SUPERLINEAR CONVERGENCE RATES FOR THE LANCZOS METHOD APPLIED TO ELLIPTIC OPERATORS

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Abstract. This paper investigates the convergence of the Lanczos method for computing the smallest eigenpair of a selfadjoint elliptic differential operator via inverse iteration (without shifts). Superlinear convergence rates are established, and their sharpness is investigated for a simple model problem. These results are illustrated numerically for a more difficult problem.

Key words. Lanczos method, superlinear convergence, Lommel polynomials.

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1. Introduction. The power iteration method is a very well-known tool for approximating the largest eigenvalue of a symmetric, positive definite matrix. It has a linear rate of convergence, where the convergence factor is given by the ratio of subdominant over dominant eigenvalue. However, with essentially the same amount of work (i.e., the same number of matrix vector multiplies) the Lanczos method [8] always yields better approximations of this eigenvalue, and at the same time provides some information about the remainder of the spectrum of the given matrix.

Although being a close relative of the conjugate gradient iteration for solving linear systems of equations, the convergence theory for the Lanczos method is less developed. Essentially, there are only the error bounds by Kaniel and Saad, as presented for instance in Parlett's book [10]. These bounds improve on the convergence factor of the power method, but still, the established rate of convergence is only linear. On the other hand the conjugate gradient method is known to converge superlinearly, and hence, at least under appropriate assumptions on the distribution of the given eigenvalues one may also expect superlinear convergence of the Lanczos approximations.

In this paper the performance of the Lanczos method is considered, when applied to a compact selfadjoint operator K with eigenvalues λ_n, which decay like

$$\lambda_n \sim n^{-s}, \qquad n \to \infty ;$$

here $s > 0$ is a prescribed number. This may correspond to applications where one is interested in the smallest eigenvalue(s) of a selfadjoint elliptic differential operator L of order s, in which case one would choose K to be the inverse of L on its range. Ericsson and Ruhe [4] have shown that the Lanczos method is a very efficient algorithm for this kind of eigenvalue problem; cf. Weinberger [13] for a number of corresponding applications.

The bounds that will be established below imply a superlinear rate of the form

$$(q/k)^{2sk} \qquad \text{with some } \; q > 0 \,, \tag{1.1}$$

as the number k of Lanczos iterations tends to infinity. A good way to think of this is as of a linear rate with a convergence factor decreasing like k^{-2s} during the iteration. Note that this is worse than the Rayleigh quotient iteration (cf., e.g., [10]), which is known to have a cubic convergence rate locally. However, as the numerical results in

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[4] and in Section 4 show, the convergence rate of the Lanczos method is sufficiently rapid to ensure that only few Lanczos iterations are required for an accuracy up to the order of the discretization error. On the other hand, an implementation of the Rayleigh quotient iteration may suffer from the use of different shifts μ_k in each iteration, by which the shifted operator $L - \mu_k I$ becomes indefinite and almost singular, with increasing numerical difficulties in the solution of the associated linear systems. For computing eigenvalues of differential operators, direct multigrid techniques as described by Hackbusch [7, Chapter 12] will typically be superior.

The main emphasis of this paper, however, is not on superlinear upper bounds, but rather on lower bounds for the Lanczos method. In Section 3 it will be shown for a one-dimensional example, namely $Lu = -u''$, that the established upper bound (1.1) is sharp up to a slight overestimation of the factor q. For this example the *precise asymptotic behaviour* of the approximation error after k Lanczos steps is determined by using the connection between the Lanczos iteration and orthogonal polynomials. The corresponding polynomials can be expressed explicitly in terms of (modified) Lommel polynomials, and the required asymptotic behaviour of these polynomials will be derived to obtain the desired result.

It should be emphasized that this theoretical analysis presumes exact arithmetic, and also does not take the discretization error into account. It is well-known that in practice the Lanczos method may slow down due to round-off errors. Concerning this important topic the reader is referred to Cullum and Willoughby [3], or to the proceedings of the Lanczos Centenary Conference [1] for more recent references. To pay tribute to these practical considerations, however, numerical results for a two dimensional partial differential operator of second order have been included in Section 4. These results illustrate the rapid convergence of the eigenvalue approximations even with finite precision arithmetic.

2. A general superlinear upper bound. In the following some basic properties of the Lanczos process are recollected for the ease of presentation; see Golub and Van Loan [5] or Parlett [10] for further details. It shall be assumed throughout that K is a compact, selfadjoint and positive definite operator in a Hilbert space $\mathcal{X}$. Let $\{x_n\}$ and $\{\lambda_n\}$, respectively, denote the normalized eigenfunctions and eigenvalues of K and, without loss of generality, let $\{\lambda_n\}$ be in strictly decreasing order. Given any

$$y = \sum_{n=1}^{\infty} \eta_n x_n \ \in \mathcal{X} \,,$$

with infinitely many $\eta_n \neq 0$, a (discrete) inner product

$$[\varphi, \psi] := \sum_{n=1}^{\infty} \eta_n^2 \varphi(\lambda_n)\psi(\lambda_n), \qquad \varphi, \psi \in \Pi \,, \tag{2.1}$$

can be defined in the space Π of polynomials over $\mathbb{R}$.

The Lanczos method with starting vector $v_0 = y/\|y\|$ generates an orthonormal basis $\{v_j\}_{j=0}^{k-1}$ of the kth Krylov subspace

$$\mathcal{K}_k(K; y) = \operatorname{span}\{y, Ky, K^2 y, \ldots, K^{k-1} y\} \subset \mathcal{X} \tag{2.2}$$

via the iteration

$$\beta_{j+1} v_{j+1} = (K - \alpha_j I) v_j - \beta_j v_{j-1}, \quad j = 0, 1, \ldots, k-1 \,; \tag{2.3}$$

here, $\beta_{j+1} > 0$ is implicitly defined so as to normalize v_{j+1}, and one has $\alpha_j = \langle v_j, Kv_j \rangle$ because of the orthogonality requirement. For notational convenience let $v_{-1} = 0$. Introducing

$$V_k = (v_0, v_1, \ldots, v_{k-1}) ,$$

one can rewrite (2.3) formally in short terms as

$$KV_k = V_k T_k + \beta_k v_k e_k^T , \tag{2.4}$$

where e_k is the kth Cartesian coordinate vector and T_k is the $k \times k$ tridiagonal matrix of the recursion coefficients,

$$T_k = \begin{pmatrix} \alpha_0 & \beta_1 & & 0 \\ \beta_1 & \alpha_1 & \ddots & \\ & \ddots & \ddots & \beta_{k-1} \\ 0 & & \beta_{k-1} & \alpha_{k-1} \end{pmatrix} .$$

By multiplying (2.4) formally from the left with V_k^* it becomes evident that the matrix

$$T_k = V_k^* K V_k = (\langle v_i, Kv_j \rangle)_{i,j=0}^{k-1}$$

is a representation of the orthogonal projection of K onto the Krylov space $\mathcal{K}_k(K; y)$, and it makes sense to consider the eigenvalues of T_k as approximate eigenvalues of K.

The results in this paper strongly rely on the following connection to the theory of orthogonal polynomials. As is obvious from the definition (2.2), the basis vector $v_j \in \mathcal{K}_{j+1}(K; y)$ can be rewritten as

$$v_j = p_j(K)y , \tag{2.5}$$

where $p_j \in \Pi_j$, i.e., the subset of polynomials of degree j or less. Moreover, from the orthonormality of the $\{v_j\}$ and the definition of the inner product (2.1) follows

$$\delta_{ij} = \langle v_i, v_j \rangle = \langle p_i(K)y, p_j(K)y \rangle = \sum_{n=1}^{\infty} \eta_n^2 p_i(\lambda_n) p_j(\lambda_n) = [p_i, p_j] .$$

In other words, the polynomials $\{p_j\}_{j \geq 0}$ form a sequence of orthonormal polynomials with respect to the inner product (2.1). These polynomials satisfy a three-term recurrence relation, and it is obvious from (2.3) and (2.5) that the same coefficients appear as in (2.3), i.e.,

$$\beta_{j+1} p_{j+1}(\lambda) = (\lambda - \alpha_j) p_j(\lambda) - \beta_j p_{j-1}(\lambda), \quad j = 0, 1, \ldots, k-1 , \tag{2.6}$$

with $p_{-1} \equiv 0$ and $p_0 \equiv 1/\|y\|$. Consequently, the matrix T_k is just the principal $k \times k$ submatrix of the semiinfinite Jacobi matrix corresponding to this inner product.

It is well-known that the eigenvalues of T_k are the roots of the kth orthogonal polynomial p_k, and that an eigenvector $\mathbf{u}$ corresponding to such a root λ is given by

$$\mathbf{u} = \big(p_0(\lambda), p_1(\lambda), \ldots, p_{k-1}(\lambda)\big)^T . \tag{2.7}$$

The roots of p_k (also called *Ritz values*) shall be denoted by

$$\lambda_{1,k} > \lambda_{2,k} > \ldots > \lambda_{k,k} .$$

At this point it is worth mentioning a well-known a posteriori bound for the error between eigenvalues of T_k and K, cf. [10, Section 13-2]. To this end let $\lambda \in \{\lambda_{j,k}\}_{j=1}^{k}$, and $\mathbf{u}$ be the corresponding eigenvector (2.7) of T_k; then there is an eigenvalue λ_n of K with

$$|\lambda_n - \lambda| \le \varepsilon_k := \frac{\beta_k p_{k-1}(\lambda)}{\left(p_0^2(\lambda) + \ldots + p_{k-1}^2(\lambda)\right)^{1/2}} . \tag{2.8}$$

This follows readily from (2.4) and standard perturbation theory.

To formulate the asymptotic results two different notations will be used: the statement $a_n \sim b_n$ means that a_n/b_n and b_n/a_n are bounded as $n \to \infty$; if, moreover, $a_n/b_n \to 1$ as $n \to \infty$ then this is denoted by $a_n \simeq b_n$. The following result states an upper bound for the superlinear convergence rate of the Lanczos method.

THEOREM 2.1. *Let $\lambda_n \sim n^{-s}$ for some $s > 0$, and assume that y has a component along x_1, i.e., $\eta_1 \neq 0$. Then there are some $q > 0$ and $c > 0$ such that*

$$0 < \lambda_1 - \lambda_{1,k} \le c(q/k)^{2sk}, \qquad k = 1, 2, \ldots \tag{2.9}$$

Proof. For any element $\mathbf{u} \in \mathbb{R}^k$ one has $V_k\mathbf{u} \in \mathcal{K}_{k-1}(K; y)$, and hence there is a polynomial p of degree $k-1$ or less with

$$V_k\mathbf{u} = p(K)y . \tag{2.10}$$

Vice versa, any polynomial of degree $k-1$ can be identified with an element of $\mathbb{R}^k$ via (2.10). This yields the following well-known variational characterization of the largest Ritz value,

$$\lambda_{1,k} = \max_{\mathbf{u}\neq\mathbf{0}} \frac{\mathbf{u}^T T_k \mathbf{u}}{\mathbf{u}^T\mathbf{u}} = \max_{\mathbf{u}\neq\mathbf{0}} \frac{\langle V_k\mathbf{u}, KV_k\mathbf{u}\rangle}{\langle V_k\mathbf{u}, V_k\mathbf{u}\rangle} = \max_{0\neq p\in\Pi_{k-1}} \frac{\langle p(K)y, Kp(K)y\rangle}{\langle p(K)y, p(K)y\rangle} ,$$

which can be rewritten in terms of the inner product (2.1) as

$$\lambda_{1,k} = \max_{0\neq p\in\Pi_{k-1}} \frac{[p, \lambda p]}{[p, p]} . \tag{2.11}$$

It should be mentioned that (2.11) is also known in the orthogonal polynomial literature (cf., e.g., Szegö [11, Section 7.72]), and has already been the starting point for the error analysis of Kaniel and Saad (cf. [10, Section 12-4]). Here, let

$$p(\lambda) := \prod_{j=2}^{k} \Big(1 - \frac{\lambda}{\lambda_j}\Big) \in \Pi_{k-1} ,$$

i.e., p vanishes at all eigenvalues λ_2 through λ_k, and – by monotonicity – is bounded by $p(0) = 1$ in $[0, \lambda_k]$. Then it follows from (2.11) and (2.1) that

$$\lambda_{1,k} \ge \frac{[p, \lambda p]}{[p, p]} \ge \frac{\eta_1^2 \lambda_1 p^2(\lambda_1)}{\eta_1^2 p^2(\lambda_1) + \sum_{n=k+1}^{\infty} \eta_n^2} .$$

Since $\{\eta_n\} \in \ell^2$ is square summable the series in the denominator is bounded, e.g., by $\|y\|^2$, and hence one has

$$\lambda_1 - \lambda_{1,k} \le \lambda_1 \big(\frac{\|y\|}{\eta_1}\big)^2 p^{-2}(\lambda_1) .$$

To complete the proof an estimate of $p(\lambda_1)$ is required. By assumption, $\lambda_1/\lambda_n \geq \varepsilon n^s$ for some $\varepsilon > 0$, and hence,

$$|p(\lambda_1)| = \prod_{j=2}^{k} \frac{\lambda_1}{\lambda_j} \Big| \frac{\lambda_j}{\lambda_1} - 1 \Big| \geq \varepsilon^{k-1} \big(1 - \frac{\lambda_2}{\lambda_1}\big)^{k-1}, \ {}^s(k+1) \,. \tag{2.12}$$

The assertion now follows from Stirling's formula. □

It must be mentioned that the use of polynomials with prescribed zeros in some of the eigenvalues of K has already been suggested in [10, p. 247] to obtain useful error bounds for clustered spectra; however, there seems to be no bound like (2.9) in the literature. Note how (2.9) illuminates the sensitivity of the rate of convergence on the decay rate of the eigenvalues. If the eigenvalues converge rapidly to zero then one can think of the dominating eigenvalue(s) to be more isolated. Note that this need not affect the convergence rate of the power method.

The technique used in the proof of Theorem 2.1 is not restricted to the largest eigenvalue only. For example, to estimate $\lambda_2 - \lambda_{2,k}$ one has to impose a prescribed zero in $\lambda_{1,k}$ for the polynomials $p \in \Pi_{k-1}$ to be used in (2.11). The resulting bound is the same as (2.9), but with some larger q and c. For an estimation of q see the following section, i.e., (3.2).

Finally, it should be mentioned that similar techniques have been applied by Nevanlinna in his monograph [9] to estimate the superlinear convergence rate of conjugate gradient type methods for solving linear equations. Although not obvious right away, it turns out that the rate of convergence for the eigenvalue approximations is similar (up to a square root) to the one for solving the linear system $(I + K)x = y$, cf. [9, Theorem 5.8.10].

3. A model problem. In this section the sharpness of Theorem 2.1 will be investigated. To this end consider the problem of approximating the smallest eigenvalue of the differential operator

$$Lu = -u'', \qquad \mathcal{D}(L) = \mathcal{H}^2(0,1) \cap \mathcal{H}_0^1[0,1] \subset \mathcal{L}^2(0,1) \,. \tag{3.1}$$

As is well-known the normalized eigenfunctions $x_n(t)$ of L are the sines $\sqrt{2}\sin n\pi t$ corresponding to eigenvalues $\mu_n = (n\pi)^2$, $n = 1, 2, \ldots$. Let $y(t) = t$ be the initial function for the Lanczos process to be considered in $\mathcal{L}^2(0,1)$. Note that in each step of (2.3) a boundary value problem

$$Lw_j = v_j \,, \qquad w_j(0) = w_j(1) = 0 \,,$$

has to be solved for w_j, and then

$$\beta_{j+1} v_{j+1} = w_j - \alpha_j v_j - \beta_j v_{j-1} \,.$$

Since

$$y(t) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{2}{n\pi} \sin n\pi t, \quad \text{a.e. in } (0,1) \,,$$

the inner product (2.1) corresponds to a discrete measure with point masses $\eta_n^2 = 2(\pi n)^{-2}$ at $\lambda_n = (\pi n)^{-2}$, $n \in \mathbb{N}$. Consequently, this problem meets the setting of

Theorem 2.1 with $s = 2$. Note that with this more detailed information the evaluation of (2.12) yields the upper bound

$$\lambda_1 - \lambda_{1,k} \le \frac{2}{3}\Big(\frac{k}{k+1}\Big)^2,\ {}^{-4}(k+1) \simeq \frac{1}{6\pi^2}\,k^{-2}(e/k)^{4k} \tag{3.2}$$

for the error of the Ritz values.

The reason for introducing this particular problem as a model problem is that one can determine the orthogonal polynomials with respect to (2.1) explicitly in this case. Still, this does not mean that their zeros are known, but their asymptotic behavior can be determined on the basis of the following (general) observation.

LEMMA 3.1. *Let μ be a discrete measure with point masses at $\{\lambda_n\}_{n=1}^{\infty}$, where λ_n is monotonically decreasing to zero. If $\{p_k\}$ is a sequence of orthogonal polynomials with respect to $d\mu$ and $\lambda_{1,k}$ the largest zero of p_k then*

$$\lambda_1 - \lambda_{1,k} \simeq \frac{p_k(\lambda_1)}{p_k'(\lambda_1)}\,, \qquad k \to \infty\,. \tag{3.3}$$

Proof. Since $\lambda_{j,k}$ are the zeros of p_k one can rewrite

$$p_k(\lambda) = p_k(0)\prod_{j=1}^{k}\Big(1 - \frac{\lambda}{\lambda_{j,k}}\Big)\,,$$

which yields

$$p_k'(\lambda) = p_k(\lambda)\sum_{j=1}^{k}\frac{1}{\lambda - \lambda_{j,k}}\,,$$

i.e.,

$$\frac{p_k'(\lambda_1)}{p_k(\lambda_1)} = \sum_{j=1}^{k}\frac{1}{\lambda_1 - \lambda_{j,k}}\,. \tag{3.4}$$

Recall that between any two mass points of μ there is at most one root of p_k (cf. [11, Theorem 3.41.2]), and hence,

$$\lambda_1 - \lambda_2 \le \lambda_1 - \lambda_{j,k} \le \lambda_1\,, \qquad 2 \le j \le k\,.$$

Consequently, since $\lambda_{1,k}$ converges with superlinear rate to λ_1 one can conclude from (3.4) that

$$\frac{p_k'(\lambda_1)}{p_k(\lambda_1)} = (\lambda_1 - \lambda_{1,k})^{-1} + O(k) \simeq (\lambda_1 - \lambda_{1,k})^{-1}\,,$$

which was to be shown. □

Consider now the Lommel polynomials $\{h_{k,\nu}\}_{k=0}^{\infty}$ for $\nu > 0$, cf., e.g., Watson [12, Section 9·6], or Chihara [2, Section VI.6]; the present notation is adopted from [2]. For $\nu > 0$ the Lommel polynomials are orthogonal with respect to a discrete measure with masses $j_{n,\nu-1}^{-2}$ at $\pm j_{n,\nu-1}^{-1}$, where $j_{n,\nu-1}$ denotes the nth positive zero of the Bessel function $J_{\nu-1}$ of order $\nu - 1$. The three-term recurrence relation is

$$h_{k+1,\nu}(\lambda) = 2\lambda(k+\nu)h_{k,\nu}(\lambda) - h_{k-1,\nu}(\lambda), \quad k = 0, 1, 2, \ldots\,, \tag{3.5}$$

with $h_0 \equiv 1$ and $h_{-1} \equiv 0$. Of particular interest for the present setting is the case $\nu = 3/2$, because $J_{1/2}(z) = (2/\pi z)^{1/2} \sin z$, and hence, $j_{n,\nu-1} = n\pi$ for $\nu = 3/2$. Therefore, using a well established technique (cf., e.g., [2, Section I.8]) it follows that the "squared" polynomials

$$p_k(\lambda) = h_{2k,3/2}(\sqrt{\lambda}), \qquad k = 0, 1, 2, \ldots, \tag{3.6}$$

are orthogonal with respect to the inner product (2.1) corresponding to the model problem introduced above. (Note, however, that p_k of (3.6) is not normalized; the orthonormal multiple $\check{p}_k$ is given in (3.15) below). The following result states the asymptotic behavior of $h_{k,\nu}$ at a mass point.

LEMMA 3.2. *Let $\nu > 0$ and $1/\lambda$ be a zero of $J_{\nu-1}$. Then, for $k \to \infty$,*

$$h_{k,\nu}(\lambda) = \frac{J_{\nu+k}(1/\lambda)}{J_\nu(1/\lambda)} \simeq \big(\frac{1}{2\lambda}\big)^{k+\nu}, \, {}^{-1}(k+\nu+1) J_\nu^{-1}\big(\frac{1}{\lambda}\big), \tag{3.7}$$

$$h'_{k,\nu}(\lambda) \simeq -\frac{1}{\lambda^2} J_{\nu-2}\big(\frac{1}{\lambda}\big), \, (k+\nu)(2\lambda)^{k+\nu-1}. \tag{3.8}$$

Proof. Recall that the Bessel functions of order $\nu+k$ satisfy the recurrence relation

$$J_{\nu+k+1}(z) = \frac{2(k+\nu)}{z} J_{\nu+k}(z) - J_{\nu+k-1}(z), \quad k = 0, 1, 2, \ldots. \tag{3.9}$$

Since $J_{\nu-1}$ vanishes at $z = 1/\lambda$ by assumption, a comparison of this recursion with (3.5) yields that $h_{k,\nu}(\lambda) = J_{\nu+k}(1/\lambda)/J_\nu(1/\lambda)$ for every $k \in \mathbb{N}$. (Note, cf. [12], that the positive zeros of the Bessel functions J_ν and $J_{\nu-1}$ interlace, and hence, $J_\nu(1/\lambda) \neq 0$). The second part of (3.7) is the well-known asymptotic behavior of the Bessel function with fixed argument.

The proof of the second assertion (3.8) requires the following identity from [12, Section 9·63] for the derivative of a Lommel polynomial,

$$h'_{k,\nu}(\lambda) = -\frac{1}{\lambda^2}\big(\lambda(k+2)h_{k,\nu}(\lambda) + h_{k+1,\nu-1}(\lambda) - h_{k+1,\nu}(\lambda)\big), \tag{3.10}$$

and Hurwitz' theorem concerning the asymptotic behavior of a Lommel polynomial at a point λ which is not a mass point, cf. [12, Section 9·65]:

$$h_{k,\nu-1}(\lambda) \simeq J_{\nu-2}(1/\lambda), \, (k+\nu-1)(2\lambda)^{k+\nu-2}, \qquad k \to \infty. \tag{3.11}$$

Since λ is a mass point corresponding to the polynomials $\{h_{k,\nu}\}$, λ is no mass point for the measure corresponding to $\{h_{k,\nu-1}\}$, and hence, (3.7), (3.10) and (3.11) yield

$$h'_{k,\nu}(\lambda) \simeq -\frac{1}{\lambda^2} h_{k+1,\nu-1}(\lambda) \simeq -\frac{1}{\lambda^2} J_{\nu-2}(1/\lambda), \, (k+\nu)(2\lambda)^{k+\nu-1},$$

as $k \to \infty$. □

After these preliminaries the strong asymptotic behavior of the error of the Lanczos approximation to the smallest eigenvalue of L can be determined.

THEOREM 3.3. *Let L be as in (3.1) with smallest eigenvalue $\mu_1 = \pi^2$, and $1/\lambda_{1,k}$ be the corresponding approximation after k Lanczos steps with initial function y. Then,*

$$\frac{1}{\lambda_{1,k}} - \mu_1 \simeq \frac{\pi^4}{64} k^{-3} \big(\frac{\pi e}{4k}\big)^{4k}, \qquad k \to \infty. \tag{3.12}$$

Proof. It only remains to assemble the previous results. First, from (3.6), Lemma 3.2, and Stirling's formula one has

$$p_k(1/\mu_1) = h_{2k,3/2}(1/\pi) \simeq \frac{\pi}{16}\, J_{3/2}^{-1}(\pi) k^{-2} (\frac{\pi e}{4k})^{2k} .$$

Since $J_{-1/2}(z) = (2/\pi z)^{1/2} \cos z$ and $J_{3/2}(\pi) = -J_{-1/2}(\pi) = \sqrt{2}/\pi$ by (3.9), this gives

$$p_k(1/\mu_1) \simeq \frac{\pi^2}{16\sqrt{2}}\, k^{-2} (\frac{\pi e}{4k})^{2k} . \tag{3.13}$$

Second, since $p_k'(\lambda) = h_{2k,3/2}'(\sqrt{\lambda})/2\sqrt{\lambda}$, Lemma 3.2 and Stirling's formula yield

$$p_k'(1/\mu_1) \simeq -2\pi^3 J_{-1/2}(\pi) k (\frac{4k}{\pi e})^{2k} = 2\sqrt{2}\pi^2 k (\frac{4k}{\pi e})^{2k} .$$

Consequently, one has

$$\frac{p_k'(1/\mu_1)}{p_k(1/\mu_1)} \simeq 64 k^3 (\frac{4k}{\pi e})^{4k} , \tag{3.14}$$

and a final application of Lemma 3.1 completes the proof. □

Comparing (3.12) with (3.2) it follows that Theorem 2.1 is quite sharp, at least as far as powers of k^{-k} are concerned. The two values of q for (1.1) as calculated in (3.2) and (3.12) only differ by as little as an extra factor of $\pi/4$. Numerically, this difference can hardly be seen due to the dominating growth of k^{4k}. As of today, it is not clear how to improve the technique in the proof of Theorem 2.1 to end up with the optimal value of q.

Finally, consider the sharpness of the a posteriori estimate ε_k of (2.8). To this end the recursion coefficients of the orthonormal multiples of p_k are required. As shown, e.g., by Grosjean [6], the polynomials $\{\sqrt{2k+3}\, h_{k,3/2}\}$ are orthonormal with respect to the Lommel measure; concerning the inner product (2.1) this implies that

$$\check{p}_k(\lambda) = \sqrt{4k+3}\, h_{2k,3/2}(\sqrt{\lambda}), \qquad k = 0, 1, 2, \ldots , \tag{3.15}$$

are the orthonormal polynomials corresponding to the Lanczos process. Inserting this into (3.5) one can compute the coefficients α_j and β_j from (2.6), namely $\alpha_0 = 1/15$, and, for $j \geq 1$,

$$\alpha_j = \frac{2}{(4j+1)(4j+5)}, \quad \beta_j = \frac{1}{(4j+1)\sqrt{(4j+3)(4j-1)}} . \tag{3.16}$$

To determine $\check{p}_{k-1}(\lambda_{1,k})$ one can use the convexity of $\check{p}_{k-1}$ in $[\lambda_{1,k-1}, \lambda_1]$ to obtain that

$$\check{p}_{k-1}(\lambda_{1,k}) \geq \check{p}_{k-1}(\lambda_1) - (\lambda_1 - \lambda_{1,k}) \check{p}_{k-1}'(\lambda_1) .$$

From this inequality and Lemma 3.1 follows that

$$\big|1 - \frac{\check{p}_{k-1}(\lambda_{1,k})}{\check{p}_{k-1}(\lambda_1)}\big| \leq (\lambda_1 - \lambda_{1,k}) \frac{\check{p}_{k-1}'(\lambda_1)}{\check{p}_{k-1}(\lambda_1)} \simeq \frac{\lambda_1 - \lambda_{1,k}}{\lambda_1 - \lambda_{1,k-1}} .$$

Since the right-hand side goes to zero by Theorem 3.3 it has been shown that

$$\check{p}_{k-1}(\lambda_{1,k}) \simeq \check{p}_{k-1}(\lambda_1) \simeq \sqrt{2}k^{1/2}(\frac{\pi e}{4k})^{2k} , \tag{3.17}$$

cf. (3.15) and (3.13).

The remaining factor in (2.8) is just the square root of the weight in the kth Gaussian quadrature rule for the inner product (2.1). This weight converges to the mass of the associated measure at λ_1, i.e.,

$$\Big(\sum_{j=0}^{k-1} \check{p}_j^2(\lambda_{1,k})\Big)^{-1} \longrightarrow \frac{2}{\pi^2} , \qquad k \to \infty . \tag{3.18}$$

Inserting now (3.16), (3.17) and (3.18) into (2.8) one obtains that

$$\varepsilon_k \simeq \frac{1}{8\pi}\, k^{-3/2}(\frac{\pi e}{4k})^{2k} .$$

As can be seen from Theorem 3.3 this is essentially the square root of (3.12). Note that this is in nice agreement with the stronger perturbation error estimate

$$\frac{1}{\mu_1} - \lambda_{1,k} \approx \varepsilon_k^2/\gamma ,$$

stated in [10, Section 13-2], where γ is the gap between $\lambda_{1,k}$ and $\lambda_{2,k}$.

It should be mentioned that the same model problem appears as Example 5.2.8 in Nevanlinna [9], where lower and upper bounds are obtained for the superlinear convergence rate of the conjugate gradient iteration applied to solving $(I+L^{-1})u = f$. These bounds are approximately the square root of the eigenvalue approximation error (3.12). While the upper bounds are obtained with similar techniques as in Section 2, Nevanlinna uses a lemma from analytic function theory to derive his lower bound. If $f = t$ a.e. in $(0,1)$, however, then the precise asymptotic convergence rate of the residual norm $\|f - (I + L^{-1})u_k\|$ can be computed by similar means as above.

4. Numerical examples. To illustrate the results of the previous section the Lanczos method has been used to compute the smallest eigenvalue $\mu_1 = \pi^2$ of the differential operator L of Section 3. The operator is approximated by finite differences, which gives the tridiagonal matrix $A = n^2 \cdot \mathit{tridiag}(-1, 2, -1)$ of size $(n-1)\times(n-1)$. It is the reciprocal $\tilde{\lambda}_1$ of the smallest eigenvalue of A, i.e.,

$$\tilde{\lambda}_1 \;=\; \frac{1}{4n^2}\sin^{-2}\frac{\pi}{2n} \;=\; \frac{1}{\pi^2} + \frac{1}{12}\,n^{-2} + \ldots ,$$

to which the Lanczos approximations will converge.

For $n = 128$, Table 4.1 presents the results of the first six Lanczos iterations: the second column shows the approximation $\lambda_{1,k}$ of the Lanczos method after k iterations, and the third column contains the approximation error $\tilde{\lambda}_1 - \lambda_{1,k}$. The numbers in the fourth column are the a posteriori error bounds ε_k defined in (2.8), while the last column contains the reciprocals of the a priori estimate (3.14), which describes the exact asymptotic behavior of the approximation error. For comparison, the last line shows the true eigenvalue $\lambda_1 = \pi^{-2}$ of L^{-1}.

Note that only three iterations are required to obtain all significant digits of λ_1 within the discretization error. It can also be seen by counting the zeros in the error

TABLE 4.1
Model problem $Lu = -u''$

k	approximations	absolute errors	a posteriori bound	estimate (3.14)
1	0.067 449 951	0.033 876 319	0.043 298 950	0.324 606 700
2	0.100 622 293	0.000 703 977	0.007 638 242	0.003 292 797
3	0.101 323 064	0.000 003 206	0.000 542 465	0.000 009 764
4	0.101 326 266	0.000 000 004	0.000 020 379	0.000 000 011
5	0.101 326 270	0	0.000 000 481	0
6	0.101 326 270	0	0.000 000 008	0
π^{-2}	0.101 321 184			

numbers that an algorithm with quadratic or even cubic convergence would not be significantly faster. As predicted by the asymptotic analysis of the previous section, the a posteriori bounds ε_k are significantly larger than the true errors, but somewhat smaller than their square roots.

The second example is a more realistic problem. Let

$$Lu = -\mathrm{div}(a\,\mathrm{grad}u)$$

be an elliptic differential operator over the square $[0,1]\times[0,1]$ with $\mathcal{D}(L) = \mathcal{H}^2 \cap \mathcal{H}_0^1 \subset \mathcal{L}^2$, and with piecewise constant coefficient function

$$a(x,y) = \begin{cases} 100 & 0 \le x, y \le 0.5\,, \\ 1 & \text{elsewhere}\,. \end{cases}$$

The aim is to determine the smallest eigenvalues of L. As described in the beginning of Section 3, these eigenvalues can be computed with the Lanczos process, solving a differential equation $Lw_j = v_j$ in each iteration. The following results correspond to $y \equiv 1$ as initial function. The differential equations have been solved with a full multigrid $V(2,2)$-cycle (called nested iteration in [7]) using two pre and post Jacobi smoothing steps, respectively, and bilinear finite elements over 128×128 squares on the finest level. Note that this means that L^{-1} is implemented by an algorithm, and not via a matrix vector multiply (although in exact arithmetic the algorithm implicitly corresponds to some matrix). As a consequence the errors in the computation are much larger than in the previous example, which leads to a certain loss of orthogonality in the Lanczos vectors. This is manifested by so-called "spurious" (or ghost) eigenvalues of the resulting Jacobi matrix. Spurious eigenvalues can be identified with a technique due to Cullum and Willoughby [3]. With their approach the first spurious eigenvalue of T_k has been detected after $k = 7$ iterations, with a second one occurring after nine iterations. Table 4.2 shows the remaining four dominant eigenvalues of T_k for $k = 1, \ldots, 10$. Note the loss of monotonicity in these columns at $k = 7$ and $k = 9$, which is due to the elimination of the spurious eigenvalues.

The last column of Table 4.2 shows the decay of the numbers ε_k of (2.8) corresponding to the dominant eigenvalue. Similarly, the final row contains the respective numbers ε_{10} for the four largest eigenvalues of T_{10}.

Again, essentially three to four iterations are required to approximate the smallest eigenvalue of L within the discretization error, and two more iterations to obtain the next one. Note that according to the a posteriori bounds ε_{10} in the last row it is not

TABLE 4.2
Problem $Lu = -div(a\ grad u)$

k	approximations				a posteriori bound
1	0.013980				0.012071
2	0.025811	0.001674			0.002749
3	0.026269	0.009937	0.000742		0.000615
4	0.026289	0.012185	0.004675	0.000458	0.000106
5	0.026289	0.012695	0.007539	0.002489	0.000010
6	0.026289	0.012731	0.008085	0.004657	0.000004
7	0.026289	0.012716	0.007807	0.003244	0.000004
8	0.026290	0.012718	0.007843	0.004459	0.000010
9	0.026291	0.012718	0.007856	0.003327	0.000004
10	0.026291	0.012718	0.007971	0.005331	0.000004
ε_{10}	0.000004	0.000005	0.003623	0.002657	

quite clear whether the third eigenvalue has converged after 10 iterations. A couple of more iterations, however, establish 0.0078 as the first few significant digits of λ_3. Anyway, after 10 iterations one has

$$\mu_1 = 38.0, \quad \mu_2 = 78.6, \quad \text{and} \quad \mu_3 \approx 125$$

as final approximations of the three smallest eigenvalues of L.

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