VARATIONS OF RITZ AND LEHMANN BOUNDS

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ABSTRACT. Eigenvalue estimates that are optimal in some sense have self-evident appeal and leave estimators with a sense of virtue and economy. So, it is natural that ongoing searches for effective strategies for difficult tasks such as estimating matrix eigenvalues that are situated well into the interior of the spectrum revisit from time to time methods that are known to yield optimal bounds. This article reviews a variety of results related to obtaining optimal bounds to matrix eigenvalues — some results are well-known; others are less known; and a few are new. We focus especially on Ritz and harmonic Ritz values, and right- and left-definite variants of Lehmann’s method.

1. RITZ AND RELATED VALUES

Let $K$ and $M$ be $n \times n$ real symmetric positive definite matrices and consider the eigenvalue problem

$$Kx = \lambda Mx \quad (1.1)$$

Label the eigenvalues from the edges toward the center (following [16]) as

$$\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_{-3} \leq \lambda_{-2} \leq \lambda_{-1}$$

with labeling inherited by the associated eigenvectors: $x_1, x_2, \ldots, x_{-2}, x_{-1}$.

Solutions to (1.1) are evidently eigenvalue/eigenvector pairs of the matrix $M^{-1}K$, which is non-symmetric on the face of it. However, $M^{-1}K$ is self-adjoint with respect to both the $M$-inner product, $x^tMx$, and the $K$-inner product, $x^tKx$. Denote by $x^m$ the $M$-adjoint of a vector $x$, $x^m = x^tM$, and by $x^K$ the $K$-adjoint, $x^K = x^tK$. “Self-adjointness” of $M^{-1}K$ amounts to the assertion that for all $x$ and $y$, $x^m(M^{-1}Ky) = (M^{-1}Kx)^my$ and $x^K(M^{-1}Ky) = (M^{-1}Kx)^Ky$. Self-adjointness with respect to the $M$- and $K$-inner products implies that the matrix representation of $M^{-1}K$ with respect to any $M$-orthogonal or $K$-orthogonal basis will be symmetric.

For a given subspace $P$ of dimension $m < n$, the Rayleigh-Ritz method proceeds by selecting a basis for $P$, say constituting the columns of a matrix $P \in \mathbb{R}^{n \times m}$, and then considering the (smaller) eigenvalue problem

$$P^tKPy = \Lambda P^tMPy \quad (1.2)$$

This will yield $m$ eigenvalues (called Ritz values) labeled similarly to $\{\lambda_i\}$ as

$$\Lambda_1 \leq \Lambda_2 \leq \Lambda_3 \leq \cdots \leq \Lambda_{-3} \leq \Lambda_{-2} \leq \Lambda_{-1}$$
with corresponding eigenvectors \( y_1, y_2, \ldots, y_{-2}, y_{-1} \). Vectors in \( P \) given as \( u_k = Py_k \) are Ritz vectors associated with the Ritz values \( \Lambda_k \). Since \( \mathbb{R}^m = \text{span}(y_1, y_2, \ldots, y_{-2}, y_{-1}) \), the full set of Ritz vectors evidently forms a basis for \( P \), which is both \( K \)-orthogonal and \( M \)-orthogonal and may be presumed to be \( M \)-normalized without loss of generality: \( u_k^T u_j = 0 \) for \( i \neq j \), and \( u_k^T u_i = 1 \).

Harmonic Ritz values \([7]\) result from applying the Rayleigh-Ritz method to the eigenvalue problem

\[
KM^{-1}Kx = \lambda Kx,
\]

which is equivalent to \((1.1)\) — it has the same eigenvalues and eigenvectors. If we use the same subspace \( P \), the harmonic Ritz values are then the eigenvalues of the \( m \times m \) problem

\[
P^T KM^{-1}KPy = \tilde{\Lambda} P^T KPy,
\]

yielding

\[
\tilde{\Lambda}_1 \leq \tilde{\Lambda}_2 \leq \tilde{\Lambda}_3 \leq \cdots \leq \tilde{\Lambda}_{-3} \leq \tilde{\Lambda}_{-2} \leq \tilde{\Lambda}_{-1}.
\]

Just as Ritz values are weighted means of the eigenvalues of the matrix, harmonic Ritz values are harmonic means of the eigenvalues of the matrix.

Quantities which will be introduced here (for lack of a better name) as dual harmonic Ritz values result from applying the Rayleigh-Ritz method to the eigenvalue problem

\[
Mx = \lambda MK^{-1}Mx,
\]

which is also equivalent to \((1.1)\), in the sense of having the same eigenvalues and eigenvectors. If we use the same approximating subspace \( P \), the dual harmonic Ritz values are the eigenvalues of the \( m \times m \) problem

\[
P^T MPy = \tilde{\tilde{\Lambda}} P^T MK^{-1}MPy,
\]

yielding

\[
\tilde{\tilde{\Lambda}}_1 \leq \tilde{\tilde{\Lambda}}_2 \leq \tilde{\tilde{\Lambda}}_3 \leq \cdots \leq \tilde{\tilde{\Lambda}}_{-3} \leq \tilde{\tilde{\Lambda}}_{-2} \leq \tilde{\tilde{\Lambda}}_{-1}.
\]

Dual harmonic Ritz values are also harmonic means of the matrix eigenvalues, however with a different weighting than for harmonic Ritz values.

Both harmonic Ritz and dual harmonic Ritz values were known even 50 years ago and found to be useful in differential eigenvalue problems — Collatz \([2]\) referred to the harmonic Ritz problem \((1.4)\) as Grammel’s equations (citing Grammel’s earlier work \([8]\)) and viewed the Rayleigh quotients for the Ritz problem \((1.2)\), the harmonic Ritz problem \((1.4)\), and the dual harmonic Ritz problem \((1.6)\), all as elements of an infinite monotone sequence of “Schwarz quotients” that could be generated iteratively.

As long as \( K \) and \( M \) are positive definite, all three of Ritz, harmonic Ritz, and dual harmonic Ritz values provide “inner” bounds to the “outer” eigenvalues of the pencil \( K - \lambda M \) (that is, of the problem \((1.1)\)). In comparing the three types of approximations using the same subspace \( P \), harmonic Ritz
values provide the best bounds of the three to the upper eigenvalues of \([1,1]\); dual harmonic Ritz values provide the best bounds of the three to the lower eigenvalues. As an example, Figure 1 shows bounds obtained for a sequence of nested Krylov subspaces taken for \(P\), with \(K = \text{diag}([1 : 2 : 100])\), \(M = I\), and a starting vector of all ones (the example of [17]).
Theorem 1.1. Suppose $K$ and $M$ are positive definite. Then

$$
\lambda_k \leq \tilde{\Lambda}_k \leq \Lambda_k \quad \text{for} \quad k = 1, 2, \ldots
$$

$$
\tilde{\Lambda}_{-\ell} \leq \Lambda_{-\ell} \leq \tilde{\Lambda}_{-\ell} \leq \lambda_{-\ell} \quad \text{for} \quad \ell = 1, 2, \ldots
$$

Proof: The min-max characterization yields

$$
\lambda_k = \min_{\dim S = k} \max_{x \in S} \frac{x^t K x}{x^t M x} \leq \min_{\dim S = k} \max_{x \in S} \frac{x^t K x}{x^t M x}
$$

and likewise,

$$
\lambda_k = \min_{\dim S = k} \max_{x \in S} \frac{x^t K M^{-1} K x}{x^t K x} \leq \min_{\dim S = k} \max_{x \in S} \frac{x^t K M^{-1} K x}{x^t K x}
$$

A similar argument shows $\lambda_k \leq \tilde{\Lambda}_k$. By repeating the argument for the eigenvalue problem $-Kx = (-\lambda)Mx$, one finds $-\lambda(\Lambda, M) \leq -\Lambda_{-\ell}$ (where $\lambda(A, B)$ is used to denote an eigenvalue of the pencil $A - \lambda B$). Notice that $-\lambda_{-\ell}(K, M) = \lambda_{-\ell}(K, M)$. Thus, $\Lambda_{-\ell} \leq \lambda_{-\ell}$ and $\tilde{\Lambda}_{-\ell} \leq \lambda_{-\ell}$.

For any $x \in \mathbb{R}^n$, the Cauchy-Schwarz inequality implies

$$
(x^t K x)^2 = (x^t K M^{-1/2} M^{1/2} x)^2 \leq x^t K M^{-1/2} K x x^t M x
$$

and

$$
(x^t M x)^2 = (x^t M K^{-1/2} K^{1/2} x)^2 \leq x^t M K^{-1/2} K x x^t K x
$$

Thus,

$$
\frac{x^t M x}{x^t M K^{-1} M x} \leq \frac{x^t K x}{x^t M x} \leq \frac{x^t K M^{-1} K x}{x^t K x},
$$

which then implies for each $k = 1, 2, \ldots, m$

$$
0 < \lambda_k \leq \tilde{\Lambda}_k = \min_{\dim S = k} \max_{x \in S} \frac{x^t M x}{x^t M K^{-1} M x} \leq \min_{\dim S = k} \max_{x \in S} \frac{x^t K x}{x^t M x} = \Lambda_k \leq \min_{\dim S = k} \max_{x \in S} \frac{x^t K M^{-1} K x}{x^t K x} = \tilde{\Lambda}_k
$$

The situation is somewhat different if $K$ is indefinite. The Ritz estimates are still “inner” bounds, that is $\lambda_k \leq \Lambda_k$ and $\Lambda_{-\ell} \leq \lambda_{-\ell}$. However, both harmonic Ritz and dual harmonic Ritz values now provide “outer” bounds (lower bounds) to negative eigenvalues of (1.1) and no simple relationship is known that would predict which of the three bounds is best (essentially owing
to there being no simple analog of the Cauchy-Schwarz inequality for indefinite inner products).

Despite the differences in behavior described above, Ritz, harmonic Ritz, and dual harmonic Ritz values each provide optimal bounds – obviously each with respect to a slightly different notion of optimality. For the Ritz problem, the matrices $P^tKP$ and $P^tMP$ provide a “sampling” of the full matrices $K$ and $M$ on the subspace $P$. Whatever spectral information about the original eigenvalue problem (1.1) that we are able to deduce by examining the Rayleigh-Ritz problem (1.2) we must draw the same conclusions for all matrix pencils that are “aliased” by the Rayleigh-Ritz sampling. Define the following set of such $n \times n$ matrix pairs:

$$
C(P) = \left\{ (A, B) \mid \begin{array}{l}
A \text{ and } B \text{ are positive definite} \\
P^t(A - K)P = 0 \\
P^t(B - M)P = 0
\end{array} \right\}
$$

**Theorem 1.2.** For any choice of positive integers $\nu$, $\pi$ with $\nu + \pi = m$ and any choice of matrix pairs $(A, B) \in C(P)$

$$
\lambda_k(A, B) \leq \Lambda_k \text{ for } k = 1, 2, \ldots, \nu \\
\Lambda_{-\ell} \leq \lambda_{-\ell}(A, B) \text{ for } \ell = 1, 2, \ldots, \pi.
$$

Furthermore, for each index pair $\nu$, $\pi$, there exists a matrix pair $(\hat{A}, \hat{B}) \in C(P)$ such that

$$
\lambda_k(\hat{A}, \hat{B}) = \Lambda_k \text{ for } k = 1, 2, \ldots, \nu \\
\Lambda_{-\ell} = \lambda_{-\ell}(\hat{A}, \hat{B}) \text{ for } \ell = 1, 2, \ldots, \pi.
$$

So, no better bounds are possible with only the information available to the Rayleigh-Ritz method as described by (1.2).

**Proof:** The first assertion is a restatement of Theorem 1.1 for the matrix pencil $A - \lambda B$. To show optimality, define the matrix of Ritz vectors: $U = [u_1, u_2, \ldots, u_\nu, u_{-\pi}, \ldots, u_{-2}, u_{-1}]$. Notice that $U$ is an $M$-orthonormal basis for $P$: $U^tMU = I$. Define also the diagonal matrix of Ritz values

$$
D = \begin{bmatrix}
\Lambda_1 \\
& \ddots \\
& & \Lambda_\nu \\
& & & \Lambda_{-\pi} \\
& & & & \ddots \\
& & & & & \Lambda_{-2} \\
& & & & & & \Lambda_{-1}
\end{bmatrix}
$$

and fix $\hat{A} = \frac{1}{\nu}(\Lambda_\nu + \Lambda_{-\pi})$. Now, consider

$$
\hat{A} = MUDU^tM + \hat{A}(M - MUU^tM) \quad \text{and} \quad \hat{B} = M.
One may verify that all required conditions are satisfied, in particular
\[(\hat{A} - \lambda \hat{B})U = MU(D - \lambda I)\]
and for any \(v \in \mathbb{R}^n\) with \(v^tMU = 0\),
\[(\hat{A} - \lambda \hat{B})v = Mv(\hat{\Lambda} - \lambda).\]
\[\blacksquare\]

A similar construction can be used to show the (analogously defined) optimality of harmonic Ritz values and dual harmonic Ritz values.

As we will see in following sections, Ritz values, harmonic Ritz values, and dual harmonic Ritz values are limiting cases of parameterized families of bounds arising from “left-definite” and “right-definite” Lehmann intervals.

2. LEHMANN’S OPTIMAL INTERVALS

Each of the Ritz-related methods discussed above will have certain advantages in estimating the extreme eigenvalues of \((1.1)\). None are particularly effective in estimating interior eigenvalues, however. Usual strategies for obtaining accurate estimates to the eigenvalues of \((1.1)\) lying close to a given value \(\rho\) involve a spectral mapping that turns the spectrum “inside out” around \(\rho\) — mapping interior eigenvalues in the neighborhood of \(\rho\) to extreme eigenvalues that are more accessible. “Shift and invert” strategies typically use the spectral mapping \(\lambda \mapsto \frac{1}{\lambda - \rho}\). A variant used especially for buckling problems (where \(M\) may be singular) utilizes instead the spectral mapping \(\lambda \mapsto \frac{\lambda}{\lambda - \rho}\). As we shall see, both of these spectral mappings play a fundamental role in the optimal bounds discovered by Lehmann \((11), (12), (13)\). The derivation used here is in the spirit of that given by Maehly in \((14)\) and the associated methods are sometimes called Lehmann-Maehly methods.

Fix a scalar \(\rho\) that is not an eigenvalue of \((1.1)\) and define the index \(r\) to satisfy
\[(2.1)\]
\(\lambda_{r-1} < \rho < \lambda_r.\)

The right-definite Lehmann method follows first from considering the spectral mapping \(\lambda \mapsto \frac{1}{\lambda - \rho}\) and an associated eigenvalue problem equivalent to
(1.1):
\[ (1.1) \quad M(K - \rho M)^{-1}Mx = \frac{1}{\lambda - \rho}Mx, \]

which has eigenvalues distributed as
\[
\frac{1}{\lambda_{r-1} - \rho} \leq \frac{1}{\lambda_{r-2} - \rho} \leq \cdots \leq 0 \leq \cdots \leq \frac{1}{\lambda_{r+1} - \rho} \leq \frac{1}{\lambda_{r} - \rho}.
\]

Notice that eigenvalues of (1.1) flanking \( \rho \) are mapped to extremal eigenvalues of (2.2). Now use an \( m \)-dimensional subspace \( S = \text{Ran}(S) \) to generate Rayleigh-Ritz estimates for the eigenvalues of (2.2):
\[ (2.2) \quad [S^t M(K - \rho M)^{-1}MS]y = R [S^t MS]y, \]
where \( S \in \mathbb{R}^{n \times m} \). Suppose (2.3) has \( \nu \) negative eigenvalues \( R_1 \leq \cdots \leq R_\nu < 0 \) and \( \pi = m - \nu \) positive eigenvalues \( 0 < R_{-\pi} \leq \cdots \leq R_{-1} \). Regardless of the subspace \( S \) that is chosen, the min-max principle (or Theorem 1.1) guarantees that for each \( k = 1, 2, \ldots, \nu \) and \( \ell = 1, 2, \ldots, \pi \)
\[
\frac{1}{\lambda_{r-k} - \rho} \leq R_k \quad \text{and} \quad R_{-\ell} \leq \frac{1}{\lambda_{r+\ell-1} - \rho}.
\]

Rearrange and introduce \( \Lambda^{(R)}_k \) and \( \Lambda^{(R)}_\ell \) defined by
\[ (2.4) \quad \Lambda^{(R)}_{-k} \overset{\text{def}}{=} \rho + \frac{1}{R_k} \leq \lambda_{r-k} \quad \text{and} \quad \lambda_{r+\ell-1} \leq \rho + \frac{1}{R_{-\ell}} \overset{\text{def}}{=} \Lambda^{(R)}_{\ell} \]
for \( k = 1, 2, \ldots, \nu \) and \( \ell = 1, 2, \ldots, \pi \). Notice that labeling of \( \Lambda^{(R)}_k \) is arranged relative to \( \rho \):
\[
\ldots \Lambda^{(R)}_{-3} \leq \Lambda^{(R)}_{-2} \leq \Lambda^{(R)}_{-1} < \rho < \Lambda^{(R)}_1 \leq \Lambda^{(R)}_2 \leq \Lambda^{(R)}_3 \ldots
\]

An equivalent statement combining (2.1) and (2.4) is

Each of the intervals \( [\Lambda^{(R)}_{-k}, \rho] \) and \( (\rho, \Lambda^{(R)}_{\ell}] \) contain respectively \( k \) and \( \ell \) eigenvalues of (1.1) for \( k = 1, 2, \ldots, \nu \) and \( \ell = 1, 2, \ldots, \pi \).

To avoid the need in (2.3) for solving linear systems having the indefinite coefficient matrix \( (K - \rho M) \), change variables in (2.3) as \( P = (K - \rho M)^{-1}MS \) — which then \textit{implicitly} determines \( S \) via a choice of \( P \). (2.3) can then be rewritten as
\[ (2.5) \quad [P^t(K - \rho M)P]y = R [P^t(K - \rho M)M^{-1}(K - \rho M)P]y \]

When \( \dim P = 1 \), (2.4) becomes Temple’s inequality
\[
\rho + \frac{p^t(K - \rho M)M^{-1}(K - \rho M)p}{p^t(K - \rho M)p} = \frac{p^t(KM^{-1}K - \rho K)p}{p^t(K - \rho M)p} \leq \lambda_{r-1}
\]

Some additional notation will reduce the impending clutter of symbols. Introduce matrices of \textit{Schwarz constants}:
\[ H_0 = [P^tKM^{-1}K], \quad H_1 = [P^tKP], \quad \text{and} \quad H_2 = [P^tMP]. \]
Then expanding out the various terms, (2.5) becomes
\[(H_1 - \rho H_2)y = R [H_0 - 2\rho H_1 + \rho^2 H_2]y\]
which may be rearranged to obtain
\[(H_0 - \rho H_1)y = \Lambda^{(R)} [H_1 - \rho H_2]y\]
(2.7)

Notice that (2.7) could be written in terms of the $M$-inner product as
\[P_m [(M^{-1})^2 - \rho(M^{-1})]Py = \Lambda^{(R)} P_m [(M^{-1}) - \rho I]Py\]
(2.8)
or in terms of the $K$-inner product as
\[P_k [(M^{-1}) - \rho I]Py = \Lambda^{(R)} P_k [I - \rho(M^{-1})^{-1}]Py\]
(2.9)

The left-definite Lehmann method can be obtained by considering the spectral mapping $\lambda \mapsto \frac{\lambda}{\lambda - \rho}$ and an associated eigenvalue problem — also equivalent to (1.1):
\[K(K - \rho M)^{-1}Kx = \frac{\lambda}{\lambda - \rho}Kx\]
(2.10)
which has eigenvalues distributed as
\[\frac{\lambda_{r-1}}{\lambda_{r-1} - \rho} \leq \frac{\lambda_{r-2}}{\lambda_{r-2} - \rho} \leq \cdots < 0 \text{ and } 1 \leq \cdots \leq \frac{\lambda_{r+1}}{\lambda_{r+1} - \rho} \leq \frac{\lambda_r}{\lambda_r - \rho}\]
(2.11)
(as long as both $K$ and $M$ are positive definite, no eigenvalue gets mapped into the interval $[0, 1]$). Again the eigenvalues of (1.1) flanking $\rho$ are mapped to extremal eigenvalues of (2.10). Using an $m$-dimensional subspace $T = \text{Ran}(T)$, one may generate Rayleigh-Ritz estimates for the eigenvalues of (2.10):
\[|T^tK(K - \rho M)^{-1}Kx| = L[T^tKT]y,\]
(2.12)
where $T \in \mathbb{R}^{n \times m}$.

If (2.12) has $\nu$ negative eigenvalues $L_1 \leq L_2 \leq \cdots \leq L_\nu < 0$ and $\pi = m - \nu$ positive eigenvalues $1 \leq L_{-\pi} \leq \cdots \leq L_{-2} \leq L_{-1}$, then regardless of the subspace $T$ that is chosen, the min-max principle (or again, Theorem 1.1) guarantees that
\[\frac{\lambda_{r-k}}{\lambda_{r-k} - \rho} \leq L_k \text{ and } L_{-\ell} \leq \frac{\lambda_{r+\ell-1}}{\lambda_{r+\ell-1} - \rho}\]
(2.13)
or equivalently
\[\Lambda^{(L)}_{-k} \overset{def}{=} \rho - \frac{\rho}{1 - L_k} \leq \lambda_{r-k} \text{ and } \lambda_{r+\ell-1} \leq \rho - \frac{\rho}{1 - L_{-\ell}} \overset{def}{=} \Lambda^{(L)}_{\ell}\]
(2.14)
for $k = 1, 2, \ldots, \nu$ and $\ell = 1, 2, \ldots, \pi$. Just as for $\Lambda^{(R)}$, the labeling of $\Lambda^{(L)}$ is done relative to $\rho$:
\[\ldots \Lambda^{(L)}_{-3} \leq \Lambda^{(L)}_{-2} \leq \Lambda^{(L)}_{-1} < \rho < \Lambda^{(L)}_1 \leq \Lambda^{(L)}_2 \leq \Lambda^{(L)}_3 \ldots\]
An equivalent statement combining (2.1) and (2.14) is

Each of the intervals \([\Lambda_L^{(L)}(\rho), \rho)\) and \((\rho, \Lambda_L^{(L)})\) contain respectively \(k\) and \(\ell\) eigenvalues of (1.1) for \(k = 1, 2, \ldots, \nu\) and \(\ell = 1, 2, \ldots, \pi\).

As before, in order to avoid solving systems with the coefficient matrix \((K - \rho M)\), change variables in (2.12) as \(P = (K - \rho M)^{-1}K T\) which then implicitly determines \(T\) via a choice of \(P\). (2.12) can then be rewritten as

\[
(P^t(K - \rho M)P)y = L[P^t(K - \rho M)K - 1(K - \rho M)P]y.
\]

(2.15)

Introduce

\[
H_3 = [P^tMK^{-1}MP].
\]

Then (2.15) becomes

\[
[H_1 - \rho H_2]y = L[H_1 - 2\rho H_2 + \rho^2 H_3]y.
\]

(2.16)

which may be rearranged to get

\[
[H_1 - \rho H_2]y = \Lambda^{(L)}[H_2 - \rho H_3]y.
\]

(2.17)

Observe that both (2.15) and (2.16) are Hermitian definite pencils with the same left-hand side. By the Sylvester Law of Inertia, they each have the same number of negative (and hence positive) eigenvalues. If a shift of \(\rho = 0\) is chosen in (2.7), the harmonic Ritz problem (1.4) is obtained and \(\Lambda^{(L)} = \Lambda^{(L)}_\ell|_{\rho = 0}\). As \(\rho \to \pm\infty\), (2.7) reduces to the Ritz problem (1.2). Similarly, if a shift of \(\rho = 0\) is chosen in (2.17), the Ritz problem (1.2) is obtained and \(\Lambda^{(L)} = \Lambda^{(L)}_\ell|_{\rho = 0}\). As \(\rho \to \pm\infty\), (2.17) reduces to the dual harmonic Ritz problem (1.6).

The left- and right-definite Lehmann bounds, \(\Lambda^{(L)}\) and \(\Lambda^{(R)}\), that are below the parameter \(\rho\) are monotone increasing with respect to \(\rho\). This is easy to show for \(\rho\) satisfying (2.1), however as \(\rho\) is increased further, \(r\) changes and the labeling of \(\Lambda^{(L)}\) and \(\Lambda^{(R)}\) shifts. This more complicated circumstance is discussed in [18] where a proof of monotonicity in the general case may be found.

Notice that (2.17) could be obtained formally from the right-definite method expressed in (2.9) by direct substitution of the \(M\)-inner product for the \(K\)-inner product.

\[
P^m((M^{-1} K) - \rho I)P y = \Lambda^{(L)} P^m[I - \rho(M^{-1} K)^{-1}]P y.
\]

(2.18)

Such a substitution also converts the harmonic Ritz problem into a Ritz problem and the Ritz problem, then into a dual harmonic Ritz problem. This provides some impetus to call the “left-definite Lehmann” method the “harmonic Lehmann” method, but Lehmann himself referred to this method as “left-definite” and besides the correspondences are a bit backward since
(right-definite) Lehmann is to Ritz as “dual harmonic Ritz” is to “harmonic Lehmann.”

3. An Alternative Formulation

Kahan developed a formulation of Lehmann’s right-definite method that is particularly well-suited to many computational settings for matrix eigenvalue problems (cf. [16], Chap. 10). We review the development here and extend it to Lehmann’s left-definite method. For a given \( m \)-dimensional subspace \( \mathcal{P} \), suppose the columns of \( Q_1 \) provide an \( M \)-orthonormal basis for \( \mathcal{P} \): \( \text{span}(Q_1) = \mathcal{P} \) and \( Q_1^T Q_1 = Q_1^T M Q_1 = I \). Define \( H \) from the “residual orthogonality” condition

\[
(M^{-1} K Q_1 - Q_1 H)^T M Q_1 = 0
\]

so that \( H = Q_1^T K Q_1 \) and observe (say, from the Gram-Schmidt process) that there is an upper triangular matrix \( C \) and a matrix \( Q_2 \) with \( M \)-orthonormal columns so that

\[
Q_2 C = M^{-1} K Q_1 - Q_1 H.
\]

Pick \( Q_3 \) to fill out an \( M \)-orthonormal basis for \( \mathbb{R}^n \) in conjunction with \( Q_1 \) and \( Q_2 \). Then with \( Q = [Q_1, Q_2, Q_3] \), we have \( Q^T M Q = I \) and

\[
M^{-1} K Q = Q \begin{bmatrix} H & C^T & 0 \\ C & V_{11} & V_{21} \\ 0 & V_{21} & V_{22} \end{bmatrix}
\]

where \( H \) is \( m \times m \) and \( V_{11} \) is \( k \times k \).

While this shows how \( H \) and \( C \) might be constructed (essentially one step of a block Lanczos process), there may be other situations of interest when \( H \) and \( C \) are known \emph{a priori}. In any case, we assume that the bottom right block \( 2 \times 2 \) submatrix, \( V \), is either unknown or at least unpleasant to deal with. With additional unitary massage, \( \text{rank}(C) = k \) could be assumed (possibly resulting in a smaller \( V_{11} \)), though it isn’t necessary in what follows. The situation \( \text{rank}(C) = k \ll m \ll n \) is common. What follows is a \emph{deus ex machina} development of Kahan’s formulation of Lehmann bounds that offers brevity but little of the insight and revelation that one may find in the excellent discussion of ([16], Chapter 10).

Apply the right-definite Lehmann bounds from (2.5) using \( P = Q_1 \). Then, \( (K - \rho M) P = Q_1 (H - \rho I) + Q_2 C \) and the right-definite Lehmann problem (2.6) appears as

\[
(H - \rho I) y = R \left[ (H - \rho I)^2 + C^T C \right] y
\]

The associated right-definite bound is \( \Lambda^{(R)} = \rho + 1/R \) and we may manipulate (3.1) to get an equivalent condition on \( \Lambda^{(R)} \):

\[
0 = \left[ (H - \rho I)(H - \Lambda^{(R)} I) + C^T C \right] y
\]
One may recognize that the coefficient matrix of (3.2) is a Schur complement of the 
\((m + k) \times (m + k)\) matrix

\[
Y(\Lambda^{(R)}) = \begin{bmatrix}
- (H - \rho I)(H - \Lambda^{(R)} I) & C^t \\
C & I
\end{bmatrix}.
\]

Hence, (3.2) has a non-trivial solution if and only if \(Y(\Lambda^{(R)})\) is singular. Suppose that neither \(\rho\) nor \(\Lambda^{(R)}\) are eigenvalues of \(H\) for the time being and define

\[
L_1 = \begin{bmatrix}
I \\
C(H - \rho I)^{-1}(H - \Lambda^{(R)} I)^{-1} & 0
\end{bmatrix},
\]

\[
L_2 = \begin{bmatrix}
I \\
C(H - \Lambda^{(R)} I)^{-1} & 0
\end{bmatrix},
\]

and

\[
D(\Lambda^{(R)}) = \begin{bmatrix}
-(H - \rho I)^{-1} & 0 \\
0 & (\rho - \Lambda^{(R)}) I
\end{bmatrix}.
\]

Then

\[
L_2 D(\Lambda^{(R)}) L_1 Y(\Lambda^{(R)}) L_1^t L_2^t = \begin{bmatrix}
H - \Lambda^{(R)} I & C^t \\
C & \rho I + C(H - \rho I)^{-1} C^t - \Lambda^{(R)} I
\end{bmatrix}.
\]

Thus \(\Lambda^{(R)}\) is an eigenvalue of the \((m + k) \times (m + k)\) matrix

\[
\begin{bmatrix}
H \\
C & \rho I + C(H - \rho I)^{-1} C^t
\end{bmatrix}
\]

if and only if either \(D(\Lambda^{(R)})\) is singular or \(Y(\Lambda^{(R)})\) is singular, which is to say, if and only if either \(\Lambda^{(R)}\) is a right-definite Lehmann bound satisfying (3.2) or \(\Lambda^{(R)} = \rho\) (which will occur with multiplicity \(k\)). A limiting argument can be mustered to handle the exceptional cases where either \(\rho\) or \(\Lambda^{(R)}\) are eigenvalues of \(H\). In situations where either the smaller eigenvalues of (1.1) are of interest or \(\|C\|\) is much smaller than \(\|H\|\), finding the eigenvalues of (3.3) is likely to yield substantially more accurate results for \(\Lambda^{(R)}\) than a direct attack on (3.1). A similar formulation for left-definite Lehmann problems will be described below.

Consider the application of the left-definite problem (2.16) with \(P = Q_1\). Note that \(KQ_1 = Q_1 H + Q_2 C\) implies that

\[
K^{-1} Q_1 = Q_1 H^{-1} - K^{-1} Q_2 C H^{-1}
\]

so then

\[
Q_1^t K^{-1} Q_1 = H^{-1} + H^{-1} C^t W C H^{-1}
\]

where \(W = Q_2^t K^{-1} Q_2\) has been introduced. (2.16) becomes

\[
(H - \rho I)y = L \left[ (H - \rho I) - \rho(I - \rho(H^{-1} + H^{-1} C^t W C H^{-1})) \right] y.
\]
The associated left-definite bound is \( \Lambda^{(L)} = -\rho L/(1 - L) \) and we may manipulate (3.5) to get an equivalent condition on \( \Lambda^{(L)} \):

\[
0 = \left[ (H - \rho I)(H - \Lambda^{(L)} I)H + \rho \Lambda^{(L)} C^t WC \right] y.
\]

(3.6) has a non-trivial solution if and only if the \((m + k) \times (m + k)\) matrix

\[
\hat{Y}(\Lambda^{(L)}) = \begin{bmatrix}
-H - \rho I & H - \Lambda^{(L)} I & \Lambda^{(L)} C^t \\
\rho C & W^{-1}
\end{bmatrix}
\]
is singular. Suppose that neither \( \rho \) nor \( \Lambda^{(L)} \) are eigenvalues of \( H \) and define

\[
F = (H - \rho I)^{-1} (H - \Lambda^{(L)} I)^{-1} H^{-1}
\]

\[
\hat{L}_1 = \begin{bmatrix} I & 0 \\ \rho CF & I \end{bmatrix}, \quad \hat{U}_1 = \begin{bmatrix} I & \Lambda^{(L)} FC^t \\ 0 & I \end{bmatrix},
\]

\[
\hat{L}_2 = \begin{bmatrix} I \\ C(H - \Lambda^{(L)} I)^{-1} I \end{bmatrix},
\]

and \( \hat{D}(\Lambda^{(L)}) = \begin{bmatrix} -H - \rho I^{-1} & 0 \\ 0 & (\rho - \Lambda^{(L)}) / \rho I \end{bmatrix} \).

Then

\[
(3.7) \quad \hat{L}_2 \hat{D}(\Lambda^{(L)}) \hat{L}_1 \hat{Y}(\Lambda^{(L)}) \hat{U}_1 L_2^t = \begin{bmatrix} H - \Lambda^{(L)} I & \rho \Lambda^{(L)} C^t \\ C & \rho \Lambda^{(L)} N_1 + \Lambda^{(L)} M_1 \end{bmatrix},
\]

where \( N_1 = W^{-1} + CH^{-1} C^t \) and \( N_2 = C(H - \rho I)^{-1} C^t \). Thus \( \Lambda^{(L)} \) is an eigenvalue of an auxiliary \((m + k) \times (m + k)\) matrix pencil — not unlike the right-definite case. This matrix pencil will be definite when \( N_1 - N_2 \) is positive-definite, which in turn can be guaranteed when the \((r - 1)st\) Ritz value is a sufficiently accurate approximation to \( \lambda_{r-1} \):

**Theorem 3.1.** Suppose \( \rho \) is not an eigenvalue of \( [L]\). Each interval \([\Lambda^{(L)}_{-i}, \rho]\) and \((\rho, \Lambda^{(L)}_j]\) contains respectively at least \( i \) and \( j \) eigenvalues of \( [L]\), where

\[
0 < \Lambda^{(L)}_{-i} \leq \cdots \leq \Lambda^{(L)}_{-2} \leq \Lambda^{(L)}_{-1} < \rho < \Lambda^{(L)}_1 \leq \Lambda^{(L)}_2 \leq \cdots
\]

are the positive eigenvalues of the \((m + k) \times (m + k)\) matrix pencil

\[
(3.8) \quad \begin{bmatrix} H & C^t \\ C & N_1 \end{bmatrix} - \Lambda^{(L)} \begin{bmatrix} I & 0 \\ 0 & M_1 \end{bmatrix},
\]

where

\[
M_1 = \frac{1}{\rho} (N_1 - N_2)
\]

\[
N_1 = W^{-1} + CH^{-1} C^t, \quad \text{and}
\]

\[
N_2 = C(H - \rho I)^{-1} C^t.
\]

\( \rho \) is an eigenvalue of (3.8) with multiplicity \( k \). If the Ritz value \( \lambda_{r-1} < \rho \), then \( M_1 \) is positive definite and (3.8) is a Hermitian definite pencil.
PROOF: The first assertion follows immediately from (3.7), since then \( \Lambda^{(L)} \) is an eigenvalue of (3.8) if and only if either \( \hat{D}(\Lambda^{(L)}) \) is singular or \( \hat{Y}(\Lambda^{(L)}) \) is singular. As before a limiting argument handles the exceptional cases where either \( \rho \) or \( \Lambda^{(L)} \) are eigenvalues of \( H \).

For the second statement, note that \( \Lambda_{r-1} < \rho \) implies from the way that \( r \) was chosen in (2.1) that \( H - \rho I \) has precisely \( r - 1 \) negative eigenvalues. Note then that \( N_1 - N_2 \) is positive-definite if and only if the matrix

\[
\begin{bmatrix}
\frac{1}{\rho}(H - \rho I)H & 0 \\
0 & N_1 - N_2
\end{bmatrix}
\]  

has precisely \( r - 1 \) negative eigenvalues. Define

\[
\hat{L}_1 = \begin{bmatrix}
I \\
\rho CH^{-1}(H - \rho I)^{-1} & 0
\end{bmatrix},
\hat{L}_2 = \begin{bmatrix}
I & -C^tW \\
0 & I
\end{bmatrix}, \quad \text{and} \quad \hat{D} = \begin{bmatrix}
\rho H^{-1} & 0 \\
0 & I
\end{bmatrix}.
\]

and calculate with \( \tilde{F} = \hat{D}\hat{L}_2\hat{L}_1 \)

\[
\tilde{F}
\begin{bmatrix}
\frac{1}{\rho}(H - \rho I)H & 0 \\
0 & N_1 - N_2
\end{bmatrix}
\tilde{F}^t = \begin{bmatrix}
\rho(I - \rho P^tK^{-1}P) & 0 \\
0 & W^{-1}
\end{bmatrix}.
\]

Suppose (3.9) had more than \( r - 1 \) negative eigenvalues. Then (3.10) has more than \( r - 1 \) negative eigenvalues and therefore \( I - \rho P^tK^{-1}P \) has more than \( r - 1 \) negative eigenvalues. Equivalently, this means that \( P^tK^{-1}P \) has \( r \) or more eigenvalues above \( 1/\rho \). Since the eigenvalues of \( P^tK^{-1}P \) provide inner bounds to the outer eigenvalues of \( K^{-1} \), this implies in turn that \( K^{-1} \) must have \( r \) or more eigenvalues above \( 1/\rho \). But this contradicts the choice of \( \rho \) made in (2.1).
The inequalities of (2.13) remain valid if $\hat{L}_k$ replaces $L_k$ and $\hat{L}_{-\ell}$ replaces $L_{-\ell}$. Likewise if we define $\hat{\Lambda}^{(L)}(\hat{L}) = -\rho\hat{L}_{-i}/(1 - \hat{L}_{-i})$, the usual labeling is retained $$\ldots \hat{\Lambda}^{(L)}_{-3} \leq \hat{\Lambda}^{(L)}_{-2} \leq \hat{\Lambda}^{(L)}_{-1} < \rho < \hat{\Lambda}^{(L)}_1 \leq \hat{\Lambda}^{(L)}_2 \leq \hat{\Lambda}^{(L)}_3 \ldots,$$
and $\hat{\Lambda}^{(L)}_{-k} \leq \hat{\Lambda}^{(L)}_{-k}$ for each $k = 1, \ldots, \nu$. The situation regarding the positively indexed $\hat{\Lambda}^{(L)}$ that yield bounds above $\rho$ is slightly more complicated since it may occur that $\hat{L}_{-\ell} < 1 < \hat{L}_{-\ell}$ which would then imply that $\hat{\Lambda}^{(L)}_{-\ell} < 0$. In effect, $\hat{\Lambda}^{(L)}_{-\ell}$ has “wrapped around” the point at infinity, yielding only trivial bounds for $\lambda_{r+\ell-1}$. Nontrivial bounds are retained whenever $\hat{\Lambda}^{(L)}_{-\ell} > 0$, however.

Now, much the same development that yielded Theorem 3.1 may be followed with $\hat{W}$ replacing $W$. This is summarized as

**Theorem 3.2.** Suppose $\rho$ is not an eigenvalue of $[L, \hat{L}]$. Each interval $[\hat{\Lambda}^{(L)}_{-i}, \rho]$ and $(\rho, \hat{\Lambda}^{(L)}_j]$ contains respectively at least $i$ and $j$ eigenvalues of $[L, \hat{L}]$, where

$$0 < \hat{\Lambda}^{(L)}_{-\nu} \leq \cdots \leq \hat{\Lambda}^{(L)}_{-2} \leq \hat{\Lambda}^{(L)}_{-1} < \rho < \hat{\Lambda}^{(L)}_1 \leq \hat{\Lambda}^{(L)}_2 \leq \hat{\Lambda}^{(L)}_3 \ldots,$$

are the positive eigenvalues of the $(m + k) \times (m + k)$ matrix pencil

$$\begin{bmatrix} H & C^t \\ C & N_1 \end{bmatrix} - \Lambda^{(L)} \begin{bmatrix} I & 0 \\ 0 & M_1 \end{bmatrix},$$

where $M_1 = \frac{1}{\rho}(\hat{N}_1 - N_2)$

$$\hat{N}_1 = \hat{W}^{-1} + CH^{-1}C^t,$$

$$N_2 = C(H - \rho I)^{-1}C^t,$$

and $\hat{W}$ is any positive-definite matrix satisfying $\hat{W} \geq W = Q_2^tK^{-1}Q_2$. $\rho$ is an eigenvalue of (2.13) with multiplicity $k$.

Goerisch ([4],[6],[7]) discovered this approach and developed a very flexible framework for applying this critical approximation step for the original left-definite Lehmann formulation (2.16) in a PDE setting. He called it the $\{X, b, T\}$ method (referring to an auxiliary vector space $X$, an auxiliary bilinear form $b$, and an auxiliary linear operator $T$ that he introduces) but most others refer to this approach simply as the Lehmann-Goerisch method. To give a simple example, suppose a lower bound to $K$ is known: $\kappa \|x\|^2 \leq x^tKx$, and suppose we have obtained an approximate solution $Z_2$ to the matrix equation $KZ = Q_2$. Let $R = Q_2 - KZ_2$ be the associated residual matrix. Then one may verify that

$$W = Q_2^tK^{-1}Q_2 = R^tK^{-1}R + Z_2^tR + Q_2^tZ_2$$

$$\leq \frac{1}{\kappa}R^tR + Z_2^tR + Q_2^tZ_2 \overset{def}{=} \hat{W}.$$
Note that $\hat{W}$ contains the nominal estimate of $W$, $Q_2^tK^{-1}Q_2^t = Q_2^tZ_2$, together with correction terms that ensure $\hat{W} \geq W$ and that can be made small by solving $KZ = Q_2$ more accurately.

4. A Left-Right Comparison

For the general eigenvalue problem (1.1), application of either right- or left-definite Lehmann bounds involve solving linear systems having either $M$ (for right-definite problems) or $K$ (for left-definite problems) as a coefficient matrix. If one system is very much simpler than the other (e.g., if $M = I$) one may feel compelled to choose the simpler path. But is there a difference in accuracy? Goerisch and coworkers in Braunschweig and Clausthal (see for example, [5] and [6]) have observed that for many applications in PDE settings, left-definite Lehmann bounds often were superior to right-definite bounds — even if an extra level of approximation is included as described in Theorem 3.2. Along similar lines, Knyazev [10] has produced error estimates for Lehmann methods that suggest left-definite bounds might be better than right-definite bounds asymptotically.

We explore this issue here. Define

$$J_0 = H_0 - \rho H_1, \quad J_1 = H_1 - \rho H_2, \quad \text{and} \quad J_2 = H_2 - \rho H_3.$$  

The matrix pencils associated with (2.6) and (2.16) may be written as

$$(4.1) \quad J_1 - R(J_0 - \rho J_1)$$

and

$$(4.2) \quad J_1 - L(J_1 - \rho J_2)$$

for right-definite and left-definite problems, respectively.

The following lemma and theorem incorporate some unpublished results of Goerisch\footnote{Friedrich Goerisch died suddenly in 1995 after a brief illness. The loss of his passion and insight is still deeply felt among his colleagues and friends.}

**Lemma 4.1.** Let $G = \begin{bmatrix} J_0 & J_1 \\ J_1 & J_2 \end{bmatrix} \in \mathbb{R}^{2m \times 2m}$. $G$ has no more than $r - 1$ negative eigenvalues.

**Proof:** Suppose that $G$ has $r$ or more negative eigenvalues. Then there is an $r$-dimensional subspace $Z$ of $\mathbb{R}^{2m}$ such that $z^tGz < 0$ for all $z \in Z$ with $z \neq 0$. Define the linear mapping $T : Z \rightarrow \mathbb{R}^n$ by

$$T(z) = \sum_{i=1}^{m} z_iKp_i + \sum_{i=1}^{m} z_{i+m}Mp_i$$

Elementary manipulations verify that for $z \in Z$ with $z \neq 0,$

$$(4.3) \quad z^tGz = T(z)^tM^{-1}T(z) - \rho T(z)^tK^{-1}T(z) < 0$$
In particular, this means that \( T(z) = 0 \) implies that \( z = 0 \), so \( \text{null}(T) = 0 \) and \( \text{rank}(T) = \dim Z = r \).

Since \( K \) is positive-definite \( u^tK^{-1}u > 0 \) for all \( u \in \mathbb{R}^n \) so (4.3) implies 
\[
\lambda > \frac{u^tM^{-1}u}{u^tK^{-1}u} < \rho \text{ for all } u \in \text{Ran}(T) \text{ with } u \neq 0.
\]

Now \( \lambda \) is an eigenvalue of (4.1) if and only if it is also an eigenvalue of 
\[
M^{-1}v = \lambda K^{-1}v,
\]
so by the min-max principle
\[
\lambda_r = \min_{\dim \mathcal{P} = r} \max_{u \in \mathcal{P}} \frac{u^tM^{-1}u}{u^tK^{-1}u} \leq \max_{u \in \text{Ran}(T)} \frac{u^tM^{-1}u}{u^tK^{-1}u} < \rho
\]
which contradicts \( \lambda_{r-1} < \rho < \lambda_r \). Thus, \( \dim Z < r \). ■

**Theorem 4.2.** If the harmonic Ritz value \( \Lambda_{r-1} \) from (4.3) satisfies \( \Lambda_{r-1} < \rho \) then left-definite Lehmann bounds will be uniformly better than right-definite Lehmann bounds:
\[
(4.4) \quad \Lambda_{-k}^{(R)} \leq \Lambda_{-k}^{(L)} \leq \lambda_{r-k} \quad \text{for } k = 1, \ldots, r - 1
\]
\[
(4.5) \quad \lambda_{r+\ell-1} \leq \Lambda_{\ell}^{(L)} \leq \Lambda_{\ell}^{(R)} \quad \text{for } \ell = 1, \ldots, m - r + 1
\]

**Proof:** To show that (4.4) and (4.5) are true, it is sufficient to show
\[
L_k \leq 1 + \rho R_k \text{ for } k = 1, 2, \ldots, r - 1 \text{ and that } 1 + \rho R_{-\ell} \leq L_{-\ell} \text{ for } \ell = 1, 2, \ldots, m - r + 1
\]
From (4.3), one finds that 1 + \( \rho R_k \) and 1 + \( \rho R_{-\ell} \) are eigenvalues of
\[
(4.6) \quad J_0 - (1 + \rho R)(J_0 - \rho J_1)
\]

Since \( \Lambda_{r-1} \leq \tilde{\Lambda}_{r-1} < \rho \), both \( J_0 \) and \( J_1 \) have \( r - 1 \) negative eigenvalues. This implies that both (4.1) and (4.2) have \( r - 1 \) negative eigenvalues. Premultiplication of (4.6) by \( J_1J_0^{-1} \) yields an equivalent matrix pencil:
\[
J_1 - (1 + \rho R)(J_1 - \rho J_1J_0^{-1}J_1)
\]

Consider
\[
G = \begin{bmatrix} J_0 & J_1 \\ J_1 & J_2 \end{bmatrix} = \begin{bmatrix} I & 0 \\ J_1J_0^{-1} & I \end{bmatrix} \begin{bmatrix} J_0 & 0 \\ 0 & J_2 - J_1J_0^{-1}J_1 \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & J_1^{-1}J_1 \end{bmatrix}.
\]

By the lemma and the Sylvester law of inertia, \( J_0 \oplus J_2 - J_1J_0^{-1}J_1 \) can have no more than \( r - 1 \) negative eigenvalues. Since \( J_0 \) has exactly \( r - 1 \) eigenvalues by hypothesis, \( J_2 - J_1J_0^{-1}J_1 \) must be positive semi-definite and
\[
0 < x^t(J_1 - \rho J_2)x < x^t(J_1 - \rho J_1J_0^{-1}J_1)x
\]
for all nontrivial \( x \). Hence, for \( k = 1, 2, \ldots, r - 1 \),
\[
1 + \rho R_k = \min_{\dim S = k} \max_{x \in S} \frac{x^tJ_1x}{x^t(J_1 - \rho J_1J_0^{-1}J_1)x} \geq \min_{\dim S = k} \max_{x \in S} \frac{x^tJ_1x}{x^t(J_1 - \rho J_2)x} = L_k
\]
and for $\ell = 1, 2, \ldots, m - r + 1$,

$$-(1 + \rho R_{-\ell}) = \min_{\dim S = \ell} \max_{x \in S} \frac{-x^t J_1 x}{x^t (J_1 - \rho J_1 J_0^{-1} J_1) x} \geq \min_{\dim S = \ell} \max_{x \in S} \frac{-x^t J_1 x}{x^t (J_1 - \rho J_2) x} = -L_{-\ell}.$$  

Since there will be subspaces of dimension up to $r - 1$ for which $x^t J_1 x < 0$ and subspaces of dimension up to $m - r + 1$ for which $x^t J_1 x > 0$, we may restrict ourselves to $x$ for which the numerators in the above expressions are strictly negative with no loss of generality.

5. A Ritz-Lehmann Comparison

One may hope that the role spectral mapping played in the derivation of both left- and right-definite variants of Lehmann’s method might lead to significant improvements beyond the straightforward application of the Rayleigh-Ritz method. Indeed, spectral mapping has been used for some time with Lanczos methods (e.g., [3]) with sometimes spectacular effect and so encouraged, some have considered the use of right-definite Lehmann bounds using Krylov subspaces generated in the course of an ordinary Lanczos process (e.g., [15] and [17]). By and large, results along these lines have been disappointing when compared with what “shift-and-invert” methods offer (albeit at a much higher price). One may instead seek to compare the expected outcomes of Lehmann methods with those of Rayleigh-Ritz methods. Observe that each method makes optimal use of the information required in the sense that no better bounds are possible with the information used, so in a certain manner of speaking we are really comparing the utility of various types of information in extracting eigenvalue information.

Zimmerman [18] proved that the error in left-definite Lehmann bounds is no worse than proportional to the error in Ritz bounds and may be smaller. Thus, left-definite Lehmann bounds carry the potential of greater accuracy than Ritz bounds. We probably shouldn’t expect them to be much better, though. In [10], Knyazev states that eigenvector approximations provided by either the right- or left-definite variants of Lehmann’s method will asymptotically approach the corresponding Ritz vectors as they close upon the true eigenvectors. Thus, Lehmann methods appear to recover invariant subspace information with about the same efficiency as Rayleigh-Ritz methods.

It is important to note that Lehmann methods provide eigenvalue bounds that often are difficult to obtain in other ways. For example, Behnke [1] combined right-definite Lehmann methods with interval techniques in order to deduce guaranteed bounds to matrix eigenvalue problems and his approach appears to be competitive with the best known interval algorithms for this problem.
For the remainder of this section, we will consider the application of a left-definite Lehmann method within a Lanczos process for resolving a large-scale matrix eigenvalue problem. Since left-definite Lehmann methods are known to be superior to right-definite Lehmann methods (at least to the extent claimed in Section 4), one may seek to improve upon the results of Morgan [15] by using left-definite Lehmann-Goerisch bounds as formulated in Theorem 3.2.

Specifically, let \( M = I \) in (1.1) and let \( T \) be a tridiagonal matrix that is similar to \( K \) – so that \( K = QTQ^t \) for some \( n \times n \) unitary matrix \( Q \). For any index \( 1 \leq \ell \leq n \), let \( T_{\ell} \) denote the \( \ell \)th principal submatrix of \( T \):

\[
T_{\ell} = \begin{bmatrix}
\alpha_1 & \beta_1 & \beta_2 & \cdots & \beta_{\ell-1} \\
\beta_1 & \alpha_2 & \beta_2 & \cdots & \cdots \\
\beta_2 & \alpha_3 & \cdots & \beta_{\ell-1} & \alpha_{\ell} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
&&&&
\end{bmatrix}
\]

and define \( V \) via a partitioning of \( T \) as

\[
T = \begin{bmatrix}
T_{\ell} & \beta_t e_\ell e^t_1 \\
\beta_t e_1 e^t_\ell & V
\end{bmatrix}
\]

Let \( Q_\ell \) denote a matrix containing the first \( \ell \) columns of \( Q \): \( Q_\ell = [q_1, \ldots, q_\ell] \).

The Lanczos algorithm builds up the matrices \( T \) and \( Q \) one column at a time starting with the vector \( q_1 \). Only information on the action of \( K \) on selected vectors in \( \mathbb{R}^n \) is used. Different choices for \( q_1 \) produce distinct outcomes for \( T \), if all goes well. Extracting useful information when not all goes well is fundamental to modern approaches – a discussion may be found in [10].

At the \( \ell \)th step, the basic Lanczos recursion appears as

\[
KQ_\ell = Q_\ell T_\ell + \beta_{\ell+1} q_{\ell+1} e^t_1
\]

In exact arithmetic, the first \( \ell \) steps yields a matrix \( Q_\ell \) that satisfies \( Q^t_\ell Q_\ell = I \) and

\[
\text{Ran}(Q_\ell) = \text{span}\{q_1, Aq_1, \ldots, A^{\ell-1} q_1\} = K_\ell(A, q_1),
\]

a Krylov subspace of order \( \ell \). The application of Theorem 3.2 is straightforward:

**Theorem 5.1.** Let \( M = I \) and suppose \( \rho \) is not an eigenvalue of (1.1). Each interval \([\Lambda_{-1}(\ell), \rho]\) and \((\rho, \Lambda_1(\ell)]\) contains respectively at least \( i \) and \( j \) eigenvalues of the matrix \( K \), where

\[
0 < \Lambda_{-1}(\ell) \leq \Lambda_{-2}(\ell) \leq \Lambda_{-3}(\ell) \leq \cdots \leq \Lambda_{-j}(\ell) \leq \Lambda_{-j+1}(\ell) < \rho \leq \Lambda_{j}(\ell) \leq \Lambda_{j+1}(\ell) \leq \cdots
\]

are the positive eigenvalues of the tridiagonal matrix pencil

\[
(5.1) \quad \begin{bmatrix}
T_\ell & \beta_t e_\ell \\
\beta_t e_1 e^t_\ell & \omega_{k+1}^{-1} + \beta_k^2 e_\ell e^t_1 T_{k-1} e_\ell
\end{bmatrix} - \Lambda^{(L)} \begin{bmatrix}
I & 0 \\
0 & (\rho \omega_{k+1})^{-1} - \beta_k^2 \delta_{k+1}(\rho)
\end{bmatrix}
\]
where \( \omega_{k+1} \) is any number that satisfies

\[
\omega_{k+1} \geq q_{k+1}K^{-1}q_{k+1} \quad \text{and} \quad \delta_{k+1}(\rho) = e_k^T T_k^{-1} (T_k - \rho)^{-1} e_k.
\]

Note that \( \rho \) is a simple eigenvalue of (5.1)

We apply this directly to the numerical example considered in \([17]\) and in Section 1. Figure 2 shows the convergence history both for Ritz bounds and for left-definite Lehmann bounds, for the seventh through tenth eigenvalues of the matrix. We also apply a shift and invert Lanczos method using the spectral transformation \( \lambda \mapsto \frac{\lambda}{\lambda - \rho} \). A few features are apparent. The first is that the Lehmann bounds aren’t nearly as good as the shift and invert bounds to which they are closely related. Paige, Parlett, and van der Vorst \([17]\) observed this disappointing behaviour for right-definite Lehmann methods (in their context, harmonic Ritz on a shifted matrix) — the left-definite Lehmann method does not fare much better. Knyazev’s observations \([10]\) relating convergence of Lehmann eigenvectors to Ritz vectors suggest that spectral information for interior matrix eigenvalues will not be picked up any more rapidly with Lehmann methods than for Ritz methods. This is in stark contrast with shift and invert strategies which will produce approximate eigenvectors that are rapidly drawn into invariant subspaces associated with eigenvalues close to \( \rho \).

The second observation is that, nonetheless, the Lehmann bounds do appear to approach the exact eigenvalues at a rate comparable to that of the Ritz bounds — consistent with the results of Zimmerman discussed above. Furthermore, one can see that the Lehmann bounds appear to pass through a series of stagnation points en route to their limit, and the farther they lie from \( \rho \), the more abrupt the transition between stagnation points. These stagnation points appear to be close to the exact matrix eigenvalues.

The following simple Bauer-Fike style perturbation result lends some insight to this behaviour.

**Theorem 5.2.** Let \( \Lambda^{(L)} \) be any left-definite Lehmann bound and denote with \( \Lambda_i \) the Ritz values from (5.2). Then

\[
\min_i \left( \frac{|\Lambda_i - \rho|}{\rho} \right) \left( \frac{|\Lambda_i - \Lambda^{(L)}|}{\Lambda^{(L)}} \right) \Lambda_i \leq \|W\| \|C\|^2 (5.2)
\]

**Proof:** If either \((H - \rho I)\) or \((H - \Lambda^{(L)} I)\) is singular then (5.2) holds trivially. Suppose then that \((H - \rho I)\) and \((H - \Lambda^{(L)} I)\) are nonsingular. Rearrange the expression (5.6) to get

\[
y = -\rho \Lambda^{(L)} (H - \rho I)^{-1} (H - \Lambda^{(L)} I)^{-1} H^{-1} C^T W C y
\]

Take norms on each side and simplify:

\[
1 \leq \rho \Lambda^{(L)} \|(H - \rho I)^{-1}(H - \Lambda^{(L)} I)^{-1} H^{-1}\| \|W\| \|C\|^2 (5.3)
\]
Then notice that

\[
\| (\mathbf{H} - \rho \mathbf{I})^{-1} (\mathbf{H} - \Lambda^{(L)} \mathbf{I})^{-1} \mathbf{H}^{-1} \| = \max_i \left( \frac{1}{|\Lambda_i - \rho|} \right) \left( \frac{1}{|\Lambda_i - \Lambda^{(L)}|} \right) \frac{1}{\Lambda_i}
\]

\[
= 1/ \min_i (|\Lambda_i - \rho| |\Lambda_i - \Lambda^{(L)}| \Lambda_i),
\]

which may be combined with (5.3) to get (5.2).

Notice that the right hand side of (5.2) has a magnitude related to the size of the Ritz residual \( \mathbf{KQ}_1 - \mathbf{Q}_1 \mathbf{H} \) and is independent of which Lehmann bound \( \Lambda^{(L)} \) is chosen. Suppose the right hand side of (5.2) is moderately small and choose a Lehmann bound \( \Lambda^{(L)} \). If \( \Lambda^{(L)} \) is not close to \( \rho \) then any Ritz value \( \Lambda_i \) that is close to \( \Lambda^{(L)} \) will not be close to \( \rho \) either. Thus any \( \Lambda^{(L)} \) chosen far from \( \rho \) is constrained by (5.2) to be nearer to at least one \( \Lambda_i \) then it would be were \( \Lambda^{(L)} \) chosen closer to \( \rho \). A qualitative interpretation that one might take from this is that Lehmann bounds \( \Lambda^{(L)} \) far from \( \rho \) tend to occur in the neighborhood of Ritz values \( \Lambda_i \). Furthermore, Lehmann bounds \( \Lambda^{(L)} \) far from \( \rho \) that are also situated toward the edges of the spectrum will tend to aggregate in the neighborhood of exact eigenvalues since the attracting Ritz values themselves will be approximating extreme eigenvalues fairly well.

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