Upper bounds for convergence rates of acceleration methods with initial iterations *

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GMRES(n, k), a version of GMRES for the solution of large sparse linear systems, is introduced. A cycle of GMRES(n, k) consists of n Richardson iterations followed by k iterations of GMRES. Such cycles can be repeated until convergence is achieved. The advantage in this approach is in the opportunity to use moderate k, which results in time and memory saving. Because the number of inner products among the vectors of iteration is about $k^2/2$, using a moderate k is particularly attractive on message-passing parallel architectures, where inner products require expensive global communication. The present analysis provides tight upper bounds for the convergence rates of GMRES(n, k) for problems with diagonalizable coefficient matrices whose spectra lie in an ellipse in $\mathbb{C} \setminus \{0\}$. The advantage of GMRES(n, k) over GMRES(k) is illustrated numerically.

1. Introduction

Let s be the solution to the nonsingular linear $N \times N$ system Bx = f, which we choose to write equivalently in the possibly preconditioned form

$$Ax = b. \tag{1.1}$$

With x_0 picked arbitrarily, we generate the vectors x_1, x_2, \ldots :

$$x_{j+1} = (I - A)x_j + b, \quad j = 0, 1, \dots$$
 (1.2)

If $r \equiv \rho(I - A)$, the spectral radius of I - A, then the error $x_n - s$ tends to zero practically as r^n for $n \to \infty$ provided r < 1.

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In most cases of interest that occur in practice r may be very close to 1, and this causes the sequence $\{x_j\}_{j=0}^{\infty}$ to converge very slowly. An efficient way of overcoming this problem is to use Krylov subspace methods (see, for example, [2,3,8,11,13,14, 20,33,36–38]). As a representative of these methods we use here the generalized minimum residual method (GMRES) of Saad and Schultz [21], which is particularly attractive because of its numerical stability. The mathematical equivalence of Krylov subspace methods and vector extrapolation methods such as the Minimal Polynomial Extrapolation (MPE) and the Reduced Rank Extrapolation (RRE) (see [6,10,18]) is treated in detail in [27].

Krylov subspace methods require the computation of inner products among the vectors of iteration for the orthogonalization of residuals with respect to some inner product or bilinear form. For the Krylov subspace methods mentioned above, the number of inner products computed and the storage requirements increase with the iteration number k (the dimension of the Krylov subspace used) like $k^2/2$ and k, respectively. For even moderately large k, the storage requirements may be prohibitively large, and the time consumption of the acceleration may dominate that of the matrixvector products required in the iteration. This is especially pronounced when the system is sparse but unstructured so that no well parallelized, well vectorized preconditioners are available and, therefore, only simple preconditioners such as that of the Jacobi iteration are allowed. In such cases, the orthogonalization phase may form the "bottle-neck" in the algorithm, namely, the most time consuming part. For example, for message-passing parallel architectures with mesh-connected processor arrays, the inner products required for the orthogonalization involve global communication among all the processors and, thus, are far more time consuming than the basic Jacobi iteration, which uses immediate neighbor communication only. Therefore, GMRES is often used in cycling mode, that is, it is restarted after every k iterations (with a moderate k, usually $k \leq 20$), the last iteration of a cycle serving as the initial guess for the next one. This approach is commonly referred to as GMRES(k). Of course, the total number of iterations required for convergence is larger than that in GMRES; still, it is attractive when GMRES cannot be used or is inefficient because of the above-mentioned problems.

There are several ways to preprocess the sequence of vectors of iteration before using GMRES(k) in order to increase the efficiency of the acceleration (see, for example, [4,9,16,19]). The GMRES(n, k) method proposed here may also be considered a preprocessing, in which GMRES(k) is preceded by n Richardson iterations. Each cycle of GMRES(n, k) thus consists of n initial iterations x_1, x_2, \ldots, x_n as in (1.2) followed by k iterations of GMRES applied to x_n . (In particular, GMRES(0, k) is the same as GMRES(k).) The result of any one cycle (denoted hereafter by $s_{n,k}$) serves as the initial guess x_0 for the next cycle. (In the sequel, we may also use the notation $s_{n,k}$ when the method of Arnoldi [2] is used rather than GMRES, see [31].)

It was observed in [28] that, for the vector extrapolation methods MPE and RRE that are mathematically equivalent to the above-mentioned Krylov subspace methods, using n > 0 (even with moderate values of n) may substantially improve the

convergence behavior. Our purpose in the present work is to provide a rigorous explanation of this interesting and useful phenomenon. We also illustrate numerically that GMRES(n, k) with n > 0 is superior to GMRES(k).

Since n and k are fixed in GMRES(n, k), it is clear that the analysis of GMRES(n, k) necessitates the study of $s_{n,k}$ for fixed n and k. We mention that the analysis of the sequences $\{s_{n,k}\}_{n=0}^{\infty}$ with fixed k has been given in [26,29,30]. It should be emphasized, however, that the results of these papers concern the behavior of $s_{n,k}$ for $n \to \infty$ and thus are asymptotic in nature. Therefore, they cannot be used to explain the behavior of $s_{n,k}$ with small or moderately large values of n and arbitrary values of k, which is what we need for the analysis of GMRES(n, k).

The contents of the paper are as follows. In section 2, upper bounds for the convergence rates of GMRES(n, k) are introduced. In section 3, explicit formulas for these upper bounds are derived for some model cases. In section 4, it is shown numerically that these bounds are tight and decrease rapidly as functions of n and k. In section 5, numerical comparisons between GMRES, GMRES(k) and GMRES(n, k) are made.

2. Derivation of upper bounds

Define the residual vector r(x) associated with an arbitrary vector x by

$$r(x) = b - Ax.$$

Let $\|\cdot\|$ denote the vector l_2 -norm induced by the Euclidean inner product in \mathbb{C}^N and the operator norm induced by this vector norm. For any matrix G, denote the condition number of G, $\|G\| \|G^{-1}\|$, by $\kappa(G)$ and the spectrum of G by spect(G).

Define

$$\Pi_k = \left\{ q(\lambda) = \sum_{i=0}^k a_i \lambda^i : q(0) = 1 \right\}.$$

Then, for any $Q_k \in \Pi_k$, we have for GMRES

$$\left\| r(s_{n,k}) \right\| \leqslant \left\| Q_k(A) r(x_n) \right\|. \tag{2.1}$$

The result in (2.1) follows from the analysis in [11] and the mathematical equivalence that is proved in [27]. In [27], a unified approach is presented from which both (2.1) and a similar estimate for the method of Arnoldi [2] can be obtained simultaneously.

Hereafter we assume that A is diagonalizable. This assumption is needed for the analysis only, not for the application of the present method.

We shall denote the matrix that diagonalizes A by R, so that

$$A = R\Lambda R^{-1}, \quad \Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_N).$$

Note that R is not uniquely defined; it can be replaced by RD, where D is a nonsingular diagonal matrix. The matrix D can be chosen so that $\kappa(RD)$ is minimal. For A normal, this minimum is obtained by requiring that RD be orthogonal.

We shall also define

$$\mathcal{P}_k = \left\{ q(\lambda) = \sum_{i=0}^k a_i \lambda^i \colon q(1) = 1 \right\}.$$

Because r(x) = A(s - x),

$$x_n - s = (I - A)(x_{n-1} - s) = \dots = (I - A)^n (x_0 - s), \text{ for all } n \ge 1.$$

Therefore, for any $Q_k \in \Pi_k$, we have for GMRES

$$\left\|r(s_{n,k})\right\| \leq \left\|Q_k(A)(I-A)^n\right\| \left\|r(x_0)\right\| \leq \kappa(R) \left\|Q_k(\Lambda)(I-\Lambda)^n\right\| \left\|r(x_0)\right\|.$$

A similar bound can be obtained for the method of [2] and the methods that are mathematically equivalent to it (see [27] for the details). (It is also shown in [32] that the above coefficient $\kappa(R)$ could be omitted if the above norm were accordingly redefined.) Consequently, for GMRES

$$\left\| r(s_{n,k}) \right\| \leqslant \kappa(R) \Gamma_{n,k}^{\operatorname{spect}(I-A)} \left\| r(x_0) \right\|,$$

where, for any set D of complex numbers,

$$\Gamma_{n,k}^{D} \equiv \min_{p \in \mathcal{P}_{k}} \max_{z \in D} \left| p(z) z^{n} \right|.$$
(2.2)

Clearly, for n > 0, $\Gamma_{n,k}^D = \Gamma_{n,k}^{D \setminus \{0\}}$. Furthermore, $D \subset D'$ implies $\Gamma_{n,k}^D \leqslant \Gamma_{n,k}^{D'}$. These properties are used in the next section to derive upper bounds for $\Gamma_{n,k}^{\text{spect}(I-A)}$.

3. Bounds for $\Gamma_{n,k}^{\text{spect}(I-A)}$

From the definition of $\Gamma_{n,k}^{\text{spect}(I-A)}$ given in (2.2), it is obvious that precise knowledge of it requires complete information on the spectrum of A, which is not available in general. We may, however, obtain reasonably good bounds on $\Gamma_{n,k}^{\text{spect}(I-A)}$ for n > 0if we know that the nonzero part of the spectrum of I - A is contained in a set $D \subset \mathbb{C} \setminus \{1\}$. (If 1 is an eigenvalue of I - A, the system in (1.1) is singular, contrary to our assumption in the introduction.) Then, for n > 0,

$$\Gamma_{n,k}^{\text{spect}(I-A)} \leqslant \min_{q \in \mathcal{P}_k} \max_{\lambda \in D} \left| \lambda^n q(\lambda) \right| = \Gamma_{n,k}^D.$$
(3.1)

If D is a domain, then, by the maximum modulus theorem for analytic functions,

$$\Gamma_{n,k}^{\text{spect}(I-A)} \leqslant \Gamma_{n,k}^{D} = \min_{q \in \mathcal{P}_k} \max_{\lambda \in \partial D} \left| \lambda^n q(\lambda) \right| = \Gamma_{n,k}^{\partial D},$$
(3.2)

where ∂D denotes the boundary of D.

In general, the min-max problems of (3.1) and (3.2) cannot be solved analytically in a simple way. When n = 0, some analytic solutions are known, however. The best known is the one for the case in which D is a finite real interval $[\alpha, \beta]$ with $\alpha < \beta < 1$, α being arbitrary otherwise. In this case the optimal polynomial $q^*(\lambda)$ is $T_k(g(\lambda))/T_k(g(1))$, with $g(\lambda) = (2\lambda - \alpha - \beta)/(\beta - \alpha)$, where $T_k(z)$ is the Chebyshev polynomial of the first kind of degree k. Consequently,

$$\Gamma_{0,k}^{D} = \frac{1}{T_{k}((2 - \alpha - \beta)/(\beta - \alpha))}.$$
(3.3)

This result can be found in, e.g., Varga [35]. The analytical solution of the min-max problem for n = 0 and $D = \{\lambda: \lambda = i\xi, -\beta \leq \xi \leq \beta, \beta > 0 \text{ real}\}$ has been provided recently by Freund and Ruscheweyh [12], who also give a numerical method for the case in which D is any line segment in $\mathbb{C} \setminus \{1\}$.

Note that the min-max problems in (3.1) and (3.2) are constrained best uniform approximation problems by incomplete polynomials. The problem relevant to the present case is the one in (3.1), which now reads

$$\Gamma_{n,k}^{D} = \min_{\sum_{i=0}^{k} a_{i}=1} \max_{\lambda \in D} \left| \sum_{i=0}^{k} a_{i} \lambda^{n+i} \right|.$$
(3.4)

Uniform approximation on the real interval [0, 1] by incomplete polynomials has been studied by Lorentz [17] and, in a series of papers, by Saff and Varga [22–25]. From [22, proposition 3], it follows that the solution of (3.1) for n = 1 and arbitrary k and $D = [\alpha, \beta], 0 < \alpha < \beta < 1$ real, is

$$q^{*}(\lambda) = \frac{T_{k+1}((1-\eta)\lambda/\beta + \eta)}{T_{k+1}((1-\eta)/\beta + \eta)}$$

and, hence,

$$\Gamma_{1,k}^{[0,\beta]} = \frac{1}{T_{k+1}((1-\eta)/\beta + \eta)}$$

where $\eta = -\cos(\pi/2(k+1))$. (This result applies to the method in [15], which is equivalent to using n = 1.) For general n, we shall not attempt to determine $q^*(\lambda)$ analytically. We could determine $q^*(\lambda)$ numerically by the Remes algorithm, see [7], although this would not provide us with an analytical upper bound for $\Gamma_{n,k}^{\text{spect}(I-A)}$. Instead of doing this we shall try to give an analytical upper bound on $\Gamma_{n,k}^{D}$ in terms of orthogonal polynomials with respect to the weight function λ^{2n} .

3.1. D is a domain or a curve in the complex plane

Let $\{\phi_{n,j}(\lambda)\}_{j=0}^{\infty}$ be the sequence of polynomials orthogonal with respect to the non-negative weight function $|\lambda|^{2n}$, in the sense

$$\int_{\Omega} |\lambda|^{2n} \overline{\phi_{n,i}(\lambda)} \phi_{n,j}(\lambda) \,\mathrm{d}\Omega = \nu_j \delta_{ij}.$$

Here Ω stands for *D* when *D* is a curve or a domain (or ∂D in case *D* is a domain) and δ_{mk} is the Kronecker delta. As a result, $d\Omega$ is the line element on Ω if Ω is a curve, or the area element if Ω is a domain. By (3.1) and theorem A.4 in the appendix, we have

$$\left\{c\sum_{j=0}^{k} \left|\phi_{n,j}(1)\right|^{2} / \nu_{j}\right\}^{-1/2} \leqslant \Gamma_{n,k}^{D} \leqslant \frac{\max_{\lambda \in D} \left|\lambda^{n} \phi_{n,k}(\lambda)\right|}{\left|\phi_{n,k}(1)\right|},\tag{3.5}$$

where $c = \int_{\Omega} d\Omega$.

Of course, in order to determine these bounds we need to find the polynomials $\phi_{n,k}(\lambda)$ numerically, possibly through the 3-term recursion relation that they satisfy. In addition, this recursion relation needs to be determined numerically too.

3.2. D is an interval in the complex plane

Important simplifications take place when $D = [\alpha, \beta] \subset \mathbb{C} \setminus \{1\}$. (Note that α and β may be complex.) In this case, by theorem A.3 in the appendix,

$$\max_{\lambda \in D} \left| \lambda^n \phi_{n,k}(\lambda) \right| = \max\left(\left| \alpha^n \phi_{n,k}(\alpha) \right|, \left| \beta^n \phi_{n,k}(\beta) \right| \right).$$
(3.6)

When $D = [\alpha, \beta] \subset [0, \beta]$, it is possible to bound $\Gamma_{n,k}^D$ by $\Gamma_{n,k}^{[0,\beta]}$. The motivation for this is that, for large n, $\Gamma_{n,k}^{[0,\beta]}$ will not be too different from $\Gamma_{n,k}^D$, since the weight $|\lambda|^n$ in the interval $[0, \alpha]$ is negligible compared to its average value in the interval $[\alpha, \beta]$, hence, there cannot be a great difference between the solutions of the two min-max problems on $[\alpha, \beta]$ and on $[0, \beta]$. Furthermore, explicit lower and upper bounds for $\Gamma_{n,k}^{[0,\beta]}$ exist. Hence, this case deserves special treatment.

3.3. The case $D = [0, \beta] \subset \mathbb{C} \setminus \{1\}$

Here $\phi_{n,k}(\lambda)$ is expressible in terms of Jacobi polynomials. In fact, $\phi_{n,k}(\lambda)$, which now is the *k*th orthogonal polynomial with respect to the weight function $|\lambda|^{2n}$ and the measure $|d\lambda|$ on $[0,\beta]$, is a constant multiple of $P_k^{(0,2n)}(2\lambda/\beta-1)$ by (A.4) in the appendix.

By (A.2) and (A.3) from the appendix, we have, respectively,

$$\int_{0}^{\beta} |\lambda|^{2n} \left| P_{k}^{(0,2n)}(2\lambda/\beta - 1) \right|^{2} |\mathrm{d}\lambda| = \frac{|\beta|^{2n+1}}{2n + 2k + 1}$$
(3.7)

and

$$P_k^{(0,2n)}(2\lambda/\beta - 1)\big|_{\lambda=\beta} = P_k^{(0,2n)}(1) = 1.$$
(3.8)

Using (3.7) and (3.8) to make the appropriate substitutions in (3.5) and (3.6), we now obtain an upper and a lower bound for $\Gamma_{n,k}^D$, which are expressible in terms of Jacobi polynomials and, hence, are easily computable. These are given in theorem 3.1 below.

Theorem 3.1. Let $D = [0, \beta] \subset \mathbb{C} \setminus \{1\}$. Then $\Gamma_{n,k}^D$ satisfies the inequalities

$$\frac{|\beta|^n}{\left\{\sum_{j=0}^k (2n+2j+1)|P_j^{(0,2n)}(2/\beta-1)|^2\right\}^{1/2}} \leqslant \Gamma_{n,k}^D \leqslant \frac{|\beta|^n}{\left|P_k^{(0,2n)}(2/\beta-1)\right|}.$$
 (3.9)

If, in addition, β is real, $\beta < 1$, and $\beta \neq 0$, then $2/\beta - 1 > 1$ or $2/\beta - 1 < -1$. Thus, by theorem A.1 in the appendix, the sequence $\{|P_j^{(0,2n)}(2/\beta - 1)|\}_{j=0}^{\infty}$ is monotonically increasing. We can use this to replace the lower bound on $\Gamma_{n,k}^D$ by a weaker but more informative one presented in the following corollary.

Corollary 3.2. Let $D = [0, \beta]$, where $\beta < 1$, $\beta \neq 0$. Then $\Gamma_{n,k}^D$ satisfies the following weaker form of (3.9):

$$\frac{1}{\sqrt{(k+1)(2n+2k+1)}} \cdot \frac{|\beta|^n}{|P_k^{(0,2n)}(2/\beta-1)|} \leqslant \Gamma_{n,k}^D \leqslant \frac{|\beta|^n}{|P_k^{(0,2n)}(2/\beta-1)|}.$$
 (3.10)

As can be seen from (3.10), the upper and lower bounds on $\Gamma_{n,k}^D$ differ from each other at most by a factor $\sqrt{(k+1)(2n+2k+1)}$ and this implies that the upper bound is quite tight (especially for moderate values of n and k), as will be demonstrated numerically later.

Remark. Using (A.1), one may substitute in (3.9) and (3.10)

$$P_k^{(0,2n)}(2/\beta - 1) = \beta^{-k} \sum_{j=0}^k \binom{k}{j} \binom{2n+k}{j} (1-\beta)^j.$$
(3.11)

From this one obtains that, for $-1 \leq \beta < 1$, the upper bound in (3.9)–(3.10) is a monotonically decreasing function of n and k (see the proof of theorem A.1 in the appendix). This is a desirable property for an upper bound, since it holds for $\Gamma_{n,k}^D$ itself.

Note that when n = 0 the Jacobi polynomial $P_k^{(0,2n)}(z)$ reduces to the Legendre polynomial of degree k. This causes the upper bound to be slightly inferior to that obtained from the corresponding Chebyshev polynomial as in (3.3).

3.4. The case $D = [-\beta, \beta] \subset \mathbb{C} \setminus \{1\}$

Here we assume again that β is a complex number. Again, the orthogonal polynomials $\phi_{n,k}(\lambda)$ can be expressed in terms of Jacobi polynomials. Using the substitution $\lambda = \beta x$ in (A.5) in the appendix, we have,

$$\phi_{n,k}(\lambda) = \begin{cases} P_{\nu}^{(0,n-1/2)} (2(\lambda/\beta)^2 - 1) & \text{if } k = 2\nu, \\ (\lambda/\beta) P_{\nu}^{(0,n+1/2)} (2(\lambda/\beta)^2 - 1) & \text{if } k = 2\nu + 1, \end{cases}$$
(3.12)

i.e., $\phi_{n,k}(\lambda)$ is an even or odd function of λ , depending on whether k is even or odd, respectively. As a result of (3.12), we obtain

$$\phi_{n,k}(\beta) = 1$$
 for all n and k

and

$$\nu_j = \int_{-\beta}^{\beta} |\lambda|^{2n} |\phi_{n,j}(\lambda)|^2 |\mathrm{d}\lambda| = \frac{|\beta|^{2n+1}}{n+j+1/2} \quad \text{for all } n \text{ and } j.$$

Combining all these in (3.5) and (3.6), we obtain:

Theorem 3.3. Let $D = [-\beta, \beta] \subset \mathbb{C} \setminus \{1\}$. Then $\Gamma_{n,k}^D$ satisfies the inequalities

$$\frac{|\beta|^n}{\left\{\sum_{j=0}^k (2n+2j+1)|\phi_{n,j}(1)|^2\right\}^{1/2}} \leqslant \Gamma_{n,k}^D \leqslant \frac{|\beta|^n}{|\phi_{n,k}(1)|}.$$
(3.13)

Using (A.7) in the appendix (with $x = 1/\beta$ there), one may substitute

$$\frac{|\beta|^n}{|\phi_{n,k}(1)|} = \frac{|\beta|^{n+k}}{\left|\sum_{j=0}^{\nu} {\nu \choose j} {n+\mu-1/2 \choose j} (1-\beta^2)^j\right|},$$
(3.14)

with

$$\nu = \left\lfloor \frac{k}{2} \right\rfloor \quad \text{and} \quad \mu = \left\lfloor \frac{k+1}{2} \right\rfloor,$$
(3.15)

as follows from (A.7) and (A.8).

If, in addition, β^2 is real and $-1 \leq \beta^2 < 1$, then theorem A.2 applies, and, therefore, the sequence $\{|\phi_{n,j}(1)|\}_{j=0}^{\infty}$ is monotonically increasing. With the help of this property, we can replace (3.13) by the weaker but more informative form presented in the following corollary.

Corollary 3.4. Let $D = [-\beta, \beta]$, where $-1 \leq \beta^2 < 1$. Then $\Gamma_{n,k}^D$ satisfies

$$\frac{1}{\sqrt{(k+1)(2n+2k+1)}} \cdot \frac{|\beta|^n}{|\phi_{n,k}(1)|} \leqslant \Gamma^D_{n,k} \leqslant \frac{|\beta|^n}{|\phi_{n,k}(1)|}$$

Assuming again that β^2 may be complex, we note that the upper bound given by (3.13) and (3.14) can be improved somewhat as follows: by the fact that $|\lambda|^n$ is symmetric with respect to the origin in $D = [-\beta, \beta]$, we see that the solution of the min-max problem in (3.1) is even or odd depending on whether k is even or odd, respectively. Thus

$$\Gamma_{n,k}^{D} = \min_{q \in \mathcal{P}_{k}} \max_{\lambda \in [-\beta,\beta]} \left| \lambda^{n} q(\lambda) \right| = \begin{cases} \min_{h \in P_{\nu}} \max_{\lambda \in [0,\beta]} \left| \lambda^{n} h\left(\lambda^{2}\right) \right| & \text{if } k = 2\nu, \\ \min_{h \in P_{\nu}} \max_{\lambda \in [0,\beta]} \left| \lambda^{n+1} h\left(\lambda^{2}\right) \right| & \text{if } k = 2\nu + 1. \end{cases}$$

Making now the change of variable $\lambda^2 = \tau$, we have

$$\Gamma_{n,k}^{D} = \begin{cases} \min_{h \in P_{\nu}} \max_{\tau \in [0,\beta^{2}]} |\tau^{n/2}h(\tau)| & \text{if } k = 2\nu, \\ \min_{h \in P_{\nu}} \max_{\tau \in [0,\beta^{2}]} |\tau^{(n+1)/2}h(\tau)| & \text{if } k = 2\nu + 1. \end{cases}$$

We finally employ theorem 3.1 to obtain

$$\frac{|\beta|^{n}}{\left\{\sum_{j=0}^{\nu}(n+2j+1)|P_{j}^{(0,n)}(2/\beta^{2}-1)|^{2}\right\}^{1/2}} \leqslant \Gamma_{n,2\nu}^{D} \leqslant \frac{|\beta|^{n}}{|P_{\nu}^{(0,n)}(2/\beta^{2}-1)|}$$

$$\frac{|\beta|^{n+1}}{\left\{\sum_{j=0}^{\nu}(n+2j+2)|P_{j}^{(0,n+1)}(2/\beta^{2}-1)|^{2}\right\}^{1/2}} \leqslant \Gamma_{n,2\nu+1}^{D} \leqslant \frac{|\beta|^{n+1}}{|P_{\nu}^{(0,n+1)}(2/\beta^{2}-1)|}.$$
(3.16)

As in (3.11), the upper bounds on $\Gamma_{n,k}^D$ can be unified to read

$$\Gamma_{n,k}^{D} \leqslant \frac{|\beta|^{n+k}}{\left|\sum_{j=0}^{\nu} {\nu \choose j} {n+\mu \choose j} (1-\beta^{2})^{j}\right|}$$
(3.17)

with ν and μ as defined in (3.15). Comparing the upper bound in (3.17) with that of (3.13) and (3.14) for the case $-1 \leq \beta^2 < 1$, we see that the former is slightly smaller than the latter. Both, however, have the desirable property of being monotonically decreasing functions of n and k. For $\beta^2 < -1$, this is not necessarily true. In this case, it is only guaranteed that both upper bounds have the property that the sequences obtained by taking the upper bounds for either $\Gamma_{n,2\nu}^D$ or $\Gamma_{n,2\nu+1}^D$ are monotonically decreasing functions of ν (see theorems A.1 and A.2 in the appendix).

3.5. *D* is an ellipse in $\mathbb{C} \setminus \{1\}$

In this case we can extend our previous results to obtain bounds on $\Gamma_{n,k}^D$ in conjunction with Bernstein's theorem, which is stated below.

Theorem 3.5 (Bernstein). Let p(z) be a polynomial of degree at most k. Denote by \mathcal{E}_{τ} the ellipse with foci at ± 1 , semi-major axis $\frac{1}{2}(\tau + \tau^{-1})$ and semi-minor axis $\frac{1}{2}(\tau - \tau^{-1})$, where $\tau > 1$. Then

$$\max_{z \in \mathcal{E}_{\tau}} \left| p(z) \right| \leqslant \tau^k \max_{z \in [-1,1]} \left| p(z) \right|.$$

As a result of this theorem, we see that if the foci of the ellipse are at α and β , then the above upper bounds for the case $D = [\alpha, \beta]$ need to be multiplied by τ^{n+k} for some $\tau > 1$, whose size depends on the size of the ellipse. Of course, this will be so provided 1 lies outside the ellipse. The thinner the ellipse, the closer τ is to 1.

4. Numerical computation of the bounds

We would now like to demonstrate by actual computation that the bounds that were presented in sections 3.3 and 3.4 are very close to $\Gamma_{n,k}^D$. We also computed the upper bounds obtained from (3.3), namely,

$$\Gamma_{n,k}^{D} \leqslant \frac{|\beta|^{n}}{T_{k}((2-\alpha-\beta)/(\beta-\alpha))} \equiv \Gamma_{n,k}^{\text{Ch}}.$$
(4.1)

The inequality in (4.1) is actually an equality when n = 0 as follows from (3.3). As mentioned previously, these bounds do not explain the behavior of $s_{n,k}$ for n > 0. They are given only for the sake of comparison. Finally, we computed the lower bounds on $\Gamma_{n,k}^D$ in order to verify that the upper bounds are indeed quite tight. All the computations reported in this section were done on an IBM-370 computer in double precision arithmetic.

Tables 1 and 2 contain the lower and upper bounds for $\Gamma_{n,k}^D$ and the Chebyshev polynomial bounds given in (4.1) for the cases D = [0, 0.96] and D = [-0.96, 0.96], respectively. The values considered are n = 0, 50, 100 and $k = 0, 2, 4, \dots, 20$. Note

Table 1 Bounds for $\Gamma_{n,k}^D$ when D = [0, 0.96]. "Ib" is the lower bound defined in (3.9), "ub" is the upper bound defined in (3.9) and $\Gamma_{n,k}^{Ch}$ is the Chebyshev bound defined in (4.1). Note that $\Gamma_{0,k}^D = \Gamma_{0,k}^{Ch}$ for this case.

k	n = 0			n = 50			n = 100		
	lb	ub	$\Gamma^{\mathrm{Ch}}_{n,k}$	lb	ub	$\Gamma^{\mathrm{Ch}}_{n,k}$	lb	ub	$\Gamma^{\rm Ch}_{n,k}$
0	1.00D+00	1.00D+00	1.00D+00	1.29D-02	1.30D-01	1.30D-01	1.19D-03	1.69D-02	1.69D-02
2	2.83D-01	7.93D-01	7.42D-01	6.46D-04	6.88D-03	9.64D-02	2.15D-05	3.13D-04	1.25D - 02
4	1.24D-01	5.00D - 01	3.80D-01	7.71D-05	8.66D-04	4.94D-02	1.24D-06	1.86D - 05	6.41D-03
6	5.66D-02	2.77D-01	1.74D-01	1.30D-05	1.52D-04	2.26D-02	1.16D-07	1.78D-06	2.94D-03
8	2.57D-02	1.43D-01	7.79D-02	2.66D-06	3.25D-05	1.01D-02	1.42D-08	2.25D-07	1.31D-03
10	1.16D-02	7.16D-02	3.47D-02	6.22D-07	7.85D-06	4.50D-03	2.12D-09	3.42D-08	5.85D-04
12	5.20D-03	3.50D-02	1.54D-02	1.60D - 07	2.08D - 06	2.00D-03	3.61D-10	5.97D-09	2.60D - 04
14	2.32D-03	1.68D-02	6.85D-03	4.39D-08	5.88D-07	8.90D-04	6.85D-11	1.16D-09	1.16D-04
16	1.04D-03	8.00D-03	3.04D-03	1.28D-08	1.75D-07	3.95D-04	1.42D-11	2.43D-10	5.14D-05
18	4.62D-04	3.77D-03	1.35D-03	3.89D-09	5.47D-08	1.76D-04	3.13D-12	5.48D-11	2.28D-05
20	2.06D-04	1.77D-03	6.01D-04	1.23D-09	1.77D-08	7.81D-05	7.35D-13	1.31D-11	1.01D-05

Table 2

Bounds for $\Gamma_{n,k}^D$ when D = [-0.96, 0.96]. "Ib" is the lower bound defined in (3.16), "ub" is the upper bound defined in (3.16) and $\Gamma_{n,k}^{Ch}$ is the Chebyshev bound defined in (4.1). Note that $\Gamma_{0,k}^D = \Gamma_{0,k}^{Ch}$ for this

k	n = 0			n = 50			n = 100		
	lb	ub	$\Gamma^{\mathrm{Ch}}_{n,k}$	lb	ub	$\Gamma^{\mathrm{Ch}}_{n,k}$	lb	ub	$\Gamma^{\mathrm{Ch}}_{n,k}$
0	1.00D+00	1.00D+00	1.00D+00	1.82D-02	1.30D-01	1.30D-01	1.68D-03	1.69D-02	1.69D-02
2	4.42D-01	8.55D-01	8.55D-01	3.24D-03	2.39D-02	1.11D-01	1.71D-04	1.74D-03	1.44D-02
4	2.41D-01	6.44D-01	5.75D-01	8.31D-04	6.38D-03	7.47D-02	2.83D-05	2.94D-04	9.70D-03
6	1.38D-01	4.44D-01	3.45D-01	2.55D-04	2.03D-03	4.48D-02	6.02D-06	6.37D-05	5.82D-03
8	7.92D-02	2.90D-01	1.98D-01	8.78D-05	7.18D-04	2.57D-02	1.49D-06	1.61D-05	3.34D-03
10	4.54D-02	1.83D-01	1.12D-01	3.26D-05	2.74D-04	1.46D-02	4.14D-07	4.54D-06	1.89D-03
12	2.58D-02	1.13D-01	6.33D-02	1.28D-05	1.11D-04	8.22D-03	1.25D-07	1.39D-06	1.07D-03
14	1.47D-02	6.89D-02	3.56D-02	5.26D-06	4.65D-05	4.63D-03	4.01D-08	4.54D-07	6.01D-04
16	8.30D-03	4.15D-02	2.00D-02	2.23D-06	2.02D-05	2.60D-03	1.36D-08	1.56D-07	3.38D-04
18	4.69D-03	2.48D - 02	1.13D-02	9.77D-07	9.02D-06	1.46D-03	4.81D-09	5.61D-08	1.90D - 04
20	2.65D-03	1.47D-02	6.34D-03	4.37D-07	4.12D-06	8.24D-04	1.76D-09	2.09D-08	1.07D-04

the closeness of the lower and upper bounds, which implies that both are close to $\Gamma_{n,k}^D$. Note also that both bounds decrease at an increasing rate as n increases.

5. Numerical examples

Consider the 2-dimensional convection-diffusion equation

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} + \gamma \left(x \frac{\partial u}{\partial x} + y \frac{\partial u}{\partial y} \right) + \beta u = f \quad \text{in } \Omega, \qquad u = g \quad \text{on } \partial\Omega, \quad (5.1)$$

where Ω is the unit square $(0, 1) \times (0, 1)$. f and g are chosen such that the solution of (5.1) is u = xy. The linear system obtained by discretizing this equation has been used as a test problem for vector extrapolation methods and Krylov subspace methods on nonsymmetric and/or indefinite systems. See, e.g., Gander et al. [13].

Let $x_i = i\delta x$, $0 \le i \le M_x + 1$, and $y_j = j\delta y$, $0 \le j \le M_y + 1$, where $\delta x = 1/(M_x + 1)$ and $\delta y = 1/(M_y + 1)$ for some positive integers M_x and M_y . We discretize this equation by replacing all the partial derivatives at (x_i, y_j) by central differences.

For all our computations we took a random vector as the initial vector.

Observing that the matrix of the linear system above is consistently ordered, we can use the strategy that was proposed in [28, section 7] to reduce the computational cost, reducing the storage requirements by almost a half at the same time. According to this strategy, vector extrapolation methods are applied to the vector sequence obtained by using the double Jacobi iteration technique. With x_0 given, and I - A being the matrix of the Jacobi iteration method, the double Jacobi iteration produces the vectors x_1, x_2, \ldots , in accordance with

$$x_{j+1} = (I - A)((I - A)x_j + b) + b, \quad j = 0, 1, 2, \dots$$
(5.2)

We then expect cycling with the double Jacobi iteration using $s_{n,k}$ to produce results similar to those produced by cycling with the (single) Jacobi iteration using $s_{2n,2k}$. Obviously, the number of single Jacobi iterations actually performed in both cases is almost the same, although the computational cost and storage requirements for it are much lower with the double Jacobi iteration.

The acceleration method used in conjunction with this iterative technique is GM-RES in the GMRES(n, k) cycling mode for some n and k, namely, a cycle consists of n double Jacobi iterations and then k iterations of GMRES with the preconditioner corresponding to the double Jacobi iteration.

In our experiments, we pick $\gamma = 125$ and $\beta = -100$. We first picked $M_x =$ $M_y = 31$ so that the number of unknowns is $N = M_x M_y = 961$. The convergence criterion is the reduction of the l_2 -norm of the initial residual by 12 orders of magnitude. The residual is recalculated after each iteration to check whether the convergence criterion is met. (It was also checked that the l_{∞} norm of the error is reduced at about the same rate as the l_2 -norm of the residual.) The results are as follows. GMRES(20) converges in 13 cycles (figure 2). GMRES(20, 20) converges in 2 cycles (figure 1). This shows the superiority of GMRES(n, k) with n > 0 in comparison with GMRES(k). For this example, GMRES converges in 56 iterations; this requires storage of 58 arrays, which is usually prohibitive for large systems arising, for example, from 3-D PDEs. GMRES(50, 20) converges in 4 cycles, which is inferior to GMRES(20,20). This is probably because of roundoff errors; the coefficient matrix is not an *M*-matrix and, hence, the basic double Jacobi iteration diverges. The 50 initial iterations might yield very large residuals and significant roundoff errors in the subsequent GMRES iteration. Interestingly, GMRES(40) is also inferior to GMRES(20, 20): it requires 3 cycles for convergence (figure 3). The reason for this is probably also numerical instability.



Figure 1. GMRES(20, 20) for the convection–diffusion equation (5.1) on a 31×31 grid. Residual reduction (on a logarithmic scale) vs. the total number of double Jacobi iterations (including those performed within the GMRES iteration).



Figure 2. GMRES(20) for the convection–diffusion equation (5.1) on a 31×31 grid. Residual reduction (on a logarithmic scale) vs. the total number of double Jacobi iterations (including those performed within the GMRES iteration).



Figure 3. GMRES(40) for the convection–diffusion equation (5.1) on a 31×31 grid. Residual reduction (on a logarithmic scale) vs. the total number of double Jacobi iterations (including those performed within the GMRES iteration).



Figure 4. GMRES(20, 20) for the convection-diffusion equation (5.1) on a 63×63 grid. Residual reduction (on a logarithmic scale) vs. the total number of double Jacobi iterations (including those performed within the GMRES iteration).



Figure 5. GMRES(50,20) for the convection–diffusion equation (5.1) on a 63×63 grid. Residual reduction (on a logarithmic scale) vs. the total number of double Jacobi iterations (including those performed within the GMRES iteration).



Figure 6. GMRES(40) for the convection–diffusion equation (5.1) on a 63×63 grid. Residual reduction (on a logarithmic scale) vs. the total number of double Jacobi iterations (including those performed within the GMRES iteration).

We then turned to the same problem on a larger grid: $M_x = M_y = 63$. The convergence criterion is the reduction of the l_2 -norm of the initial residual by 8 orders of magnitude. Again, the double Jacobi iteration is used. The results are as follows. GMRES(20, 20) converges in 8 cycles (figure 4). GMRES(50, 20) converges in 3 cycles (figure 5). GMRES(20) stagnates. GMRES(40) converges in 15 cycles (figure 6). GMRES with no restarting converges in 65 iterations.

We have also tested the circulating convection example of Brandt and Yavneh [5]

$$\sin(\pi(y-0.5))\cos(\pi(x-0.5))u_x - \sin(\pi(x-0.5))\cos(\pi(y-0.5))u_y = 0.$$

The domain is the unit square $(0, 1) \times (0, 1)$ with a $(\delta x/2) \times (\delta y/2)$ hole at the middle of it (corresponding to a 1×1 hole at the middle of the grid). Homogeneous Dirichlet boundary conditions are imposed on the outer boundary and on this hole. The scheme is as in [5], that is, isotropic artificial viscosity is used, the amount of which is locally chosen to be the minimal amount required for diagonal dominance. $M_x = M_y = 31$ is used. The convergence criterion is the reduction of the l_2 -norm of the initial residual by 12 orders of magnitude. Again, the double Jacobi iteration is used. The results are as follows. GMRES(20) converges in 51 cycles. GMRES(20, 20) converges in 12 cycles. GMRES(60, 20) converges in 5 cycles. GMRES converges in 140 iterations, which is again prohibitive on most computers in terms of storage for large systems arising in practice. Again, the superiority of GMRES(n, k) with n > 0 over GMRES(k) and GMRES is clear.

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Appendix

A.1. A collection of useful formulas and results for Jacobi polynomials

The Jacobi polynomials $P_k^{(\alpha,\beta)}(x)$ are defined by

$$P_k^{(\alpha,\beta)}(x) = \sum_{j=0}^k \binom{k+\alpha}{k-j} \binom{k+\beta}{j} \left(\frac{x-1}{2}\right)^j \left(\frac{x+1}{2}\right)^{k-j}$$
(A.1)

with $\alpha > -1$ and $\beta > -1$. They are orthogonal with respect to the weight function $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$ on [-1, 1], i.e.,

$$\int_{-1}^{1} (1-x)^{\alpha} (1+x)^{\beta} P_m^{(\alpha,\beta)}(x) P_k^{(\alpha,\beta)}(x) dx$$
$$= \delta_{mk} \frac{2^{\alpha+\beta+1}}{2k+\alpha+\beta+1} \cdot \frac{\Gamma(k+\alpha+1)\Gamma(k+\beta+1)}{\Gamma(k+1)\Gamma(k+\alpha+\beta+1)}, \tag{A.2}$$

where δ_{mk} is the Kronecker delta. $P_k^{(\alpha,\beta)}(x)$ are normalized such that

$$P_k^{(\alpha,\beta)}(1) = \binom{k+\alpha}{k}.$$
(A.3)

For a and b complex numbers, polynomials orthogonal on [a, b] with respect to the weight function $w(z) = |(b - z)^{\alpha}(z - a)^{\beta}|$ and the measure |dz| are

$$p_k(z) = P_k^{(\alpha,\beta)} \left(2\frac{z-a}{b-a} - 1 \right).$$
 (A.4)

This result is obtained by a change of variables in the original Jacobi polynomials.

Polynomials orthogonal on [-1, 1] with respect to the weight function $w(x) = |x|^{2n}$ are given by

$$p_k(x) = \begin{cases} P_{\nu}^{(0,n-1/2)} (2x^2 - 1) & \text{if } k = 2\nu, \\ x P_{\nu}^{(0,n+1/2)} (2x^2 - 1) & \text{if } k = 2\nu + 1. \end{cases}$$
(A.5)

The normalization condition given in (A.3) is the one that has been widely accepted in the literature of orthogonal polynomials. Thus (A.1)–(A.3) can be found in many books. See, e.g., [1, chapter 22] or [34]. For (A.5) see [34, pp. 59–60].

Theorem A.1. For x > 1 or x < -1 fixed and $\alpha, \beta \ge 0$, the sequence $\{|P_k^{(\alpha,\beta)}(x)|\}_{k=0}^{\infty}$ is monotonically increasing.

Proof. We start with the case x > 1. First, all the terms in the summation on the right hand side of (A.1) are positive for x > 1. Next, the *j*th term of $P_k^{(\alpha,\beta)}(x)$ in (A.1) is strictly less than the corresponding term of $P_{k+1}^{(\alpha,\beta)}(x)$. The result now follows. As for x < -1, we first recall that

$$P_k^{(\alpha,\beta)}(-x) = (-1)^k P_k^{(\beta,\alpha)}(x),$$
(A.6)

and then apply the result for x > 1, which we have already proved, to the polynomials $P_k^{(\beta,\alpha)}(x)$.

Theorem A.2. The polynomials $p_k(x)$ that are defined in (A.5) are such that, for x real and |x| > 1, or for x pure imaginary and $|x| \ge 1$, the sequence $\{|p_k(x)|\}_{k=0}^{\infty}$ is monotonically increasing. For x pure imaginary and |x| < 1 the sequences $\{|p_{2\nu}(x)|\}_{\nu=0}^{\infty}$ and $\{|p_{2\nu+1}(x)|\}_{\nu=0}^{\infty}$ are monotonically increasing.

Proof. We observe that, by proper manipulation of (A.1), $p_k(x)$ can be expressed in the unified form

$$p_k(x) = \sum_{j=0}^{\nu} {\binom{\nu}{j}} {\binom{n+\mu-1/2}{j}} {\binom{x^2-1}{j}}^j x^{k-2j},$$
(A.7)

where

$$\nu = \left\lfloor \frac{k}{2} \right\rfloor \quad \text{and} \quad \mu = \left\lfloor \frac{k+1}{2} \right\rfloor.$$
(A.8)

Note that both ν and μ are monotonically nondecreasing in k, and that one of them is always increasing. Letting now x be real and x > 1, we see that all the terms in the summation on the right hand side of (A.7) are positive. Next, the *j*th term of $p_k(x)$ in (A.7) is strictly less than the corresponding term of $p_{k+1}(x)$. The result now follows for x > 1. For x < -1, we note that $p_k(-x) = (-1)^k p_k(x)$, and apply the result for x > 1, which we have already proved, to the polynomials $p_k(x)$. For the case in which x is pure imaginary, i.e., $x = i\xi$, ξ real, the factor $(x^2 - 1)^j x^{k-2j}$ in the *j*th term of $p_k(x)$ becomes $i^k(\xi^2 + 1)^j \xi^{k-2j}$. The proof for the case $|x| \ge 1$ can now be completed as before. The proof of the case |x| < 1 can be done by employing theorem A.1 in conjunction with (A.5).

A.2. A result on monotonic weight functions

Theorem A.3. Let $\{p_n(z)\}_{n=0}^{\infty}$ be the sequence of polynomials orthogonal on [a, b] (for a and b complex numbers) with respect to the non-negative weight function w(z) and the measure |dz|. Assume that w(z) is nondecreasing on [a, b]; that is, for any two points $z_1, z_2 \in [a, b]$

$$|z_1 - b| < |z_2 - b| \Rightarrow w(z_1) \ge w(z_2).$$

Then the functions $\sqrt{w(z)}|p_n(z)|$ attain their maximum on [a, b] for z = b. A corresponding statement holds for any subinterval $[z_0, b]$ of [a, b], where w(z) is nondecreasing.

Proof. For a and b real, the proof is given in [34, theorem 7.2, p. 163]. For a and b complex, let T be the affine mapping which maps [-1, 1] onto [a, b]. Since w(Tx) is nondecreasing on $[T^{-1}z_0, T^{-1}b]$, the theorem follows by applying it to the orthogonal polynomials $p_n(Tx)$ on [-1, 1] with respect to the weight function w(Tx) and the measure |dx|.

A.3. A lower bound for a best polynomial l_{∞} -approximation problem

Theorem A.4. Let $\{p_n(z)\}_{n=0}^{\infty}$ be the sequence of orthonormal polynomials on a compact set Ω of the complex *z*-plane with respect to the real non-negative weight function w(z) on Ω , i.e.,

$$\int_{\Omega} w(z) \overline{p_m(z)} p_n(z) \, \mathrm{d}\Omega = \delta_{m,n},\tag{A.9}$$

where $d\Omega$ stands for the area element if Ω is a domain *D*, and for the line element if Ω is the boundary of a domain *D* or an arbitrary rectifiable curve. Let $\phi^*(z)$ be the solution of the constrained min-max problem

$$\min_{\phi} \max_{z \in \Omega} \left| \sqrt{w(z)} \phi(z) \right|, \quad \phi(z) \text{ polynomial of degree } \leqslant k,$$
subject to $M(\phi) = 1,$
(A.10)

where M is a bounded linear functional on the space of functions continuous on Ω . Then

$$\max_{z\in\Omega} \left| \sqrt{w(z)} \phi^*(z) \right| \ge \left\{ c \sum_{j=0}^k \left| M(p_j) \right|^2 \right\}^{-1/2}, \quad c = \int_{\Omega} d\Omega.$$
(A.11)

Proof. We start by observing that, for any function f(z) that is continuous on Ω , we have

$$\max_{z \in \Omega} \left| f(z) \right| \ge \left\{ c^{-1} \int_{\Omega} \left| f(z) \right|^2 \mathrm{d}\Omega \right\}^{1/2}.$$
(A.12)

Letting now $f(z) = \sqrt{w(z)}\phi(z)$ in (A.12), where $\phi(z)$ is a polynomial of degree at most k satisfying $M(\phi) = 1$, and minimizing both sides of (A.12) with respect to ϕ , we obtain

$$\max_{z\in\Omega} \left| \sqrt{w(z)}\phi^*(z) \right| \ge \min_{M(\phi)=1} \left\{ c^{-1} \int_{\Omega} w(z) \left| \phi(z) \right|^2 \mathrm{d}\Omega \right\}^{1/2}.$$
(A.13)

Since $\phi(z)$ is a polynomial of degree k, it can be written as

$$\phi(z) = \sum_{i=0}^{k} \alpha_i p_i(z), \qquad (A.14)$$

so that the minimization problem on the right-hand side of (A.13) becomes

$$\min_{\alpha_i} \sum_{i=0}^k |\alpha_i|^2$$
(A.15)
subject to $\sum_{i=0}^k \alpha_i M(p_i) = 1.$

The solution of (A.15) can be achieved, e.g., by using the method of Lagrange multipliers, and is given by

$$\alpha_j = \frac{\overline{M(p_j)}}{\sum_{i=0}^k |M(p_i)|^2}, \quad j = 0, 1, \dots, k.$$
 (A.16)

Combining (A.16) with (A.13)–(A.15), (A.11) follows.

Obviously, in case $\Omega = [a, b]$, a finite real interval, we have $d\Omega = dx$ and c = b - a.

Also, if M is a point evaluation functional, i.e., $M(\phi) = \phi(\xi)$ for some ξ , then $M(p_i) = p_i(\xi)$ in (A.11).

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