RITZ VALUE BOUNDS THAT EXPLOIT QUASI-SPARSITY

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Abstract. Absolute and relative perturbation bounds for Ritz values of complex square matrices are presented. The bounds exploit quasi-sparsity of the eigenvectors, apply to specified eigenvalues, and do not use the entire matrix. The bounds are tighter than existing bounds when eigenvectors are quasi-sparse. The bounds are customized for Hermitian banded and tridiagonal matrices. A bound for the (relative) accuracy of the relative Ritz value separation is also derived.

Key words. eigenvalue, Ritz value, relative error, eigenvalue separation

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1. Introduction. The perturbation bounds in this paper were motivated by the Quasi-Sparse Eigenvector (QSE) method [9]. The QSE method computes the eigenvalues with (algebraically) smallest real part of extremely large, possibly infinite Hamiltonian matrices in quantum physics.

More specifically, a QSE iteration approximates eigenvalues with smallest real part of a Hamiltonian matrix

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

by the eigenvalues of a 'truncation' H_{11}, whose dimension is small compared to that of H. Ideally, the relative separation of the computed eigenvalues should have 5 percent accuracy.

We derive perturbation bounds to estimate how well the eigenvalues of H_{11}, which are Ritz values of H, approximate a desired eigenvalue of H. There are three reasons why existing bounds are not sufficient for this purpose.

First, numerical experiments show that the QSE method tends to be fast for matrices whose eigenvectors are quasi-sparse, i.e. have many elements of small magnitude. Existing perturbation bounds for Ritz values, both absolute [10, §11], [8, 12] and relative [1, 3], don't exploit quasi-sparsity.

Second, traditional Ritz value bounds don't have control over which eigenvalues they approximate, and may not give a bound for the desired eigenvalue. Suppose one wants to approximate the smallest eigenvalue $\lambda_1(H) \approx 1$ of

$$H = \begin{pmatrix} 100 & \epsilon \\ \epsilon & 1 \end{pmatrix}, \qquad 0 \leq \epsilon < 1$$

by the eigenvalue 100 of $H_{11} = 100$. The Ritz value bound [10, Theorem (11-5-1)] only gives a bound for the large eigenvalue $\lambda_2(H) \approx 100$, $|100 - \lambda_2(H)| \leq \|H_{12}\| = \epsilon$. It does not give information about the accuracy of the small eigenvalue, $|100 - \lambda_1(H)|$.

Third, many eigenvalue perturbation bounds depend on the entire matrix. But when a matrix is extremely large or infinite, one can afford to work with only a small piece (in this sense our motivation is similar to that of the Residual Interlace

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Theorem [10, §10.4]). For instance, Weyl's theorem for Hermitian matrices [10, Fact 1-11] implies

$$\left|\lambda_i(H) - \lambda_i \begin{pmatrix} H_{11} & 0 \\ 0 & H_{22} \end{pmatrix}\right| \le \|H_{12}\|,$$

where $\lambda_i(\cdot)$ denotes the ith smallest eigenvalue of a matrix and $\|\cdot\|$ the (Euclidean) two-norm. When H is extremely large or infinite, H_{22} may not be available or may not even be known. Instead we need a bound for $|\lambda_i(H) - \lambda_i(H_{11})|$. Fortunately, the matrices in the problems from [9] are often banded, so H_{12} and H_{21} have few non-zero elements and can be part of a bound.

Overview. Perturbation bounds for the approximation of any eigenvalue by a Ritz value are derived in §2. The bounds depend on the magnitude of eigenvector components, and can be considered an extension of Ritz value bound for Hermitian matrices to general, complex matrices. The bounds are specialized to Hermitian matrices in §3, Hermitian banded matrices in §4 and Hermitian tridiagonal matrices in §5. In all cases the bounds for the smallest eigenvalue are stronger than the ones for the larger eigenvalues. The bounds are tighter than existing Ritz value bounds for Hermitian matrices when the relevant eigenvectors are quasi-sparse. Relative bounds for general complex matrices and Hermitian matrices are presented in §6. Again, the bound for the smallest eigenvalue requires the fewest assumptions. Perturbation bounds for the relative separation of real eigenvalues are derived in in §7. At last, in §8 simultaneous bounds for several eigenvalues are discussed, which require a stronger measure of quasi-sparsity. The bounds are tighter when the eigenvalues are real.

Notation. A complex matrix V has transpose V^T and conjugate transpose V^*. The identity matrix is I, the *ith* column is e_i. The eigenvalues of a complex square matrix A are denoted by $\lambda_i(A)$. $\|\cdot\|$ denotes the Euclidean two-norm, and $\|\cdot\|_F$ the Frobenius norm.

2. Diagonalizable Matrices. We derive perturbation bounds for the approximation of *any* eigenvalue by an eigenvalue of a leading principal submatrix. The bounds depend on the magnitude of eigenvector components.

Let H be a complex square matrix with eigenvalues λ_j and corresponding eigenvectors v_j, i.e. $Hv_j = \lambda_j v_j$. Partition

$$H = \begin{matrix} & m & \\ m & \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \end{matrix}, \qquad v_j = \begin{pmatrix} v_j^{(1)} \\ v_j^{(2)} \end{pmatrix}.$$

The eigenvalues of H_{11} are θ_i, $1 \le i \le m$. We want to approximate any eigenvalue λ_j of H by an eigenvalue θ_i of H_{11}. Most bounds in this paper are based on the following approach.

Idea. Write the first block row in $(H - \lambda_j I)v_j = 0$ as $(H_{11} - \lambda_j I)v_j^{(1)} = -H_{12}v_j^{(2)}$ and take norms. If $v_j^{(2)} \ne 0$, divide by $\|v_j^{(2)}\|$. This yields the factor $\rho_j \equiv \|v_j^{(2)}\|/\|v_j^{(1)}\|$ in the upper bound. If λ_j is non-derogatory, it has an eigenspace of dimension one. Then ρ_j is well-defined and unique, and the next definition is justified.

DEFINITION 2.1. *The quantity*

$$\rho_j \equiv \|v_j^{(2)}\|/\|v_j^{(1)}\|$$

measures the quasi-sparsity of a vector v_j *with regard to the partition* $v_j = \begin{pmatrix} v_j^{(1)} \\ v_j^{(2)} \end{pmatrix}$.
For a given partition, v_j *is quasi-sparse if* $\rho_j < 1$.

If $v_j^{(1)} = 0$ then λ_j is an eigenvalue of H_{22}. We do not consider this case here. If $v_j^{(2)} = 0$, i.e. $\rho_j = 0$, then λ_j is an eigenvalue of H_{11}. Necessary and sufficient conditions for λ_j to be a Ritz value are discussed in [6]. Our perturbation bounds for an eigenvalue λ_j depend on the quasi-sparsity ρ_j of its eigenvectors. The bounds are tighter than existing Ritz value bounds when the corresponding eigenvectors are quasi sparse, i.e. $\rho_j < 1$.

The bound below extends the Ritz value bound for Hermitian matrices [10, Theorem (11-5-1)] to general, complex matrices.

FACT 1. *If* H_{11} *is diagonalizable with eigenvector matrix* W*, and* λ_j *is non-derogatory (and* $\rho_j < \infty$*) then*

$$\min_{1 \le i \le m} |\theta_i - \lambda_j| \le \kappa(W)\, \|H_{12}\|\, \rho_j,$$

where $\kappa(W) \equiv \|W\|\, \|W^{-1}\|$.

The bound for the eigenvalue λ_j decreases with the quasi-sparsity ρ_j of its eigenvectors v_j. The bound does not depend on the eigenvector condition number of H, only on that of the principal submatrix H_{11}.

3. Hermitian Matrices. We consider the bounds in §2 for Hermitian matrices, where we can say more about the accuracy of the smallest Ritz value.

Label the eigenvalues in ascending order, $\lambda_1 \le \lambda_2 \le \ldots$, and $\theta_1 \le \ldots \le \theta_m$. The traditional Ritz value bound [10, Theorem (11-5-1)] implies that there are m eigenvalues λ_{i_j} of H such that

$$|\theta_j - \lambda_{i_j}| \le \|H_{12}\|, \qquad 1 \le j \le m. \tag{3.1}$$

The bound below is tighter than (3.1) if the eigenvectors are quasi-sparse.

FACT 2 (Hermitian Matrices). *Let* H *be Hermitian.*

If λ_1 *is distinct (and* $\rho_1 < \infty$*) then*

$$0 \le \theta_1 - \lambda_1 \le \|H_{12}\|\, \rho_1,$$

If λ_j *is distinct (and* $\rho_j < \infty$*) then*

$$\min_{1 \le i \le m} |\theta_i - \lambda_j| \le \|H_{12}\|\, \rho_j, \qquad j \ge 2.$$

Proof. This follows from Fact 1 and the bound for λ_1 from the Cauchy interlace theorem [10, §10-1]. □

In contrast to Fact 2, the traditional bound (3.1) may not give any information about the smallest eigenvalue λ_1. For instance, the eigenvalues of

$$H = \begin{pmatrix} 100 & \epsilon \\ \epsilon & 1 \end{pmatrix}, \qquad 0 \le \epsilon < 1$$

satisfy, according to Weyl's theorem [10, Fact 1-11],

$$1 - \epsilon \le \lambda_1 \le 1 + \epsilon, \qquad 100 - \epsilon \le \lambda_2 \le 100 + \epsilon.$$

With $H_{11} = 100$ and $\theta_1 = 100$, (3.1) gives $|\theta_1 - \lambda_2| \leq \|H_{12}\| = \epsilon$, but it does not bound $\theta_1 - \lambda_1$. In contrast, Fact 2 yields

$$\rho_1 \leq \frac{99+\epsilon}{\epsilon} \qquad \text{and} \qquad \theta_1 - \lambda_1 \leq \|H_{12}\|\,\rho_1 = 99+\epsilon.$$

The upper bound is the same as the one implied by Weyl's theorem, $99-\epsilon \leq \theta_1 - \lambda_1 \leq 99+\epsilon$.

Below is a bound on the quasi-sparsity. It confirms the observation in [9, §3] that eigenvectors are likely to be quasi-sparse if the spacing between eigenvalues is not too small compared to the size of the off-diagonal entries.

FACT 3 (Quasi-Sparsity). *If H is Hermitian, and λ_j distinct and not an eigenvalue of H_{22} (and $\rho_j < \infty$) then*

$$\rho_j \leq \frac{\|H_{12}\|}{\min_k |\lambda_k(H_{22}) - \lambda_j|}, \qquad j \geq 1.$$

This implies a quadratic bound similar to [10, Theorem (11-7-1)],

$$\min_{1\leq i\leq m} |\theta_i - \lambda_j| \leq \frac{\|H_{12}\|^2}{\min_k |\lambda_k(H_{22}) - \lambda_j|}, \qquad j \geq 1, \tag{3.2}$$

provided λ_j is distinct and not an eigenvalue of H_{22}, and $\rho_j < \infty$. This bound is a consequence of Fact 2 and can therefore never be better. In fact, it can be a lot worse.

EXAMPLE 1. *The quadratic bound for θ_1 in (3.2),*

$$0 \leq \theta_1 - \lambda_1 \leq \frac{\|H_{12}\|^2}{\min_k |\lambda_k(H_{22}) - \lambda_1|},$$

can be arbitrarily worse than the bound in Fact 2.

The Hermitian matrix

$$H = \begin{pmatrix} \theta & \eta & \\ \bar{\eta} & 1 & \\ & & \lambda_1 + \epsilon \end{pmatrix}, \qquad 0 < \epsilon < 1, \quad \theta < |\eta|^2 \text{ real},$$

has eigenvalues $\lambda_1 \equiv \frac{1}{2}(\theta + 1 - \delta) < 1$, as well as $\lambda_1 + \epsilon$ and $\frac{1}{2}(\theta + 1 + \delta) > 1$, where $\delta \equiv \sqrt{4|\eta|^2 + (\theta-1)^2}$.

Choose $m = 1$, so $H_{11} = \theta$ and $H_{12} = \begin{pmatrix} \eta & 0 \end{pmatrix}$. Eigenvectors associated with λ_1 are multiples of $v_1 = \begin{pmatrix} 1 & -\frac{1}{2\eta}(\theta - 1 + \delta) & 0 \end{pmatrix}^T$. From $1 - \lambda_1 > 1$ follows $\rho_1 = |\eta|/(1-\lambda_1) < \eta$; and from $\lambda_1 + \epsilon < \lambda_1 + 1 < 1$ follows $\epsilon = \min_k |\lambda_k(H_{22}) - \lambda_1|$. Fact 2 implies $\theta - \lambda_1 \leq |\eta|^2$, but the quadratic bound in Fact 3.2 amounts to $\theta - \lambda_1 \leq |\eta|^2/\epsilon$, which is much worse for small ϵ.

4. Banded Hermitian Matrices. When a Hermitian matrix is banded one can exploit quasi-sparsity and tighten the bounds, especially the one for the smallest eigenvalue. A matrix H with elements h_{ij} has half-bandwidth w if $h_{ij} = 0$ for $i > j + w$.

DEFINITION 4.1. *The quantities*

$$\rho_1^w \equiv \frac{\|v_{m-w+1:m,1}\|\,\|v_{m+1:m+w,1}\|}{\|v_{1:m,1}\|^2}, \qquad \rho_j^w \equiv \frac{\|v_{m+1:m+w,j}\|}{\|v_{1:m,j}\|}, \quad j \geq 2$$

measure the quasi-sparsity of a vector v_j with regard to the partition

$$v_j = (v_{1:m,j}^T \quad v_{m+1:m+w,j}^T \quad \dots)^T$$

of a matrix with half-bandwidth $w \leq m$. For a given partition, v_j is quasi-sparse if $\rho_j^w < 1$.

Note that the quasi-sparsity measure for the smallest eigenvalue is stricter than that of the larger eigenvalues. In general $\rho_j^w \leq \rho_j$, because only w rather than all components of $v_j^{(2)}$ participate in the numerator of ρ_j. Hence, the bounds below can be tighter than those for general Hermitian matrices in Fact 2.

FACT 4 (Banded Matrices). *Let H be Hermitian with half-bandwidth $w \leq m$.*

If λ_1 is distinct (and $\rho_1^w < \infty$) then

$$0 \leq \theta_1 - \lambda_1 \leq \|H_{12}\| \, \rho_1^w.$$

If λ_j is distinct (and $\rho_j^w < \infty$) then

$$\min_{1 \leq i \leq m} |\theta_i - \lambda_j| \leq \|H_{12}\| \, \rho_j^w, \qquad j \geq 2.$$

Proof. Use the fact that $H_{12} = \begin{pmatrix} 0 & 0 \\ L & 0 \end{pmatrix}$ where L is order w. Because $H_{11} - \lambda_1 I$ is positive semi-definite, $(\theta_1 - \lambda_1)\|v_1^{(1)}\|^2 \leq (v_1^{(1)})^*(H_{11} - \lambda_1 I)v_1^{(1)}$. □

5. Hermitian Tridiagonal Matrices. We adapt the bounds for banded matrices to tridiagonal matrices and derive expressions for the Ritz value errors.

Let

$$T \equiv \begin{pmatrix} \alpha_1 & \beta_1 & & \\ \bar{\beta}_1 & \alpha_2 & \beta_2 & \\ & \bar{\beta}_2 & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix}$$

be an unreduced Hermitian tridiagonal matrix, i.e. $\beta_i \neq 0$. The eigenvalues λ_j of T are distinct [10, Lemma (7-7-1)]. Leading and trailing principal submatrices of T are denoted by

$$T_m \equiv \begin{pmatrix} \alpha_1 & \beta_1 & & \\ \bar{\beta}_1 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_{m-1} \\ & & \bar{\beta}_{m-1} & \alpha_m \end{pmatrix}, \qquad \hat{T}_{m+1} \equiv \begin{pmatrix} \alpha_{m+1} & \beta_{m+1} & & \\ \bar{\beta}_{m+1} & \alpha_{m+2} & \beta_{m+2} & \\ & \bar{\beta}_{m+2} & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix},$$

so that

$$T = \begin{pmatrix} T_m & \beta_m e_m e_1^* \\ \bar{\beta}_m e_1 e_m^* & \hat{T}_{m+1} \end{pmatrix},$$

where e_i denotes the ith column of an identity matrix. The leading principal submatrix T_m is also an unreduced tridiagonal with eigenvalues $\theta_1 < \ldots < \theta_m$.

A tridiagonal matrix has half-bandwidth $w = 1$, and the measures for quasi-sparsity are

$$\tau_1 \equiv \rho_1^1 = \frac{|v_{m,1}| \, |v_{m+1,1}|}{\|v_{1:m,1}\|^2}, \qquad \tau_j \equiv \rho_j^1 = \frac{|v_{m+1,j}|}{\|v_{1:m,j}\|}, \quad j \geq 2.$$

Since an unreduced Hermitian tridiagonal has distinct eigenvalues, all eigenspaces are one-dimensional, and the leading component of each eigenvector is non-zero [10, Theorem (7-9-5)], i.e. $v_{1:m,j} \neq 0$. Therefore τ_j is always well-defined. Moreover, all elements of an eigenvector v_1 for the smallest eigenvalue are nonzero [10, Theorem (7-9-5)], hence $\tau_1 > 0$.

FACT 5 (Tridiagonal Matrices). *Let T be unreduced Hermitian tridiagonal. Then*

$$0 \leq \theta_1 - \lambda_1 = c_1\, |\beta_m|\, \tau_1, \qquad \min_{1 \leq i \leq m} |\theta_i - \lambda_j| = c_j\, |\beta_m|\, \tau_j, \quad j \geq 2,$$

where $0 \leq c_j \leq 1$, $j \geq 1$, *and*

$$c_1 \equiv \frac{\sum_{i=1}^m |\gamma_{i1}|^2}{|\gamma_{m1}|\, \prod_{i=2}^m |\theta_i - \lambda_1|}, \qquad c_j \equiv \frac{(\sum_{i=1}^m |\gamma_{ij}|^2)^{1/2}}{\prod_{i=1, i\neq k}^m |\theta_i - \lambda_j|}, \quad j \geq 2,$$

$\gamma_{1j} \equiv \beta_1 \cdots \beta_{m-1}$,

$$\gamma_{ij} \equiv \beta_i \cdots \beta_{m-1}\, \det(\lambda_j I - T_{i-1}), \qquad 2 \leq i \leq m-1,$$

and $\gamma_{mj} = \det(\lambda_j - T_{m-1})$.

Proof. An eigenvector v_j is a multiple of [10, §7-10], [14, §5.48]

$$\begin{pmatrix} \gamma_{1j} & \ldots & \gamma_{m-1,j} & \gamma_{mj} & \frac{\det(\lambda_j I - T_m)}{\beta_m} & \frac{\det(\lambda_j I - T_{m+1})}{\beta_m \beta_{m+1}} & \ldots \end{pmatrix}^T.$$

If λ_j is an eigenvalue of T_m then $\tau_j = 0$, and the desired equalities hold. Now assume that λ_j is not an eigenvalue of T_m.

Using the above expression in τ_1 yields

$$\tau_1 = \frac{|v_{m,1}|\, |v_{m+1,1}|}{\|v_{1:m,1}\|^2} = \frac{|\gamma_{m1}|\, |\det(\lambda_1 I - T_m)|}{|\beta_m|\, \sum_{i=1}^m |\gamma_{i1}|^2} = \frac{|\gamma_{mj}|\, |\theta_1 - \lambda_1| \cdots |\theta_m - \lambda_1|}{|\beta_m|\, \sum_{i=1}^m |\gamma_{ij}|^2}.$$

Solving for $\theta_1 - \lambda_1$ gives $\theta_1 - \lambda_1 = c_1 |\beta_m| \tau_1$, where $c_1 \geq 0$. Since all elements of v_1 are non-zero [10, Theorem (7-9-5)], $\gamma_{m1} \neq 0$ and c_1 is well-defined. The proof for $j \geq 2$ is similar.

Fact 4 implies $\min_{1 \leq i \leq m} |\theta_i - \lambda_j| \leq |\beta_m|\, \tau_j$, which means $c_j \leq 1$. ∎

If T is almost decoupled, i.e. $|\beta_m|$ is small, and if v_j is quasi-sparse then some Ritz value θ_i is close to λ_j. The quantity c_j indicates the tightness of the bound in Fact 4 for tridiagonal matrices,

$$\min_{1 \leq i \leq m} |\theta_i - \lambda_j| \leq |\beta_m|\, \tau_j.$$

The bound can be loose if λ_j is well separated from all but one eigenvalue of T_m.

As in Fact 3, one can bound the quasi-sparsity.

FACT 6. *If T is an unreduced Hermitian tridiagonal and λ_j is not an eigenvalue of $\hat{T}_{m+1}$ then*

$$\tau_1 = |\beta_m|\, \frac{|v_{m,1}|^2}{\|v_{1:m,1}\|^2}\, e_1^*(\hat{T}_{m+1} - \lambda_1 I)^{-1} e_1$$

and

$$\tau_j = |\beta_m|\, \frac{|v_{m,j}|}{\|v_{1:m,j}\|}\, |e_1^*(\hat{T}_{m+1} - \lambda_j I)^{-1} e_1|, \qquad j \geq 2.$$

Thus $\tau_j \leq |\beta_m||e_1^*(\hat{T}_{m+1} - \lambda_j I)^{-1} e_1|$. This means, an eigenvector v_j is quasi-sparse if the off-diagonal part β_m and the leading diagonal element of $(\hat{T}_{m+1} - \lambda_j I)^{-1}$ are small in magnitude.

Example 1 illustrates that the quadratic bounds (3.2) for general Hermitian matrices can be much worse than the quasi-sparsity bounds in Fact 2. This is not true for tridiagonal matrices: the quadratic bounds below are equal to the quasi-sparse bounds in Fact 5 because the expression for τ_j in Fact 6 holds with equality,

$$\theta_1 - \lambda_1 \leq |\beta_m|^2 \frac{|v_{m,1}|^2}{\|v_{1:m,1}\|^2} e_1^*(\hat{T}_{m+1} - \lambda_1 I)^{-1} e_1 \tag{5.1}$$

$$\min_{1 \leq i \leq m} |\theta_i - \lambda_j| \leq |\beta_m|^2 \frac{|v_{m,j}|}{\|v_{1:m,j}\|} |e_1^*(\hat{T}_{m+1} - \lambda_j I)^{-1} e_1|, \qquad j \geq 2, \tag{5.2}$$

provided λ_j is not an eigenvalue of $\hat{T}_{m+1}$.

Example 2 (Toeplitz Matrices). *The real symmetric tridiagonal Toeplitz matrix*

$$T \equiv \begin{pmatrix} \alpha & \beta & & \\ \beta & \alpha & \ddots & \\ & \ddots & \ddots & \beta \\ & & \beta & \alpha \end{pmatrix}, \qquad \beta > 0,$$

of order n *has as smallest eigenvalue [11, §2.6.2]* $\lambda_1 = \alpha + 2\beta \cos\left(\frac{n\pi}{n+1}\right)$ *and eigenvector*

$$v_1 = \frac{2}{\sqrt{n+1}} \left(\sin\left(\tfrac{1\pi}{n+1}\right) \quad \sin\left(\tfrac{2\pi}{n+1}\right) \quad \ldots \quad \sin\left(\tfrac{n\pi}{n+1}\right) \right)^T.$$

For $m \ll n$ *approximate* $\sin x \approx x$ *and* $\cos x \approx 1 - \frac{x^2}{2}$. *Then the error in the smallest Ritzvalue is*

$$\theta_1 - \lambda_1 = 2\beta \left(\cos \frac{\pi}{n+1} - \cos \frac{\pi}{m+1} \right) \approx \beta \frac{\pi^2}{(m+1)^2},$$

while Fact 5 gives the bound

$$\beta \, \tau_1 \approx \frac{6\beta}{2m+1}.$$

That is, the error is proportional to β/m^2 *and the bound is proportional to* β/m. *Therefore the error bound predicts correctly that the error is proportional to the magnitude* β *of the offdiagonal elements.*

6. Relative Bounds. We derive perturbation bounds on the relative error for eigenvalues of a leading principal submatrix of H. Relative eigenvalue bounds are surveyed in [5].

The relative error bound below corresponds to the absolute bound in Fact 1. It resembles the relative bounds in [4, §5] but exploits quasi-sparsity.

Fact 7. *If* H_{11} *is non-singular and diagonalizable with eigenvector matrix* W, *and* λ_j *is non-derogatory (and* $\rho_j < \infty$*) then*

$$\min_{1 \leq i \leq m} \left| \frac{\theta_i - \lambda_j}{\theta_i} \right| \leq \kappa(W) \, \|H_{11}^{-1} H_{12}\| \, \rho_j,$$

where $\kappa(W) \equiv \|W\|\,\|W^{-1}\|$.

Proof. Write the first block row of $(H-\lambda_j I)v_j = 0$ as $(I-\lambda_j H_{11}^{-1})v_j^{(1)} = -H_{11}^{-1}H_{12}v_j^{(2)}$. □

Like the absolute bound in Fact 1, the relative bound decreases with the quasi-sparsity. The bound itself is also relative in the sense that the off-diagonal part H_{12} is 'normalized' by H_{11}.

When H is Hermitian one can bound the relative error between jth eigenvalue and Ritz value for the m smallest eigenvalues of H (m is the dimension of H_{11}), provided the error is sufficiently small compared to the eigenvalue separation. To prove the relative bounds we define the eigenvalue separation as

$$\Delta_k \equiv \frac{\lambda_{k+1}-\lambda_k}{\max\{|\lambda_k|,\, |\lambda_{k+1}|\}}, \qquad k \geq 1.$$

First we derive a bound that holds without regard to quasi-sparsity.

FACT 8 (m Smallest Eigenvalues). *Let H be Hermitian and H_{11} be nonsingular; and let the m smallest eigenvalues $\lambda_1 < \ldots < \lambda_m$ of H be distinct and non-zero. Let $\lambda_i = \theta_i(1+\epsilon_i)$.*

If $|\epsilon_1| < 1$ then

$$|\epsilon_1| = \min_{1\leq i\leq m}\left|\frac{\theta_i-\lambda_1}{\theta_i}\right|.$$

If for some $2 \leq i \leq m$,

$$|\epsilon_k| < \min\left\{\frac{1}{2}\Delta_{k-1},\, \frac{1}{2}\Delta_k,\, 1\right\}, \qquad 1 \leq k \leq i,$$

then[1]

$$|\epsilon_i| = \min_{1\leq l\leq m}\left|\frac{\theta_l-\lambda_i}{\theta_l}\right|.$$

Proof. The Cauchy interlace theorem [10, §10-1] implies for the m smallest eigenvalues of H, $\lambda_i \leq \theta_i$, $1 \leq i \leq m$. The case $\lambda_i < 0 < \theta_i$ cannot occur because $1 < 1-\frac{\lambda_i}{\theta_i}$ contradicts the assumption $|\epsilon_i| < 1$.

$i = 1$. For $\lambda_1 > 0$ or $\theta_1 < 0$ one gets, respectively,

$$0 \leq 1-\frac{\lambda_1}{\theta_1} \leq 1-\frac{\lambda_1}{\theta_i} \qquad \text{or} \qquad 0 \geq 1-\frac{\lambda_1}{\theta_1} \geq 1-\frac{\lambda_1}{\theta_i}, \qquad i \geq 2.$$

Thus

$$\left|\frac{\theta_1-\lambda_1}{\theta_1}\right| = \min_{1\leq i\leq m}\left|\frac{\theta_i-\lambda_1}{\theta_i}\right|.$$

$i = 2$. As above one shows

$$\left|\frac{\theta_2-\lambda_2}{\theta_2}\right| = \min_{2\leq i\leq m}\left|\frac{\theta_i-\lambda_2}{\theta_i}\right|.$$

[1]The boundary conditions are $|\epsilon_1| \leq \min\{\frac{1}{2}\Delta_1, 1\}$ and $|\epsilon_m| \leq \min\{\frac{1}{2}\Delta_{m-1}, 1\}$.

It remains to show that θ_2 is closer to λ_2 than θ_1.

For $\lambda_1 > 0$ or $\lambda_2 < 0$ the assumption $|\epsilon_1| < \Delta_1$ implies $\theta_1 < \lambda_2$. For $\theta_1 < 0$ and $\lambda_2 > 0$ this is true automatically. Therefore $\lambda_1 \leq \theta_1 < \lambda_2 \leq \theta_2$. Hence

$$\frac{\lambda_2 - \theta_1}{\theta_1} = z + \frac{\theta_2 - \lambda_2}{\theta_2},$$

where

$$z \equiv \frac{\lambda_2 - \theta_1}{\theta_1} - \frac{\theta_2 - \lambda_2}{\theta_2} = \frac{\lambda_2 - \lambda_1}{\lambda_1} + \frac{\lambda_2}{\lambda_1}\,\epsilon_1 + \epsilon_2.$$

If $\theta_2 < 0$ then $z < 0$. When $\lambda_1 > 0$ write

$$z = \frac{\lambda_2}{\lambda_1}\left(\frac{\lambda_2 - \lambda_1}{\lambda_2} + \epsilon_1 + \frac{\lambda_1}{\lambda_2}\,\epsilon_2\right)$$

which shows $z > 0$. If $\theta_1 < 0 < \lambda_2$ then

$$\frac{\lambda_2 - \theta_1}{|\theta_1|} > 1 > |\epsilon_2|.$$

Therefore

$$\left|\frac{\theta_2 - \lambda_2}{\theta_2}\right| = \min_{1 \leq i \leq m} \left|\frac{\theta_i - \lambda_2}{\theta_i}\right|.$$

$i \geq 3$. The proof proceeds by induction and is similar to the case $i = 2$. ▯

Therefore, if the relative distances between the first $i-1$ eigenvalues and Ritz values are sufficiently small (compared to the separation of the adjacent eigenvalues) then θ_i is the Ritz value closest to λ_i in the relative sense. As in the case of absolute bounds, the bound for the smallest eigenvalue requires the fewest assumptions. If H is Hermitian positive-definite the condition on ϵ_k simplifies to

$$|\epsilon_k| \leq \frac{\lambda_{k+1} - \lambda_k}{\lambda_{k+1}}.$$

Now we add quasi-sparsity.

Corollary 6.1. *Let H be Hermitian and H_{11} be nonsingular; and let the m smallest eigenvalues $\lambda_1 < \ldots < \lambda_m$ of H be distinct and non-zero.*

If $\|H_{11}^{-1}H_{12}\|\rho_1 < 1$ then

$$\left|\frac{\theta_1 - \lambda_1}{\theta_1}\right| \leq \|H_{11}^{-1}H_{12}\|\rho_1.$$

If for some $2 \leq i \leq m$,

$$\|H_{11}^{-1}H_{12}\|\rho_k \leq \min\left\{\frac{1}{2}\Delta_{k-1},\, \frac{1}{2}\Delta_k,\, 1\right\}, \qquad 1 \leq k \leq i,$$

then[2]

$$\left|\frac{\theta_i - \lambda_i}{\theta_i}\right| \leq \|H_{11}^{-1}H_{12}\|\rho_i.$$

Proof. Follows from Facts 7 and 8. ▯

Therefore, if the bound in Fact 7 is small compared to the eigenvalue separation, then Fact 7 bounds the relative distance between ith Ritzvalue and eigenvalue.

[2]The boundary conditions are $\|H_{11}^{-1}H_{12}\|\rho_1 \leq \min\{\frac{1}{2}\Delta_1, 1\}$ and $\|H_{11}^{-1}H_{12}\|\rho_m \leq \min\{\frac{1}{2}\Delta_{m-1}, 1\}$.

7. Relative Separation. One of the requirements for the QSE method [9] is that the computed eigenvalues have a relative separation that is accurate to at least 5 percent. We present a perturbation bound for the relative separation of the Ritz values, when eigenvalues and Ritz values are real.

We use the same stringent concept of separation as in the previous section,

$$\Delta_k(\lambda) \equiv \frac{\lambda_{k+1}-\lambda_k}{\max\{|\lambda_k|,\, |\lambda_{k+1}|\}}, \qquad \Delta_k(\theta) \equiv \frac{\theta_{k+1}-\theta_k}{\max\{|\theta_k|,\, |\theta_{k+1}|\}},$$

where $\lambda_k \leq \lambda_{k+1}$ and $\theta_k \leq \theta_{k+1}$. The relative accuracy of $\Delta_k(\theta)$ is

$$\left|\frac{\Delta_k(\lambda)-\Delta_k(\theta)}{\Delta_k(\lambda)}\right|.$$

FACT 9. *Let $\lambda_1 < \lambda_2$ and $\theta_1 < \theta_2$ be real and non-zero with $\lambda_1 = \theta_1(1+\epsilon_1)$ and $\lambda_2 = \theta_2(1+\epsilon_2)$ where $|\epsilon_1|, |\epsilon_2| < \epsilon$ for some $0 \leq \epsilon < 1$.*

Then

$$\left|\frac{\Delta_1(\lambda)-\Delta_1(\theta)}{\Delta_1(\lambda)}\right| \leq \frac{1}{1-\frac{\mu}{M}}\,\frac{2\epsilon}{1-\epsilon},$$

where $\mu \equiv \min\{|\lambda_1|,\, |\lambda_2|\}$ and $M \equiv \max\{|\lambda_1|,\, |\lambda_2|\}$.

Proof. The assumption $|\epsilon_i| < 1$ assures that λ_i and θ_i have the same sign. □

The factor $1/(1-\frac{\mu}{M})$ is a condition number for the relative separation. It's basically the same as the condition number for subtraction. The condition number is close to one, if the relative separation between λ_1 and λ_2 is large. The accuracy requirement of 5 percent for the QSE method is not so hard to achieve, as the following example illustrates. Suppose λ_1 and λ_2 are accurate to 8 digits, $\epsilon \leq 10^{-8}$. To obtain a relative accuracy of at least .05 for the relative separation, it suffices to have $\lambda_1 \leq (1-10^{-6})\lambda_2$.

COROLLARY 7.1. *Let H be Hermitian and H_{11} be nonsingular; and let the m smallest eigenvalues $\lambda_1 < \ldots < \lambda_m$ of H be distinct and non-zero.*

If $\|H_{11}^{-1}H_{12}\|\rho_i < 1$, $1 \leq i \leq m$, then

$$\left|\frac{\Delta_i(\lambda)-\Delta_i(\theta)}{\Delta_i(\lambda)}\right| \leq \frac{1}{1-\frac{\mu_i}{M_i}}\,\frac{2\epsilon_i}{1-\epsilon_i}, \qquad 1 \leq i \leq m-1,$$

where $\epsilon_i \equiv \|H_{11}^{-1}H_{12}\|\ \max\{\rho_i, \rho_{i+1}\}$, and

$$\mu_i \equiv \min\{|\lambda_i|,\, |\lambda_{i+1}|\}, \qquad M_i \equiv \max\{|\lambda_i|,\, |\lambda_{i+1}|\}.$$

Therefore, if the Ritz values are sufficiently accurate then the accuracy of the Ritz value separation is comparable to the accuracy of the Ritz values. Note that the conditions for an accurate Ritz value separation are less stringent than the ones in Corollary 6.1 that guarantee the pairing up of a Ritz value with the corresponding eigenvalue.

8. Several Eigenvalues. We present simultaneous error bounds for all eigenvalues of H_{11}.

Let $\lambda_1, \ldots, \lambda_m$ be distinct eigenvalues of a complex square matrix H. Set

$$\Lambda \equiv \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_m \end{pmatrix}, \qquad V \equiv (\, v_1 \quad \ldots \quad v_m \,),$$

where v_j is an eigenvector for λ_j, so $HV = V\Lambda$. Partition V conformally with H, $V = \begin{pmatrix} V_{11} \\ V_{21} \end{pmatrix}$.

The quantities $\|V_{21}\|\|V_{11}^{-1}\|$, and $\|V_{21}V_{11}^{-1}\|$ for Hermitian matrices, measure the block quasi-sparsity of the vectors V with regard to the partition $\begin{pmatrix} V_{11}^T & V_{21}^T \end{pmatrix}^T$. They appear to represent a more stringent measure of quasi-sparsity then ρ_j from Definition 2.1 because

$$\min_{1\leq i\leq m} \rho_i \leq \frac{1}{\sqrt{m}}\|V_{21}V_{11}^{-1}\| \leq \frac{1}{\sqrt{m}}\|V_{21}\|\,\|V_{11}^{-1}\|.$$

The bound below extends [10, Theorem (11-5-7)] from Hermitian to diagonalizable matrices. Although neither H nor H_{11} are normal, the bound contains no eigenvector condition numbers.

Fact 10. *If $\lambda_1, \ldots, \lambda_m$ are distinct eigenvalues of H, and V_{11} is non-singular, then there is a permutation $\sigma(\cdot)$ so that*

$$\left(\sum_{i=1}^m |\theta_{\sigma(i)} - \lambda_i|^2\right)^{1/2} \leq \sqrt{m}\,\|H_{12}\|_F\,\|V_{21}\|\,\|V_{11}^{-1}\|.$$

Proof. Write the first block row of $H\begin{pmatrix} V_{11} \\ V_{21} \end{pmatrix} = \begin{pmatrix} V_{11} \\ V_{21} \end{pmatrix}\Lambda$ as

$$V_{11}^{-1}H_{11}V_{11} - \Lambda = -V_{11}^{-1}H_{12}V_{21}.$$

Since Λ is normal, [13, Theorem 1.1], [2, Problem VI.8.11] imply that there is a permutation $\sigma(\cdot)$ so that

$$\begin{aligned}\left(\sum_{i=1}^m |\theta_{\sigma(i)} - \lambda_i|^2\right)^{1/2} &= \left(\sum_{j=1}^m |\lambda_{\sigma(i)}(V_{11}^{-1}H_{11}V_{11}) - \lambda_i|^2\right)^{1/2} \\ &\leq \sqrt{m}\,\|H_{12}\|_F\,\|V_{21}\|\,\|V_{11}^{-1}\|.\end{aligned}$$

□

For a block of vectors to be quasi-sparse, V_{11} must be well-conditioned with respect to inversion and $\|V_{21}\|$ must be small. Unfortunately $\|V_{21}\|\,\|V_{11}^{-1}\|$ is not invariant under column scaling. The bound can be improved when the desired eigenvalues are real.

Fact 11 (Real Eigenvalues). *If $\lambda_1 < \ldots < \lambda_m$ are real, and V_{11} is non-singular then*

$$\left(\sum_{i=1}^m |\theta_i - \lambda_i|^2\right)^{1/2} \leq \sqrt{2}\,\|H_{12}\|_F\,\|V_{21}\|\,\|V_{11}^{-1}\|,$$

where $\Re(\theta_1) \leq \ldots \leq \Re(\theta_m)$.

If, in addition, H_{11} is Hermitian then

$$\left(\sum_{i=1}^m |\theta_i - \lambda_i|^2\right)^{1/2} \leq \sqrt{2}\,\|H_{12}\|_F\,\|V_{21}V_{11}^{-1}\|.$$

Proof. For the first inequality write

$$V_{11}^{-1} H_{11} V_{11} - \Lambda = -V_{11}^{-1} H_{12} V_{21},$$

where Λ is Hermitian. For the second inequality write

$$H_{11} - V_{11} \Lambda V_{11}^{-1} = -H_{12} V_{21} V_{11}^{-1},$$

where H_{11} is Hermitian. Apply [7, §0, (ii)], [2, Problem VI.8.7]. □

The quasi-sparsity measure $\|V_{21} V_{11}^{-1}\|$ in the second bound has the advantage of being invariant under column scaling. Since the eigenvalues λ_j are assumed to be distinct, the quasi-sparsity measure for Hermitian matrices is unique.

The bounds in this section are tighter than [10, Theorem (11-5-7)] when the eigenvectors are quasi-sparse, i.e. $\|V_{21}\| \, \|V_{11}^{-1}\| < 1$ or $\|V_{21} V_{11}^{-1}\| < 1$. However, the eigenvalues of H in [10, Theorem (11-5-7)] are not known, while here we can pick them to our liking.

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