BOUNDS ON THE CONVERGENCE OF RITZ VALUES FROM KRYLOV SUBSPACES TO INTERIOR EIGENVALUES OF HERMITEAN MATRICES

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Abstract. We consider bounds on the convergence of Ritz values from a sequence of Krylov subspaces to interior eigenvalues of Hermitean matrices. These bounds are useful in regions of low spectral density, for example near voids in the spectrum, as is required in many applications. Our bounds are obtained by considering the usual Kaniel–Paige–Saad formalism applied to the shifted and squared matrix.

Key words. Lanczos, Krylov, spectrum, eigensolvers, linear algebra

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1. Introduction. In this paper we derive a bound on how well an eigenvalue of a Hermitean matrix is approximated by the corresponding Ritz value obtained from its restriction to a Krylov subspace. Such bounds are useful in practice because no Krylov space based method for determining eigenpairs (such as Arnoldi or Lánczos algorithms) can do better than this even in exact arithmetic.

We shall show that the eigenvalues \( \lambda_\alpha \) of an \( N \times N \) Hermitean matrix \( A \) are approximated by its Ritz values \( \theta_\alpha \) from the Krylov space \( K_n(A,v) \) with an error bounded by

\[
0 \leq \lambda_\alpha - \theta_\alpha \leq \min_{\Lambda} \frac{2(\lambda'_j - \lambda'_N)(K'_j \tan \angle'_j)^2 e^{-2(n-2j)\mu'_j} + O(\mu'_j^2)}{|\lambda_\alpha - \Lambda|}
\]

where \( \lambda'_1 \geq \lambda'_2 \geq \cdots \geq \lambda'_N \) are the eigenvalues of \( A' \equiv -(\Lambda - A)^2 \) with \( j \) such that \( \lambda'_j = -(\Lambda - \lambda_\alpha)^2 \),

\[
K'_j \approx \prod_{i=1}^{j-1} \frac{\lambda'_i - \lambda'_N}{\lambda'_i - \lambda'_j}, \quad \mu'_j = \sqrt{\frac{\lambda'_j - \lambda'_{j+1}}{\lambda'_{j+1} - \lambda'_N}},
\]

and \( \angle'_j \) is the angle between the projection of \( v \) onto \( \text{span}(z_{j+1}, \ldots, z_N) \) and \( z_j \) where \( z_i \) is an eigenvector of \( A' \) (and thus also of \( A \)) belonging to the eigenvalue \( \lambda'_j \).

In section §2 we briefly indicate why the problem of finding approximations to interior eigenvalues of large Hermitean matrices is important in a variety of physical applications. In §3 we review some basic properties of Hermitean matrices introducing the notation to be used throughout the paper, and in §4 we review some useful bounds on Ritz values for general subspaces. Section §5.1 derives the bounds on the convergence of extremal eigenvalues due to Kaniel [2], Paige [4] and Saad [7]. We then present a straightforward but apparently new generalization that gives bounds for the interior eigenvalues close to “voids” in the spectrum in §5.2 followed by some examples illustrating the application of our bounds.

2. Applications. The problem of finding good approximations to interior eigenvalues in low-density regions of the spectrum of a Hermitean matrix is common to
many areas of computational science, but the particular application that led us to consider this problem [3] is that of evaluating the Neuberger operator for lattice QCD (Quantum Chromodynamics being the quantum field theory of the strong nuclear force). This requires us to evaluate the \textit{signum} function of the “Hermitean Dirac operator” $\gamma_5 D$, which is defined by diagonalizing this matrix and taking the sign ($\pm 1$) of each of its eigenvalues. It is far too expensive to carry out the full diagonalization, so we use a Zolotarev rational approximation for the signum function as this can be evaluated just using matrix addition, multiplication, and inversion (using a multi-shift solver for its stable partial fraction expansion). This approximation is expensive for very small eigenvalues of $\gamma_5 D$, and as there are only a relatively small number of these we want to deflate them and take their sign explicitly. While the Neuberger operator is Hermitean, it is not positive; furthermore, for physically interesting parameters its spectrum has a large void around zero, with perhaps only a few “topological” or “defect” modes leading to discrete eigenvalues within this void. The relevant numerical problem is therefore to find the eigenpairs within or close to this void.

Previously [1] such eigenpairs had been found by finding the extremal eigenpairs of the square of the Neuberger operator, but this then required further effort to separate artificial degeneracies of the squared matrix arising from (almost) degenerate positive and negative eigenvalues of the original matrix. We observed that there is in fact no need to square the matrix, as the desired eigenpairs converge rapidly for the Neuberger operator itself, despite the fact that the eigenvalues are far from either end of the spectrum and thus the usual Kaniel–Paige–Saad bounds are not applicable. We used a new algorithm based on the Lánczos algorithm with selective orthogonalization (LANSO) method of Parlett and Scott [6] (which avoids the appearance of duplicates of eigenvalues due to rounding errors in finite-precision arithmetic computations) that allows us to find eigenpairs with eigenvalues of a Hermitean matrix $A$ that lie within a specified interval. We shall describe this algorithm in a forthcoming publication.

The fact that such interior eigenpairs converged rapidly led us to consider how to find realistic bounds in this case, and we were led to use the Kaniel–Paige–Saad bounds for the extremal eigenvalues of the shifted and squared matrix $-(\Lambda - A)^2$ to give bounds on the convergence of the original matrix $A$.

We do not believe that applications in which such interior eigenvalues in low-density spectral regions are important are unusual. To give just one more example, we may consider the Hamiltonian for an electron in a metal, semiconductor, or insulator, which may be approximated by a large Hermitean matrix with “conduction bands” separated by large “band gaps”. The details of the eigenvalues deep within the bands are not too important: for example their separation is related to the inverse (macroscopic) volume of the system under consideration, but the eigenpairs at the edges of and between the bands determine many physically important properties.

3. Basic Properties of Hermitean Matrices. In this section we summarize the basic properties of Hermitean (symmetric) matrices, with the goal of specifying our notation.

A matrix $A$ is \textit{Hermitean} (with respect to a sesquilinear inner product) if $A = A^\dagger$, which means $(u, Av) = (A^\dagger u, v) = (Au, v) = (v, Au)^*$, or equivalently $u^\dagger \cdot Av = (A^\dagger u)^\dagger \cdot v = (Au)^\dagger \cdot v = (v^\dagger \cdot Au)^*$. An eigenvalue $\lambda$ of $A$ satisfies $Az = \lambda z$ where $z \neq 0$ is the corresponding eigenvector. The eigenvalues are real

$$\lambda = \frac{(z, Az)}{(z, z)} = \frac{(z, A^\dagger z)}{(z, z)} = \frac{(z, A^* z)}{(z, z)} = \frac{(z, Az)^*}{(z, z)} = \lambda^*,$$
and the eigenvectors corresponding to different eigenvalues are orthogonal: \( \lambda(z', z) = (z', Az) = (Az', z) = \lambda^*(z', z) = \lambda' (z', z) \), hence \((\lambda' - \lambda)(z', z) = 0\), so \( \lambda \neq \lambda' \Rightarrow (z', z) = 0 \). We can choose eigenvectors belonging to the same eigenvalue to be orthonormal, for example by using the Gram–Schmidt procedure, as any linear combination of such eigenvectors is also an eigenvector.

Since any matrix can be reduced to triangular form \( T \) by a unitary (orthogonal) transformation\(^1\) (change of basis), \( A = UTU^{-1} = UTU^\dagger \), and \( T^\dagger = (U^\dagger AU)^\dagger = U^\dagger A^\dagger U = U^\dagger AU = T \), it follows that \( T \) is real and diagonal, and thus \( AU = UT \) so the columns of \( U \) furnish the orthonormal eigenvectors.

4. Subspace Bounds.

4.1. Rayleigh Quotient. We consider how the eigenvalues and eigenvectors of an approximation to a matrix \( A \) are related to the actual eigenpairs. Consider the Rayleigh quotient which has the spectral representation

\[
\rho(u, A) = \frac{(u, Au)}{(u, u)} = \sum_j \lambda_j \frac{|(z_j, u)|^2}{\sum_k |(z_k, u)|^2}.
\]

This is a weighted mean of eigenvalues, so it satisfies the inequalities \( \lambda_1 \geq \rho(u, A) \geq \lambda_N \), where \( N = \text{dim } A \) and we have ordered the eigenvalues such that \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N \).

4.2. Ritz Pairs. The extrema of the Rayleigh quotient may be found by varying the components \( u_j = (z_j, u) \) of \( u \) subject to the constraint that \( ||u|| = 1 \). Introducing a Lagrange multiplier \( \mu \) we find \((A - \mu)u = 0\), whose solutions are the eigenpairs \( \mu = \lambda_j \) with \( u = z_j \) for \( j = 1, \ldots, N \). If we restrict \( u \) to an \( m \)-dimensional subspace \( X \subseteq \mathbb{R}^N \) then the extrema of the Rayleigh quotient are the Ritz pairs \( \mu = \theta_j \) with \( u = y_j \) for \( j = 1, \ldots, m \). The Ritz pairs are the eigenvalues and eigenvectors of the restriction of \( A \) to the subspace, \( H = Q^\dagger AQ \), that is \( \text{Hs}_j = \theta_j \text{s}_j \). Here \( Q \) is an \( N \times m \) matrix with orthonormal columns \( (QQ^\dagger = 1) \) and \( QQ^\dagger \) is an orthogonal projector onto \( X \). Note that the vectors \( y_j = Qs_j \in \mathbb{R}^N \) are not eigenvectors of \( A \), although \( Q^\dagger(A - \theta_j)y_j = 0 \), since the residual \( R = AQ - QH \neq 0 \) in general. The Rayleigh quotient \( \rho(u \in X, A) \) restricted to the subspace \( X \) is a weighted mean of Ritz values so \( \theta_1 \geq \rho(u \in X, A) \geq \theta_m \) where we have ordered the Ritz values \( \theta_1 \geq \theta_2 \geq \cdots \geq \theta_m \).

For large matrices our strategy is to compute the Ritz pairs of \( A \) for suitably chosen subspaces \( X \); we are interested in how well these may approximate the eigenvalues of \( A \) itself.

4.3. MaxMin and MinMax Bounds. Let \( S_j \subseteq X \) be an arbitrary subspace of dimension \( j \), and \( C_{j-1} \subseteq X \) another arbitrary subspace of codimension \( j - 1 \), i.e., a subspace of dimension \( m - j + 1 \) if \( m < \infty \). There must be a non-zero vector \( \mathbf{v} \in S_j \cap C_{j-1} \), where of course \( \mathbf{v} \) depends upon \( S_j \) and \( C_{j-1} \); therefore \( \min_{u \in S_j} \rho(u, A) \leq \rho(\mathbf{v}, A) \leq \max_{u \in C_{j-1}} \rho(u, A) \). Hence, for any pair of subspaces \( S_j \) and \( C_{j-1} \), \( \min_{u \in S_j} \rho(u, A) \leq \max_{u \in C_{j-1}} \rho(u, A) \). Taking the maximum over all \( S_j \) and the minimum over all \( C_{j-1} \) we obtain \( \max_{S_j \subseteq X} \min_{u \in S_j} \rho(u, A) \leq \min_{C_{j-1} \subseteq X} \max_{u \in C_{j-1}} \rho(u, A) \). For the particular subspace \( S_j = \text{span}(y_1, \ldots, y_j) \) the

\(^1\)This is “Schur normal form”, which follows from the Cayley–Hamilton theorem that every matrix satisfies its characteristic equation, and the fundamental theorem of algebra which states that the characteristic polynomial \( p(\lambda) = \det(A - \lambda) \) has exactly \( \dim A \) complex roots, counting multiplicity.
shall assume that the initial vector is not orthogonal to the eigenvector, \( (v) \) this would be very unlikely for a randomly chosen \( \mathbf{x} \). The central inequality following from the inclusion bound gives the first and last inequalities in 5.1. Kaniel–Paige–Saad Bounds. This would be very unlikely for a randomly chosen \( \mathbf{x} \). The central inequality following from the inclusion bound gives the first and last inequalities in 5.1. Kaniel–Paige–Saad Bounds. 

**4.4. Krylov Spaces.** An interesting family of subspaces are the Krylov spaces

\[
K_n(A, \mathbf{v}) = \text{span}(\mathbf{v}, A\mathbf{v}, A^2\mathbf{v}, \ldots, A^{n-1}\mathbf{v})
\]

where \( \mathbf{v} \neq 0 \) is some arbitrary vector. The Ritz values of \( A \) in a Krylov space are non-degenerate, as otherwise we could construct a Ritz vector \( \mathbf{y} \neq 0 \) such that \( (\mathbf{y}, \mathbf{v}) = 0 \): this would imply that \( (\mathbf{y}, A^k\mathbf{v}) = \theta^k(\mathbf{y}, \mathbf{v}) = 0 \) \( \forall k \geq 0 \) contradicting the assumption that \( \mathbf{y} \in K_n(A, \mathbf{v}) \).

A similar argument shows that for Ritz pairs \( \theta, \mathbf{y} \) and \( \theta', \mathbf{y}' \) there is a unit vector \( \mathbf{u} \in \text{span}(\mathbf{y}, \mathbf{y}') \) with \( (\mathbf{u}, \mathbf{v}) = 0 \), for which \( (\mathbf{u}, A^k\mathbf{v}) \propto (\theta - \theta')\|\mathbf{v}\| \), indicating that although we may find good approximations in a Krylov space for nearly-degenerate eigenvalues, we should not expect the same to be true for the corresponding eigenvectors.

**5. Error Bounds.**

**5.1. Kaniel–Paige–Saad Bounds.** In this section we briefly survey the derivation of the Kaniel–Paige–Saad bounds on the extremal eigenvalues of Hermitian matrices. Our notation is similar but not identical to that of Parlett [5].

Let us now study how rapidly we may expect eigenvalues to converge to a given accuracy in the sequence of Krylov spaces of increasing dimension. We shall follow the method introduced by Kaniel [2] and corrected and extended by Paige [4] and Saad [7]. Consider the angle \( \angle(\mathbf{z}_j, \mathbf{u}) \) between an eigenvector \( \mathbf{z}_j \) and a vector \( \mathbf{u} \in K_n(A, \mathbf{v}) \). We shall assume that the initial vector is not orthogonal to the eigenvector, \( (\mathbf{z}_j, \mathbf{v}) \neq 0 \): this would be very unlikely for a randomly chosen \( \mathbf{v} \). Indeed, we expect than on average \( |(\mathbf{z}_j, \mathbf{v})| \approx 1/\sqrt{N} \) if \( \mathbf{v} \) is a random unit vector.

Consider the subspace \( X \subseteq K_n(A, \mathbf{v}) \subseteq \mathbb{R}^N \), with \( X = \text{span}(\mathbf{y}_j, \mathbf{y}_{j+1}, \ldots, \mathbf{y}_n) \) where the \( \mathbf{y}_i \) are Ritz vectors for \( K_n(A - \lambda_j, \mathbf{v}) = K_n(A, \mathbf{v}) \) for which the MaxMin bound gives the first and last inequalities in

\[
\theta_j - \lambda_j = \max_{S_j \subseteq \lambda A} \min_{u \in S_j} \rho(\mathbf{u}, A - \lambda_j) \leq \max_{S_j \subseteq \mathbb{R}^n} \min_{u \in S_j} \rho(\mathbf{u}, A - \lambda_j) = 0,
\]

the central inequality following from the inclusion \( X \subseteq \mathbb{R}^N \). \( \rho(\mathbf{u} \in X, A) \leq \theta_j \) as it is a weighted mean of \( \theta_j, \theta_{j+1}, \ldots, \theta_n \), hence \( \rho(\mathbf{u} \in X, A - \lambda_j) \leq \theta_j - \lambda_j \), or equivalently

\[
0 \leq \lambda_j - \theta_j \leq \rho(\mathbf{u} \in X, \lambda_j - A).
\]

Any \( \mathbf{u} \) in the Krylov space can be written as \( \mathbf{u} = p(A)\mathbf{v} \) where \( p \) is a polynomial of degree \( \deg p \leq n - 1 \). A sufficient condition for \( \mathbf{u} = p(A)\mathbf{v} \) to be in \( X \) is that the polynomial \( p \) has the Ritz values \( \theta_1, \theta_2, \ldots, \theta_{n-1} \) as roots, \( p(\theta_i) = 0 \) for \( i < j \). If \( p(A) = (A - \theta_i)q(A) \) with \( q \) some polynomial of degree \( \leq n - 2 \) then \( (\mathbf{y}_i, \mathbf{u}) = (\mathbf{y}_i, p(A)\mathbf{v}) = (\mathbf{y}_i, (A - \theta_i)q(A)\mathbf{v}) = ((A - \theta_i)\mathbf{y}_i, q(A)\mathbf{v}) = (\mathbf{w}, q(A)\mathbf{v}) = 0 \), where \( \mathbf{w} \) is a vector orthogonal to \( K_n(A, \mathbf{v}) \) and hence to \( q(A)\mathbf{v} \in K_{n-1}(A, \mathbf{v}) \). Therefore a sufficient condition for \( \mathbf{u} \in X \) is that \( p(x) = q(x)l(x) \) with \( \deg q \leq n - j \) and \( l(x) = \prod_{i=1}^{j-1} \frac{x - \theta_i}{\theta_j - \theta_i} \). Although we do not need it here it is easy to prove that this is also a necessary condition.
The Rayleigh quotient for a vector $u = p(A)v = \sum_{k=1}^{N} p(\lambda_k)z_k(v, v)$ is
\[
\rho(u \in X, \lambda_j - A) = \frac{u, (\lambda_j - A)u}{u, u} = \frac{\sum_{k=1}^{N} |p(\lambda_k)(z_k, v)|^2(\lambda_j - \lambda_k)}{\sum_{k=1}^{N} |p(\lambda_k)(z_k, v)|^2}.
\]

The terms in the numerator for $k < j$ are all negative, so we may bound $\rho$ above by dropping them; likewise we only increase the bound by replacing $\lambda_j - \lambda_k$ by $\lambda_j - \lambda_N$ for the remaining terms in the numerator, and dropping all the terms with $k \neq j$ in the denominator, leading to
\[
\rho(u \in X, \lambda_j - A) \leq (\lambda_j - \lambda_N) \frac{\sum_{k=j+1}^{N} |p(\lambda_k)(z_k, v)|^2}{|p(\lambda_j)(z_j, v)|^2}.
\]

From this we immediately obtain the desired bound using Kaniel’s choice of $q$ as the Chebyshev polynomial $T_{n-j} \circ \gamma_j$, where
\[
\gamma_j(\lambda) = 2\frac{\lambda - \lambda_N}{\lambda_{j+1} - \lambda_N} - 1 = 1 + 2\frac{\lambda - \lambda_{j+1}}{\lambda_{j+1} - \lambda_N}
\]
maps the interval $[\lambda_N, \lambda_{j+1}] \mapsto [-1, 1]$, hence (q.v., Appendix A)
\[
\max_{\lambda \in [\lambda_N, \lambda_{j+1}]} |q(\lambda)| = \max_{x \in [-1, 1]} |T_{n-j}(x)| \leq 1
\]
Furthermore $l(\lambda_j) = 1$, so if we define $K_j \equiv |l(\lambda_N)| \geq \max_{\lambda \in [\lambda_N, \lambda_{j+1}]} |l(\lambda)|$ we obtain
\[
\rho(u \in X, \lambda_j - A) \leq (\lambda_j - \lambda_N)(K_j \tan \angle_j)^2
\]

Here $(\tan \angle_j)^2 = \frac{\sum_{k=j+1}^{N} |(z_k, v)|^2}{\sum_{k=j+1}^{N} |(z_k, v)|^2}$, so $\angle_j$ is the angle between the projection of $v$ onto $\text{span}(z_{j+1}, \ldots, z_N)$ and $z_j$. Note that in the interesting case where $\theta_i \approx \lambda_i$ for $i \leq j$
\[
K_j = \prod_{i=1}^{j-1} \frac{\theta_i - \lambda_N}{\theta_i - \lambda_j} \approx \prod_{i=1}^{j-1} \frac{\lambda_i - \lambda_N}{\lambda_i - \lambda_j}.
\]

From the bounds on Chebyshev polynomials given in Appendix A we get
\[
0 \leq \lambda_j - \theta_j \leq 4(\lambda_j - \lambda_N)(K_j \tan \angle_j)^2 e^{-4(n-j)\mu_j + O(\mu_j^2)}
\]
where $\gamma_j(\lambda_j) = 1 + 2\mu_j^2$ with $\mu_j = \sqrt{\frac{\lambda_{j+1} - \lambda_N}{\lambda_{j+1} - \lambda_N}}$, and thus $\ln \left(\gamma_j(\lambda_j) + \sqrt{\gamma_j(\lambda_j)^2 - 1}\right) = 2\mu_j + O(\mu_j^2)$.

5.2. Bounds for Interior Eigenvalues. We will produce a bound for an interior eigenvalue by introducing a shift $\Lambda$ and considering the spectrum of the shifted and squared matrix $A' \equiv - (A - \Lambda)^2$. The parameter $\Lambda$ is only needed for our error bound and has no effect on the Krylov space Ritz values; hence the best bound will just be the minimum over all possible values of $\Lambda$; a practical bound can be found by a judicious choice of $\Lambda$.

Notice that the “interior” eigenvalues of $A$ near $\Lambda$ are the largest eigenvalues of $A'$. Furthermore, the Krylov space for $A'$ is contained within that for $A$, albeit with twice the size (but the same number of applications of $A$): $K_n(- (A - \Lambda)^2, v) \subseteq K_{2n}(A, v)$. 
We will establish that the Kaniel–Paige–Saad bounds for $K_n(A', v)$ must therefore also hold for the latter.

Suppose that the spectrum of $A$ has an interior eigenvalue $\lambda_\alpha$. As usual, we shall write the eigenvalues in decreasing order $\lambda_1 \geq \cdots \geq \lambda_{\alpha-1} \geq \lambda_\alpha \geq \cdots \geq \lambda_N$, as we shall do for the corresponding eigenvalues of $A'$, $\lambda'_1 \geq \cdots \geq \lambda'_{\alpha-1} \geq \lambda'_\alpha \geq \cdots \geq \lambda'_N$. The smallest eigenvalue of $A'$ is $\lambda'_N = \min((-\lambda_1 - \Lambda)^2, -(\lambda_N - \Lambda)^2)$. We apply the Kaniel–Paige–Saad bound to the matrix $A'$ in the Krylov space $K_n(A', v)$ whose Ritz pairs are $\theta'_j, y'_j$ for $j = 1, \ldots, n$. Following the arguments of the preceding section we find that the Ritz value $\theta'_j$ satisfies $\lambda'_j \geq \theta'_j \geq \rho(u \in X', A')$ for any vector $u \in X' \equiv \text{span}(y'_j, y'_{j+1}, \ldots, y'_n)$ and the Rayleigh quotient is bounded by choosing $u = p'(A')v$ for the polynomial

$$p'(x) = T_{n-j} \left( \frac{x - \lambda'_N}{\lambda'_{j+1} - \lambda'_N} - 1 \right) \prod_{i=1}^{j-1} \frac{\theta'_i - x}{\theta'_i - \lambda'_j}.$$  

This leads to $0 \leq \lambda'_j - \theta'_j \leq \rho(u \in X', \lambda'_j - A')$ with

$$\rho(u \in X', \lambda'_j - A') \leq 4(\lambda'_j - \lambda'_N) (K'_j)^2 e^{-4(n-j)\mu'_j + O(\mu'_j^2)} \equiv \varepsilon'_\Lambda,$$

where

$$K'_j \equiv \prod_{i=1}^{j-1} \frac{\theta'_i - \lambda'_N}{\theta'_i - \lambda'_j} \approx \prod_{i=1}^{j-1} \frac{\lambda'_i - \lambda'_N}{\lambda'_i - \lambda'_j},$$

$$\mu'_j = \sqrt{\frac{\lambda'_j - \lambda'_{j+1}}{\lambda'_{j+1} - \lambda'_N}},$$

and $\varepsilon'_j$ is analogous to $\varepsilon_j$ (the eigenvectors of $A'$ are the same as those of $A$ but their ordering is different).

Let $\nu \equiv |\lambda_\alpha - \Lambda|$, $\xi \equiv \sqrt{-\theta'_j} > 0$ (recall that with our conventions both $\lambda'_j \leq 0$ and $\theta'_j \leq 0$), and $\delta \equiv \lambda'_j - \theta'_j = -\nu^2 + \xi^2 = (\xi - \nu)(\xi + \nu)$ with $0 \leq \delta \leq \varepsilon'_\Lambda$. Then $\xi - \nu = \frac{\varepsilon'_\Lambda}{2\nu} \leq \delta \leq \frac{\varepsilon'_\Lambda}{2\nu}$ since $\delta \geq 0 \Rightarrow \xi - \nu \geq 0 \Rightarrow \xi + \nu = (\xi - \nu) + 2\nu \geq 2\nu$. Hence we obtain the following bound on the error in the Ritz value $\tilde{\theta}_\alpha = \Lambda \pm \sqrt{-\theta'_j}$ of $A$ corresponding to the eigenvalue $\lambda_\alpha$ of $A$ obtained from the Ritz value $\theta'_j$ of $A'$ in the Krylov space $K_n(A', v)$:

$$\left| \lambda_\alpha - \tilde{\theta}_\alpha \right| = \min_{\pm} |\lambda_\alpha - (\Lambda \pm \sqrt{-\theta'_j})| = \xi - \nu \leq \frac{\varepsilon'_\Lambda}{2\nu} = \frac{\varepsilon'_\Lambda}{2|\lambda_\alpha - \Lambda|}.$$  

Furthermore, since $K_n(A', v) \subseteq K_{2n}(A, v) \subseteq \mathbb{R}^N$ the MaxMin inequalities

$$\max_{S \subseteq K_n(A', v)} \min_{u \in S} \rho(u, A) \leq \max_{S \subseteq K_{2n}(A, v)} \min_{u \in S} \rho(u, A) \leq \max_{S \subseteq \mathbb{R}^N} \min_{u \in S} \rho(u, A)$$

imply that $\tilde{\theta}_\alpha \leq \theta_\alpha \leq \lambda_\alpha$. This means that the bound (5.2) on the error of the Ritz value $\theta_\alpha$ from the Krylov space $K_n(A', v)$ bounds that of the Ritz value $\theta_\alpha$ from the Krylov space $K_{2n}(A, v)$, $\lambda_\alpha - \tilde{\theta}_\alpha \geq \lambda_\alpha - \theta_\alpha \geq 0$.

5.3. Discussion. The advantage of the bound given by equations (5.1) and (5.2) is that although the exponents $\mu'$ will in general be smaller than those from the original Kanell–Paige–Saad bound the prefactor $K'$ may be far smaller in the interior of the spectrum.
Furthermore, μ′ may not be much smaller than μ for eigenvalues in low density parts of the spectrum for a good choice of the parameter Λ. For example, suppose that λ,, is just below a large void in the spectrum of width Δ, but not necessarily immediately adjacent to it, and is also close to λ,+. We can choose Λ near the middle of void such that λ'=+ = (λ, − Λ)2. For notational simplicity let us also assume that λ' = −(λN − Λ)2, so

\[
\mu_j^2 = \frac{λ'_j - λ'_j+1}{λ'_j+1 - λ'_j} = -\frac{(λa - Λ)^2 + (λa+1 - Λ)^2}{(λa+1 - Λ)^2 + (λN - Λ)^2} = \frac{(λa - λa+1)(2Λ - λa - λa+1)}{(λa+1 - λN)(2Λ - λa+1 - λN)}.
\]

Now, 2Λ − (λa + λa+) ∼ Δ, hence

\[
μ_j' = μ_j\sqrt{\frac{2Λ - λa - λa+1}{2Λ - λa+1 - λN}} \approx μ_j\sqrt{\frac{Δ}{2Λ - λa+1 + λN}} \geq μ_j\sqrt{\frac{Δ}{λa - λN}},
\]

which is only slightly smaller than μj if Δ is a significant fraction of the spectrum.

The limit on how far Λ can be from λa and λa+1 is that when it gets closer to a dense band of eigenvalues the opposite side of the void the ordering of the eigenvalues of A′ will change and λj+1 ′ < −(λa+1 − Λ)2. A few eigenvalues within the void do not matter, as they can be “removed” by a suitable zero in the polynomial p′, at the cost of a smaller K′ factor and a slightly smaller factor n − j in the exponent.

Amusingly, for (near) extremal eigenvalues μ = μ′ as we may take Λ → ±∞. Nevertheless, there is always an extra factor of two in the exponent arising from the fact the Krylov space K2n(A, v) is twice as large as K_n(A′, v), so asymptotically for large n the original bound is always better. This is not too important for two reasons: firstly because we are usually interested in getting approximations within some specified error rather than in the limit where the error tends to zero, and secondly since the Ritz values are exactly equal to the eigenvalues for n = N in exact arithmetic (or for smaller values of n if the spectrum of A is degenerate) there is a natural upper limit on the dimension n of the Krylov space.

6. Examples.

6.1. Qualitative Example. As our first example, consider an N × N matrix A whose spectrum lies in the unit interval. This matrix has k bands, each containing N/k eigenvalues, and each band is separated by a “void” of size Δ. Within each band the eigenvalues are separated uniformly by δ = 1 − (k − 1)Δ/N.

If Δ = 0 then all the eigenvalues are uniformly spaced, so μj ∝ √δ = 1/√N for any λj, and the Kaniel–Paige–Saad bound shows that to resolve the eigenvalues we require a Krylov space of dimension n ∝ √N. For eigenvalues in the interior of the spectrum the Kj factors become large, of course.

If δ = 0 then A has k eigenvalues each with a degeneracy of N/k, and there are only k Ritz pairs. If δ ∼ 1 then the error in the Ritz values |θ − λ| ≈ δ for n ∼ k, but we require n ∝ 1/√δ in order to resolve the eigenvalues within each band (at least until the Ritz values become exact for n = N).

If Δ ∼ δ then the exponent μ′ ∝ √δ for an interior eigenvalue λ close to a void for shift Λ ≈ λ ∓ Δ/k, so to resolve it we also need n ∝ √N. This is the same scaling behaviour as for the usual bound, but the key difference between our bound and the usual one is that K′ ≪ K. As Δ → δ the scaling behaviour crosses over to n ∝ N since μ′ ∝ μ2. Perhaps this should not be too surprising as the Ritz values become exact for n = N.
6.2. Quantitative Example. Our second example is more quantitative. We consider a matrix with two bands of closely-spaced eigenvalues and a few other eigenvalues well-separated from these bands. In order to determine the value of the shift Λ we need to specify the value of n — the dimension of the Krylov space $K_n(A, v)$ — at which the bounds are to be evaluated. We do this implicitly by choosing the value of Λ for which a bound of some specified magnitude, in this case $10^{-8}$, is achieved for the smallest n. We compute an approximation to such a Λ by minimizing the exponent $\mu'$. To do this we note that since $d\mu'/d\Lambda \neq 0$ anywhere $\mu'$ can only have an extremum as a function of Λ when two eigenvalue of $A'$ become degenerate, as at such points the correspondence between the eigenvalues of A and those of $A'$ changes so as to maintain the correct order of the $\lambda'$. We stress that these approximations merely mean that we may not have chosen quite the optimal value for Λ, nevertheless the bounds obtained are still valid since they hold for any Λ.

The convergence of the Ritz values is illustrated in Figure 6.1. This clearly shows that our new bounds (solid lines) are significantly tighter than the usual Kaniel–Paige–Saad bounds (dashed lines) for the well-separated interior eigenvalues, although as expected the original bounds are better for the extremal eigenvalues.
This example illustrates some other interesting properties of the bounds. Observe that the lowest eigenvalue in this example, \( \lambda_{46} = -13.2 \), is almost degenerate with the second-lowest eigenvalue, \( \lambda_{45} = -13.1 \). This means that its bounds correctly indicate that it will only converge slowly. Interestingly the bound for latter is better than that for the former because this small gap appears in the coefficient \( K_2 \) rather than the exponent \( \mu_1 \) of the extremal bounds for \(-A\).

If we did not know the spectrum beforehand, but tried to determine the bounds from the Ritz values from \( K_n(A, \mathbf{v}) \) for some large value of \( n \), we might be misled into thinking that the lowest eigenvalue was exactly degenerate, and thus obtain a much tighter bound on its convergence, and this bound would seem to agree with the empirical convergence of the Ritz value. Only when \( n \) becomes sufficiently large to resolve the splitting is this bound violated, there being a “plateau” in the error for this Ritz value until the Krylov space is able to separate the actual eigenpairs. The fact that the eigenvalue is nearly degenerate may be determined even for small \( n \) by “restarting”, that is constructing the Krylov space \( K_n(A, \mathbf{v}') \) for some different initial vector \( \mathbf{v}' \), but this is insufficient to distinguish between exact and near degeneracies.

It is often the case in applications that we are interested in finding eigenvalues and their eigenspaces up to some specified accuracy: for example, the matrix may be derived from a model that is only valid up to this accuracy. In such cases the bounds determined from the approximate spectrum may be more useful than the “exact” bounds, as might the “exact” bounds obtained from the approximate spectrum in which nearly degenerate eigenvalues are collapsed into exactly degenerate ones. This situation is common to both our shifted and squared bounds and to the original “extremal” bounds.

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Appendix A. Chebyshev Polynomials.

Chebyshev polynomials of the first kind may be defined as \( T_n(x) = \cos(n \cos^{-1} x) \), so it is immediately obvious that \( |T_n(x)| \leq 1 \) for \( |x| \leq 1 \). It is perhaps surprising that it is a polynomial in \( x \), but application of the binomial theorem shows that

\[
T_n(x) = \sum_{j=0}^{[n/2]} \sum_{\ell=0}^{j} \binom{n}{j} \binom{j}{\ell} (-1)^{j+\ell} x^{n+2(\ell-j)},
\]

so it is indeed a polynomial of degree \( n \). Moreover it is also easy to see that

\[
T_n(x) = \frac{1}{2} \left[ e^{n \ln(\sqrt{x^2+1}) - (x-1)\sqrt{x^2-1}} + e^{n \ln(\sqrt{x^2+1}) - (x+1)\sqrt{x^2-1}} \right] ;
\]

we thus deduce that \( T_n(x) \geq \frac{1}{2} e^{n \ln(\sqrt{x^2+1})} \) for \( x \geq 1 \).

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