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Approximate Solutions and Eigenvalue Bounds from Krylov Subspaces

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The first and third authors dedicate this to Beresford Parlett and Velvel Kahan — not only in recognition of their exceptional abilities in general, and contributions to this topic in particular, but also for the friendship, ideas and encouragement they have given us, and above all for the impeccable character and style they have both consistently exhibited.

Approximations to the solution of a large sparse symmetric system of equations are considered. The conjugate gradient and minimum residual approximations are studied without reference to their computation. Several different bases for the associated Krylov subspace are used, including the usual Lanczos basis. The zeros of the iteration polynomial for the minimum residual approximation (*harmonic* Ritz values) are characterized in several ways and, in addition, attractive convergence properties are established. The connection of these harmonic Ritz values to Lehmann's optimal intervals for eigenvalues of the original matrix appears to be new.

KEY WORDS Krylov subspace, Lanczos process, symmetric matrix, conjugate gradients, minimum residual, Lehmann intervals

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1. Introduction

Krylov subspaces are useful for approximating eigenvalues and for solving sparse linear systems of equations. When the matrix in question is real and symmetric the Lanczos algorithm provides an efficient method for producing an orthonormal sequence of vectors which provides a basis for an appropriate Krylov subspace [7,15].

Both the conjugate gradient algorithm (CG) and the minimum residual algorithm (MR) are available to solve the appropriate linear system $Ax = b$, see for example [5,14]. However CG is only guaranteed to exist and be stable when A is positive definite. The properties of the CG and MR approximations, their error bounds, residuals and iteration polynomials, are usually derived as consequences of the algorithms themselves. What we do in this paper, for clarity and emphasis, is to discuss the CG and MR approximations from a Krylov subspace *without any reference to how these approximations are to be computed.* This leads us to some insights that appear to be new as well as simple explanations of known phenomena. We ignore the complications produced by rounding errors; for the effect of these on the Lanczos process see for example [6,12,13,15].

It is known, at least to experts, that the so called *Ritz values* for A from the Krylov subspace govern the accuracy of CG [16]. We illustrate here how local peaks in the error norm of the CG approximation occur when a Ritz value lands close to zero on its way to an eigenvalue. The corresponding quantities for MR were studied in [4,10]. Since they are Ritz values, but associated with A^{-1}, we call them *harmonic* Ritz values rather than use overworked adjectives such as pseudo or generalized as used in [4,10,11], and [3] in French. The smallest positive harmonic Ritz value approaches the smallest positive eigenvalue of A monotonically *from above* and the largest negative harmonic Ritz value approaches the largest negative eigenvalue of A monotonically *from below* as the dimension increases. We discovered that, when appropriate shifts are used, these harmonic Ritz values yield the 'optimal' error bounds on A's eigenvalues that Lehmann derived in the 1950s and 1960s [8,9]. There are several different ways to characterize the harmonic Ritz values either via a pseudo-Lanczos algorithm using an indefinite product $[u, v] \equiv v^t Au$ or as a banded generalized eigenvalue problem. Nevertheless, using Kahan's reformulation of Lehmann's intervals, see [15], one can compute them from a carefully chosen symmetric tridiagonal matrix which has the Lanczos tridiagonal matrix as a leading submatrix. Consequently ordinary Ritz values interlace harmonic Ritz values.

The next section establishes notation and then the Galerkin solution is considered (the CG solution when A is positive definite). Most, perhaps all, of these initial results are known, but not as well as they should be. Section 4. summarizes our experiments illustrating the irregular behavior of the CG error norm for matrices that are not positive definite.

In Section 5. the minimum residual approximation is analyzed and the harmonic Ritz values are introduced. Section 6. describes the pseudo-Lanczos algorithm and finally in Section 7. the connection with the Lehmann/Kahan bounds is established.

2. Notation for Krylov Subspaces

Let A denote a real symmetric $n \times n$ matrix. Krylov subspaces, defined in (2.1) below, arise naturally in a variety of methods. A sequence of vectors is generated, one at a time, and the subspaces they span form a nested sequence. Suitable linear combinations of the vectors yield approximate solutions to linear systems $Ax = b$ and also approximate eigenvectors. The subspaces are defined for each $j \leq n$ by

$$\mathcal{K}^j = \mathcal{K}^j(A; b) \equiv \text{span}\{b, Ab, \ldots, A^{j-1}b\}. \tag{2.1}$$

An orthonormal basis $\{v_1, v_2, \ldots, v_j\}$, called the Lanczos basis, may be obtained by applying the Gram-Schmidt process to the Krylov (or power) basis $\{b, Ab, \ldots, A^{j-1}b\}$. Define $V_j \in \mathbb{R}^{n \times j}$ by

$$V_j \equiv [v_1, \ldots, v_j]. \tag{2.2}$$

In practice, however, V_j is computed by a three-term recurrence relation that avoids most of the work needed for the Gram-Schmidt process. Since we are avoiding algorithmic details in this paper we simply state the relations satisfied by the generated quantities. See [5] or [15] for a full development.

starting vector: $$b = v_1 ||b|| = v_1 \beta_1, \tag{2.3}$$

orthonormality: $$V_j^t V_j = I_j, \text{ the } j \times j \text{ identity matrix}, \tag{2.4}$$

3-term recurrence: $$AV_j = V_{j+1}\hat{T}_j = V_j T_j + v_{j+1}\beta_{j+1}(e_j^{(j)})^t \tag{2.5}$$

where

$$T_j = \text{tridiag} \begin{pmatrix} & \beta_2 & & \bullet & & \bullet & & \beta_j & \\ \alpha_1 & & \alpha_2 & & \bullet & & \alpha_{j-1} & & \alpha_j \\ & \beta_2 & & \bullet & & \bullet & & \beta_j & \end{pmatrix}, \tag{2.6}$$

$$(e_j^{(j)})^t = (0, 0, \ldots, 0, 1), \tag{2.7}$$

and the superscript (j) gives the dimension and $\hat{T}_j \in \mathbb{R}^{(j+1)\times j}$, where $\hat{T}_j$ is T_j supplemented with an extra row $(0, 0, ..., 0, \beta_{j+1})$.

The Lanczos vectors are computed by equating the last columns on each side of (2.5) and noting that all quantities are known except for β_{j+1} and v_{j+1}.

The construction of the Lanczos basis is shift-invariant, that is using $A - \mu I$ instead of A one obtains

$$(A - \mu I)V_j = V_j(T_j - \mu I_j) + v_{j+1}\beta_{j+1}(e_j^{(j)})^t,$$

with all the same quantities as before.

One nice feature is that if $\dim \mathcal{K}^j < j$ then $\mathcal{K}^j$ is invariant under A, and in that case the approximations discussed in the rest of this paper are exact solutions. Consequently there is no loss of generality in assuming that $\dim \mathcal{K}^j = j$, and hence that the quantities $\beta_2, \ldots, \beta_n$ defined below are all positive.

The spectral factorization of T_j is written as

$$T_j = S_j \Theta_j S_j^t,$$

where

$$S_j^{-1} = S_j^t, \quad \Theta_j = \text{diag}\,(\theta_1^{(j)}, \ldots, \theta_j^{(j)}). \tag{2.8}$$

With the quantities in (2.8) one can define a third basis for $\mathcal{K}^j$, the Ritz basis $\{y_1^{(j)}, \ldots, y_j^{(j)}\}$, and the matrix $Y_j \equiv V_j S_j$, where

$$y_i^{(j)} \equiv V_j s_i, \quad i = 1, 2, \ldots, j, \tag{2.9}$$

with s_i the ith column of S_j and s_{ki} is its kth entry. In contrast to the Lanczos basis the whole Ritz basis changes at each step. The pairs $(\theta_i^{(j)}, y_i^{(j)})$, $i = 1, \ldots, j$ are the Rayleigh-Ritz approximations to eigenpairs of A from $\mathcal{K}^j$ and this set of pairs is, in a precise sense, see [15], the best set of approximate eigenpairs from $\mathcal{K}^j$. Indeed the $(\theta_i^{(j)}, y_i^{(j)})$ are the eigenpairs of the projection of A onto $\mathcal{K}^j$. The full dimension assumption makes the $\{\theta_i^{(j)}\}$ distinct and we order them by

$$\theta_1^{(j)} < \theta_2^{(j)} < \ldots < \theta_j^{(j)}. \tag{2.10}$$

For brevity the $\{\theta_i^{(j)}\}$ are called Ritz values of A.

The Lanczos algorithm computes the $\{v_i\}$ in turn and builds up T_j at the same time from (2.5). In this paper we make use of four bases for $\mathcal{K}^j$: the Lanczos basis $\{v_1, \ldots, v_j\}$, the Ritz basis $\{y_1^{(j)}, \ldots, y_j^{(j)}\}$, the power basis $\{b, Ab, \ldots, A^{j-1}b\}$, and a basis introduced in Section 5. called the harmonic Ritz basis. Each has its merits.

The power basis shows the one-one correspondence between $\mathbb{P}_{j-1}$, the space of real polynomials of degree strictly less than j, and $\mathcal{K}^j(b; A)$ given by

$$\phi \in \mathbb{P}_{j-1} \longleftrightarrow \phi(A)b \in \mathcal{K}^j. \tag{2.11}$$

It is helpful to keep the polynomials ϕ and the vectors $\phi(A)b$ simultaneously in mind when reading the sections that follow.

The following elementary but important lemma shows an attractive feature of Krylov subspaces which will be used in several places. The proof simply exploits the tridiagonal form of T_j.

Lemma 1 *Let $\varphi(\lambda) = \gamma_j\lambda^j + \ldots + \gamma_1\lambda + \gamma_0$ have exact degree j. Then*

$$\varphi(A)b = V_j\varphi(T_j)e_1^{(j)}\beta_1 + v_{j+1}\gamma_j\bar{\beta}_{j+1} \in \mathcal{K}^{j+1}, \text{ not } \mathcal{K}^j,$$

where $\bar{\beta}_m \equiv \beta_1\beta_2\cdots\beta_m$.

Proof We drop the superscript (j) on all the $e_i^{(j)}$. Define $u_1 \equiv e_1$, and for $k = 2, \ldots, j$, $u_k \equiv T_j u_{k-1} = T_j^{k-1}e_1$, then since T_j is tridiagonal (2.6) shows that u_k has only its first k entries nonzero, the kth being $\beta_2\cdots\beta_k$ for $k > 1$. ¿From (2.5)

$$\begin{aligned}
AV_je_1 &= V_jT_je_1 = V_ju_2,\\
A^2V_je_1 &= AV_ju_2 = V_jT_ju_2 = V_ju_3 = V_jT_j^2e_1,\\
A^kV_je_1 &= AV_ju_k = V_jT_ju_k = V_ju_{k+1} = V_jT_j^ke_1 \qquad \text{if } k < j,\\
A^jV_je_1 &= AV_ju_j = (V_jT_j + v_{j+1}\beta_{j+1}e_j^t)u_j = V_jT_j^je_1 + v_{j+1}\beta_2\cdots\beta_{j+1}.
\end{aligned} \tag{2.12}$$

Thus, for $\varphi \in I\!P_j$,

$$\varphi(A)v_1 = V_j\varphi(T_j)e_1 + v_{j+1}\gamma_j\beta_2\cdots\beta_{j+1},$$

and the lemma follows on multiplying by β_1. ■

Corollary 1 *The only nonzero vectors in $\mathcal{K}^{j+1}$ that are orthogonal to $\mathcal{K}^j$ have the form $\varphi(A)b$ where the $\varphi(\lambda)$ are scalar multiples of $\pi_j(\lambda) \equiv det\,(\lambda I_j - T_j)$; $v_{j+1} = \pi_j(A)b/\bar{\beta}_{j+1}$.*

Proof If $\rho_k(\lambda) = \gamma_k\lambda^k + \ldots$ has exact degree $k < j$ then from (2.12) $\rho_k(A)b$ has a nonzero component along $v_{k+1} \in \mathcal{K}^j$, and so cannot be orthogonal to $\mathcal{K}^j$.
Now $\pi_j(\lambda)$ is monic of degree j, and by the Cayley-Hamilton theorem $\pi_j(T_j) = 0$. So from the lemma, for $\alpha \in I\!R$, $\alpha\pi_j(A)b = v_{j+1}\bar{\beta}_{j+1}\alpha \perp \mathcal{K}^j$. Since any polynomial of degree j that is not a multiple of π_j may be written as $\alpha\pi_j + \rho_k$ with ρ_k of degree $k < j$ we see that

$$(\alpha\pi_j + \rho_k)(A)b = v_{j+1}\bar{\beta}_{j+1}\alpha + \rho_k(A)b$$

which is not orthogonal to $\mathcal{K}^j$. ■
The monic polynomial π_j is called the Lanczos polynomial of degree j. By (2.8)

$$\pi_j(\lambda) = \prod_{i=1}^{j}(\lambda - \theta_i^{(j)}) \tag{2.13}$$

and this product representation gives more insight than an expansion in the power basis. In fact the $\{\pi_i\}$ are a sequence of polynomials orthogonal with respect to a certain inner product. However we do not make use of the properties of such polynomials in this essay.

3. The Galerkin (conjugate gradient) Approximation

This section considers the Galerkin (or weak) solution x_j^w from $\mathcal{K}^j$ to $Ax = b$, for $j < n$. It is what CG delivers. In general it satisfies

$$(Ax_j^w, u) = (b, u) \quad \text{for all } u \in \mathcal{K}^j,$$

or equivalently

$$r_j^w \equiv b - Ax_j^w \perp \mathcal{K}^j. \tag{3.14}$$

which is why x_j^w may be called a Galerkin approximation; $\mathcal{K}^j$ comprises the test vectors as well as the trial vectors. Next we give representations for x_j^w and r_j^w in the three bases exhibited in Section 2.. Justification and discussion come afterwards since the results are quite well known. We use $||.||$ to denote the vector 2-norm throughout.

$$\text{Lanczos basis:} \quad x_j^w = V_jT_j^{-1}e_1||b||, \tag{3.15}$$

$$||r_j^w|| = \beta_{j+1}|e_j^tT_j^{-1}e_1| \cdot ||b||, \tag{3.16}$$

$$(r_j^w)^tA^{-1}r_j^w = b^tA^{-1}b - \beta_1^2e_1^tT_j^{-1}e_1. \tag{3.17}$$

$$\text{Ritz basis:} \quad x_j^w = Y_j \Theta_j^{-1} (S_j^t e_1) ||b|| = ||b|| \sum_{i=1}^{j} y_i^{(j)} (s_{1i}/\theta_i^{(j)}), \tag{3.18}$$

$$(r_j^w)^t A^{-1} r_j^w = b^t A^{-1} b - ||b||^2 \sum_{i=1}^{j} s_{1i}^2/\theta_i^{(j)}. \tag{3.19}$$

$$\text{Krylov basis:} \quad x_j^w = \left[\left(\frac{\pi_j(0) - \pi_j(\lambda)}{\lambda \pi_j(0)} \right)_{\lambda = A} \right] b, \tag{3.20}$$

$$r_j^w = \pi_j(A) b / \pi_j(0), \tag{3.21}$$

where π_j is the jth Lanczos polynomial.

Justification

The Ritz representation is less well known than the other two. All three forms show that the existence of T_j^{-1} is a necessary and sufficient condition for existence and uniqueness of x_j^w. The Lanczos representation follows readily from (2.5) using (2.3) and (2.4). The Ritz representation follows from (2.8) and $T_j^{-1} = S_j \Theta_j^{-1} S_j^t$. To obtain (3.19) from (3.18) it is only necessary to note that $Y_j = V_j S_j$ gives

$$Y_j^t Y_j = V_j^t S_j^t S_j V_j = I_j, \qquad b = \beta_1 V_j e_1 = \beta_1 Y_j S_j^t e_1,$$

and since $r_j^w \perp x_j^w$,

$$(r_j^w)^t A^{-1} r_j^w = b^t A^{-1} b - 2 b^t x_j^w + (x_j^w)^t A x_j^w = b^t A^{-1} b - b^t x_j^w.$$

The Ritz representation (3.18) shows clearly that to have a good approximation to $A^{-1}b$ by x_j^w requires that the Ritz pairs $(\theta_i^{(j)}, y_i^{(j)})$ associated with the eigenvalues close to zero be good approximations too. In many applications the small eigenvalues are closely clustered and the large eigenvalues are relatively well separated, and consequently good approximations to the small eigenvalues occur for much larger values of j than good approximations to the large eigenvalues, see for example [15, Ch. 12]. This explains the puzzling phenomenon that it is often 'easier' to approximate several large eigenvalues of A than to approximate $A^{-1}b$, the solution to one linear system.

The elegant result (3.21) follows from the corollary to Lemma 1 in Section 2.. We included that proof because it seems to be the most elementary derivation of (3.21). Since $x_j^w \in \mathcal{K}^j$, $r_j^w = b - A x_j^w \in \mathcal{K}^{j+1}(A; b)$, and from (2.11) $r_j^w = \varphi(A) b$, $\varphi \in I\!P_j$. It is the special nature of Krylov spaces that yields

$$\varphi(A) b = V_j \varphi(T_j) e_1 \beta_1 + v_{j+1} \gamma_j \bar{\beta}_{j+1},$$

and only the choice $\varphi = \alpha \pi_j, \quad \alpha \in I\!R$, eliminates the components of the residual $\varphi(A)b$ in $\mathcal{K}^j$. To determine α we see from $\alpha \pi_j(A) b = b - A x_j^w$ that $\alpha \pi_j(0) = 1$, so the unique residual polynomial for a Galerkin solution from $\mathcal{K}^j$ is $\pi_j(\lambda)/\pi_j(0)$. The expression (3.20) follows from $x_j^w = A^{-1}(b - r_j^w) = A^{-1}[\pi_j(0) I - \pi_j(A)] b / \pi_j(0)$ on

noting $\pi_j(0) - \pi_j(\lambda)$ has no constant term. Observe that

$$\pi_j(0) = \det\ [0 \cdot I_j - T_j] = \prod_{i=1}^{j}(-\theta_i^{(j)}),$$

so that if $\theta_i^{(j)}$ vanishes there is no weak solution for this value of j. Consequently the Galerkin solution may not be worth computing whenever T_j is ill-conditioned.
Comments

Since T_j represents the projection of A onto $\mathcal{K}^j$ the Ritz values, for each j, are confined to the convex hull of A's eigenvalues, i.e. the smallest interval containing A's spectrum. When A is indefinite A's spectral interval contains zero, and transient peaks in the graph of $||r_j^w||$ as a function of j occur only when a Ritz value lands close to zero on its way to one of A's eigenvalues. The experiments in the next section illustrate these comments.

The gradient of the functional $(b - Ax)^t A^{-1}(b - Ax)$ is $-2(b - Ax)^t$ and thus, on $\mathcal{K}^j$, this functional is stationary at $x = x_j^w$. The second derivative (or Hessian) matrix is $2A$ and so for positive definite A this critical point is actually a minimum over $x \in \mathcal{K}^j$, and this functional may be written as

$$||r||^2_{A^{-1}} \quad \text{or} \quad ||A^{-1}b - x||^2_A$$

because both A^{-1} and A induce valid norms. The conjugate gradient algorithm (CG) is a popular way of computing x_j^w in the positive definite case. Indeed the algorithm is often presented as a way to minimize the A-norm of the error at each step.

Even when CG is presented with a symmetric indefinite matrix it may well succeed in producing a satisfactory approximation. Nevertheless stability cannot be guaranteed in this case since breakdown is possible. There is a minor variation of the usual CG implementation that can, when necessary, take a double step and avoid the explicit computation of x_j^w when T_j is ill-conditioned. Such algorithms are under study by the second author. Algorithms in [14] can do this, but are more expensive than CG. For nonsymmetric A a look-ahead variant of bi-CG has been developed by R. Bank in [1].

4. An Experiment with Conjugate Gradients

Here we show how the CG error tends to behave for indefinite matrices. An illustration of similar residual behavior is given in [14], but here we explain why the observed behavior occurs. For nonsingular A the error has the same iteration polynomial (applied to x, the initial error) as the residual has (applied to b, the initial residual), since from (3.21)

$$x - x_j^w = A^{-1}r_j^w = A^{-1}\pi_j(A)b/\pi_j(0) = \pi_j(A)x/\pi_j(0). \tag{4.22}$$

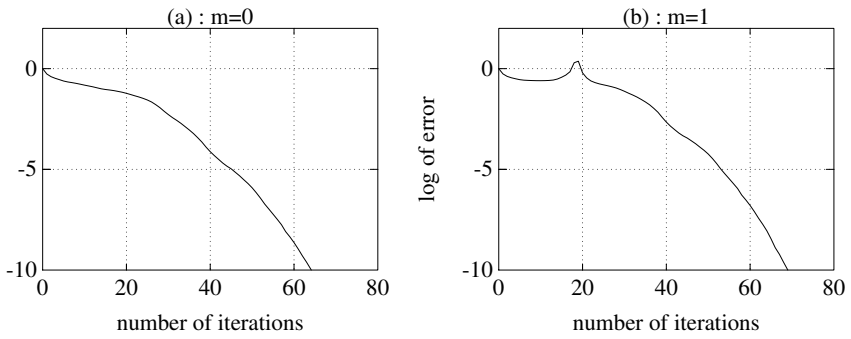

Figure 1. Convergence of CG for $m = 0, 1$.

A clear understanding of the behavior follows from the form of this error. From (2.13) we see the components of the error are proportional to

$$\pi_j(\lambda_i)/\pi_j(0) = (1 - \lambda_i/\theta_1^{(j)}) \ldots (1 - \lambda_i/\theta_k^{(j)}) \ldots (1 - \lambda_i/\theta_j^{(j)}), \quad i = 1, \ldots, n.$$

If for any j there is a Ritz value $\theta_k^{(j)} \approx 0$, this ensures $\pi_j(\lambda_i)/\pi_j(0)$ will be large for reasonably sized λ_i not well approximated by some Ritz value, and so a very small $\theta_k^{(j)}$ can give some very large error components.

Our numerical experiment has been carried out with a diagonal matrix (which is not a loss of generality) of dimension 100, with m some integer in $[0, 100]$:

$$A = \mathrm{diag}(1 - 2m, 3 - 2m, ..., 197 - 2m, 199 - 2m), \tag{4.23}$$

so that A has m negative eigenvalues. The right hand side has been chosen so that $x = (1, 1, ..., 1)^t$, and $x_0 = 0$.

For $m = 0$, we have that A is positive definite, and the convergence history plotted in Figure 1(a) will therefore not come as a surprise.

For $m = 1$, we observed the convergence history as shown in Figure 1(b). The peak at the 19th step can be explained as follows. When for some j the Ritz value $\theta_1^{(j)}$ comes close to the origin (on its way towards $\lambda_1 = -1$), which happens for $j = 19$, most of the $\pi_j(\lambda_i)/\pi_j(0)$ may be expected to be large. Hence the error can take a large value. Note that $\theta_2^{(j)}$ converges to $\lambda_2 = 1$, so that it can happen only during a relatively short phase in the iteration process that a Ritz value may come close to the origin. After such a phase, i.e., when $\theta_1^{(j)}$ has arrived in the neighborhood of λ_1, we may expect the process to behave as a process in which λ_1 plays no role. That means that the process behaves as a process determined by positive eigenvalues only [2,16]. It may then be no surprise to see a convergence behavior very similar to the situation for $m = 0$ when $j > 20$ in Figure 1(b).

Likewise, for $m = 2$, we may expect two phases where a Ritz value is close to the origin (hence two peaks, see Figure 2(a)), and for $m = 3$ we see three peaks, as might have been anticipated. Obviously we have been lucky enough to avoid the rare event of singular T_j. However, for indefinite matrices Ritz values may come

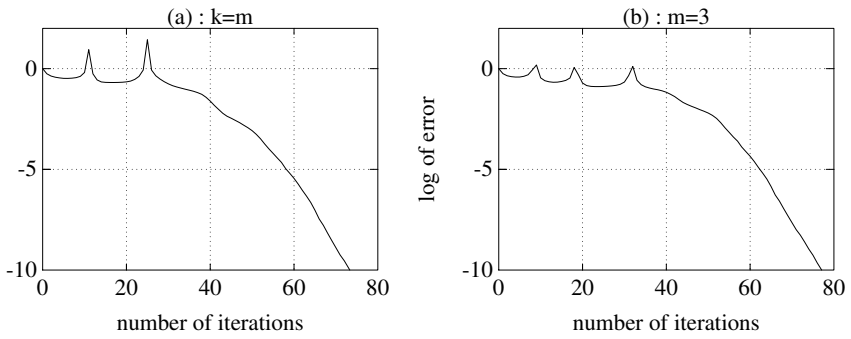

Figure 2. Convergence of CG for $m = 2, 3$.

arbitrarily close to the origin, so that the peaks can be very high indeed. We must not give the impression that there will always be m peaks, i.e. local maxima, in the graph of $||r_j^{mr}||$ when there are m negative eigenvalues. However m is an upper bound on that number when $b^t Ab \gg 0$.

5. The Minimal Residual Approximation

The Galerkin solution to $Ax = b$ discussed in Section 3. neglects the quantity β_{j+1} which is, in practice, knowable after j steps of an appropriate Krylov subspace method. With the aid of β_{j+1} it is possible to find the unique vector x_j^{mr} in $\mathcal{K}^j$ that minimizes $||b - Ax||$. Thus $r_j^{mr} \equiv b - Ax_j^{mr}$ is characterized by

$$||r_j^{mr}|| = \min \ ||b - Au|| \ \text{ over } u \in \mathcal{K}^j(b; A). \tag{5.24}$$

We may also call x_j^{mr} the least squares (LS) solution to $Ax = b$ in $\mathcal{K}^j$.

Recall from (2.5) that the Lanczos algorithm delivers $V_j \in \mathbb{R}^{n \times j}$ where $AV_j = V_{j+1}\hat{T}_j$. The accuracy of the Galerkin solution in $\mathcal{K}^j$ is governed by the eigenvalues of T_j and, by analogy, we might expect the accuracy of the MR solution in $\mathcal{K}^j$ to be governed by the singular values of $\hat{T}_j$. This is not correct, but is close to the truth. The appropriate quantities, which we are tempted to call the *harmonic* Ritz values, turn out to be the reciprocals of the (ordinary or weak) Ritz values of A^{-1} from $A\mathcal{K}^j$. ¿From (2.5) and (2.8) $T_j = S_j \Theta_j S_j^t = V_j^t A V_j$, so if A has eigendecomposition $A = X\Lambda X^t$ we see $\Theta_j = W_j^t \Lambda W_j$, $W_j \equiv X^t V_j S_j$, and the (ordinary) Ritz values $\theta_i^{(j)}$ (of A) are all weighted *arithmetic* means of A's eigenvalues. At the end of this section we will show the harmonic Ritz values are all weighted *harmonic* means of A's eigenvalues, which led to this terminology.

The singular values of $\hat{T}_j$ are the eigenvalues of the symmetric positive definite matrix M_j where

$$M_j^2 = \hat{T}_j^t \hat{T}_j = T_j^2 + \beta_{j+1}^2 e_j e_j^t = T_j(I + \beta_{j+1}^2 f_j f_j^t)T_j, \tag{5.25}$$

this last expression holding if T_j is nonsingular and $T_j f_j = e_j$.

Before we say more about the harmonic Ritz values we present x_j^{mr} in terms of the Lanczos basis. We will prove all these results later in this section.

$$\begin{aligned} x_j^{mr} &= V_j \hat{T}_j^{+} e_1^{(j+1)} \beta_1 \\ &= V_j M_j^{-2} T_j e_1^{(j)} \beta_1, \end{aligned} \tag{5.26}$$

where $\hat{T}_j^{+}$ denotes the Moore-Penrose generalized inverse of $\hat{T}_j$. Further

$$r_j^{mr} = V_{j+1} w \, w(1) \beta_1, \quad ||r_j^{mr}|| = |w(1)| \, \beta_1, \tag{5.27}$$

where w is the normalized left null vector of $\hat{T}_j$; $w^t \hat{T}_j = 0^t$ and $w(1)$ is its first entry. We also show

$$|w(1)| = \beta_{j+1} |f_j(1)| / (1 + \beta_{j+1}^2 ||f_j||^2)^{1/2}, \tag{5.28}$$

giving the improvement in the residual of MR over the weak solution:

$$||r_j^{mr}|| = ||r_j^{w}|| / (1 + \beta_{j+1}^2 ||f_j||^2)^{1/2}. \tag{5.29}$$

Next we introduce the monic MR polynomial, and justify this definition later:

$$\begin{aligned} \chi_j(\lambda) &\equiv \det \left[\lambda I_j - T_j^{-1} M_j^2 \right] \\ &= \det \left[\lambda I_j - T_j - f_j e_j^t \beta_{j+1}^2 \right] \\ &= \prod_{i=1}^{j} (\lambda - \tilde{\theta}_i^{(j)}). \end{aligned} \tag{5.30}$$

In terms of the Krylov basis and this MR polynomial we will show

$$r_j^{mr} = \chi_j(A) b / \chi_j(0), \tag{5.31}$$

$$x_j^{mr} = \left(\frac{\chi_j(0) - \chi_j(\lambda)}{\lambda \chi_j(0)} \bigg|_{\lambda = A} \right) b. \tag{5.32}$$

These $\{\tilde{\theta}_i^{(j)}\}$ are the *harmonic* Ritz values. Associated with them are *harmonic* Ritz vectors

$$\tilde{y}_i^{(j)} \equiv V_j \tilde{s}_i, \quad i = 1, \ldots, j, \tag{5.33}$$

where

$$T_j^{-1} M_j^2 \tilde{s}_i = \tilde{s}_i \tilde{\theta}_i^{(j)}, \quad ||\tilde{s}_i|| = 1. \tag{5.34}$$

Since $T_j \tilde{s}_i = M_j^2 \tilde{s}_i / \tilde{\theta}_i^{(j)}$ it follows that the set $\{\tilde{s}_i\}$ is M_j^2-orthogonal and hence linearly independent. In particular with obvious notation

$$M_j^{-2} T_j \tilde{S}_j = \tilde{S}_j \tilde{\Theta}_j^{-1}. \tag{5.35}$$

In terms of the harmonic Ritz basis $\{\tilde{y}_1^{(j)}, \ldots, \tilde{y}_j^{(j)}\}$, $\tilde{y}_i^{(j)} \equiv V_j \tilde{s}_i$, $i = 1, \ldots, j$,

$$x_j^{mr} = \beta_1 \sum_{i=1}^{j} \tilde{y}_i^{(j)} (\gamma_{i1} / \tilde{\theta}_i^{(j)}), \qquad \gamma_{i1} \equiv e_i^t \tilde{S}_j^{-1} e_1. \tag{5.36}$$

In view of (5.36) it is significant that the largest interval around zero that is free of eigenvalues of A is also free of harmonic Ritz values.

Justification

Recall that

$$AV_j = V_{j+1} \hat{T}_j \quad \text{and} \quad V_n^{-1} = V_n^t.$$

For any vector $V_j c$ in $\mathcal{K}^j$,

$$\begin{aligned} r &= b - AV_j c \\ &= V_n e_1^{(n)} \beta_1 - V_n \begin{pmatrix} \hat{T}_j \\ 0 \end{pmatrix} c. \end{aligned}$$

Since V_n is orthogonal

$$\begin{aligned} ||r|| &= ||e_1^{(n)} \beta_1 - \begin{pmatrix} \hat{T}_j \\ 0 \end{pmatrix} c||, \\ &= ||e_1^{(j+1)} \beta_1 - \hat{T}_j c||, \quad \text{discarding null rows.} \end{aligned}$$

In terms of the Moore-Penrose generalized inverse the least squares solution is

$$\begin{aligned} c_j^{mr} &= (\hat{T}_j^{+}) e_1^{(j+1)} \beta_1 \\ &= (\hat{T}_j^t \hat{T}_j)^{-1} \hat{T}_j^t e_1^{(j+1)} \beta_1 \\ &= M_j^{-2} T_j e_1^{(j)} \beta_1, \end{aligned}$$

using the special form of $\hat{T}_j$. This gives (5.26). Now since w spans the left null space of $\hat{T}_j$, the projector onto range$(\hat{T}_j)$ is

$$\hat{T}_j \hat{T}_j^{+} = \hat{T}_j M_j^{-2} \hat{T}_j^t = I_{j+1} - ww^t$$

giving

$$\begin{aligned} Ax_j^{mr} &= AV_j \hat{T}_j^{+} e_1^{(j+1)} \beta_1 \\ &= V_{j+1} (\hat{T}_j \hat{T}_j^{+}) e_1^{(j+1)} \beta_1 \\ &= V_{j+1} (I - ww^t) e_1^{(j+1)} \beta_1, \end{aligned}$$

Thus

$$r_j^{mr} = b - Ax_j^{mr} = V_{j+1} ww^t e_1^{(j+1)} \beta_1,$$

as claimed in (5.27). Note that $||r_j^{mr}|| = |w(1)| \beta_1$, and if T_j is nonsingular

$$w(1)^2 = 1 - e_1^t T_j M_j^{-2} T_j e_1 = 1 - e_1^t (I_j + \beta_{j+1}^2 f_j f_j^t)^{-1} e_1,$$

and using $(I+uu^t)^{-1} = I - u(1+u^tu)^{-1}u^t$ gives (5.28) and so (5.29).

The derivation of χ_j is more interesting. Recall from Section 3. that

$$V_j^t \pi_j(A) b = 0$$

where π_j is the monic Lanczos polynomial. Now from (5.24) we see $r_j^{mr} = b - AV_j z_j$ where z_j is chosen so that $(AV_j)^t r_j^{mr} = 0$. Thus for the residual to have the form $\alpha\chi(A)b$ we seek $\chi \in I\!P_j$ such that $V_j^t A\chi(A)b = 0$. We can create monic $A\chi(A)$ from $\pi_j(A)$ and $\pi_{j+1}(A)$ since

$$V_{j+1}^t \pi_{j+1}(A) b = 0$$

implies, a fortiori, that $V_j^t \pi_{j+1}(A)b = 0$. All we need for $\lambda\chi(\lambda)$ is a monic polynomial in $I\!P_{j+1}$ with no constant term, and having the right orthogonality properties. The unique solution is

$$\lambda\chi(\lambda) = \pi_{j+1}(\lambda) - \pi_j(\lambda)\pi_{j+1}(0)/\pi_j(0).$$

This defines χ_j but does not give an expression in terms of T_j and β_{j+1}. To obtain (5.31) we use the Schur complement of $\lambda I_j - T_j$ in $\lambda I_{j+1} - T_{j+1}$ and take determinants:

$$\pi_{j+1}(\lambda) = \det\,[\lambda I_{j+1} - T_{j+1}] = \pi_j(\lambda)\det\,[\lambda - \alpha_{j+1} - \beta_{j+1}^2 e_j^t(\lambda I_j - T_j)^{-1}e_j],$$

$$\pi_{j+1}(0) = \pi_j(0)[-\alpha_{j+1} + \beta_{j+1}^2 e_j^t T_j^{-1} e_j].$$

Fortunately the 'unknown' term α_{j+1} will disappear from χ:

$$\pi_{j+1}(\lambda) - \pi_j(\lambda)\pi_{j+1}(0)/\pi_j(0) = \pi_j(\lambda)[\lambda - \beta_{j+1}^2 e_j^t\{(\lambda I_j - T_j)^{-1} + T_j^{-1}\}e_j].$$

Now invoke the following identity (called Hilbert's first resolvent condition in Functional Analysis)

$$U^{-1} - V^{-1} = U^{-1}(V-U)V^{-1}$$

so that $T_j^{-1} + (\lambda - T_j)^{-1} = \lambda(\lambda - T_j)^{-1}T_j^{-1}$. Hence

$$\begin{aligned}
\chi(\lambda) &= \pi_j(\lambda)[1 - \beta_{j+1}^2 e_j^t(\lambda I_j - T_j)^{-1}T_j^{-1}e_j] \\
&= \det\,[I_j - \beta_{j+1}^2 T_j^{-1}e_j e_j^t(\lambda I_j - T_j)^{-1}]\pi_j(\lambda) \\
&= \det\,[\lambda I_j - T_j - \beta_{j+1}^2 f_j e_j^t],
\end{aligned}$$

as claimed. In the final lines we used the fact that $\det(I + xy^t) = 1 + y^t x$ and the standard result on products. The zeros $\tilde{\theta}_i^{(j)}$ of χ are eigenvalues of $T_j + \beta_{j+1}^2 T_j^{-1} e_j e_j^t$ and govern the accuracy of MR.

To justify (5.36) we see from (5.35) that $M_j^{-2}T_j = \tilde{S}_j\tilde{\Theta}_j^{-1}\tilde{S}_j^{-1}$, and after substituting this in (5.26) we obtain the desired result

$$\begin{aligned}
x_j^{mr} &= V_j\tilde{S}_j\tilde{\Theta}_j^{-1}\tilde{S}_j^{-1}e_1^{(j)}\beta_1 \\
&= \tilde{Y}_j\tilde{\Theta}_j^{-1}(\tilde{S}_j^{-1}e_1)\beta_1.
\end{aligned}$$

In [4] Freund, and in [11] Morgan, essentially use this rank one modification of

T_j to compute the $\tilde{\theta}_i$ but we offer a simpler method which is given in Section 7..

The A^{-1} connection

It remains to connect the $\{\tilde{\theta}_i^{(j)}\}$ with A^{-1}. Since A^{-1} maps $A\mathcal{K}^j$ into $\mathcal{K}^j$ we may consider the (orthogonal) projection of A^{-1} onto $A\mathcal{K}^j$. A convenient basis is $\{Av_1, \ldots, Av_j\}$ but it is not orthonormal. However the columns of $AV_j M_j^{-1}$ do form an orthonormal basis and in it the representation of the projection is

$$H_j \equiv M_j^{-1}(AV_j)^t A^{-1}(AV_j)M_j^{-1} = M_j^{-1}T_j M_j^{-1}$$

which is similar to $M_j^{-2}T_j$ as claimed, showing the inverses of the harmonic Ritz values are weighted means of the inverses of A's eigenvalues. The last section gives a simple way to compute the $\{\tilde{\theta}_i^{(j)}\}$ from a symmetric tridiagonal matrix.

The A^{-1} connection has also been noticed by Morgan [11]:Section 2. The viewpoint taken in that paper is to minimize a Rayleigh quotient for A^{-1}.

6. A Pseudo-Lanczos Algorithm

Given the equation $Ax = b$ and the Lanczos basis in $V_j = [v_1, \ldots, v_j]$, one can consider the projection of the equation onto $\mathcal{K}^j(b; A)$, namely

$$(V_j V_j^t A V_j V_j^t)u = V_j V_j^t b$$

or

$$V_j T_j V_j^t u = V_j T_j c = V_j e_1 \beta_1, \quad x \simeq V_j V_j^t u = V_j c, \quad c \in I\!R^j.$$

This yields the Galerkin (CG) solution

$$x_j^w = V_j T_j^{-1} e_1 \beta_1.$$

An alternative approach is to consider the normal equations $A^2 x = Ab$, since $A^t = A$, and the projection on $\mathcal{K}^j$, namely

$$V_j(V_j^t A^2 V_j)(V_j^t u) = V_j V_j^t Ab$$

or

$$V_j M_j^2 V_j^t u = V_j M_j^2 c = V_j T_j e_1 \beta_1, \quad x \simeq V_j V_j^t u = V_j c.$$

This yields the LS or MR solution

$$x_j^{mr} = V_j M_j^{-2} T_j e_1 \beta_1.$$

Suppose that T_j is invertible and admits the triangular factorization

$$T_j = L_j \Delta_j L_j^t,$$

where lower bidiagonal L_j has ones on the diagonal. It is a subtle and useful property of Krylov subspaces that M_j^2 is reduced to tridiagonal form $\check{T}_j$ by the *same*

congruence that reduces T_j to Δ_j, so that as we will show,

$$M_j^2 - \lambda T_j = L_j(\check{T}_j - \lambda\Delta_j)L_j^t. \tag{6.37}$$

The only undesirable feature is that since T_j is not positive definite its triangular factorization might be unstable, but it will exist if $T_1, \ldots, T_j$ are all nonsingular, which is the necessary and sufficient condition for the pseudo-Lanczos process below to be successful.

One way to understand the reduction in (6.37) is as a byproduct of a pseudo-Lanczos algorithm applied to A which differs from the standard algorithm only by replacing the Euclidean inner product $(f, g) = g^t f$ by an *indefinite* inner product

$$[f, g] \equiv g^t A f. \tag{6.38}$$

It is only the failure of the positivity axiom that prevents $[\cdot, \cdot]$ from being a true inner product. Initially

$$\tilde{v}_1 = v_1, \quad \omega_1 = [\tilde{v}_1, \tilde{v}_1], \quad \tilde{\alpha}_1 = [A\tilde{v}_1, \tilde{v}_1], \quad \tilde{v}_2 = A\tilde{v}_1 - \tilde{v}_1\tilde{\alpha}_1/\omega_1.$$

The ith step of this pseudo-Lanczos algorithm is

$$\begin{aligned} \omega_i &\equiv [\tilde{v}_i, \tilde{v}_i], \\ t &\equiv A\tilde{v}_i - \tilde{v}_{i-1}\omega_i/\omega_{i-1}, \\ \tilde{\alpha}_i &\equiv [t, \tilde{v}_i], \\ \tilde{v}_{i+1} &\equiv t - \tilde{v}_i\tilde{\alpha}_i/\omega_i. \end{aligned}$$

$$\text{If} \quad \tilde{T}_j \equiv \text{tridiag} \begin{pmatrix} & \omega_2 & & & \omega_j \\ \tilde{\alpha}_1 & & \bullet & & & \tilde{\alpha}_j \\ & \omega_2 & & \bullet & \omega_j \end{pmatrix}, \tag{6.39}$$

then after j successful steps (i.e. $\omega_i \neq 0$) the matrix $\tilde{V}_j = [\tilde{v}_1, \ldots, \tilde{v}_j]$ satisfies

$$\tilde{V}_j^t A\tilde{V}_j = [\tilde{V}_j, \tilde{V}_j] = \Omega_j = \text{diag}\,(\omega_1, \ldots, \omega_j),$$

$$A\tilde{V}_j - \tilde{V}_j\Omega_j^{-1}\tilde{T}_j = \tilde{v}_{j+1}e_j^t.$$

Consequently

$$\tilde{V}_j^t A^2\tilde{V}_j = [\tilde{V}_j, A\tilde{V}_j] = \tilde{T}_j.$$

By construction, $\tilde{v}_i \in \mathcal{K}^i$ for each i, and thus

$$V_j = \tilde{V}_j R_j \tag{6.40}$$

for some invertible upper triangular matrix R_j. In particular $[\tilde{V}_j, \tilde{V}_j] = \Omega_j$ gives

$$R_j^t\Omega_j R_j = R_j^t\tilde{V}_j^t A\tilde{V}_j R_j = V_j^t A V_j = T_j$$

which is tridiagonal. Consequently R_j must be bidiagonal. Next comes

$$R_j^t\tilde{T}_j R_j = R_j^t\tilde{V}_j^t A^2\tilde{V}_j R_j = V_j^t A^2 V_j = M_j^2 = \hat{T}_j^t\hat{T}_j,$$

this last from Section 5.. Thus we have obtained

$$M_j^2 - \lambda T_j = R_j^t[\tilde{T}_j - \lambda\Omega_j]R_j, \tag{6.41}$$

and (6.41) differs from (6.37) only by a diagonal scaling $R_j = D_j L_j^t$. But the eigenvalues of the pencil $M_j^2 - \lambda T_j$ are the zeros of $\chi(\lambda)$ in (5.30), and so therefore are the eigenvalues of the pencil $\tilde{T}_j - \lambda\Omega_j$, where these are just the "Ritz values" of this pseudo-Lanczos process.

Finally by substituting the above expressions for M_j^2 and T_j in (5.26) we see

$$x_j^{mr} = V_j M_j^{-2} T_j e_1\beta_1 = \tilde{V}_j R_j (R_j^t \tilde{T}_j R_j)^{-1} R_j^t \Omega_j R_j e_1\beta_1 = \tilde{V}_j \tilde{T}_j^{-1} e_1\omega_1||b||,$$

since $R_j e_1 = e_1$ from (6.40) and $\tilde{v}_1 = v_1$, so the MR solution can be found from this pseudo-Lanczos process in the same way the weak solution was found from the standard Lanczos process via (3.15).

We hasten to add that in practice we would not compute the Harmonic Ritz values or the MR solution from this pseudo-Lanczos process — it is essentially of theoretical interest.

7. Harmonic Ritz Values and Lehmann's Intervals

We recall two standard results from eigenvalue theory. An $m \times m$ matrix H is said to be a *section* of an $n \times n$ A if $H = Q^t A Q$ for some $Q \in \mathbb{R}^{n\times m}$ with $Q^t Q = I_m$, $m < n$.

(I) Interlacing
Any intervals $(-\infty, s]$ and $[t, +\infty)$ contain at least as many eigenvalues of A as they do eigenvalues of a section H.

(II) Nesting
The convex hull of the Ritz values (for A) of a subspace $\mathcal{S}$ contains the Ritz values (for A) of any proper subspace of $\mathcal{S}$.

The Krylov methods build up a nested sequence of subspaces. By (II) the extreme Ritz values min and max must converge monotonically to the extreme eigenvalues as the dimension increases. Applying this result to A^{-1} we see that when A has eigenvalues of both signs then the smallest positive harmonic Ritz value approximates the smallest positive eigenvalue of A *from above*. Similarly the largest negative harmonic Ritz value approximates the largest negative eigenvalue of A *from below*. In other words any interval containing zero and free of A's eigenvalues is also free of harmonic Ritz values.

In practice, for Krylov subspaces of modest dimension (such as 30), the extreme Ritz values are good approximations to the extreme eigenvalues of A. Now since the harmonic Ritz values are reciprocals of the Ritz values of A^{-1} from $A\mathcal{K}^j$, we might guess that the smallest (in absolute value) harmonic Ritz values would also be good approximations to A's smallest eigenvalues, and approximate these much sooner than the Ritz values would. Unfortunately this is not borne out by our example below. Clearly the Ritz values of A^{-1} from $A\mathcal{K}^j$ do not behave the way we would hope Ritz values of A^{-1} from $\mathcal{K}^j$ to behave.

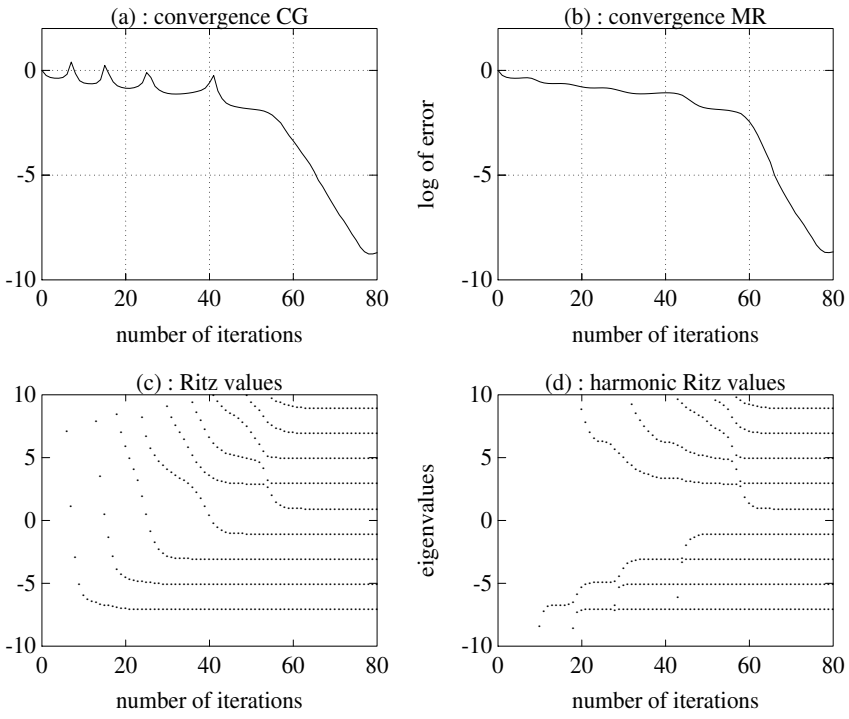

Figure 3. Convergence of CG and MR and the Ritz values for $m = 4$.

In Figure 3(a) we have plotted the convergence history of CG for the case $m = 4$ in (4.23), and we see four peaks, as anticipated. In Figure 3(c) we see how the Ritz values converge to "their" eigenvalues. Note that we do have four phases in which a Ritz value is close to zero, and these phases correspond to the peaks in Figure 3(a).

In Figure 3(b) we have displayed the convergence history for the minimum residual process, which is smooth as one might expect: because of the minimization of $\|r_j^{mr}\|_2$ over the current Krylov subspace, we know this cannot increase. ¿From the polynomial point of view we know that no harmonic Ritz value can come close enough to the origin to blow up the MR-polynomial in (5.31).

In Figure 3(d) we see the convergence of the harmonic Ritz values for the corresponding pseudo-Lanczos process, i.e., the Lanczos process carried out with the bilinear form given in (6.38). Note that the smallest positive harmonic Ritz value converges monotonically from above to the smallest positive eigenvalue, and also that the largest negative harmonic Ritz value (the negative value closest to zero) converges monotonically from below to the largest negative eigenvalue. But we see these small eigenvalues are still only found at about the same stage as in Figure 3(c). However, as we show below, these harmonic Ritz values do provide optimal eigenvalue intervals. The $\{\theta_i^{(j)}\}$ interlace the $\{\tilde{\theta}_i^{(j)}\} \cup \{0\}$ which interlace the $\{\theta_i^{(j+1)}\} \cup \{\pm\infty\}$, the sign on ∞ depends on α_{j+1}. It follows that each $\tilde{\theta}_i^{(j)}$ lies between a $\theta^{(j)}$ and a $\theta^{(j+1)}$. Consequently the $\theta^{(j)}$ and the $\tilde{\theta}^{(j)}$ stabilize (on

eigenvalues) at about the same value of j.

We also observe that the minimum residual process converges much faster after the smallest positive eigenvalue and the largest negative one have been approximated sufficiently well, see [1] for more details. This happens at about the same phase in the iteration process of CG, which is not that amazing, since it may be expected that as soon as the CG convergence behavior is determined by the positive eigenvalues only, the corresponding error norm $(x_j^w - x)^t A(x_j^w - x)$, with the error restricted to the subspace spanned by the "positive" eigenvectors, must be expected to reduce about as fast as $(x_j^{mr} - x)^t A^2 (x_j^{mr} - x)$, see [11] for more details. Since the MR approximation makes use of the value β_{j+1} it would seem preferable to the weak (CG) approximation. However it proved hard to find an efficient implementations of MR that could compete with CG. See [14] for further discussion of practical aspects of the two approaches.

As far as solving $Ax = b$ is concerned we have no more to say about harmonic Ritz values. However it turns out that the computable error bounds on eigenvalues developed by N.J. Lehmann in the 1950s and 1960s are directly related to harmonic Ritz values. The key fact is the shift invariance of Krylov subspace methods. The three term recurrence relation (2.5) may be applied to $A - \mu I$ instead of A to obtain

$$(A - \mu I)V_j = V_j(T_j - \mu I_j) + v_{j+1}\beta_{j+1}e_j^t \tag{7.42}$$

with the same Lanczos vectors $\{v_1, \ldots, v_j\}$ as before. The Ritz values from $\mathcal{K}^j = \text{range}(V_j)$ for $A - \mu I$ are just $\theta_i^{(j)} - \mu$, but the harmonic Ritz values change in a much more complicated way since from the eigenproblem (5.34) we have

$$[(T_j - \mu I_j)^2 + \beta_{j+1}^2 e_j e_j^t]u = \tilde{\theta}(T_j - \mu I_j)u. \tag{7.43}$$

So, when necessary, we write $\tilde{\theta}_i^{(j)}(\mu), \quad i = 1, \ldots, j$, to indicate this dependence on μ. We assume that μ is not an eigenvalue of T_j.

Note that the two $\tilde{\theta}_i^{(j)}(\mu)$ closest to μ converge monotonically to the two eigenvalues of A closest to μ.

Readers familiar with Lehmann's results will recognize (7.43) as a possible formulation of his $[t, \tau]$ (here $[\mu, \mu + \tilde{\theta}]$) intervals in [8]. Let us index the solutions of (7.43) as follows and drop the dependence on μ:

$$\tilde{\theta}_{-r}^{(j)} < \ldots < \tilde{\theta}_{-1}^{(j)} < 0 < \tilde{\theta}_1^{(j)} < \tilde{\theta}_{j-r}^{(j)}. \tag{7.44}$$

Theorem (Lehmann, 1966)
Each interval $[\mu, \mu + \tilde{\theta}_i^{(j)}]$, $i = 1, \ldots, j-r$ *contains at least* i *eigenvalues of* A. *Each interval* $[\mu + \tilde{\theta}_{-i}^{(j)}, \mu]$, $i = 1, \ldots, r$ *contains at least* i *eigenvalues of* A. *Moreover, in the absence of extra information no smaller intervals have this property.*

It comes as no great surprise that the polynomial χ_μ corresponding to the minimum residual $||b-(A-\mu)x||$ should have zeros which are reasonable approximations to the eigenvalues of A closest to μ. The equation (7.43) can be reformulated as

$$\det\,[(T_j - \mu I_j)(T_j - \langle \mu + \tilde{\theta} \rangle I_j) + \beta_{j+1}^2 e_j e_j^t] = 0, \tag{7.45}$$

and it was from (7.45) that Lehmann advocated computing $\tilde{\theta}$.

Nevertheless there is a simpler and more accurate way to find the $\tilde{\theta}_i^{(j)}(\mu)$, $i = 1, \ldots, j$. It was found by Kahan and presented in [15, Ch. 10]. Consider the $(j+1) \times (j+1)$ tridiagonal matrix $\bar{T}_{j+1}$ obtained from $T_{j+1} - \mu I_{j+1}$ by replacing the $(j+1, j+1)$ entry by β_{j+1}^2/δ_j where $\delta_j^{-1} = e_j^t(T_j - \mu I_j)^{-1}e_j$ is the reciprocal of the (j,j) element of Δ_j in the triangular factorization $T_j - \mu I_j = L_j \Delta_j L_j^t$. It will be shown that $\bar{T}_{j+1}$ has zero as a simple eigenvalue and the remaining eigenvalues yield the $\tilde{\theta}_i^{(j)}(\mu)$, $i = 1, \ldots, j$. The derivation makes use of the same facts as were used at the end of Section 5. when justifying expression (5.30).

$$\bar{T}_{j+1} - \tilde{\theta} I = \left[\begin{array}{c|c} T_j - \mu I - \tilde{\theta} I & \beta_{j+1} \\ \hline \beta_{j+1} & \beta_{j+1}^2/\delta_j - \tilde{\theta} \end{array}\right] \tag{7.46}$$

$$\begin{aligned} \det\,[\bar{T}_{j+1} - \tilde{\theta} I] &= \det\,(T_j - \mu I - \tilde{\theta} I) * \\ &\quad [\beta_{j+1}^2/\delta_j - \tilde{\theta} - \beta_{j+1}^2 e_j^t (T_j - \mu - \tilde{\theta})^{-1} e_j] \\ &= \det\,(T_j - \mu - \tilde{\theta})[\beta_{j+1}^2 e_j^t \{(T_j - \mu)^{-1} - (T_j - \mu - \tilde{\theta})^{-1}\} e_j - \tilde{\theta}] \\ &= \det\,(T_j - \mu - \tilde{\theta})[-\tilde{\theta}\beta_{j+1}^2 e_j^t (T_j - \mu - \tilde{\theta})^{-1}(T_j - \mu)^{-1} e_j - \tilde{\theta}] \\ &= (-\tilde{\theta}) \det\,(T_j - \mu - \tilde{\theta})[1 + \beta_{j+1}^2 e_j^t (T_j - \mu - \tilde{\theta})^{-1}(T_j - \mu)^{-1} e_j] \\ &= (-\tilde{\theta}) \det\,(T_j - \mu - \tilde{\theta}) \det\,[I + \beta_{j+1}^2 (T_j - \mu)^{-1} e_j e_j^t (T_j - \mu - \tilde{\theta})^{-1}] \\ &= (-\tilde{\theta}) \det\,[(T_j - \mu - \tilde{\theta})(T_j - \mu) + \beta_{j+1}^2 e_j e_j^t]/\det\,(T_j - \mu). \end{aligned}$$

Thus the eigenvalues of $\bar{T}_{j+1}$ are zero and the solutions of (7.45).

Note that the eigenvalues of $T_j - \mu I$, i.e. the shifted Ritz values, strictly interlace those of $\bar{T}_{j+1}$. Adding μ to these shows, with appropriate indexing shown in 7.44,

$$\ldots < \mu + \tilde{\theta}_{-1}^{(j)}(\mu) < \theta_{-1}^{(j)} < \mu < \theta_1^{(j)} < \mu + \tilde{\theta}_1^{(j)}(\mu) < \ldots,$$

so the Ritz values lie strictly within the corresponding Lehmann intervals.

8. Conclusions

We have shown that the zeros of the iteration polynomial (5.30) associated with the minimum residual method for symmetric indefinite systems satisfy interesting convergence properties. In particular, these zeros (the harmonic Ritz values) converge to the eigenvalues of A monotonically towards the origin (from both sides for indefinite A). By considering different shifts in $A - \mu I$, we have shown the corresponding zeros give us the Lehmann $[t, \tau]$ intervals for bounding eigenvalues of A. This could be an alternative to using inverse iteration via iterative solution of equations. Our observations also help in understanding local convergence behavior in the conjugate gradient and minimum residual methods.

The contribution of this study is largely a theoretical one. It points out useful connections between what we have called the harmonic Ritz values of A, the minimum residual method and its iteration polynomial, the pseudo-Lanczos process in

Section 6. and its Ritz values, and the Lehmann eigenvalue intervals, as well as explaining results we observe in practice. This increased understanding could facilitate the study and design of methods for finding internal eigenvalues or solving linear systems involving large matrices. In [11] it has been suggested that the harmonic Ritz vectors offer better possibilities for restarting purposes when searching for internal eigenvalues.

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