ideas in [20] we write*

$$\begin{aligned} \mathbf{P}_1^{-1}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T}\mathbf{w}_1 &= \mu_1\mathbf{w}_1, \\ \textit{as} \qquad (\mathbf{A} - \sigma^{(i)}\mathbf{I})\widetilde{\mathbf{w}} = \mu_1\mathbf{P}_1\mathbf{P}_1^T\widetilde{\mathbf{w}} &= \mu_1(\mathbf{A} - \mathbf{E})\widetilde{\mathbf{w}}, \end{aligned}$$

where $\widetilde{\mathbf{w}} = \mathbf{P}_1^{-T}\mathbf{w}_1$*. So*

$$(\mathbf{A} + \frac{\mu_1}{1-\mu_1}\mathbf{E})\widetilde{\mathbf{w}} = \frac{\sigma^{(i)}}{1-\mu_1}\widetilde{\mathbf{w}}.$$

Now comparing with $\mathbf{A}\mathbf{v}_1 = \lambda_1\mathbf{v}_1$ *the Bauer-Fike Theorem gives*

$$\left|\frac{\sigma^{(i)}}{1-\mu_1} - \lambda_1\right| \le \left|\frac{\mu_1}{1-\mu_1}\right| \|\mathbf{E}\|$$

and hence, since $\lambda_1 > 0$ *and* $\|\mathbf{E}\| < \lambda_1$ *by the assumptions above,*

$$\lambda_1 - \|\mathbf{E}\| \le \frac{|\lambda_1 - \sigma^{(i)}|}{|\mu_1|} \le \lambda_1 + \|\mathbf{E}\| . \tag{59}$$

Thus in both examples considered here we can say that, under suitable assumptions,

$$|\lambda_1|\, C' \le \frac{|\lambda_1 - \sigma^{(i)}|}{|\mu_1|} \le |\lambda_1|\, C \tag{60}$$

for some positive constants C' and C independent of i.

3.2 Inner Iterations for Unpreconditioned MINRES

Consider now the use of (52) to help understand the behaviour of MINRES in inexact inverse iteration. For simplicity we shall consider in detail the case where λ_1 is the smallest eigenvalue of $\mathbf{A}$, but the theory can be extended to any well-separated simple eigenvalue. Let λ_1 satisfy $\lambda_1 < \lambda_2 \le \lambda_3 \ldots \le \lambda_n$, and assume that any shift $\sigma^{(i)}$ satisfies (4) so that we can regard $\lambda_1 - \sigma^{(i)}$ as well-separated from $\lambda_j - \sigma^{(i)}, j = 2, \ldots, n$.

For unpreconditioned MINRES we take $\mathbf{B} = (\mathbf{A} - \sigma^{(i)}\mathbf{I})$, $\mathbf{b} = \mathbf{x}^{(i)}$, and

$$\mathbf{res}_{k^{(i)}}^{(i)} := \mathbf{x}^{(i)} - (\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}_{k^{(i)}}^{(i)}, \tag{61}$$

where $\mathbf{y}_{k^{(i)}}^{(i)}$ denotes the $k^{(i)}$th iterate of MINRES. Using case (a) in Lemma 3.1, and $\delta = 1$ in (52) we find that to achieve (11) it is sufficient for $k^{(i)}$ to satisfy

$$k^{(i)} \ge 1 + \left\{\log 2|\lambda_1 - \lambda_n| + \log \frac{|s^{(i)}|}{|\lambda_1 - \sigma^{(i)}|\tau^{(i)}}\right\} / \log q_e^{-1}. \tag{62}$$

The theory in Section 2.3 assumed the upper bounds $\tau^{(i)} \leq C_2|s^{(i)}|^\beta$ and $|\lambda_1 - \sigma^{(i)}| \leq C_1|s^{(i)}|^\alpha$. Now, in addition, assume the two sided bounds

$$C_1'|s^{(i)}|^\alpha \leq |\lambda_1 - \sigma^{(i)}| \leq C_1|s^{(i)}|^\alpha, \quad C_2'|s^{(i)}|^\beta \leq \tau^{(i)} \leq C_2|s^{(i)}|^\beta, \tag{63}$$

where the constants are positive and independent of i. These are easily seen to be satisfied in the cases of interest here, namely, for a fixed shift or a Rayleigh quotient shift (7), and a constant tolerance or decreasing tolerance based on the eigenvalue residual (8). Using the lower bounds for $\tau^{(i)}$ and $|\lambda_1 - \sigma^{(i)}|$ in (63) we see that (11) is satisfied if

$$k^{(i)} \quad \geq \quad 1 + \left\{ \log \frac{2|\lambda_1 - \lambda_n|}{C_1'C_2'} + (\alpha + \beta - 1) \log |s^{(i)}|^{-1} \right\} / \log q_e^{-1}. \tag{64}$$

We have thus proved the following Lemma.

Lemma 3.2 *(a) Assume Algorithm 1 is used to compute the smallest eigenvalue of* $\mathbf{A}$ *using unpreconditioned MINRES for the inexact solves. Assume in addition that the lower bounds given by (63) hold. If*

$$k^{(i)} \quad \geq \quad 1 + \left\{ \log \frac{2|\lambda_1 - \lambda_n|}{C_1'C_2'} + (\alpha + \beta - 1) \log |s^{(i)}|^{-1} \right\} / \log(q_e^{-1}),$$

then $\mathbf{res}^{(i)}$ *defined by (61) satisfies* $\|\mathbf{res}^{(i)}\| \leq \tau^{(i)}$ *and Algorithm 1 converges with a rate predicted by Theorem 2.2.*

(b) In particular, for convergence to occur in the inexact Rayleigh Quotient methods of Theorem 2.1 we see that for a decreasing tolerance (case (a)) it is sufficient that

$$k^{(i)} \quad \geq \quad 1 + \left\{ \log C + 2 \log |s^{(i)}|^{-1} \right\} / \log(q_e^{-1}) \tag{65}$$

for some C *independent of* i*. (This is the case of* $\alpha = 2, \beta = 1$*). Moreover for a fixed tolerance (case(b)) it is sufficient that*

$$k^{(i)} \quad \geq \quad 1 + \left\{ \log C + \log |s^{(i)}|^{-1} \right\} / \log(q_e^{-1}) \tag{66}$$

for some C *independent of* i*. (This is the case of* $\alpha = 2, \beta = 0$*).*

We note that if $\alpha + \beta = 1$ (i.e. linear convergence in Theorem 2.2) then the condition on $k^{(i)}$ does not grow. This is confirmed by numerical results in Example 3.3. However, for **RQId** and **RQIf**, Lemma 3.2, case (b), predicts an increase in the number of inner iterations required for each outer iteration, with **RQId** being more expensive than **RQIf**. This behaviour is indeed observed in Table 1. Significantly, we see that the effect of letting $\sigma^{(i)}$ converge quadratically to λ_1 produces only logarithmic growth in the number of inner iterations needed to achieve convergence, so that we need not be concerned that the Krylov solver is applied to a matrix which is becoming more and more singular. The explanation lies in the interplay between the choices of shift, tolerance and right hand side. For unpreconditioned solves the term $\log \dfrac{\|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\|}{|\mu_1|\tau}$ in the bound for k given by (52) produces the $\log \dfrac{s^{(i)}}{|\lambda_1 - \sigma^{(i)}|\tau^{(i)}}$ term in (62), which provides nothing worse than logarithmic growth in $|s^{(i)}|^{-1}$.

It is well known that the bound given by (51) is, at best, descriptive and is unlikely to be sharp. As a consequence (64) is unlikely to provide a realistic estimate for $k^{(i)}$ and should only be used in a descriptive sense as above. Nevertheless, descriptive bounds such as this play a key role in the appraisal of the practical value of various iterative methods, especially when applied to discretizations of PDEs.

A similar analysis can be carried out if one wishes to calculate an interior eigenvalue of a general matrix $\mathbf{A}$. We do not repeat this analysis here but a bound similar to (64) is obtained with the main difference that the factor q_e is replaced by q_i given by (50). However the comments about the likely increase in the number of inner iterations remain valid.

3.3 Inner Iterations for Preconditioned MINRES

In this subsection we give an analysis of the number of inner iterations for the two preconditioned methods using preconditioned MINRES with Rayleigh quotient shifts and a fixed tolerance. (The two methods are covered by Theorems 2.1 and 2.3). The main result is given in the following Lemma.

Lemma 3.3 *(a) (Standard Preconditioning) Assume Algorithm 1 with Rayleigh quotient shifts and a fixed tolerance $\tau^{(i)} = \tau^{(0)}$ is used to compute the smallest eigenvalue of $\mathbf{A}$ using preconditioned MINRES for the inexact solves. Additionally, assume $|(\lambda_1 - \sigma^{(i)})/\mu_1|$ satisfies (60). If*

$$k^{(i)} \quad \geq \quad 1 + \{\log C + 2\log |s^{(i)}|^{-1}\}/\log q_e^{-1} \tag{67}$$

where C is a known constant independent of i, then the outer iteration converges quadratically.

(b) (Simoncini-Elden Preconditioning) Assume Algorithm 2 with Rayleigh quotient shifts and a fixed tolerance $\tau^{(i)} = \tau^{(0)}$ is used to compute the smallest eigenvalue of $\mathbf{A}$ using preconditioned MINRES for the inexact solves. Additionally, assume $|(\lambda_1 - \sigma^{(i)})/\mu_1|$ satisfies (60). If

$$k^{(i)} \quad \geq \quad 1 + \{\log C' + \log |s^{(i)}|^{-1}\}/\log q_e^{-1} \tag{68}$$

where C' is a known constant independent of i then the outer iteration converges quadratically.

Proof: The standard preconditioned case is given by (in the notation of (51) and (52))

$$\mathbf{z}_k = \mathbf{P}_1^T\mathbf{y}^{(i)}, \quad \mathbf{B} = \mathbf{P}_1^{-1}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T}, \quad \mathbf{b} = \mathbf{P}_1^{-1}\mathbf{x}^{(i)}, \tag{69}$$

with, from (54), $\| \mathbf{Q}_1\mathbf{W}^T\mathbf{b} \| \leq \| \mathbf{P}_1^{-1} \|$, and in the Simoncini-Elden preconditioned form given in Algorithm 2 we have

$$\mathbf{z}_k = \mathbf{P}_1^T\mathbf{y}^{(i)}, \quad \mathbf{B} = \mathbf{P}_1^{-1}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T}, \quad \mathbf{b} = \mathbf{P}_1^T\mathbf{x}^{(i)},$$

with, from (55), $\|\mathbf{Q}_1\mathbf{W}^T\mathbf{b}\|\leq C|s^{(i)}|$, for some constant C independent of i. Here we see that the Simoncini-Elden preconditioning retains the $|s^{(i)}|$ factor in the bound on $\| \mathbf{Q}_1\mathbf{W}^T\mathbf{b} \|$. This turns out to be the main difference between the methods and will explain the improved inner iteration performance of the Simoncini-Elden preconditioning over standard preconditioning.

Proof of (a). For the standard preconditioned case we stop Algorithm 1 using the residual of the unpreconditioned system not the residual of $\mathbf{B}\mathbf{z}_{k^{(i)}} = \mathbf{b}$. Now

$$\|(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} - \mathbf{x}^{(i)}\|=\|\mathbf{P}_1(\mathbf{B}\mathbf{z}_{k^{(i)}} - \mathbf{b})\|\leq\|\mathbf{P}_1\|\|\mathbf{B}\mathbf{z}_{k^{(i)}} - \mathbf{b}\|, \tag{70}$$

and so, if $k^{(i)}$ is such that

$$\|\mathbf{B}\mathbf{z}_{k^{(i)}} - \mathbf{b}\|\leq \tau^{(i)}\ \|\mathbf{P}_1\|^{-1}, \tag{71}$$

then we satisfy

$$\|(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} - \mathbf{x}^{(i)}\|\leq \tau^{(i)}. \tag{72}$$

Using (51), (52) and (54), condition (71) holds if $k^{(i)}$ satisfies,

$$k^{(i)} \geq 1 + \left\{\log\left(2 \max_{j=2,\dots,n} |\mu_1 - \mu_j|\kappa(\mathbf{P}_1)\right) + \log\frac{1}{|\mu_1|\ \tau^{(i)}}\right\} / \log q_e^{-1}. \tag{73}$$

or, equivalently,

$$k^{(i)} \geq 1 + \left\{\log\left(2 \max_{j=2,\dots,n} |\mu_1 - \mu_j|\kappa(\mathbf{P}_1)\frac{|\lambda_1 - \sigma^{(i)}|}{|\mu_1|}\right) + \log\frac{1}{|\lambda_1 - \sigma^{(i)}|\ \tau^{(i)}}\right\} / \log q_e^{-1}. \tag{74}$$

Here q_e is given by (49). The quantity $\frac{|\lambda_1 - \sigma^{(i)}|}{|\mu_1|}$ relates the eigenvalue nearest zero of $(\mathbf{A} - \sigma^{(i)}\mathbf{I})$ to the value of the corresponding eigenvalue of $\mathbf{P}_1^{-1}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{P}_1^{-T}$. We shall assume the bound (60) for this ratio as is discussed in detail in §3.1. Note that $\tau^{(i)} = \tau^{(0)}$, a constant, and we no longer have a factor of $|s^{(i)}|$ in the numerator of the second log term in (74) compared to (62). This log term produces the $2\log|s^{(i)}|^{-1}$ term in (67).

Proof of (b). For the Simoncini-Elden preconditioned approach in Algorithm 2 the analysis proceeds similarly. To achieve

$$\|(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} - \mathbf{P}\mathbf{x}^{(i)}\|\leq \tau^{(i)}\ \|\mathbf{P}\mathbf{x}^{(i)}\| \tag{75}$$

it is sufficient that $\| \mathbf{P}_1(\mathbf{P}_1^{-1}(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{P}_1^T\widetilde{\mathbf{y}}^{(i)} - \mathbf{P}_1^T\mathbf{x}^{(i)}) \|\leq \tau^{(i)}\ \| \mathbf{P}\mathbf{x}^{(i)} \|$, where $\widetilde{\mathbf{y}}^{(i)} = \mathbf{P}_1^{-T}\mathbf{y}^{(i)}$. In the notation of Lemma 3.1, (c), condition (75) will hold if $\|\mathbf{P}_1\|\|\mathbf{B}\mathbf{z}_k - \mathbf{b}\|\leq \tau^{(i)}\ \|\mathbf{P}\mathbf{x}^{(i)}\|$ and this is achieved provided

$$k^{(i)} \geq 1 + \left\{\log\left(2 \max_{j=2,\dots,n} |\mu_1 - \mu_j|\frac{|\lambda_1 - \sigma^{(i)}|\ \|\mathbf{P}_1\|}{|\mu_1|\ \|\mathbf{P}\mathbf{x}^{(i)}\|}\right) + \log\frac{|s^{(i)}|}{|\lambda_1 - \sigma^{(i)}|\ \tau^{(i)}}\right\} / \log q_e^{-1}. \tag{76}$$

where the second log term now has $|s^{(i)}|$ in the numerator and has the same form as the second term in the unpreconditioned inequality (62). This term produces the

$\log |s^{(i)}|^{-1}$ term in (68). $\square$

Because of the different factors multiplying the $\log |s^{(i)}|^{-1}$ terms in (67) and (68) we expect that Algorithm 2 may be less expensive in terms of the total number of inner iterations compared with preconditioned Algorithm 1. This is indeed observed in Table 2, where we compare the number of inner iterations needed by methods **RQIf** (Lemma 3.3, case (a)) and **SEf** (Lemma 3.3, case (b)) applied to the matrix in Example 2.3 to compute the interior eigenvalue. We see that both methods exhibit an increase in the number of inner iterations as the outer iteration proceeds as predicted by (67) and (68), but **RQIf** is more expensive than **SEf** with regard to the total number of inner iterations to achieve comparable accuracy which may be explained by the multiplier 2 in front of the second log term in (67), compared with the multiplier 1 in (68).

3.4 'A posteriori' bounds for preconditioned MINRES

The discussion in the previous subsection is a natural consequence of the inequality (52) on the number of inner iterations in MINRES. In this subsection we look at an alternative approach that extracts additional information available from (74) and (76) by combining the MINRES theory with the inexact inverse iteration convergence theory of §2. Note that the theory in this section does not rely on $\sigma^{(i)}$ being the Rayleigh Quotient.

In the previous sections we considered 'a priori' information about the cost of an inner solve. Here we will use 'a posteriori' information to obtain an upper bound on the overall cost of the inner solves of a convergent method. To this end we define $k_M^{(i)}$ to be the actual number of inner iterations used by MINRES at step i, that is,

$$\|\mathbf{res}^{(i)}_{k_M^{(i)}}\| \leq \tau^{(i)}, \quad \|\mathbf{res}^{(i)}_k\| > \tau^{(i)}, \ \ \forall k < k_M^{(i)}. \tag{77}$$

Now the inequalities in §3.2 and §3.3 produce sufficient conditions on the number of inner solves needed to ensure a residual tolerance is satisfied. Equally well, however, these sufficient conditions provide *upper* bounds on the actual number of inner iterations needed. This is seen in the following consequence of Corollary 3.1.

Corollary 3.2 *Let the assumptions of Corollary 3.1 hold. Define k_* by*

$$k_* := 1 + \left(\log 2(|\max_{j=2,\ldots,n} |\mu_1 - \mu_j|) + \log \frac{\|\mathbf{Q}_1 \mathbf{W}^T \mathbf{b}^{(i)}\|}{|\mu_1| \tau^{(i)}} \right) / \log q^{-1}, \tag{78}$$

and let $k_M^{(i)}$ denote the actual number of inner iterations used by MINRES to solve $\mathbf{B}\mathbf{z} = \mathbf{b}^{(i)}$ to a tolerance $\tau^{(i)}$. Then

$$k_M^{(i)} \leq k_* + 1. \tag{79}$$

Proof: The quantity k_* may not be an integer and so one needs to add 1 to ensure an upper bound on the integer $k_M^{(i)}$. $\square$

The idea in this subsection is to use the right hand side of (13) to link $k_M^{(i)}$ with $t^{(i+1)}$ as follows. Assume the inexact inverse iteration algorithm under consideration converges with the second equation in (63) with $\beta = 1$ satisfied or with $\tau^{(i)}$ fixed. So we can say

$$\frac{|s^{(i)}| + \tau^{(i)}}{|c^{(i)}| - \tau^{(i)}} \leq C_5 \tau^{(i)} \tag{80}$$

for some C_5 independent of i. Thus (13) gives

$$t^{(i+1)} \leq \frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_2 - \sigma^{(i)}|}\, C_5 \tau^{(i)}, \tag{81}$$

and hence

$$\frac{1}{|\lambda_1 - \sigma^{(i)}|\tau^{(i)}} \leq \frac{C_5}{|\lambda_2 - \sigma^{(i)}|\; t^{(i+1)}}. \tag{82}$$

Hence, taking logs we have

$$\log \frac{1}{|\lambda_1 - \sigma^{(i)}|\tau^{(i)}} \leq \log \frac{C_5}{|\lambda_2 - \sigma^{(i)}|} + \log \frac{1}{t^{(i+1)}}. \tag{83}$$

Now for standard preconditioned solves the upper bound on $k_M^{(i)}$ is given (from (78) and (79)) by

$$k_M^{(i)} \leq 2 + \left(\log (2 \max_{j=2,\ldots,n} |\mu_1 - \mu_j|\; \kappa(\mathbf{P}_1) \frac{|\lambda_1 - \sigma^{(i)}|}{|\mu_1|}) + \log \frac{1}{|\lambda_1 - \sigma^{(i)}|\tau^{(i)}} \right) / \log q_e^{-1} \tag{84}$$

and hence, using (82),

$$k_M^{(i)} \leq 2 + (\log C + \log \frac{1}{t^{(i+1)}}) / \log q_e^{-1} \tag{85}$$

where

$$C = 2 \max_{j=2,\ldots,n} |\mu_1 - \mu_j|\; \kappa(\mathbf{P}_1)\; \frac{|\lambda_1 - \sigma^{(i)}|}{\mu_1}\; \frac{C_5}{|\lambda_2 - \sigma^{(i)}|}. \tag{86}$$

Under assumptions (4) and (60), C is bounded independent of i.

Now consider Algorithm 2 with a fixed tolerance so that (39) holds with $\|\mathbf{res}^{(i)}\| \leq \tau^{(0)}\; \|\mathbf{P}\mathbf{x}^{(i)}\|$. Assuming (38) and (40) also hold and that the method is convergent, then we may write

$$t^{(i+1)} \quad \leq \quad \frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_2 - \sigma^{(i)}|} C$$

for some C independent of i using (39). Reasoning as in the standard preconditioned case we obtain a similar bound for $k_M^{(i)}$ but with the key difference that the $\|\mathbf{Q}_1 \mathbf{W}^T \mathbf{b}^{(i)}\|$ term leads to a $\log \frac{t^{(i)}}{t^{(i+1)}}$ term rather than the $\log \frac{1}{t^{(i+1)}}$ term in (85), and this provides a simplification as is shown in the following theorem.

Theorem 3.2 *(a) (Standard Preconditioning) Assume Algorithm 1 converges, where the system* $(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} = \mathbf{x}^{(i)}$ *is solved by preconditioned MINRES. Let* $k_M^{(i)}$ *denote the actual number of inner iterations used by MINRES at step* i*. Then*

$$k_M^{(i)} \;\leq\; 2 + (\log C + \log \frac{1}{t^{(i+1)}}) / \log(q_e^{-1}) \tag{87}$$

for some known positive constant C *independent of* i*. If* $\mathcal{N}$ *outer iterations are needed to reduce the error angle by* $10^{-\gamma}$*, for some* γ *then*

$$\sum_{i=0}^{\mathcal{N}-1} k_M^{(i)} \;\leq\; 2\mathcal{N} + \Big[\mathcal{N}\log C + \sum_{i=0}^{\mathcal{N}-1} \log \frac{1}{t^{(i+1)}}\Big] / \log(q_e^{-1}). \tag{88}$$

.

(b) (Simoncini-Elden Preconditioning) Assume Algorithm 2 with a fixed tolerance satisfying (40) converges, where the system $(\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} = \mathbf{P}\mathbf{x}^{(i)}$ *is solved by preconditioned MINRES with Rayleigh quotient shifts. Let* $k_M^{(i)}$ *denote the actual number of inner iterations used by MINRES at step* i *so that* $\| (\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}^{(i)} - \mathbf{P}\mathbf{x}^{(i)}\| \leq \tau^{(i)} \; \|\mathbf{P}\mathbf{x}^{(i)}\|$ *holds. Then*

$$k_M^{(i)} \;\leq\; 1 + (\log C + \log \frac{t^{(i)}}{t^{(i+1)}}) / \log(q_e^{-1}) \tag{89}$$

for some known positive constant C *independent of* i*. If* $\mathcal{N}$ *outer iterations are needed to reduce the error angle by* $10^{-\gamma}$*, for some* γ*, then*

$$\sum_{i=0}^{\mathcal{N}-1} k_M^{(i)} \;\leq\; 2\mathcal{N} + \Big[\mathcal{N}\log C + \gamma \log 10\Big] / \log(q_e^{-1}). \tag{90}$$

Comparing (90) with (88) we anticipate that the total number of inner iterations in case (b) would be significantly lower than in case (a) since $\gamma \log 10$ in (90) will be significantly smaller than $\sum_{i=0}^{\mathcal{N}-1} \log \frac{1}{t^{(i+1)}}$, the corresponding term in (88). Note also that if we take $\mathbf{P} = \mathbf{I}$ in case (b) above then the behaviour for an unpreconditioned solver is described.

The following example helps to illustrate the results of Theorem 3.2.

Example 3.3 *Consider again Example 2.3 where method* **RQIf** *is described and let us also consider the following linearly convergent method.*

FSd*: Algorithm 1 with fixed shift* $\sigma^{(i)} = \sigma^{(0)}$ *and descreasing tolerance* $\tau^{(i)} = \min\{\tau_0, \tau_1 \|\mathbf{r}^{(i)}\| / \sigma^{(0)}\}$*.*

In Table 3 we present results obtained using **FSd** *and* **RQIf** *in the calculation of the smallest eigenvalue.*

First consider the results obtained by unpreconditioned **FSd** on the left hand side of Table 3. The outer rate of convergence is linear, and so Lemma 3.2 predicts no growth in inner iterations as the outer iteration proceeds. This is indeed observed. Further, in most iterations we have $t^{(i+1)}/t^{(i)} \approx 0.1$ with an inner cost of about 90

	unprec **FSd** $\tau_1 = 0.125$		prec **FSd** $\tau_1 = 0.5$		prec **RQIf** $\tau^{(0)} = 0.9$	
	$tan\theta^{(i)}$	k^{i-1}	$tan\theta^{(i)}$	k^{i-1}	$tan\theta^{(i)}$	k^{i-1}
0	1.0e-02		1.0e-02		1.0e-02	
1	5.9e-04	56	1.3e-04	16	5.9e-03	8
2	5.4e-05	97	1.0e-05	18	1.2e-06	19
3	5.3e-06	95	1.2e-06	20	1.3e-12	30
4	5.6e-07	98	1.3e-07	22		
5	5.9e-08	91	1.4e-08	24		
6	6.3e-09	93	1.6e-09	26		
7	6.7e-10	84	1.8e-10	28		
8	7.0e-11	90	2.1e-11	30		
9	2.1e-11	30				
$\sum k^{i-1}$		734		184		57

Table 3: Numerical results showing the behaviour of $k^{(i)}$ for **FSd** and **RQIf**.

iterations, whereas the last iteration provides an improvement of $t^{(i+1)}/t^{(i)} \approx 0.33$ and costs 30 iterations, which is consistent with (89).

Using preconditioned linear solves we expect that the number of inner iterations at each outer iteration will be significantly decreased compared with the unpreconditioned case. This is indeed observed in the middle columns of Table 3. However we note that in the preconditioned case the number of inner iterations increases with the progress of the outer iteration as predicted by (87).

Further, (87) indicates that, whatever the outer rate of convergence of the standard preconditioned method the number of inner iterations $k^{(i)}$ to produce an error angle $t^{(i+1)}$ depends on $\log(1/t^{(i+1)})$ and is independent of the previous error angle. This is confirmed in Table 3 where for $i = 3$ preconditioned **FSd** needed 20 iterations to produce an error angle of 1.2×10^{-06}, whereas at $i = 2$ preconditioned **RQIf** achieved an error angle of 1.2×10^{-06} after 19 iterations, essentially the same cost, even though the previous error angles were considerably different. This shows the effect of $\log \frac{1}{t^{(i+1)}}$ in (87).

Comparing preconditioned **RQIf** with preconditioned **SEf** in Table 2 we see the superiority of **SEf** in terms of overall costs to achieve a given accuracy. This is predicted in Theorem 3.2 where for **SEf** the total cost depends on a $\gamma \log 10$ term in (90), whereas the corresponding term in (88) contains a sum of $\log \frac{1}{t^{(i+1)}}$ terms.

Finally we note that in Table 2 algorithm **RQIf** is approximating the 20th eigenvalue compared with the smallest eigenvalue as in Table 3, and hence the total number of inner iterations required is larger in Table 2 than in Table 3.

4 Stopping Conditions

As we have already remarked, we use the standard relative residual stopping condition

$$\|\mathbf{res}^{(i)}\| \leq \tau^{(i)} \, \|\mathbf{P}\mathbf{x}^{(i)}\| \tag{91}$$

in our convergence analysis, in our numerical algorithm, and in our treatment of the inner iteration performance of the iterative solver MINRES. In the paper [20] a different stopping condition is considered. There they emphasise that the ultimate aim is to improve the current estimate of the eigenvector, and this may improve even though $\|\mathbf{res}^{(i)}\|$ does not reduce. To this end a different stopping condition is suggested and this we describe below. In this section we also present some numerical results obtained using the Krylov solver MINRES to compare the two stopping conditions applied to Algorithm 2. Our results indicate that the stopping condition in [20] shows little improvement over a residual stopping condition and may, in fact, be less reliable.

Let $\mathbf{y}_k^{(i)}$ denote the approximate solution of (34) after k steps of MINRES with starting guess $\mathbf{y}^{(i)} = \mathbf{0}$, and set $\mathbf{x}_k^{(i+1)} = \mathbf{y}_k^{(i)} / \, \|\mathbf{y}_k^{(i)}\|$. In this subsection we add the subscript k to the residual so that

$$\mathbf{res}_k^{(i+1)} := \mathbf{P}\mathbf{x}^{(i)} - (\mathbf{A} - \sigma^{(i)}\mathbf{I})\mathbf{y}_k^{(i)}. \tag{92}$$

The stopping condition in [20] involves three components. For a given $\tau_{inner}^{SE} > 0$, the inner iteration should satisfy (see (7.2) in [20])

$$stop_1(k) := \frac{|\, \|\mathbf{y}_k^{(i)}\| - \|\mathbf{y}_{k-1}^{(i)}\| \,|}{\|\mathbf{y}_k^{(i)}\|} < \tau_{inner}^{SE}, \tag{93}$$

and

$$stop_2(k) := \|\mathbf{y}_k^{(i)}\| \|(\mathbf{A} - \varrho(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}_k^{(i)}\| > 1. \tag{94}$$

(See (5.3) in [20]). Finally, the whole algorithm is stopped when the relative eigenvalue residual is smaller than a required outer tolerance $\tau_{outer} > 0$

$$relr(\mathbf{x}_k^{(i+1)}) := \frac{\|(\mathbf{A} - \varrho(\mathbf{x}_k^{(i+1)})\mathbf{I})\mathbf{x}_k^{(i+1)}\|}{|\varrho(\mathbf{x}_k^{(i+1)})|} \leq \tau_{outer}. \tag{95}$$

Note that in the experiments reported here and in [20] this last condition is checked after each step of the inner iteration. This is easily accomplished using only additional inner products (adapting the approach in Appendix A in [20] to MINRES, see [1]). In summary, the overall stopping condition is

$$\{stop_1(k) \leq \tau_{inner}^{SE} \;\; AND \;\; stop_2(k) > 1\} \quad OR \quad relr(\mathbf{x}_k^{(i+1)}) \leq \tau_{outer}. \tag{96}$$

In Algorithm 2 we also use (95) but instead of (93) and (94) we use the residual test

$$\|\mathbf{res}_k^{(i)}\| \leq \tau^{(i)} \, \|\mathbf{P}\mathbf{x}^{(i)}\|, \tag{97}$$

	SEf extreme $\tau^{(0)} = 0.5$		**SEstop** extreme $\tau^{SE}_{inner} = 0.25$		**SEf** interior $\tau^{(0)} = 0.1$		**SEstop** interior $\tau^{SE}_{inner} = 0.001$	
	$tan\theta^{(i)}$	$k^{(i-1)}$	$tan\theta^{(i)}$	$k^{(i-1)}$	$tan\theta^{(i)}$	$k^{(i-1)}$	$tan\theta^{(i)}$	$k^{(i-1)}$
0	1.0e-02		1.0e-02		1.0e-03		1.0e-03	
1	6.5e-03	3	5.5e-03	4	6.1e-05	36	8.6e-05	23
2	1.2e-04	8	9.3e-05	9	5.1e-10	65	2.7e-05	26
3	9.0e-09	16	1.7e-09	18	4.3e-10	8	8.2e-11	55
4	2.8e-12	14	2.2e-12	13				
$\sum k^{(i-1)}$		41		44		109		104

Table 4: Comparison of the stopping conditions (98) and (96) using preconditioned MINRES applied to Example 2.3.

as discussed in our earlier theory. So for some $\tau^{(i)} > 0$ and $\tau_{outer} > 0$ we stop an inner solve using

$$\|\mathbf{res}_k^{(i)}\| \leq \tau^{(i)} \, \|\mathbf{P}\mathbf{x}^{(i)}\| \quad OR \quad relr(\mathbf{x}_k^{(i+1)}) \leq \tau_{outer}. \tag{98}$$

Example 4.1 Comparison of stopping conditions (96) and (98) *Again we consider the matrix in Example 2.3 and use MINRES with the same preconditioner as in Example 2.3, applied to the same Algorithm with the same starting values. We compare two versions of Algorithm 2, namely,*

(a) **SEf***: Solve (34) using preconditioned MINRES with stopping condition (98).*

(b) **SEstop***: Solve (34) using preconditioned MINRES with stopping condition (96).*

In Table 4 we present results to find λ_1*, which we call the "extreme" eigenvalue, and* $\lambda_{20} = 4.06 \times 10^5$ *the 20th smallest eigenvalue, which we call the "interior" eigenvalue. In all cases we took* $\tau_{outer} = 10^{-10}$*. The values of* $\tau^{(i)} = \tau^{(0)}$ *are given in the table.*

First, it is important to note that for the computations of both λ_1 and λ_{20} using **SEstop** in (93) we tested many values for τ^{SE}_{inner}, and in the numerical results presented here we used the *optimal* value (that is, we used the one leading to the minimum number of inner iterations). In our experience the performance of **SEstop** was quite sensitive to the choice of τ^{SE}_{inner}. In particular, when calculating the interior eigenvalue, if τ^{SE}_{inner} is chosen too large then stagnation or non-convergence can readily occur. In contrast the performance of **SEf** was rather insensitive to the choice of $\tau^{(0)}$.

The values of $\tau^{(0)}$ and the optimal τ^{SE}_{inner} for each experiment are given in Table 4. We note that for both the extreme and interior eigenvalues there is little difference in the performance of the methods **SEf** and **SEstop**, both with regard to outer iterations and the number of inner iterations required.

a) Extreme eigenvalue b) Interior eigenvalue

Figure 1: Comparison of the convergence history for the eigenvalue residuals $\mathbf{r}^{(i)}_{SEf(k)}$ (dotted), $\mathbf{r}^{(i)}_{SEstop(k)}$ (crosses) and linear solve residuals $\mathbf{res}(i)_{SEf(k)}$ (line) and $\mathbf{res}(i)_{SEstop(k)}$ (circles) against number of inner iterations.

To further compare the methods we define

$$
\begin{aligned}
\mathbf{r}^{(i)}_{SEf(k)} &:= \|(\mathbf{A} - \varrho(\mathbf{x}_k^{(i+1)})\mathbf{I})\mathbf{x}_k^{(i+1)}\|, \quad \text{using } \mathbf{SEf}, \\
\mathbf{res}^{(i)}_{SEf(k)} &:= \|\mathbf{P}\mathbf{x}^{(i)} - (\mathbf{A} - \varrho(\mathbf{x}_k^{(i+1)})\mathbf{I})\mathbf{y}_k^{(i)}\|, \quad \text{using } \mathbf{SEf},
\end{aligned}
$$

with similar definitions for $\mathbf{r}^{(i)}_{SEstop(k)}$ and $\mathbf{res}^{(i)}_{SEstop(k)}$. We compare the stopping conditions (96) and (98) in Figure 1 where we plot $\mathbf{r}^{(i)}_{SEf(k)}$ against $\mathbf{r}^{(i)}_{SEstop(k)}$, and $\mathbf{res}^{(i)}_{SEf(k)}$ against $\mathbf{res}^{(i)}_{SEstop(k)}$ for both the extreme and interior eigenvalues. In this figure the horizontal axis counts all the inner iterations. We observe that there appears little difference in the qualitative behaviour of the methods **SEf** and **SEstop** with respect to either the eigenvalue residuals, the system residuals, or as previously seen in Table 4, with respect to the total number of outer iterations required. Note that the spike in $\mathbf{r}^{(i)}_{SEf(k)}$ is caused at the start of a new outer iteration where the first inner iteration provides a poorer approximation of the sought eigenvalue due to the fact that the $(1,1)$ element in the triangular matrix formed by MINRES is zero up to round-off erro. This phenomenon was noticed by [19].

In Figure 2 we plot the values of $stop_1(k)$ given by (93) as the iteration proceeds for both the extreme and interior eigenvalues. We note that the graphs of $stop_1(k)$ are extremely erratic, especially for the interior eigenvalue. This behaviour has been observed in several other experiments and may cause the non-convergence phenomena observed for other values of τ^{SE}_{inner}.

From our experiments we conclude that though the stopping conditions (93) and (94) are motivated differently, in practice they appear to behave rather like the standard residual stopping condition (97). We emphasise that in our experiments the value of τ^{SE}_{inner} used in **SEstop** has been chosen to be the best possible value. In practice we would not know this value and if τ^{SE}_{inner} is chosen too large then **SEstop** may fail for an interior eigenvalue. In contrast the residual stopping condition (97) uses a fixed tolerance and Algorithm **SEf** performs quite similarly for a range of values of τ^0.

a) Extreme eigenvalue b) Interior eigenvalue

Figure 2: Behaviour of the stopping condition $stop_1(k)$ given by (93).

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