Eigenvalue bounds from the Schur form *

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Abstract

Computing the partial Schur form of a matrix is a common kernel in widely used software for solving eigenvalues problems. Partial Schur forms and Schur vectors also arise naturally in deflation techniques. In this paper, error bounds are proposed which are based on the Schur form of a matrix. We show how the bounds derived for the general case simplify in special situations such as those of Hermitian matrices or partially normal or nearly normal matrices. The derived bounds are similar to well-known bounds such as the Kato-Temple and the Bauer-Fike inequalities.

1 Introduction

A common issue that arises when computing eigenvalues of matrices is to provide estimates on the errors made when approximating eigenpairs given some computable quantities, such are residual norms. For example, given an approximate eigenvalue $\tilde{\lambda}$ and associated approximate eigenvector $\tilde{u}$ such that

$$A\tilde{u} = \tilde{\lambda}\tilde{u} + r$$

the question is to provide estimates for $|\lambda - \tilde{\lambda}|$, and $\sin \angle(u, \tilde{u})$, for some exact eigenpair (λ, u) in terms of the residual norm $\|r\|$. In the normal case, there are several useful results of this type. In the non-normal case, the existing bounds can be too pessimistic to have any practical value. Though it is not possible to give as accurate bounds in the non-normal case as in the normal case, it is sometimes possible and useful to provide tighter bounds that yield partial information. This can be achieved by sacrificing on the completeness of the desired information. Indeed, the idea is that a sharp bound on, say, the error $|\lambda - \tilde{\lambda}|$ is impossible to obtain but inequalities involving perhaps an unknown

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condition number could be extracted. If the condition number is estimated by some heuristic means, estimates of the error could then result. The goal of this paper is to provide such alternative inequalities by exploiting the Schur canonical form of matrices.

We now give a brief background on the Schur canonical form of general matrices. A square complex or real matrix A can be factored in the form

$$A = QRQ^H \tag{1}$$

in which R is an upper triangular matrix and Q is a unitary matrix, i.e., such that $Q^HQ = I$. The diagonal elements of R are the eigenvalues of A (repeated with their multiplicities). An important point exploited in this paper is the fact that these eigenvalues can be put in any order in the diagonal using orthogonal transformations. In other words the Schur factorization is not unique and a different factorization can be obtained for each order of the eigenvalues.

Current algorithms for solving Hermitian and non-Hermitian eigenvalue problems often use the Schur form rather than eigenvectors. Moreover, it is common to use Schur forms in deflation techniques, as is done, for example, in the following algorithm.

ALGORITHM **1.1 Schur Deflation**

Solve $Aq_1 = \lambda_1 q_1$ *with* $\|q_1\|_2 = 1$; *set* $Q_1 = [q_1]$
Do $j = 2, \ldots, p$:
  Compute the eigenpair:
    $(I - Q_{j-1}Q_{j-1}^H)Aq_j = \lambda_j q_j$, *with* $\|q_j\|_2 = 1$
  Set $Q_j = [Q_{j-1}, q_j]$
EndDo

After the algorithm has completed, the partial Schur form

$$AQ_p = Q_pR_p \tag{2}$$

can be obtained from simply computing the matrix $R_p = Q_p^HAQ_p$. Here R_p is an upper triangular matrix. Note also that

$$(I - Q_pQ_p^H)AQ_p = 0$$

An information that is immediately available from the relation (2) is that the matrix Q_p is an orthonormal basis of an invariant subspace of A and that the p eigenvalues of the matrix R_p are also eigenvalues of the matrix A. Moreover, the corresponding eigenvectors can be easily computed. If (λ_i, x_i) is an eigenpair of the matrix R_p then it can easily be shown that (λ_i, Q_px_i) is an eigenpair of the matrix A.

Consider now a particular group of eigenvalues

$$\Lambda_1 = \{\lambda_1, \lambda_2, \ldots, \lambda_p\} .$$

The factorization (1) can be partitioned accordingly as,

$$A = [Q_1, Q_2] \begin{pmatrix} R_1 & W^H \\ O & R_2 \end{pmatrix} [Q_1, Q_2]^H \tag{3}$$

with $diag(R_1) = \Lambda_1$. For example when $p = 1$, Λ_1 consists of one particular eigenvalue λ which is assumed to be simple. Then it is possible to rewrite the Schur factorization as

$$A = [q_1, Q_2] \begin{pmatrix} \lambda & w^H \\ O & R_2 \end{pmatrix} [q_1, Q_2]^H \tag{4}$$

2 General error bounds for a single eigenvalue

In this section it is assumed that the eigenvalue λ is simple. Let $\tilde{\lambda}, \tilde{u}$ an approximate eigenpair such that

$$(A - \tilde{\lambda} I)\tilde{u} = r \tag{5}$$

It is possible to express the above equality in the Q basis, defined by the Schur factorization. This will be referred to as the Schur basis in the sequel. Writing $\tilde{u}$ and r in the Q basis as

$$\tilde{u} = Q \begin{pmatrix} \alpha \\ x \end{pmatrix} \text{ and } r = Q \begin{pmatrix} \epsilon \\ s \end{pmatrix}$$

and using relations (4) and (5), we obtain the following set of equations

$$\begin{pmatrix} \lambda - \tilde{\lambda} & w^H \\ O & R_2 - \tilde{\lambda} I \end{pmatrix} \begin{pmatrix} \alpha \\ x \end{pmatrix} = \begin{pmatrix} \epsilon \\ s \end{pmatrix} . \tag{6}$$

The vector s contains the components of r in the orthogonal to the eigenvector associated with λ. Let $P = q_1 q_1^H$ be the orthogonal projector onto the first Schur basis, i.e., the orthogonal projector onto the eigenvector associated with λ. Then the following can be stated:

- $Pr = \epsilon q_1$, i.e., ϵ is the component of r in q_1 in the Q-basis.
- $(I - P)r = Q_2 s$, i.e., s is the vector of components of r in the basis $q_2, q_3, \ldots, q_n$ of the orthogonal complement of q_1.
- $R_2 - \tilde{\lambda} I$ is the matrix expression of $(I - P)(A - \tilde{\lambda} I)(I - P)$ in the Q_2 basis.
- w is the matrix expression of $PA(I - P)$, which is an operator from $span(Q_2)$ to $span(q_1)$.

The exact eigenvector associated with the eigenvalue λ is the vector q_1, or the vector e_1 in the Schur basis. If $\tilde{u}$ is the approximate eigenvector, it is interesting to consider the projection of $\tilde{u}$ onto the exact eigenvector. If we work in the Schur basis then writing $\tilde{u} = Q \begin{pmatrix} \alpha \\ x \end{pmatrix}$ and $P\tilde{u} = Q \begin{pmatrix} \alpha \\ 0 \end{pmatrix}$ yields

$$(I - P)\tilde{u} = Q \begin{pmatrix} 0 \\ x \end{pmatrix} \tag{7}$$

Consider now specifically the relation (6). The second part of the relation yields,

$$(R_2 - \tilde{\lambda} I)x = s$$

from which we obtain,

$$x = (R_2 - \tilde{\lambda} I)^{-1} s$$

In case $\tilde{\lambda}$ is an eigenvalue of R_2, then a pseudo-inverse must be used. Observing that $\|s\|_2 = \|(I-P)r\|_2$ and referring to equation (7) shows that

$$\|(I-P)\tilde{u}\|_2 = \|x\|_2 \leq \|(R_2 - \tilde{\lambda} I)^{-1}\|_2 \|(I-P)r\|_2$$

The quantity $\tilde{\gamma} = \|(R_2 - \tilde{\lambda} I)^{-1}\|_2$ is an approximation to the condition number $\gamma = \|(R_2 - \lambda I)^{-1}\|_2$ of the eigenvector associated with $\tilde{\lambda}$. Using projectors, we can rewrite $\tilde{\gamma}$ as

$$\tilde{\gamma} = \| \left[(I-P)(A - \tilde{\lambda} I)(I-P) \right]^+ \|_2$$

which approximates

$$\gamma = \| \left[(I-P)(A - \lambda I)(I-P) \right]^+ \|_2$$

This is commonly used as the condition number for the eigenvector associated with λ. Note that when A is normal, R_2 is diagonal and $\tilde{\gamma}$ is then equal to the inverse of the distance from $\tilde{\lambda}$ to the eigenvalues of A other than λ.

Since $(I-P)\tilde{u} = \sin \angle(u, \tilde{u})$ and $\|(I-P)r\|_2 \leq \|r\|_2$ the above result leads to the following bound.

Theorem 2.1 *Let $\tilde{u}$ be the computed eigenvector associated with $\tilde{\lambda}$ and $r = (A - \tilde{\lambda} I)\tilde{u}$. Then,*

$$\sin \angle(u, \tilde{u}) \leq \tilde{\gamma} \|r\|_2$$

where $\tilde{\gamma} = \| \left[(I-P)(A - \tilde{\lambda} I)(I-P) \right]^+ \|_2$ and $P = q_1 q_1^H$.

An important observation is that whether in the Hermitian or non-Hermitian case, an estimate of the angle between exact and approximate eigenvectors is readily available from the residual norm once an estimate of the condition number is available. In practice, it is not necessary to obtain rigorous bounds for estimating errors. These are impossible to obtain at a reasonable cost in the non-normal case. In the normal case an estimate of the distance between $\tilde{\lambda}$ and the other eigenvalues is usually available from the algorithm used which typically yields a good estimate or bound for γ. Estimating γ is clearly harder in the non-normal case. However, it is important to separate the difficulty inherent in estimating the condition number from that of estimating errors. Condition numbers can be estimated by heuristics [1]. A trivial point in case, would be to perturb data slightly in certain ways and recompute approximate eigenvectors.

Return to relation (6) and consider now the first equation.

$$\alpha(\lambda - \tilde{\lambda}) + w^H x = \epsilon \tag{8}$$

Assume that $\tilde{v}$ is an approximate left eigenvector of A associated with the eigenvalue $\tilde{\lambda}$,

$$\tilde{v}^H A = \tilde{\lambda} \tilde{v}^H + z^H$$

Writing $\tilde{v}$ and z in the Q basis as

$$\tilde{v} = Q \begin{pmatrix} \beta \\ y \end{pmatrix} \text{ and } z = Q \begin{pmatrix} \eta \\ t \end{pmatrix}$$

the above equation would become,

$$\begin{pmatrix} \beta & y^H \end{pmatrix} \begin{pmatrix} \lambda - \tilde{\lambda} & w^H \\ O & R_2 - \tilde{\lambda} I \end{pmatrix} = \begin{pmatrix} \eta & t^H \end{pmatrix}$$

Equating the second columns yields,

$$\beta w^H + y^H (R_2 - \tilde{\lambda} I) = t^H$$

In a number of algorithms, $\tilde{v}$ is orthogonal to r. Assume this is the case. This translates into $\beta\epsilon + y^H s = 0$ or $\epsilon\beta = -y^H s$.

From relation (8), we get,

$$\begin{aligned} \alpha\beta(\lambda - \tilde{\lambda}) &= -y^H s - \beta w^H x \\ &= -\left[y^H s + \beta w^H (R_2 - \tilde{\lambda} I)^{-1} s \right] \\ &= -\left[y^H (R_2 - \tilde{\lambda} I) + \beta w^H \right] (R_2 - \tilde{\lambda})^{-1} s \\ &= -t^H (R_2 - \tilde{\lambda})^{-1} s \end{aligned}$$

This leads to the simple equality

$$\tilde{\lambda} - \lambda = \frac{t^H (R_2 - \tilde{\lambda} I)^{-1} s}{\alpha\beta}$$

Recalling that $|\alpha| = \|P\tilde{u}\|_2$ and $|\beta| = \|P\tilde{v}\|_2$ and similarly, $\|s\|_2 = \|(I-P)r\|_2$ and $\|t\|_2 = \|(I-P)z\|_2$ then we obtain the following error bound.

Theorem 2.2 *Let $\tilde{u}$, $\tilde{v}$ be the computed right and left eigenvectors associated with $\tilde{\lambda}$, $r = (A - \tilde{\lambda} I)\tilde{u}$ and $z^H = \tilde{v}^H (A - \tilde{\lambda} I)$. If $\tilde{v} \perp r$ then*

$$|\tilde{\lambda} - \lambda| \leq \tilde{\gamma} \; \frac{\|(I-P)r\|_2 \; \|(I-P)z\|_2}{\|P\tilde{u}\|_2 \; \|P\tilde{v}\|_2} \tag{9}$$

where $\tilde{\gamma} = \| \left[(I-P)(A - \tilde{\lambda} I)(I-P) \right]^+ \|_2$ and $P = q_1 q_1^H$

Note that a slightly weaker inequality is

$$|\tilde{\lambda} - \lambda| \leq \tilde{\gamma} \; \frac{\|r\|_2 \; \|z\|_2}{\|P\tilde{u}\|_2 \; \|P\tilde{v}\|_2}$$

which indicates the well-known fact that when $\tilde{v} \perp r$ the error is of the order of the product of the left and right residual norms. The above inequality does not provide complete information on the errors made on the eigenvalues. There are three missing quantities: $\|P\tilde{u}\|_2$, $\|P\tilde{v}\|_2$ and $\tilde{\gamma}$. As before $\tilde{\gamma}$ can be estimated – e.g., by heuristics. Of the other two quantities $\|P\tilde{u}\|_2$, is normally close to one if the approximation is good enough. Finally, $\|P\tilde{v}\|_2$ is close to the cosine of the angle between the exact left and right eigenvectors, and can usually be estimated from the computations by the cosine of the approximate left and right eigenvectors.

In fact, it might be more appropriate to rewrite the above inequality in yet another form:

$$|\tilde{\lambda} - \lambda| \; \cos\angle(u, \tilde{u}) \cos\angle(u, \tilde{v}) \; \leq \tilde{\gamma} \; \|r\|_2 \; \|z\|_2.$$

3 General error bounds for a group of eigenvalues

Consider now the situation of a group of eigenvalues. Using the relation (3), rewrite the relation (5) in the general situation as

$$\begin{pmatrix} R_1 - \tilde{\lambda} I & W^H \\ O & R_2 - \tilde{\lambda} I \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \epsilon \\ s \end{pmatrix}. \tag{10}$$

The first part of the equality yields,

$$(R_1 - \tilde{\lambda} I) x_1 = \epsilon - W^H x_2$$

and from the second we obtain an expression for x_2 which is

$$x_2 = (R_2 - \tilde{\lambda} I)^{-1} s$$

Therefore,

$$(R_1 - \tilde{\lambda} I) x_1 = \epsilon - W^H (R_2 - \tilde{\lambda} I)^{-1} s \tag{11}$$

In the sequel we will exploit the upper bound

$$\|\epsilon - W^H (R_2 - \tilde{\lambda} I)^{-1} s\|_2 \leq \sqrt{1 + \|W^H (R_2 - \tilde{\lambda} I)^{-1}\|_2^2}\, \|r\|_2 \tag{12}$$

which follows from the Cauchy-Schwarz inequality. It is important to provide an interpretation to this term which is strongly related to left eigenvectors. Consider $\tilde{v} = (y_1^H, y_2^H)$ a left eigenvector associated with λ, the approximate eigenvalue closest to $\tilde{\lambda}$. Then,

$$\begin{pmatrix} y_1^H, & y_2^H \end{pmatrix} \begin{pmatrix} R_1 - \lambda & W^H \\ O & R_2 - \lambda I \end{pmatrix} = 0$$

Equating the first column of the result to zero indicates, as expected that y_1 is a left eigenvector R_1. Equating the 2nd column to zero gives,

$$y_1^H W^H + y_2^H (R_2 - \lambda I) = 0$$

or

$$y_2^H = -y_1^H W^H (R_2 - \lambda I)^{-1}$$

The matrix $-W^H (R_2 - \lambda I)^{-1}$ multiplies the left eigenvector of R_1 in order to obtain the component in the Q_2-space of the left eigenvector. It is therefore natural to keep the term $\|W^H (R_2 - \lambda I)^{-1}\|$ together instead of using upper bounds involving the norm of W^H. We will use the notation,

$$\tilde{\gamma}_w = \|W^H (R_2 - \tilde{\lambda} I)^{-1}\|_2 \,. \tag{13}$$

Define the spectrum of R_1 by $\Lambda_1 = \{\lambda_1, \lambda_2, \ldots, \lambda_p\}$ and set $\tau(\tilde{\lambda}) = \min_{i=1:p} |\lambda_i - \tilde{\lambda}|$. In the general case, i.e., when R_1 is an upper triangular matrix, the matrix R_1 can be written as $R_1 = D - N$ where D is a diagonal matrix with the λ_i's on its diagonal and N is a strictly upper triangular matrix. Then, the relation (11) yields,

$$\tau(\tilde{\lambda}) \|x_1\|_2 = \|(R_1 - \tilde{\lambda} I) x_1 + N x_1\|_2 \leq \sqrt{1 + \tilde{\gamma}_w^2}\, \|r\|_2 + \|N\|_2\, \|x_1\|_2$$

which can be written as

$$\tau(\tilde{\lambda}) \leq \frac{\sqrt{1+\tilde{\gamma}_w^2}}{\|P\tilde{u}\|_2} \|r\|_2 + \|N\|_2 \tag{14}$$

This bound can be very pessimistic for highly non-normal matrices because in these cases, the matrix N has a very large norm.

An error bound which does not involve the matrix N can be obtained. Taking norms on both sides of the relation (11) leads to

$$\|(R_1 - \tilde{\lambda}I)x_1\|_2 \leq \|\epsilon - W^H(R_2 - \tilde{\lambda}I)^{-1}s\|_2$$

Using the inequality

$$\|(R_1 - \tilde{\lambda}I)x_1\|_2 \geq \sigma_{\min}\|x_1\|_2$$

where $\sigma_{\min}$ is the smallest singular value of $R_1 - \tilde{\lambda}I$, and recalling that $\|P\tilde{u}\|_2 = \|x_1\|_2$, we obtain the following bound.

Proposition 3.1 *Let A have the Schur form of equation (3) and let $(\tilde{\lambda}, \tilde{u})$ be an approximate eigenpair with residual vector r. Define $\tilde{\gamma}_w$ as in (13). Then the smallest singular value of $R_1 - \tilde{\lambda}I$ satisfies the inequality,*

$$\sigma_{\min} \leq \frac{\sqrt{1+\tilde{\gamma}_w^2}}{\|P\tilde{u}\|_2} \|r\|_2 \ . \tag{15}$$

In the case when R_1 is diagonal then clearly $\sigma_{\min}$ is simply the distance from $\tilde{\lambda}$ to the spectrum of R_1. Note that the above inequality can be interpreted from a pseudospectrum viewpoint [7, 3]. It stipulates that the approximate eigenvalue $\tilde{\lambda}$ is located inside the ϵ pseudo-spectrum level-curve of R_1 defined for ϵ equal to the right-hand side of (15).

In the inequality (14) we could use the fact that N is a nilpotent matrix, i.e., there exists an integer k not exceeding the dimension p of the matrix R_1 such that $N^k = 0$. This integer k is the maximum index of the eigenvalues in the group $\{\lambda_1, \ldots, \lambda_p\}$ and depends on the canonical Jordan form of the matrix R_1 and therefore also on the Jordan form of A. Let Δ be the diagonal matrix $\Delta = D - \tilde{\lambda}I$. The following relation holds

$$(\Delta - N)^{-1} = \left(\sum_{i=0}^{\infty}(\Delta^{-1}N)^i\right)\Delta^{-1} = \left(\sum_{i=0}^{k}(\Delta^{-1}N)^i\right)\Delta^{-1}$$

Taking norm and using Lemma 2.3.3 from [4] the following error bound can be derived

$$\frac{\tau(\tilde{\lambda})^k}{\|N^{k-1}\|_2 + \tau(\tilde{\lambda})\|N^{k-2}\|_2 + \ldots + \tau(\tilde{\lambda})^{k-1}} \leq \frac{\sqrt{1+\tilde{\gamma}_w^2}}{\|P\tilde{u}\|_2} \|r\|_2$$

A similar inequality was pointed out in [2] (Corollary 5.1). Note that if $\|N\|_2$ tends to zero, i.e., the matrix R_1 tends to become diagonal then the left hand side is essentially equal to $\tau(\tilde{\lambda})$.

4 The Hermitian Case

When the matrix is Hermitian, it is fairly easy to derive residual bounds for approximate eigenvalues or eigenvectors. Assume that an approximate eigenpair satisfies the relation (5) where $\tilde{\lambda} = (A\tilde{u}, \tilde{u})/(\tilde{u}, \tilde{u})$. Then a well-known result [6] stipulates that there is an exact eigenvalue λ such that

$$|\lambda - \tilde{\lambda}| \leq \frac{\|r\|_2^2}{\tilde{\delta}}$$

where

$$\tilde{\delta} = \min_{\lambda_i \in \Lambda(A),\ \lambda_i \neq \lambda} |\lambda_i - \tilde{\lambda}|$$

Similarly, there is an exact eigenvector u such that

$$\sin \angle(u, \tilde{u}) \leq \frac{\|r\|_2}{\tilde{\delta}}$$

These two upper bounds are sharp and extremely useful in practice, in spite of the fact that they involve the unknown quantity $\tilde{\delta}$. Note that the first result is similar to the one derived in Theorem 2.2 except for the denominator and the second result is equivalent to the one derived in Theorem 2.1 because for Hermitian matrices, $\tilde{\gamma}$ can be approximated by the inverse of $\tilde{\delta}$. In practice, it is common that approximations to the neighboring eigenvalues are also available and a simple estimate for $\tilde{\delta}$ is provided by replacing $\tilde{\delta} = dist(\tilde{\lambda}, \Lambda(A) - \{\lambda\})$ by $dist(\tilde{\lambda}, \tilde{\Lambda}(A) - \{\tilde{\lambda}\})$, in which $\Lambda(A)$ represents the spectrum of A and $\tilde{\Lambda}(A)$ the approximate spectrum. This provides an estimate, a very useful one in practice, rather than a rigorous bound.

Rigorous upper bounds can usually be obtained by exploiting alternative inequalities. For example, assuming eigenvalues are labeled decreasingly and we are seeking λ_1, the closest approximation is $\tilde{\lambda}_1$ and we obtain

$$\tilde{\delta} = |\tilde{\lambda}_1 - \lambda_2| \geq |\tilde{\lambda}_1 - \tilde{\lambda}_2| - |\tilde{\lambda}_2 - \lambda_2|.$$

Now $|\tilde{\lambda}_1 - \tilde{\lambda}_2|$ is computable and $|\tilde{\lambda}_2 - \lambda_2|$ can be estimated using a fairly simple bound such as $|\tilde{\lambda}_2 - \lambda_2| \leq \|r_2\|$ and the following rigorous and computable upper bound can be obtained,

$$|\lambda - \tilde{\lambda}| \leq \frac{\|r_1\|_2^2}{|\tilde{\lambda}_1 - \tilde{\lambda}_2| - \|r_2\|_2}$$

provided that $|\tilde{\lambda}_1 - \tilde{\lambda}_2| > \|r_2\|_2$. Unfortunately, obtaining such rigorous bounds does not seem to be possible in the non-normal case. On the other hand it is still possible to obtain good estimates based on estimating $\tilde{\gamma}$ and other quantities.

5 Partial and Near Normality

First suppose that we are only interested in a single eigenvalue and consider the relation (8) again. We make the assumption that the vector w is zero. This is a strong assumption

that has implications on the matrix and not only the approximation. In this case, the relation (8) becomes,

$$\alpha(\lambda - \tilde{\lambda}) = \epsilon$$

and since $\alpha = \|P\tilde{u}\|_2$, and $\epsilon = \|Pr\|_2$ we obtain a remarkably simple inequality,

$$|\lambda - \tilde{\lambda}| \leq \frac{\|Pr\|_2}{\|P\tilde{u}\|_2} \leq \frac{\|r\|_2}{\|P\tilde{u}\|_2}$$

A bound of this type was also pointed out in [2] (Corollary 3.2). Except for the denominator term this is very similar to the Bauer-Fike inequality. In fact the denominator should be close to one if the eigenvector is accurate enough. Another way of rewriting the inequality is:

$$|\lambda - \tilde{\lambda}| \cos \angle(u, \tilde{u}) \leq \|r\|_2$$

Note that when $w = 0$, then the left and right eigenvectors associated with λ are identical. This also means that the right and left residuals r and z are identical. If in addition, it is assumed that $r \perp \tilde{u}$ then $\alpha\epsilon + y^H s = 0$ and as a result $\epsilon = -y^H s/\alpha$, so

$$|\tilde{\lambda} - \lambda| \leq \frac{\|(R_2 - \tilde{\lambda}I)^{-1}\|_2 \|(I - P)r\|_2^2}{\|P\tilde{u}\|_2^2}$$

This inequality can be rewritten as

$$|\lambda - \tilde{\lambda}| \ \cos^2 \angle(u, \tilde{u})| \leq \tilde{\gamma}\|r\|_2^2$$

and can be viewed as a generalization of the Kato-Temple inequality.

Now, suppose we are interested in a group of eigenvalues. In the case when R_1 is simply diagonal, then clearly

$$\tau(\tilde{\lambda})\|x_1\|_2 \leq \|(R_1 - \tilde{\lambda}I)\|_2 \ \|x_1\|_2 \leq \sqrt{1 + \tilde{\gamma}_w^2} \ \|r\|_2$$

which becomes

$$\tau(\tilde{\lambda}) \leq \frac{\sqrt{1 + \tilde{\gamma}_w^2}}{\|P\tilde{u}\|_2} \ \|r\|_2$$

If we also assume that $W = 0$, the first equation of the relation (10) becomes

$$(R_1 - \tilde{\lambda}I)x_1 = \epsilon$$

and since R_1 is a diagonal matrix we obtain the following error bound

$$\tau(\tilde{\lambda}) \leq \frac{\|r\|_2}{\|P\tilde{u}\|_2}$$

Again, this error bound is similar to the Bauer-Fike inequality.

6 Numerical Illustrations

We now illustrate the error bounds derived in the previous sections for the case when the eigenpair $(\tilde{\lambda}, \tilde{u})$ is computed by the power method and the subspace iteration method. The power method computes the dominant eigenpair of a matrix A and the subspace iteration method computes a given number, say p, of the dominant eigenpairs of A. The two algorithms are as follows.

ALGORITHM **6.1 Power Method**

1. *Choose* $\tilde{u}$ *such that* $\|\tilde{u}\|_2 = 1$
2. *Do until convergence*
3. $\quad \tilde{u} = A\tilde{u}/\|A\tilde{u}\|$
4. $\quad \tilde{\lambda} = \tilde{u}^H A\tilde{u}$
5. $\quad$ *If the stopping criterion is satisfied then exit*
6. *EndDo*

Note that the denominator in Step 3 is often replaced by a signed number whose purpose is to allow convergence in 'direction' for cases of negative (or complex) eigenvalues.

ALGORITHM **6.2 Subspace Iteration Method**

1. *Choose a* n *by* p *matrix* U *such that* $U^H U = I$
2. *Do until convergence*
3. $\quad V = AU$
4. $\quad$ *Compute the QR factorization of* V*:* $V = UR$
5. $\quad$ *Compute the eigenpairs* $\{\tilde{\lambda}_i, \tilde{x}_i\}_{i=1:p}$ *of* $B = U^H AU$
6. $\quad$ *Set* $\{\tilde{u}_i = Q\tilde{x}_i\}_{i=1:p}$
7. $\quad$ *If the stopping criterion is satisfied then exit*
8. *EndDo*

For the power method, $(\tilde{\lambda}, \tilde{u})$ will approximate the dominant eigenpair of A. In the subspace iteration method the dominant eigenpair of A is approximated by $(\tilde{\lambda}, U\tilde{x})$ where $(\tilde{\lambda}, \tilde{x})$ is the dominant eigenpair of the projected matrix B. Note that, if at each step of the subspace iteration method we compute the Schur factorization of B, i.e., $BS = ST$, then upon termination of the algorithm the matrix $Q = US$ is a basis of an invariant subspace associated with the p dominant eigenvalues of A and the matrix T is the corresponding partial Schur form. More details for both methods can be found in [4, 6].

The matrices used for the experiments are n by n matrices of the form

$$A = Q \begin{pmatrix} R_1 & W^H \\ O & R_2 \end{pmatrix} Q^H$$

The matrix Q is the unitary matrix `orthog.m` from [5] and the block matrices are given by

$$R_1 = \begin{pmatrix} n & 0 & \dots & \dots & 0 \\ 0 & n-1 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \dots & \dots & 0 & n-p+1 \end{pmatrix} + \alpha_1 N_1$$

$$R_2 = \begin{pmatrix} n-p & 0 & \dots & \dots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \dots & \dots & 0 & 1 \end{pmatrix} + \alpha_2 N_2,$$

and

$$W = \alpha_3 C$$

where N_1 and N_2 are strictly upper triangular random matrices of unit norm, C is a random matrix of unit norm and α_1, α_2 and α_3 are real numbers. Note that α_1 and α_2 are parameters for the degree of the non-normality of the p by p matrix R_1 and of the $n-p$ by $n-p$ matrix R_2. Tuning the values of the α_i parameters allows us to study matrices with different properties. For example, $\alpha_1 = \alpha_2 = \alpha_3 = 0$ models the Hermitian case. Note that the dominant eigenvalues of the matrix A are located in R_1 and the exact Schur vectors are given by the matrix Q. All the experiments have been performed for matrices of size $n = 10$ and the error bounds are given for the dominant eigenpair $(\tilde{\lambda}, \tilde{u})$. The y-axes in the figures are log-scaled.

First, suppose we are only interested in the dominant eigenpair of A, i.e., $\lambda = 10$ and that this eigenpair is computed using the power method, i.e., $p = 1$. Now, consider the case when $W^H = 0$, i.e., the matrix A is partially non-normal, and the power method is used. Since the left dominant eigenvector is orthogonal to the residual $r = A\tilde{u} - \tilde{\lambda}\tilde{u}$, the previously derived error bound becomes

$$|\tilde{\lambda} - \lambda| \leq \frac{\tilde{\gamma}\|r\|_2^2}{\|P\tilde{u}\|_2^2}, \tag{16}$$

where $\tilde{\gamma}$ is computed as $\|(R_2 - \tilde{\lambda}I)^+\|_2$ and $P\tilde{u}$ is given by $(q_1^H\tilde{u})q_1$. Figure (1) shows that the quantity $|\tilde{\lambda} - \lambda|$ (dashed line) is well approximated by the right hand side of the Kato-Temple like inequality (16) (solid line).

Now, suppose that we are interested in the group of the 5 dominant eigenvalues of the matrix A, i.e., $p = 5$ and the target eigenpair $(\tilde{\lambda}, \tilde{u})$ is computed using the subspace iteration method. Figures (2) and (3) show the history of the computation for two cases: (1) when the matrix R_1 is diagonal, i.e., $\alpha_1 = 0, \alpha_2 = \alpha_3 = 10$ and (2) for the general case, i.e., $\alpha_1 = \alpha_2 = \alpha_3 = 10$. For the first case, the analysis given in the previous section yields an error bound of the form

$$\tau(\tilde{\lambda}) \leq \frac{\sqrt{1 + \tilde{\gamma}_w^2}}{\|P\tilde{u}\|_2} \|r\|_2 \tag{17}$$

whereas for the second case we obtain an error bound such as

$$\sigma_{\min} \leq \frac{\sqrt{1 + \tilde{\gamma}_w^2}}{\|P\tilde{u}\|_2} \|r\|_2 \tag{18}$$

For the first case, we can see that the derived Bauer-Fike like upper bound (17) (solid line in Figures (2)) give a fairly good approximation for the behavior of the quantity

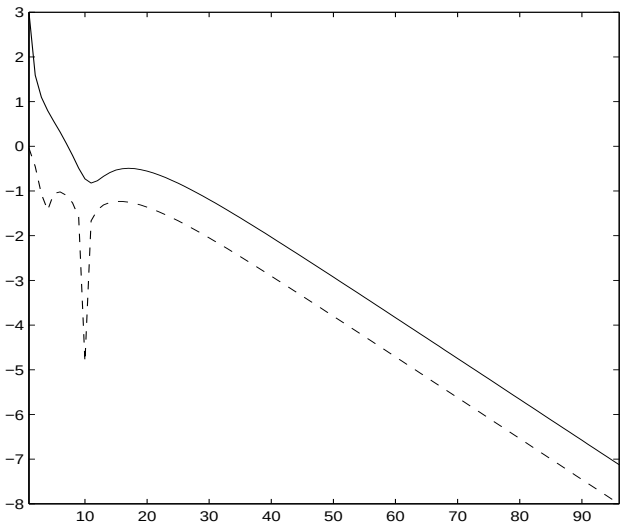

Figure 1: Error bounds versus the iteration number j of the power method when the matrix A is partially non-normal ($\alpha_2 = 10, W = 0$). The dashed line corresponds to $|\tilde{\lambda} - 10|$ while the solid line corresponds to $\tilde{\gamma}\|r\|_2^2/\|P\tilde{u}\|_2^2$.

$\tau(\tilde{\lambda})$ (dashed line in Figure (2)). The same conclusion holds for the agreement between the pseudospectra like bound (18) (solid line in Figure (3)) and the studied quantity $\sigma_{\min}$ (dashed line in Figure (3)).

7 Conclusion

In this paper we established a number of error bounds for eigenvalue problems which exploit the Schur canonical form. The information provided by these bounds is often not as complete as can be obtained in similar results in the normal case. This means that some of the parameters in the bounds are not available and must be estimated, possibly by heuristic means. On the other hand these bounds can provide a fairly accurate representation of the behavior of the approximate eigenpairs.

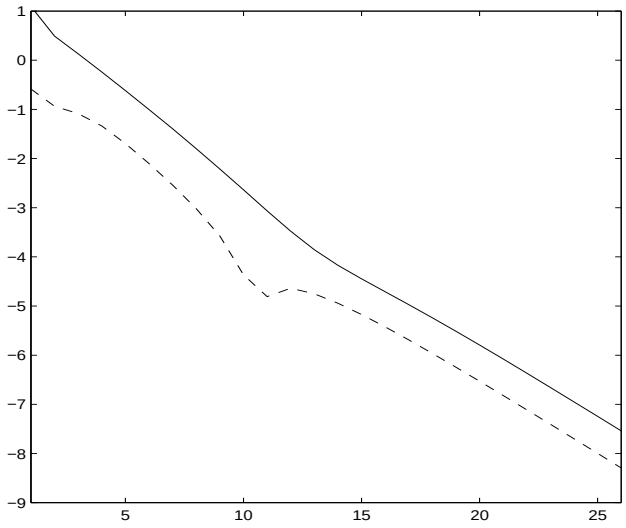

Figure 2: Error bounds versus the iteration number j of the subspace iteration method when the matrix R_1 is diagonal. The dashed line corresponds to the left-hand side of (17) and the solid like is its upper bound given by the right-hand side of (17)

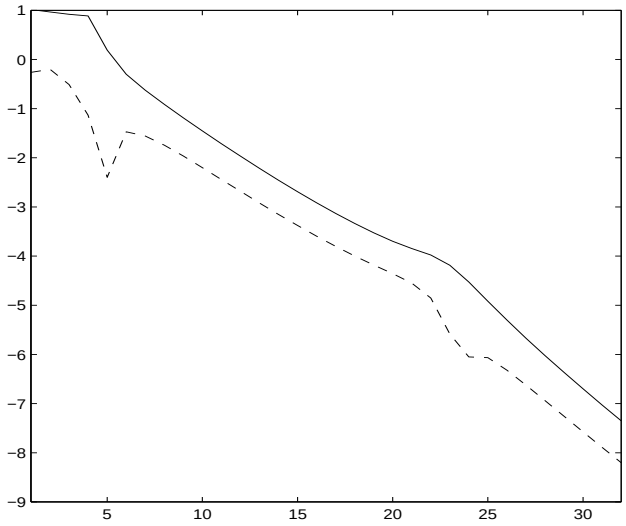

Figure 3: Error bounds versus the iteration number j of the subspace iteration method in the general case for a group of eigenvalues. The dashed line corresponds to the left-hand side of (18) and the solid like is its upper bound given by the right-hand side of (18)

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