Chapter 3

Error Bounds for CG, MINRES, and GMRES

It was shown in Chapter 2 that the CG, MINRES, and GMRES algorithms each generate the optimal approximate solution from a Krylov subspace, where "optimal" is taken to mean having an error with minimal A-norm in the case of CG or having a residual with minimal 2-norm in the case of MINRES and GMRES. In this chapter we derive bounds on the appropriate error norm for the optimal approximation from a Krylov subspace.

A goal is to derive a *sharp* upper bound on the reduction in the A-norm of the error for CG or in the 2-norm of the residual for both MINRES and GMRES—that is, an upper bound that is independent of the initial vector but that is actually attained for certain initial vectors. This describes the *worst-case* behavior of the algorithms (for a given matrix A). It can sometimes be shown that the "typical" behavior of the algorithms is not much different from the worst-case behavior. That is, if the initial vector is random, then convergence may be only moderately faster than for the worst initial vector. For certain special initial vectors, however, convergence may be much faster than the worst-case analysis would suggest. Still, it is usually the same analysis that enables one to identify these "special" initial vectors, and it is often clear how the bounds must be modified to account for special properties of the initial vector.

For *normal* matrices, a sharp upper bound on the appropriate error norm is known. This is not the case for nonnormal matrices,and a number of possible approaches to this problem are discussed in section 3.2.

3.1. Hermitian Problems—CG and MINRES.

It was shown in Chapter 2 that the A-norm of the error in the CG algorithm for Hermitian positive definite problems and the 2-norm of the residual in the MINRES algorithm for general Hermitian problems are minimized over the spaces

$$e_0 + \text{span}\{Ae_0, A^2e_0, \ldots, A^ke_0\} \quad \text{and} \quad r_0 + \text{span}\{Ar_0, A^2r_0, \ldots, A^kr_0\},$$

respectively. It follows that the CG error vector and the MINRES residual

vector at step k can be written in the form

$$e_k = P_k^C(A)e_0, \quad r_k = P_k^M(A)r_0, \tag{3.1}$$

where P_k^C and P_k^M are kth-degree polynomials with value 1 at the origin and, of all such polynomials that could be substituted in (3.1), P_k^C gives the error of minimal A-norm in the CG algorithm and P_k^M gives the residual of minimal 2-norm in the MINRES algorithm. In other words, the error e_k in the CG approximation satisfies

$$\|e_k\|_A = \min_{p_k} \|p_k(A)e_0\|_A \tag{3.2}$$

and the residual r_k in the MINRES algorithm satisfies

$$\|r_k\| = \min_{p_k} \|p_k(A)r_0\|, \tag{3.3}$$

where the minimum is taken over all polynomials p_k of degree k or less with $p_k(0) = 1$.

In this section we derive bounds on the expressions in the right-hand sides of (3.2) and (3.3) that are *independent* of the direction of the initial error e_0 or residual r_0, although they do depend on the size of these quantities. A sharp upper bound is derived involving all of the *eigenvalues* of A, and then simpler (but nonsharp) bounds are given based on knowledge of just a few of the eigenvalues of A.

Let an eigendecomposition of A be written as $A = U\Lambda U^H$, where U is a unitary matrix and $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$ is a diagonal matrix of eigenvalues. If A is positive definite, define $A^{1/2}$ to be $U\Lambda^{1/2}U^H$. Then the A-norm of a vector v is just the 2-norm of the vector $A^{1/2}v$. Equalities (3.2) and (3.3) imply that

$$\begin{aligned} \|e_k\|_A &= \min_{p_k} \|A^{1/2}p_k(A)e_0\| = \min_{p_k} \|Up_k(\Lambda)U^H A^{1/2}e_0\| \\ &\leq \min_{p_k} \|p_k(\Lambda)\| \cdot \|e_0\|_A, \end{aligned} \tag{3.4}$$

$$\|r_k\| = \min_{p_k} \|Up_k(\Lambda)U^H r_0\| \leq \min_{p_k} \|p_k(\Lambda)\| \cdot \|r_0\|, \tag{3.5}$$

with the inequalities following, because if $\hat{p}_k$ is the polynomial that minimizes $\|p_k(\Lambda)\|$, then

$$\min_{p_k} \|Up_k(\Lambda)U^H w\| \leq \|U\hat{p}_k(\Lambda)U^H w\| \leq \|U\hat{p}_k(\Lambda)U^H\| \, \|w\| = \|\hat{p}_k(\Lambda)\| \, \|w\|$$

for any vector w. Of course, the polynomial that minimizes the expressions in the equalities of (3.4) and (3.5) is *not* necessarily the same one that minimizes $\|p_k(\Lambda)\|$ in the inequalities. The MINRES and CG polynomials depend on the initial vector, while this polynomial does not. Hence it is not immediately obvious that the bounds in (3.4) and (3.5) are *sharp*, that is, that they can

actually be attained for certain initial vectors. It turns out that this is the case, however. See, for example, [63, 68, 85]. For each k there is an initial vector e_0 for which the CG polynomial at step k is the polynomial that minimizes $\|p_k(A)\|$ and for which equality holds in (3.4). An analogous result holds for MINRES.

The sharp upper bounds (3.4) and (3.5) can be written in the form

$$\|e_k\|_A/\|e_0\|_A \leq \min_{p_k} \max_{i=1,\ldots,n} |p_k(\lambda_i)| \quad \text{for CG,} \tag{3.6}$$

$$\|r_k\|/\|r_0\| \leq \min_{p_k} \max_{i=1,\ldots,n} |p_k(\lambda_i)| \quad \text{for MINRES.} \tag{3.7}$$

The problem of describing the convergence of these algorithms therefore reduces to one in approximation theory—how well can one approximate zero on the set of eigenvalues of A using a kth-degree polynomial with value 1 at the origin? While there is no simple expression for the maximum value of the minimax polynomial on a discrete set of points, this minimax polynomial can be calculated if the eigenvalues of A are known; more importantly, this sharp upper bound provides intuition as to what constitutes "good" and "bad" eigenvalue distributions. Eigenvalues tightly clustered around a single point (away from the origin) are good, for instance, because the polynomial $(1-z/c)^k$ is small in absolute value at all points near c. Widely spread eigenvalues, especially if they lie on both sides of the origin, are bad, because a low-degree polynomial with value 1 at the origin cannot be small at a large number of such points.

Since one usually has only limited information about the eigenvalues of A, it is useful to have error bounds that involve only a few properties of the eigenvalues. For example, in the CG algorithm for Hermitian positive definite problems, knowing only the largest and smallest eigenvalues of A, one can obtain an error bound by considering the minimax polynomial on the *interval* from λ_{min} to λ_{max}, i.e., the Chebyshev polynomial shifted to the interval and scaled to have value 1 at the origin.

THEOREM 3.1.1. *Let e_k be the error at step k of the CG algorithm applied to the Hermitian positive definite linear system $Ax = b$. Then*

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq 2 \left[\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} \right)^k + \left(\frac{\sqrt{\kappa}+1}{\sqrt{\kappa}-1} \right)^k \right]^{-1} \leq 2 \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} \right)^k, \tag{3.8}$$

where $\kappa = \lambda_{max}/\lambda_{min}$ is the ratio of the largest to smallest eigenvalue of A.

Proof. Consider the kth scaled and shifted Chebyshev polynomial on the interval $[\lambda_{min}, \lambda_{max}]$

$$p_k(z) = T_k\left(\frac{2z - \lambda_{max} - \lambda_{min}}{\lambda_{max} - \lambda_{min}} \right) \Big/ T_k\left(\frac{-\lambda_{max} - \lambda_{min}}{\lambda_{max} - \lambda_{min}} \right), \tag{3.9}$$

where $T_k(z)$ is the Chebyshev polynomial of the first kind on the interval $[-1, 1]$ satisfying

$$T_0(z) = 1, \quad T_1(z) = z,$$

$$T_{j+1}(z) = 2zT_j(z) - T_{j-1}(z), \quad j = 1, 2, \ldots.$$

In the interval $[-1, 1]$, we have $T_k(z) = \cos(k \cos^{-1}(z))$, so $|T_k(z)| \leq 1$ and the absolute value of the numerator in (3.9) is bounded by 1 for z in the interval $[\lambda_{min}, \lambda_{max}]$. It attains this bound at the endpoints of the interval and at $k-1$ interior points. To determine the size of the denominator in (3.9), note that outside the interval $[-1, 1]$, we have

$$T_k(z) = \cosh(k \cosh^{-1} z),$$

so if z is of the form $z = \cosh(\ln y) = \frac{1}{2}(y+y^{-1})$, then $T_k(z) = \frac{1}{2}(y^k+y^{-k})$. The argument in the denominator of (3.9) can be expressed in the form $\frac{1}{2}(y + y^{-1})$ if y satisfies

$$-\frac{\lambda_{max} + \lambda_{min}}{\lambda_{max} - \lambda_{min}} = -\frac{\kappa + 1}{\kappa - 1} = \frac{1}{2}(y + y^{-1}),$$

which is equivalent to the quadratic equation

$$\frac{1}{2}y^2 + \frac{\kappa + 1}{\kappa - 1}y + \frac{1}{2} = 0.$$

Solving this equation, we find

$$y = -\frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1} \quad \text{or} \quad y = -\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}.$$

In either case, the denominator in (3.9) has absolute value equal to

$$\frac{1}{2}\left[\left(\frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1}\right)^k + \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^k\right],$$

and from this the result (3.8) follows. □

Knowing only the largest and smallest eigenvalues of a Hermitian positive definite matrix A, bound (3.8) is the best possible. If the interior eigenvalues of A lie at the points where the Chebyshev polynomial p_k in (3.9) attains its maximum absolute value on $[\lambda_{min}, \lambda_{max}]$, then for a certain initial error e_0, the CG polynomial will be equal to the Chebyshev polynomial, and the bound in (3.8) will actually be attained at step k.

If additional information is available about the interior eigenvalues of A, one can often improve on the estimate (3.8) while maintaining a simpler expression than the sharp bound (3.6). Suppose, for example, that A has one eigenvalue much larger than the others, say, $\lambda_1 \leq \cdots \leq \lambda_{n-1} << \lambda_n$, that is, $\lambda_n/\lambda_{n-1} >> 1$. Consider a polynomial p_k that is the product of a linear factor that is zero at λ_n and the $(k-1)$st-degree scaled and shifted Chebyshev polynomial on the interval $[\lambda_1, \lambda_{n-1}]$:

$$p_k(z) = \left[T_{k-1}\left(\frac{2z - \lambda_{n-1} - \lambda_1}{\lambda_{n-1} - \lambda_1}\right) \Big/ T_{k-1}\left(\frac{-\lambda_{n-1} - \lambda_1}{\lambda_{n-1} - \lambda_1}\right)\right] \cdot \left(\frac{\lambda_n - z}{\lambda_n}\right).$$

Since the second factor is zero at λ_n and less than one in absolute value at each of the other eigenvalues, the maximum absolute value of this polynomial on $\{\lambda_1, \ldots, \lambda_n\}$ is less than the maximum absolute value of the first factor on $\{\lambda_1, \ldots, \lambda_{n-1}\}$. Using arguments like those in Theorem 3.1.1, it follows that

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq 2\left(\frac{\sqrt{\kappa_{n-1}}-1}{\sqrt{\kappa_{n-1}}+1}\right)^{k-1}, \quad \kappa_{n-1} = \frac{\lambda_{n-1}}{\lambda_1}. \tag{3.10}$$

Similarly, if the matrix A has just a few large outlying eigenvalues, say, $\lambda_1 \leq \cdots \leq \lambda_{n-\ell} << \lambda_{n-\ell+1} \leq \cdots \leq \lambda_n$ (i.e., $\lambda_{n-\ell+1}/\lambda_{n-\ell} >> 1$), one can consider a polynomial p_k that is the product of an ℓth-degree factor that is zero at each of the outliers (and less than one in magnitude at each of the other eigenvalues) and a scaled and shifted Chebyshev polynomial of degree $k-\ell$ on the interval $[\lambda_1, \lambda_{n-\ell}]$. Bounding the size of this polynomial gives

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq 2\left(\frac{\sqrt{\kappa_{n-\ell}}-1}{\sqrt{\kappa_{n-\ell}}+1}\right)^{k-\ell}, \quad \kappa_{n-\ell} = \frac{\lambda_{n-\ell}}{\lambda_1}. \tag{3.11}$$

Analogous results hold for the 2-norm of the residual in the MINRES algorithm applied to a Hermitian positive definite linear system, and the proofs are identical. For example, for any $\ell \geq 0$, we have

$$\frac{\|r_k\|}{\|r_0\|} \leq 2\left(\frac{\sqrt{\kappa_{n-\ell}}-1}{\sqrt{\kappa_{n-\ell}}+1}\right)^{k-\ell}, \quad \kappa_{n-\ell} = \frac{\lambda_{n-\ell}}{\lambda_1} \quad \text{(MINRES)}. \tag{3.12}$$

For Hermitian *indefinite* problems, a different polynomial must be considered. We derive only a simple estimate in the case when the eigenvalues of A are contained in two intervals $[a,b] \bigcup [c,d]$, where $a < b < 0 < c < d$ and $b-a = d-c$. In this case, the kth-degree polynomial with value 1 at the origin that has minimal maximum deviation from 0 on $[a,b] \bigcup [c,d]$ is given by

$$p_k(z) = T_\ell(q(z))/T_\ell(q(0)), \quad q(z) = 1 + \frac{2(z-b)(z-c)}{ad-bc}, \tag{3.13}$$

where $\ell = [\frac{k}{2}]$, $[\cdot]$ denotes the integer part, and T_ℓ is the ℓth Chebyshev polynomial. Note that the function $q(z)$ maps each of the intervals $[a,b]$ and $[c,d]$ to the interval $[-1,1]$. It follows that for $z \in [a,b] \bigcup [c,d]$, the absolute value of the numerator in (3.13) is bounded by 1. The size of the denominator is determined in the same way as before: if $q(0) = \frac{1}{2}(y + y^{-1})$, then $T_\ell(q(0)) = \frac{1}{2}(y^\ell + y^{-\ell})$. To determine y, we must solve the equation

$$q(0) = \frac{ad+bc}{ad-bc} = \frac{1}{2}(y + y^{-1})$$

or the quadratic equation

$$\frac{1}{2}y^2 - \frac{ad+bc}{ad-bc}y + \frac{1}{2} = 0.$$

This equation has the solutions

$$y = \frac{\sqrt{|ad|} - \sqrt{|bc|}}{\sqrt{|ad|} + \sqrt{|bc|}} \quad \text{or} \quad \frac{\sqrt{|ad|} + \sqrt{|bc|}}{\sqrt{|ad|} - \sqrt{|bc|}}.$$

It follows that the norm of the kth MINRES residual is bounded by

$$\frac{\|r_k\|}{\|r_0\|} \leq 2 \left(\frac{\sqrt{|ad|} - \sqrt{|bc|}}{\sqrt{|ad|} + \sqrt{|bc|}} \right)^{[k/2]} \tag{3.14}$$

In the special case when $a = -d$ and $b = -c$ (so the two intervals are placed symmetrically about the origin), the bound in (3.14) becomes

$$\frac{\|r_k\|}{\|r_0\|} \leq 2 \left(\frac{d/c - 1}{d/c + 1} \right)^{[k/2]} \tag{3.15}$$

This is the bound one would obtain at step $[k/2]$ for a Hermitian positive definite matrix with condition number $(d/c)^2$! It is as difficult to approximate zero on two intervals situated symmetrically about the origin as it is to approximate zero on a single interval lying on one side of the origin whose ratio of largest to smallest point is equal to the *square* of that in the 2-interval problem. Remember, however, that estimate (3.14) implies better approximation properties for intervals not symmetrically placed about the origin. For further discussion of approximation problems on two intervals, see [50, secs. 3.3–3.4]

3.2. Non-Hermitian Problems—GMRES.

Like MINRES for Hermitian problems, the GMRES algorithm for general linear systems produces a residual at step k whose 2-norm satisfies (3.3). To derive a bound on the expression in (3.3) that is independent of the direction of r_0, we could proceed as in the previous section by employing an eigendecomposition of A. To this end, assume that A is diagonalizable and let $A = V\Lambda V^{-1}$ be an eigendecomposition, where $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ is a diagonal matrix of eigenvalues and the columns of V are right eigenvectors of A (normalized in any desired way). Then it follows from (3.3) that

$$\|r_k\| = \min_{p_k} \|V p_k(\Lambda) V^{-1} r_0\| \leq \kappa(V) \min_{p_k} \|p_k(\Lambda)\| \cdot \|r_0\|,$$

$$\|r_k\|/\|r_0\| \leq \kappa(V) \min_{p_k} \max_{i=1,\ldots,n} |p_k(\lambda_i)|, \tag{3.16}$$

where $\kappa(V) = \|V\| \cdot \|V^{-1}\|$ is the condition number of the eigenvector matrix V. We will assume that the columns of V have been scaled to make this condition number as small as possible. As in the Hermitian case, the polynomial that minimizes $\|V p_k(\Lambda) V^{-1} r_0\|$ is not necessarily the one that minimizes $\|p_k(\Lambda)\|$, and it is not clear whether the bound in (3.16) is sharp. It turns out that if A is a *normal* matrix (a diagonalizable matrix with a complete set of orthonormal

eigenvectors), then $\kappa(V) = 1$ and the bound in (3.16) is sharp [68, 85]. In this case, as in the Hermitian case, the problem of describing the convergence of GMRES reduces to a problem in approximation theory—how well can one approximate zero on the set of *complex* eigenvalues using a kth-degree polynomial with value 1 at the origin? We do not have simple estimates, such as that obtained in Theorem 3.1.1 based on the ratio of largest to smallest eigenvalue, but one's intuition about good and bad eigenvalue distributions in the complex plane still applies. Eigenvalues tightly clustered about a single point (away from the origin) are good, since the polynomial $(1 - z/c)^k$ is small at all points close to c in the complex plane. Eigenvalues all around the origin are bad because (by the maximum principle) it is impossible to have a polynomial that is 1 at the origin and less than 1 everywhere on some closed curve around the origin. Similarly, a low-degree polynomial cannot be 1 at the origin and small in absolute value at many points distributed all around the origin.

If the matrix A is nonnormal but has a fairly well-conditioned eigenvector matrix V, then the bound (3.16), while not necessarily sharp, gives a reasonable estimate of the actual size of the residual. In this case again, it is A's eigenvalue distribution that essentially determines the behavior of GMRES.

In general, however, the behavior of GMRES cannot be determined from eigenvalues alone. In fact, it is shown in [72, 69] that *any* nonincreasing curve represents a plot of residual norm versus iteration number for the GMRES method applied to some problem; moreover, that problem can be taken to have any desired eigenvalues. Thus, for example, eigenvalues tightly clustered around 1 are not necessarily good for nonnormal matrices, as they are for normal ones.

A simple way to see this is to consider a matrix A with the following sparsity pattern:

$$\begin{pmatrix} 0 & * & 0 & \dots & 0 \\ 0 & * & * & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \\ 0 & * & * & \dots & * \\ * & * & * & \dots & * \end{pmatrix}, \tag{3.17}$$

where the $*$'s represent any values and the other entries are 0. If the initial residual r_0 is a multiple of the first unit vector $\xi_1 \equiv (1, 0, \dots, 0)^T$, then Ar_0 is a multiple of ξ_n, $A^2 r_0$ is a linear combination of ξ_n and ξ_{n-1}, etc. All vectors $A^k r_0$, $k = 1, \dots, n-1$ are orthogonal to r_0, so the optimal approximation from the space $x_0 + \text{span}\{r_0, Ar_0, \dots, A^{k-1} r_0\}$ is simply $x_k = x_0$ for $k = 1, \dots, n-1$; i.e., GMRES makes no progress until step n! Now, the class of matrices of the

form (3.17) includes, for example, all *companion matrices*:

$$\begin{pmatrix} 0 & 1 & & \\ 0 & 0 & \ddots & \\ \vdots & \vdots & & 1 \\ c_0 & c_1 & \dots & c_{n-1} \end{pmatrix}$$

The eigenvalues of this matrix are the roots of the polynomial $z^n - \sum_{j=0}^{n-1} c_j z^j$, and the coefficients $c_0, \dots, c_{n-1}$ can be chosen to make this matrix have any desired eigenvalues. If GMRES is applied to (3.17) with a different initial residual, say, a random r_0, then, while some progress will be made before step n, it is likely that a significant residual component will remain, until that final step.

Of course, one probably would not use the GMRES algorithm to solve a linear system with the sparsity pattern of that in (3.17), but the same result holds for any matrix that is unitarily similar to one of the form (3.17). Note that (3.17) is simply a permuted lower triangular matrix. Every matrix is unitarily similar to a lower triangular matrix, but, fortunately, most matrices are *not* unitarily similar to one of the form (3.17)!

When the eigenvector matrix V is extremely ill-conditioned, the bound (3.16) is less useful. It may be greater than 1 for all $k < n$, but we know from other arguments that $\|r_k\|/\|r_0\| \leq 1$ for all k. In such cases, it is not clear whether GMRES converges poorly or whether the bound (3.16) is simply a large overestimate of the actual residual norm. Attempts have been made to delineate those cases in which GMRES actually does converge poorly from those for which GMRES converges well and the bound (3.16) is just a large overestimate.

Different bounds on the residual norm can be obtained based on the field of values of A, provided $0 \notin \mathcal{F}(A)$. For example, suppose $\mathcal{F}(A)$ is contained in a disk $\mathbf{D} = \{z \in \mathbf{C} : \ |z - c| \leq s\}$ which does not contain the origin. Consider the polynomial $p_k(z) = (1 - z/c)^k$. It follows from (1.16–1.17) that

$$\mathcal{F}(I - (1/c)A) = 1 - (1/c)\mathcal{F}(A) \subseteq \{z \in \mathbf{C} : \ |z| \leq s/|c|\}$$

and hence that $\nu(I - (1/c)A) \leq s/|c|$. The power inequality (1.22) implies that $\nu((I - (1/c)A)^k) \leq (s/|c|)^k$ and hence, by (1.21),

$$\|p_k(A)\| \leq 2\left(\frac{s}{|c|}\right)^k.$$

It follows that the GMRES residual norm satisfies

$$\|r_k\|/\|r_0\| \leq 2\left(\frac{s}{|c|}\right)^k, \tag{3.18}$$

and this bound holds for the restarted GMRES algorithm GMRES(j) provided that $j \geq k$. It is somewhat stronger than the bound (2.13) for GMRES(1)

(which is the same as Orthomin(1)), because the factor 2 does not have to be raised to the kth power. Still, (3.18) sometimes gives a significant overestimate of the actual GMRES residual norm. In many cases, a disk $\mathbf{D}$ may have to be much larger than $\mathcal{F}(A)$ in order to include $\mathcal{F}(A)$.

Using the recent result (2.14), however, involving the Faber polynomials for an arbitrary convex set S that contains $\mathcal{F}(A)$ and not the origin, one can more closely fit $\mathcal{F}(A)$ while choosing S so that the Faber polynomials for S are close to the minimax polynomials. For example, suppose $\mathcal{F}(A)$ is contained in the ellipse

$$E_s(\gamma,\delta) = \{z \in \mathbf{C}: \ |z-(\delta-\gamma)| + |z-(\delta+\gamma)| \le |\gamma|(s+s^{-1})\},$$

with foci $\delta \pm \gamma$ and semi-axes $|\gamma|(s \pm s^{-1})$. Assume that $0 \notin E_s(\gamma,\delta)$. The kth Faber polynomial for E_s is just the kth Chebyshev polynomial of the first kind translated to the interval $[\delta-\gamma, \delta+\gamma]$. When this polynomial is normalized to have value one at the origin, its maximum value on E_s can be shown to be

$$|F_k(z)/F_k(0)| \le (s^k + s^{-k}) \frac{\kappa^k}{1-\kappa^{2k}}, \quad z \in E_s,$$

where

$$\kappa = \left| \frac{\delta - \sqrt{\delta^2-\gamma^2}}{\gamma} \right|$$

and the branch of the square root is chosen so that $\kappa < 1$. We assume here that $s < \kappa^{-1}$. For further details, see [38, 39].

Inequality (2.14) still does not lead to a sharp bound on the residual norm in most cases, and it can be applied only when $0 \notin \mathcal{F}(A)$. Another approach to estimating $\|p(A)\|$ in terms of the size of $p(z)$ in some region of the complex plane has been suggested by Trefethen [129]. It is the idea of *pseudo-eigenvalues.*

For any polynomial p, the matrix $p(A)$ can be written as a Cauchy integral

$$p(A) = \frac{1}{2\pi i} \int_\Gamma p(z)(zI-A)^{-1} dz, \tag{3.19}$$

where Γ is any simple closed curve or union of simple closed curves containing the spectrum of A. Taking norms on each side in (3.19) and replacing the norm of the integral by the length $\mathcal{L}(\Gamma)$ of the curve times the maximum norm of the integrand gives

$$\|p(A)\| \le \frac{\mathcal{L}(\Gamma)}{2\pi} \max_{z\in\Gamma} \|p(z)(zI-A)^{-1}\|. \tag{3.20}$$

Now, if we consider a curve Γ_ϵ on which the resolvent norm $\|(zI-A)^{-1}\|$ is constant, say, $\|(zI-A)^{-1}\| = \epsilon^{-1}$, then (3.20) implies

$$\|p(A)\| \le \frac{\mathcal{L}(\Gamma_\epsilon)}{2\pi\epsilon} \max_{z\in\Gamma_\epsilon} |p(z)|. \tag{3.21}$$

The curve on which $\|(zI - A)^{-1}\| = \epsilon^{-1}$ is referred to as the boundary of the ϵ-pseudospectrum of A:

$$\Lambda_\epsilon \equiv \{z : \|(zI - A)^{-1}\| \geq \epsilon^{-1}\}.$$

From (3.21) and the optimality of the GMRES approximation, it follows that the GMRES residual r_k satisfies

$$\|r_k\|/\|r_0\| \leq \frac{\mathcal{L}(\Gamma_\epsilon)}{2\pi\epsilon} \min_{p_k} \max_{z \in \Gamma_\epsilon} |p_k(z)| \tag{3.22}$$

for any choice of the parameter ϵ. For certain problems, and with carefully chosen values of ϵ, the bound (3.22) may be much smaller than that in (3.16). Still, the bound (3.22) is not sharp, and for some problems there is no choice of ϵ that yields a realistic estimate of the actual GMRES residual [72]. It is easy to see where the main overestimate occurs. In going from (3.19) to (3.20) and replacing the norm of the integral by the length of the curve times the maximum norm of the integrand, one may lose important cancellation properties of the integral.

Each of the inequalities (3.16), (3.18), and (3.22) provides bounds on the GMRES residual by bounding the quantity $\min_{p_k} \|p_k(A)\|$. Now, the worst-case behavior of GMRES is given by

$$\|r_k\| = \max_{\|r_0\|=1} \min_{p_k} \|p_k(A)r_0\|. \tag{3.23}$$

The polynomial p_k depends on r_0. Until recently, it was an open question whether the right-hand side of (3.23) was equal to the quantity

$$\min_{p_k} \|p_k(A)\| \equiv \min_{p_k} \max_{\|r_0\|=1} \|p_k(A)r_0\|. \tag{3.24}$$

It is known that the right-hand sides of (3.23) and (3.24) are equal if A is a normal matrix or if the dimension of A is less than or equal to 3 or if $k = 1$, and many numerical experiments have shown that these two quantities are equal (to within the accuracy limits of the computation) for a wide variety of matrices and values of k. Recently, however, it has been shown that the two quantities may differ. Faber et al. [44] constructed an example in which the right-hand side of (3.24) is 1, while that of (3.23) is .9995. Subsequently, Toh [127] generated examples in which the ratio of the right-hand side of (3.24) to that of (3.23) can be made arbitrarily large by varying a parameter in the matrix. Thus neither of the approaches leading to inequalities (3.16) and (3.22) can be expected to yield a sharp bound on the size of the GMRES residual, and it remains an open problem to describe the convergence of GMRES in terms of some simple characteristic properties of the coefficient matrix.

Exercises.

3.1. Suppose a positive definite matrix has a small, well-separated eigenvalue, $\lambda_1 << \lambda_2 \leq \cdots \leq \lambda_n$ (that is, $\lambda_1/\lambda_2 << 1$). Derive an error bound for

CG or MINRES using the maximum value of a polynomial that is the product of a linear factor that is 0 at λ_1 and a $(k-1)$st-degree Chebyshev polynomial on the interval $[\lambda_2, \lambda_n]$. Is it more advantageous to have a small, well-separated eigenvalue or a large, well-separated eigenvalue as in (3.10)? (For the derivation of many other such error bounds, see [132].)

3.2. Consider the 4-by-4 matrix

$$A = \begin{pmatrix} 1 & \epsilon & & \\ & -1 & 1/\epsilon & \\ & & 1 & \epsilon \\ & & & -1 \end{pmatrix}, \quad \epsilon > 0.$$

This is the example devised by Toh [127] to demonstrate the difference between expressions (3.23) and (3.24).

(a) Show that the polynomial of degree 3 or less with value one at the origin that minimizes $\|p(A)\|$ over all such polynomials is

$$p_*(z) = 1 - \frac{3}{5}z^2$$

and that $\|p_*(A)\| = \frac{4}{5}$, independent of ϵ. (Hint: First show that $p_*(z)$ must be even by using the uniqueness of p_* and the fact that A^T is unitarily similar to $-A$ via the matrix

$$Q = \begin{pmatrix} & & & -1 \\ & & 1 & \\ & -1 & & \\ 1 & & & \end{pmatrix},$$

which implies that $\|p(-A)\| = \|p(A^T)\| = \|p(A)\|$ for any polynomial p. Now consider polynomials p_γ of the form $1 + \gamma z^2$ for various scalars γ. Determine the singular values of $p_\gamma(A)$ analytically to show that

$$\sigma_{max}^2(\gamma) = \frac{1}{2}\left(2(\gamma+1)^2 + \gamma^2 + |\gamma|\sqrt{4(\gamma+1)^2 + \gamma^2}\right).$$

Differentiate with respect to γ and set the derivative to zero to show that $\gamma = \frac{3}{5}$ minimizes σ_{max}.)

(b) Show that for any vector b with $\|b\| = 1$ there is a polynomial p_b of degree 3 or less with $p_b(0) = 1$ such that

$$\|p_b(A)b\| \leq 4\sqrt{\epsilon} + 5\epsilon.$$

(Hint: First note that if $b = (b_1, b_2, b_3, b_4)^T$ then

$$Ab = \begin{pmatrix} b_1 \\ -b_2 + b_3/\epsilon \\ b_3 \\ -b_4 \end{pmatrix} + \epsilon \begin{pmatrix} b_2 \\ 0 \\ b_4 \\ 0 \end{pmatrix}, \quad A^2 b = b + \begin{pmatrix} b_3 \\ b_4 \\ 0 \\ 0 \end{pmatrix},$$

$$A^3 b = Ab + \begin{pmatrix} b_3 \\ -b_4 \\ 0 \\ 0 \end{pmatrix} + \epsilon \begin{pmatrix} b_4 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

If $|b_3| \geq \sqrt{\epsilon}$, take

$$p_b(z) = 1 - z - z^2 + \left(\frac{2b_4\epsilon}{b_3} + 1\right) z^3,$$

and if $|b_3| < \sqrt{\epsilon}$ take

$$p_b(z) = 1 + z - z^2 + (\epsilon - 1)z^3.)$$