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COMPUTING PROBABILISTIC BOUNDS FOR EXTREME EIGENVALUES OF SYMMETRIC MATRICES WITH THE LANCZOS METHOD*

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Abstract. We study the Lanczos method for computing extreme eigenvalues of a symmetric or Hermitian matrix. It is not guaranteed that the extreme Ritz values are close to the extreme eigenvalues—even when the norms of the corresponding residual vectors are small. Assuming that the starting vector has been chosen randomly, we compute probabilistic bounds for the extreme eigenvalues from data available during the execution of the Lanczos process. Four different types of bounds are obtained using Lanczos, Ritz, and Chebyshev polynomials. These bounds are compared theoretically and numerically. Furthermore we show how one can determine, after each Lanczos step, a probabilistic upper bound for the number of steps still needed (without performing these steps) to obtain an approximation to the largest or smallest eigenvalue within a prescribed tolerance.

Key words. symmetric and Hermitian matrices, eigenvalues, Lanczos method, Ritz values, computation of probabilistic eigenvalue bounds, misconvergence, Lanczos polynomials, Ritz polynomials

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1. Introduction.

Knowledge about the extreme eigenvalues of symmetric or Hermitian matrices is important in many applications. For example, the stability of processes involving such matrices is often governed by the location of their eigenvalues. The extreme eigenvalues can also be used to determine condition numbers, the field of values, and ε-pseudospectra of arbitrary matrices (see, e.g., [1, 12]). For small-sized matrices the eigenvalues can be computed by the QR-method (see, e.g., [2]), but this is not feasible for large matrices. A method which is often used in practice to compute a few extreme eigenvalues of large sparse symmetric or Hermitian matrices is the Lanczos method (see, e.g., [2, 7, 14]). The approximations of the eigenvalues obtained with the Lanczos method (the Ritz values) lie between the smallest and largest eigenvalue of the original matrix and one would like to know whether the largest (or smallest) Ritz value is sufficiently close to the largest (or smallest) eigenvalue of that matrix.

The classical a priori error estimates for the Lanczos method, established by Kaniel, Paige, and Saad (see, e.g., [2, 3, 6, 7, 10]) are not applicable in practice to obtain bounds on the spectrum of Hermitian matrices, because they involve knowledge about the eigenvalues and angles between the eigenvectors and the starting vector. Furthermore one should note that small residuals for the Ritz values *only* imply that these Ritz values are close to an eigenvalue, but it is not guaranteed that this eigenvalue is indeed the one we are looking for (cf., e.g., [8]). In fact, it is not possible to derive rigorous bounds on the spectrum from *any* possible starting vector: if the

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starting vector is perpendicular to the eigenvector (or eigenspace in case of multiple eigenvalues) corresponding to the largest or smallest eigenvalue, it is impossible to obtain any information regarding this eigenvalue from the Lanczos process.

In this paper we derive various a posteriori bounds for the spectrum of real symmetric matrices using a probabilistic approach. Assuming that the starting vector of the Lanczos process is chosen randomly from the uniform distribution over the unit sphere, we derive, using data available while executing the Lanczos process, for every $\varepsilon \in (0,1)$ bounds for the spectrum with probability at least $1-\varepsilon$. No intrinsic properties of the matrix (apart from being symmetric) are required to compute our bounds. Polynomials related to the Lanczos process, namely the Lanczos polynomials and Ritz polynomials, are used to derive two types of such bounds. For symmetric positive definite matrices Kuczyński and Woźniakowski [5, Theorem 3] give, for arbitrary $t > 1$, an a priori upper bound for the probability that the largest eigenvalue is greater than t times the largest Ritz value; Chebyshev polynomials of the second kind are used to obtain these bounds. This result can be used to compute a posteriori probabilistic bounds for the spectrum while executing the Lanczos process, and bounds based on [5, Theorem 3] can be used for symmetric indefinite matrices as well. The fourth kind of bounds for the spectrum is obtained with Chebyshev polynomials of the first kind. The sharpness of the different bounds is analyzed theoretically and compared numerically. It turns out that the bounds based on Lanczos polynomials are the sharpest ones in most cases; however, the Ritz polynomials sometimes provide better bounds when the Lanczos method suffers from a misconvergence (i.e., the largest (or smallest) Ritz values in consecutive Lanczos steps seem to converge, but not to an extreme eigenvalue).

Apart from the bounds on the spectrum, we also study probabilistic bounds for the number of Lanczos steps needed to get an error (or relative error) in the largest or smallest eigenvalue that is smaller than a given tolerance. In [4, Theorem 4.2] the authors present a probabilistic upper bound for the number of Lanczos steps needed to yield a relative error in the largest eigenvalue of a symmetric positive definite matrix that is smaller than a given tolerance. For this special case numerical experiments demonstrate that our bound and the one from [4, Theorem 4.2] are almost the same. Furthermore, we provide upper bounds for the number of Lanczos steps needed to guarantee with probability at least $1-\varepsilon$ that either the spectrum lies between certain prescribed bounds, or that a misconvergence has occurred.

The results in this paper deal with the Lanczos process applied to real symmetric matrices and real starting vectors. This includes the case of Hermitian matrices, because the Lanczos method applied to a complex Hermitian matrix (with a complex starting vector) can be written as the application of the Lanczos method to a related real symmetric matrix of double size with a real starting vector (see Remark 2.1 for details).

All bounds discussed in this paper are easily implemented and can be computed with little effort while executing the Lanczos process.

The paper has been organized as follows. In section 2 some notations and definitions are introduced. Bounds based on Lanczos polynomials are presented in section 3, and bounds obtained with Ritz polynomials can be found in section 4. In section 5 we derive bounds from Chebyshev polynomials. The estimates for the number of Lanczos steps still to be done for sufficiently accurate approximations can be found in section 6.1, and the estimates for the number of Lanczos steps needed to obtain prescribed bounds for the spectrum or to detect misconvergence are given in section 6.2.

Numerical experiments are presented in section 7, and the conclusions can be found in section 8.

2. Preliminaries and notation. In this section we introduce some notations and present relevant properties of the Lanczos method. For an introduction to the Lanczos method and more details, as well as implementation issues, the reader may consult, e.g., [2, 7]. Throughout this paper we do not consider the effect of rounding errors.

The standard inner product on $\mathbb{R}^n$ will be denoted by $(\cdot,\cdot)$, and $\|\cdot\|$ stands for the Euclidean norm, and I is the $n \times n$ identity matrix.

Let A be a real symmetric $n \times n$ matrix with eigenvalues

$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n. \tag{2.1}$$

The corresponding normalized eigenvectors x_j form an orthonormal basis of $\mathbb{R}^n$. We use the Lanczos method to approximate one or a few extreme eigenvalues of A. The unit starting vector is denoted by v_1 and can be written as

$$v_1 = \sum_{j=1}^{n} \gamma_j x_j. \tag{2.2}$$

If v_1 is chosen randomly from the uniform distribution with respect to the unit sphere, the dimension of the Krylov subspace

$$K_k(A, v_1) = \operatorname{span}\{v_1, Av_1, \ldots, A^{k-1}v_1\}$$

is equal to k with probability one for k less than the number of distinct eigenvalues of A.

In the Lanczos process vectors v_k are generated by the three-term recurrence

$$\delta_k v_{k+1} = Av_k - \alpha_k v_k - \beta_{k-1} v_{k-1} \qquad \text{for} \quad k = 1, 2, 3, \ldots, \tag{2.3}$$

where $v_0 = 0$, $\beta_0 = 1$, $\alpha_k = (Av_k, v_k)$, $\beta_{k-1} = (Av_k, v_{k-1})$, and $\delta_k > 0$ is chosen such that $\|v_{k+1}\| = 1$. With this choice one has $\delta_k = \beta_k$ for $k \ge 1$. The vectors $v_1, v_2, \ldots, v_k$ form an orthonormal basis of the Krylov subspace $K_k(A, v_1)$. Let V_k be the $n \times k$ matrix of which v_j is the jth column. The *Ritz values* occurring in step k of the Lanczos process are the eigenvalues of the tridiagonal $k \times k$ matrix $T_k = V_k^{\mathrm{T}} A V_k$, and are denoted by

$$\theta_1^{(k)} < \theta_2^{(k)} < \cdots < \theta_k^{(k)};$$

the Ritz values satisfy $\theta_j^{(k)} > \lambda_j$ and $\theta_{k+1-j}^{(k)} < \lambda_{n+1-j}$ $(1 \le j \le k)$. We denote the eigenvectors of T_k by $s_j^{(k)}$: $T_k s_j^{(k)} = \theta_j^{(k)} s_j^{(k)}$ and the *Ritz vectors* by $y_j^{(k)} = V_k s_j^{(k)}$, where we assume that these Ritz vectors are normalized. We also introduce the residuals

$$r_j^{(k)} = Ay_j^{(k)} - \theta_j^{(k)} y_j^{(k)}.$$

Related to the three-term recursion (2.3) are the polynomials p_k of degree k defined by $p_{-1}(t) = 0$, $p_0(t) = 1$, and

$$\beta_k p_k(t) = (t - \alpha_k) p_{k-1}(t) - \beta_{k-1} p_{k-2}(t) \qquad \text{for} \quad k = 1, 2, 3, \ldots. \tag{2.4}$$

From (2.3) with $\delta_k = \beta_k$ and (2.4) it follows that

$$v_{k+1} = p_k(A)v_1 \qquad \text{for} \quad k = 1, 2, 3, \ldots.$$

The polynomials p_k are called the *Lanczos polynomials* with respect to A and v_1. Other polynomials related to the Lanczos method are the *Ritz polynomials* $q_j^{(k)}$ of degree $k-1$, which are characterized by the fact that

$$y_j^{(k)} = q_j^{(k)}(A)v_1 \qquad \text{for} \quad j = 1, 2, \ldots, k. \tag{2.5}$$

In the following sections estimates for the eigenvalues of A, based on Lanczos and Ritz polynomials, will be studied and compared. Therefore it is important to understand the relation between these polynomials. The polynomial p_k is a scalar multiple of the characteristic polynomial of the matrix T_k (cf., e.g., [7, section 7.3]), which implies that $\theta_1^{(k)}, \theta_2^{(k)}, \ldots, \theta_k^{(k)}$ are the zeros of p_k. From [7, section 12.3] it follows that these Ritz values without $\theta_j^{(k)}$ are the zeros of $q_j^{(k)}$. Hence $p_k(t) = c_j^{(k)}\,(t - \theta_j^{(k)})q_j^{(k)}(t)$ for a certain constant $c_j^{(k)}$.[1] Because $v_{k+1} = p_k(A)v_1 = c_j^{(k)}\,(A - \theta_j^{(k)}I)q_j^{(k)}(A)v_1 = c_j^{(k)}r_j^{(k)}$, we have $c_j^{(k)} = 1/\|r_j^{(k)}\|$, which yields the following relation between the Lanczos and Ritz polynomials:

$$p_k(t) = (t - \theta_j^{(k)})q_j^{(k)}(t) \,/\, \|r_j^{(k)}\| \qquad \text{for} \quad j = 1, 2, \ldots, k. \tag{2.6}$$

REMARK 2.1. *The Lanczos method described above can also be used to determine a few extreme eigenvalues of a complex Hermitian matrix A. The results in this paper are only valid for real symmetric matrices, but the Lanczos method for Hermitian matrices can be formulated in terms of real matrices and vectors. Let* $\operatorname{Re} A$ *and* $\operatorname{Im} A$ *be the real and imaginary part of A, respectively. The Lanczos method applied to the $2n \times 2n$ real symmetric matrix*

$$B = \begin{pmatrix} \operatorname{Re} A & -\operatorname{Im} A \\ \operatorname{Im} A & \operatorname{Re} A \end{pmatrix}$$

with starting vector $\binom{\operatorname{Re} v_1}{\operatorname{Im} v_1}$ *yields the same tridiagonal matrices T_k as the Lanczos method applied to A with starting vector v_1; this can be seen from taking the real and imaginary part of the three-term recurrence* (2.3). *The numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of B, but with multiplicity twice as large as for the matrix A. Therefore (probabilistic) bounds for the spectrum of B are (probabilistic) bounds for the spectrum of A as well.*

3. Spectral bounds using the Lanczos polynomial. In this section we will give probabilistic upper and lower bounds for the spectrum of A, based on Lanczos polynomials. For each step of the Lanczos process we obtain these bounds based on the information computed so far. No assumptions on the location or separation of the eigenvalues are required.

The Lanczos polynomials p_k are a byproduct of the process. They are usually small between $\theta_1^{(k)}$ and $\theta_k^{(k)}$ and increase rapidly outside this interval. We can exploit

[1] From this relation it follows that $q_j^{(k)}$ is a scalar multiple of $\prod_{i \neq j}(t - \theta_i^{(k)})$ and that polynomial is called a reduced Ritz polynomial in [11]. The relation between these polynomials and (2.5) also follows from [11, Formula (5.14)].

this fact: assuming that the starting vector has components in the direction of x_1 and x_n, we can provide upper and lower bounds for the spectrum of A.

From

$$1 = \|v_{k+1}\|^2 = \|p_k(A)v_1\|^2 = \sum_{j=1}^{n} \gamma_j^2 \, p_k(\lambda_j)^2$$

and $p_k(\lambda_n) > 0$ it follows that

$$1 \;\geq\; |\gamma_n| \, p_k(\lambda_n).$$

If γ_n is known, this estimate provides an upper bound λ^{up} for λ_n: let λ^{up} be the largest real zero of

$$f_L(t) = p_k(t) - 1/|\gamma_n|. \tag{3.1}$$

This number λ^{up} exists and satisfies $\lambda^{\mathrm{up}} > \theta_k^{(k)}$ because p_k is strictly increasing on $(\theta_k^{(k)}, \infty)$. The number λ^{up} can be determined by Newton's method or bisection. As a starting point for the Newton process one can take $\|A\|_\infty$ (the maximal row sum of the absolute values of the entries of A) or a previously computed upper bound for λ_n.

In practice we do not know γ_n, but we can determine the probability that $|\gamma_n|$ is smaller than a given (small) constant. Let S^{n-1} denote the $(n-1)$-dimensional unit sphere in $\mathbb{R}^n$. We assume that v_1 is chosen randomly with respect to the uniform distribution over S^{n-1}. Then, as a result, $(\gamma_1, \gamma_2, \ldots, \gamma_n)$ is also random with respect to the uniform distribution over S^{n-1} (cf., e.g., [4, p. 1116]). In the following lemma we compute the probability that $|\gamma_n|$ is smaller than δ.

LEMMA 3.1. *Assume that the starting vector v_1 has been chosen randomly with respect to the uniform distribution over the unit sphere S^{n-1} and let $\delta \in [0,1]$. Then*

$$P(|\gamma_n| \leq \delta) \;=\; 2\, B(\tfrac{n-1}{2}, \tfrac{1}{2})^{-1} \cdot \int_0^{\arcsin \delta} \cos^{n-2} t \, \mathrm{d}t,$$

where B denotes Euler's Beta function: $B(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1}\mathrm{d}t$.

Proof. Define $S_\delta = \{\gamma \in S^{n-1} : |\gamma_n| < \delta\}$; we want to determine the ratio of the areas of the sets S_δ and S^{n-1}. The image of the map

$$\varphi \;:\; (-\pi, \pi) \;\times\; (-\tfrac{\pi}{2}, \tfrac{\pi}{2})^{n-2} \;\to\; S^{n-1}$$

defined by

$$\varphi : \begin{pmatrix} \alpha \\ \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{n-2} \end{pmatrix} \mapsto \begin{pmatrix} \cos\alpha \cos\psi_1 \cos\psi_2 \cdots \cos\psi_{n-3} \cos\psi_{n-2} \\ \sin\alpha \cos\psi_1 \cos\psi_2 \cdots \cos\psi_{n-3} \cos\psi_{n-2} \\ \sin\psi_1 \cos\psi_2 \cdots \cos\psi_{n-3} \cos\psi_{n-2} \\ \vdots \\ \sin\psi_{n-3} \cos\psi_{n-2} \\ \sin\psi_{n-2} \end{pmatrix}$$

equals the sphere up to a negligible set. One can check that the associated Euclidean density is given by

$$\omega(\alpha, \psi_1, \psi_2, \ldots, \psi_{n-2}) \;=\; \cos\psi_1 \cdot \cos^2\psi_2 \cdots \cos^{n-2}\psi_{n-2}.$$

Therefore we can compute the areas of S_δ and S^{n-1} by integrating this density over the respective domains. Taking the ratio of the two results, we get

$$\begin{aligned} P(|\gamma_n| \le \delta) &= P(|\psi_{n-2}| \le \arcsin\delta) \\ &= 2\int_0^{\arcsin\delta} \cos^{n-2} t \,\mathrm{d}t \,\Big/ \int_{-\pi/2}^{\pi/2} \cos^{n-2} t \,\mathrm{d}t \\ &= 2\int_0^{\arcsin\delta} \cos^{n-2} t \,\mathrm{d}t \,\Big/ B(\tfrac{n-1}{2}, \tfrac{1}{2}), \end{aligned}$$

which proves the lemma. □

Now suppose we would like to have an upper bound for the spectrum of A that is correct with probability at least $1-\varepsilon$. Then we determine the value of δ for which

$$\int_0^{\arcsin\delta} \cos^{n-2} t \,\mathrm{d}t \;=\; \tfrac{\varepsilon}{2} B(\tfrac{n-1}{2}, \tfrac{1}{2}) \quad \left(= \varepsilon \int_0^{\pi/2} \cos^{n-2} t \,\mathrm{d}t\right) \tag{3.2}$$

holds, e.g., by using Newton's method. The integrals in (3.2) can be computed using an appropriate quadrature formula. We replace $|\gamma_n|$ in (3.1) by the value δ computed from (3.2) and determine the zero $\lambda^{\mathrm{up}} > \theta_k^{(k)}$. This λ^{up} is an upper bound for the spectrum of A with probability at least $1-\varepsilon$, and we call λ^{up} a probabilistic upper bound.

A lower bound λ^{low} for the spectrum of A with probability at least $1-\varepsilon$ can be obtained in a similar way. (Note that Lemma 3.1 remains valid if $|\gamma_n|$ is replaced by $|\gamma_1|$.) The only difference is that we have to separate the cases where k, the degree of p_k, is even ($p_k(t) \to +\infty$ for $t \to -\infty$) or odd ($p_k(t) \to -\infty$ for $t \to -\infty$). Hence we have proved the following theorem.

THEOREM 3.2. *Assume that the starting vector v_1 has been chosen randomly with respect to the uniform distribution over S^{n-1} and let $\varepsilon \in (0,1)$. Then λ^{up}, the largest zero of the polynomial*

$$f_L(t) = p_k(t) - 1/\delta \tag{3.3}$$

with δ given by (3.2)*, is an upper bound for the spectrum of A with probability at least $1-\varepsilon$, and λ^{low}, the smallest zero of*

$$f_L(t) = (-1)^k p_k(t) - 1/\delta, \tag{3.4}$$

is a lower bound for the spectrum of A with probability at least $1-\varepsilon$.

Note that if we are unlucky in choosing v_1, so that $|\gamma_n| < \delta$, then the computed bounds may or may not be correct; see section 7 for an illustration.

The determination of the lower and upper bounds from Theorem 3.2 is rather cheap in general (compared with a matrix-vector multiplication with A); the computation of $f_L(t)$ (using (2.4)) costs approximately $6k$ floating point operations. Note that the Ritz values and vectors are not needed to obtain these bounds of the spectrum. For very small k one cannot expect to obtain tight bounds, so it only makes sense to compute the zeros of (3.3) and (3.4) for k of moderate size. In practice one could, e.g., compute these zeros only every second or third Lanczos step until the bounds become sufficiently sharp.

4. Spectral bounds using Ritz polynomials. We can also try to obtain probabilistic upper and lower bounds for the spectrum of A using some Ritz polynomials $q_j^{(k)}$. The degree of these polynomials is one less than the degree of p_k, but while $p_k(\theta_k^{(k)}) = 0$, the polynomial $q_k^{(k)}$ has its last zero in $\theta_{k-1}^{(k)}$ and could be a competitor of p_k to give a possibly tighter upper bound. Similarly, $q_1^{(k)}$ may be used to obtain another lower bound.

We write $\theta_j^{(k)}$ as a Rayleigh quotient:

$$\theta_j^{(k)} = (Ay_j^{(k)}, y_j^{(k)}) = \sum_{i=1}^{n} \lambda_i \gamma_i^2 \, q_j^{(k)}(\lambda_i)^2. \tag{4.1}$$

First suppose that A is positive semidefinite. Then set $j = k$ to derive the inequality $\theta_k^{(k)} \geq \lambda_n \gamma_n^2 \, q_k^{(k)}(\lambda_n)^2$. Hence the zero $\lambda^{\text{up}} > \theta_k^{(k)}$ of

$$f_R(t) = t q_k^{(k)}(t)^2 \; - \; \theta_k^{(k)}/\gamma_n^2 \tag{4.2}$$

is an upper bound for λ_n. If γ_n is not known, one can obtain a probabilistic upper bound λ^{up} of λ_n with probability at least $1 - \varepsilon$, as in the previous section. (Replace γ_n in (4.2) by δ where δ satisfies (3.2).)

As in the previous section, if we happen to choose a v_1 so that $|\gamma_n| < \delta$, then we are not certain that the computed upper bound is correct. It can even happen that the largest zero λ^{up} of f_R with γ_n replaced by δ satisfies $\lambda^{\text{up}} < \theta_k^{(k)}$! See section 7 for an illustration.

When it is not known whether A is positive definite, we can obtain a probabilistic upper bound in the following way. Let $-\sigma < 0$ be a known lower bound for the spectrum of A: then the matrix $A + \sigma I$ is positive semidefinite. We get

$$\theta_k^{(k)} + \sigma = \sum_{i=1}^{n} (\lambda_i + \sigma) \, \gamma_i^2 \, q_k^{(k)}(\lambda_i)^2$$

with $\lambda_i + \sigma \geq 0$ for all i. The rightmost zero of

$$f_R(t) = (t + \sigma) q_k^{(k)}(t)^2 \; - \; (\theta_k^{(k)} + \sigma)/\gamma_n^2 \tag{4.3}$$

is an upper bound for the spectrum of A. Again, we can replace γ_n by the δ that satisfies (3.2) to compute a probabilistic upper bound.

For a lower bound, we use the polynomial $q_1^{(k)}$. If A is negative semidefinite, it follows from $\theta_1^{(k)} \leq \lambda_1 \gamma_1^2 \, q_1^{(k)}(\lambda_1)^2$ (cf. (4.1)) that the unique zero $\lambda^{\text{low}} < \theta_1^{(k)}$ of

$$f_R(t) = t q_1^{(k)}(t)^2 \; - \; \theta_1^{(k)}/\gamma_1^2 \tag{4.4}$$

is a lower bound for λ_1. Otherwise one has to use a shift $\tau > 0$ such that $A - \tau I$ becomes negative semidefinite and modify f_R in (4.4) accordingly. Of course the shifts σ and τ should be chosen as small as possible to get the best results.

The bounds discussed in this section can be determined for example by Newton's method or bisection. In order to compute $f_R(t)$ one has to know the largest or smallest Ritz value and the corresponding eigenvector of the tridiagonal matrix T_k. Apart from that, the computation of $f_R(t)$ is cheap. The determination of the bounds based on Ritz polynomials will be more expensive in general than the determination

of the bounds based on the Lanczos polynomials. (The Ritz values and vectors are not needed in the latter case.)

It is interesting to compare the sharpness of the bounds based on Ritz polynomials and those based on Lanczos polynomials. For simplicity we assume that A is positive semidefinite and compare the largest zero of (4.2) with the largest zero of (3.1). (The other cases, including those where shifts are used, can be analyzed in a similar way.) Consider the function

$$g(t) = \sqrt{t/\theta_k^{(k)}}\, q_k^{(k)}(t) \;-\; 1/|\gamma_n|; \tag{4.5}$$

the largest zero of g is the largest zero of f_R from (4.2). After some straightforward calculations, using (2.6) with $j = k$, one obtains that (with f_L as in (3.1) and g as in (4.5))

$$f_L(t) \;<\; g(t) \qquad \text{for} \quad \theta_k^{(k)} \;\leq\; t \;\leq\; (1+c)\,\theta_k^{(k)}$$

and

$$f_L(t) \;>\; g(t) \qquad \text{for} \quad t \;\geq\; (1+c+c^2)\,\theta_k^{(k)},$$

where $c = \|r_k^{(k)}\|/\theta_k^{(k)}$. The quantity c can be interpreted as an approximation of the relative error for the largest eigenvalue, and c will be small after sufficiently many Lanczos steps. For small c the Ritz polynomial provides a smaller upper bound for λ_n *only* when this upper bound is very close to $\theta_k^{(k)}$—but in that case the Lanczos polynomial yields a very tight upper bound as well. Hence, it is not likely that the bounds based on Ritz polynomials are sharper than the bounds obtained with the Lanczos polynomials—unless c is large. Numerical experiments illustrating these observations can be found in section 7.

5. Spectral bounds using Chebyshev polynomials. Chebyshev polynomials are often used to obtain error bounds for the Lanczos method; cf., e.g., [2, 5, 7]. In this section we explain how these polynomials can be used to obtain probabilistic upper and lower bounds for the spectrum of A, based on computations with the Lanczos method. One type of bounds follows easily from a result by Kuczyński and Woźniakowski [5, Theorem 3].

Let $c_j(t) = \cos(j \arccos t)$ be the *Chebyshev polynomial (of the first kind)* of degree j, with the usual extension outside the interval $[-1, 1]$. The polynomial

$$u_{j-1}(t) = \tfrac{1}{j}\, c_j'(t)$$

of degree $j-1$ is a *Chebyshev polynomial of the second kind* (cf. [9, p. 7]).

In [5, Theorem 3], the following result has been derived for symmetric positive definite matrices. Let $t > 1$ and v_1 be chosen randomly from the uniform distribution over S^{n-1}. Then

$$P(\lambda_n \leq t\,\theta_k^{(k)}) \;\geq\; 1 \;-\; 2\left(\, B(\tfrac{n-1}{2}, \tfrac{1}{2})\,\sqrt{t-1}\,u_{2(k-1)}(\sqrt{t}\,)\,\right)^{-1}. \tag{5.1}$$

(B is the Euler Beta function.) The estimate (5.1) can be generalized for symmetric indefinite matrices by using a shift σ such that $A + \sigma I$ is positive definite. Probability estimates for lower bounds of λ_1 can be obtained similarly. Along these lines we can derive bounds for the spectrum of A with probability at least $1 - \varepsilon$, and these results are presented in the following theorem.

THEOREM 5.1. *Let $\varepsilon \in (0,1)$ and $\sigma, \tau \in \mathbb{R}$ be such that $A + \sigma I$ is positive semidefinite, and $A - \tau I$ is negative semidefinite. Consider for $t \geq 1$ the function*

$$f(t) \;=\; \tfrac{\varepsilon}{2}\, B(\tfrac{n-1}{2}, \tfrac{1}{2})\, \sqrt{t-1}\, u_{2(k-1)}(\sqrt{t}\,) \;-\; 1 \tag{5.2}$$

(B is the Euler Beta function) and let $t_k > 1$ be the (unique) zero of f. Furthermore, let v_1 be chosen randomly from the uniform distribution over S^{n-1}. Then

$$\lambda^{\mathrm{up}} \;=\; t_k\, \theta_k^{(k)} \;+\; (t_k - 1)\sigma \tag{5.3}$$

is an upper bound for the spectrum of A with probability at least $1 - \varepsilon$, and

$$\lambda^{\mathrm{low}} \;=\; t_k\, \theta_1^{(k)} \;-\; (t_k - 1)\tau \tag{5.4}$$

is a lower bound for the spectrum of A with probability at least $1 - \varepsilon$.

The quantity t_k can be determined numerically. The numbers $u_j(t)$ can be computed from the three-term recurrence $u_j(t) = 2tu_{j-1}(t) - u_{j-2}(t)$ for $j \geq 2$, $u_0(t) = 1$, $u_1(t) = 2t$ (see, e.g., [9, p. 40]). From (5.3) and (5.4) it is clear that the shifts σ and τ should be chosen as small as possible (cf. section 4).

Other bounds for the spectrum of A can be obtained as follows, using Chebyshev polynomials of the first kind. Let $a < b$ and $c_j(t; a, b) = c_j(1 + 2(t-b)/(b-a))$ be the Chebyshev polynomial of degree j with respect to the interval $[a, b]$. With σ such that $A + \sigma I$ is positive semidefinite, we define the polynomial $h(t) = c_{k-1}(t; -\sigma, \theta_k^{(k)})$ and the vector $x = h(A)v_1 \in K_k(A, v_1)$. From $\theta_k^{(k)}(x,x) \geq (Ax, x)$ it follows that[2] the largest zero of

$$f_C(t) \;=\; (t - \theta_k^{(k)}) c_{k-1}(t; -\sigma, \theta_k^{(k)})^2 \;-\; (\theta_k^{(k)} + \sigma)/\gamma_n^2 \tag{5.5}$$

is an upper bound for λ_n. With γ_n replaced by the δ computed from (3.2), as in the previous sections, one obtains an upper bound λ^{up} for the spectrum of A with probability at least $1 - \varepsilon$. A lower bound for the spectrum of A can be obtained in a similar way, using $\theta_1^{(k)}(x,x) \leq (Ax,x)$ with $x = c_{k-1}(A; \theta_1^{(k)}, \tau)v_1$, where τ is such that $A - \tau I$ is negative semidefinite.

In order to compare the bounds derived along these lines with those obtained from Theorem 5.1, we first replace γ_n in (5.5) by δ and scale the interval $[-\sigma, \theta_k^{(k)}]$ to $[0, 1]$. The largest zero λ^{up} of (5.5) satisfies the equality $\lambda^{\mathrm{up}} = \widehat{t}\,\theta_k^{(k)} + (\widehat{t} - 1)\sigma$, where $\widehat{t} > 1$ is the unique zero of

$$g(t) \;=\; \delta\, \sqrt{t-1}\, c_{k-1}(t; 0, 1) \;-\; 1.$$

One can show that $c_{k-1}(t; 0, 1) = c_{2(k-1)}(\sqrt{t}\,; -1, 1)$ $(= c_{2(k-1)}(\sqrt{t}\,))$ for $t > 0$. This means that we have to compare the zeros of (5.2) and those of

$$g(t) \;=\; \delta\, \sqrt{t-1}\, c_{2(k-1)}(\sqrt{t}\,) \;-\; 1. \tag{5.6}$$

The relation between δ and $\frac{\varepsilon}{2}B(\frac{n-1}{2}, \frac{1}{2})$ is given by (3.2). One has $\delta > \frac{\varepsilon}{2}B(\frac{n-1}{2}, \frac{1}{2})$ for all $\varepsilon \in (0,1)$ and $n > 3$, but $\delta \approx \frac{\varepsilon}{2}B(\frac{n-1}{2}, \frac{1}{2})$ for ε and n of practical interest. For

[2] Invoke (2.2): use $\sum \gamma_j^2 \leq 1$ where the summation is with respect to those j satisfying $\lambda_j \leq \theta_k^{(k)}$ and $h(\lambda_j)^2 \leq 1$ for $\lambda_j \leq \theta_k^{(k)}$.

instance, $(\delta - \frac{\varepsilon}{2}B(\frac{n-1}{2}, \frac{1}{2}))/\delta \approx 2.6 \cdot 10^{-5}$ for $\varepsilon = 1.0 \cdot 10^{-2}$ and $n = 10^3, 10^4, 10^5, 10^6$. On the other hand one has the relation

$$u_{2(k-1)}(\sqrt{t}\,) \;=\; 2\,c_{2(k-1)}(\sqrt{t}\,) \;+\; u_{2(k-2)}(\sqrt{t}\,) \qquad \text{for} \quad t > 0$$

(cf., e.g., [9, p. 9]) so that $u_{2(k-1)}(\sqrt{t}\,) > 2c_{2(k-1)}(\sqrt{t}\,)$ for $t \geq 1$ and this implies, together with $\delta \approx \frac{\varepsilon}{2}B(\frac{n-1}{2}, \frac{1}{2})$, that the zero of (5.6) is larger than the zero of (5.2) in most applications. Hence, the upper bound λ^{up} from (5.3) is in general smaller than the upper bound obtained from (5.5), so Theorem 5.1 will produce sharper bounds than the construction described above. These observations are supported by numerical experiments in section 7.

6. Upper bounds for the number of Lanczos steps.

6.1. Bounds based on Theorem 5.1. Theorem 5.1 can also be used to compute a probabilistic upper bound for the number of Lanczos steps necessary to obtain a Ritz value close enough to λ_n in a relative or absolute sense. These estimates can be obtained while executing the Lanczos process. First we investigate how many Lanczos steps are needed to obtain a relative error that is smaller than a prescribed tolerance `tol` with probability at least $1 - \varepsilon$.

Suppose k steps of the Lanczos method have been performed and $\theta_k^{(k)} > 0$; if $\theta_k^{(k)} \leq 0$ the eigenvalue λ_n can be arbitrarily close to zero and the relative error $(\lambda_n - \theta_m^{(m)})/\lambda_n$ cannot be estimated properly. Let $m \geq k$ and let t_m be the zero of the function f in (5.2) with k replaced by m. It follows from (5.3) that

$$\frac{\lambda_n - \theta_m^{(m)}}{\lambda_n} \;\leq\; \frac{(t_m - 1)(\theta_m^{(m)} + \sigma)}{\lambda_n} \;\leq\; \frac{(t_m - 1)(\lambda_n + \sigma)}{\lambda_n} \;\leq\; \frac{(t_m - 1)(\mu + \sigma)}{\mu} \tag{6.1}$$

holds with probability at least $1 - \varepsilon$; here $\mu = \theta_k^{(k)}$ if $\sigma \geq 0$, and $\mu \geq \lambda_n$ (e.g., $\mu = \|A\|_\infty$; one should not take a probabilistic upper bound for λ_n) whenever $\sigma < 0$; σ is as in Theorem 5.1. The requirement $(t_m - 1)(\mu + \sigma)/\mu \leq \texttt{tol}$ is equivalent to $t_m \leq 1 + \texttt{tol} \cdot \mu/(\mu + \sigma)$, and the smallest integer m, for which the quantity t_m from (5.2) satisfies

$$t_m \;\leq\; 1 + \texttt{tol} \cdot \mu/(\mu + \sigma), \tag{6.2}$$

is an upper bound for the number of Lanczos steps necessary to provide an approximation $\theta_m^{(m)}$ to λ_n that satisfies $(\lambda_n - \theta_m^{(m)})/\lambda_n \leq \texttt{tol}$ with probability at least $1 - \varepsilon$. Note that in case $\sigma > 0$ the right-hand side of (6.2) increases with k, so that the smallest number m satisfying (6.2) may decrease during the execution of the Lanczos process.

For symmetric positive definite matrices an upper bound m for the number of Lanczos steps which yields an approximation to the largest eigenvalue, such that the relative error is bounded by `tol` with probability at least $1 - \varepsilon$, has been given in [4, Theorem 4.2]: the number m should satisfy

$$1.648\,\sqrt{n}\,\mathrm{e}^{-(2m-1)\sqrt{\texttt{tol}}} \;\leq\; \varepsilon. \tag{6.3}$$

Numerical experiments show that (6.3) yields almost the same upper bound as (6.2) with $\sigma = 0$ (in most cases the bounds were exactly the same, while the difference was at most two steps); this is not surprising in view of the discussion in [5, p. 679]. However,

(6.2) can be used for indefinite matrices as well, as long as $\theta_k^{(k)} > 0$. Furthermore, for symmetric positive definite matrices smaller numbers m may be obtained when (6.2) is applied with $\sigma < 0$.

To estimate the number of steps, still necessary to have the absolute error $\lambda_n - \theta_m^{(m)} \leq \texttt{tol}$ with probability at least $1 - \varepsilon$, we proceed as follows. If m satisfies the requirement (cf. (6.1))

$$(t_m - 1)(\mu + \sigma) \;\leq\; \texttt{tol}, \tag{6.4}$$

with $\mu \geq \lambda_n$ (μ should not be a probabilistic upper bound), the equality $\lambda_n - \theta_m^{(m)} \leq \texttt{tol}$ holds with probability at least $1 - \varepsilon$. The smallest integer m satisfying (6.4) can be computed. Note that (6.4) is also valid when $\theta_k^{(k)} \leq 0$ and we do not have to distinguish between the cases $\sigma \geq 0$ and $\sigma < 0$.

Estimates for the number of Lanczos steps, to be done so that the (relative) error in the smallest eigenvalue is less than tol with probability at least $1 - \varepsilon$, can be derived in a similar way.

6.2. Upper bounds for the number of Lanczos steps in case of misconvergence. Suppose that after sufficiently many Lanczos steps the largest Ritz value seems to have converged to an eigenvalue: $\theta_k^{(k)} \approx \theta_{k-1}^{(k-1)}$ for several consecutive k and $\|r_k^{(k)}\|$ is small. It is known that $|\theta_k^{(k)} - \lambda_j| \leq \|r_k^{(k)}\|$ for a certain eigenvalue λ_j (see, e.g., [7, section 4.5]), and in most cases the largest Ritz value will have converged to the largest eigenvalue λ_n, but it may also happen that $\theta_k^{(k)}$ is not close to λ_n (misconvergence); this can happen, e.g., if $|\gamma_n|$ is very small. Below we show how one can determine a probabilistic upper bound for the number of Lanczos steps needed after which one can conclude that either $\lambda_n < \lambda$ holds for a given constant λ, or a misconvergence has been detected, i.e., $\lambda_n > \theta_k^{(k)} + \|r_k^{(k)}\|$.

Let $m > k$ and g be a polynomial of degree $m - 1$, and $x = g(A)v_1 \in K_m(A, v_1)$. If $\lambda_n > \theta_k^{(k)} + \|r_k^{(k)}\|$, the inequality

$$(Ag(A)v_1, g(A)v_1) \;>\; \left(\theta_k^{(k)} + \|r_k^{(k)}\|\right) (g(A)v_1, g(A)v_1) \tag{6.5}$$

is satisfied for a certain m and a suitable polynomial g: the Ritz polynomial $q_m^{(m)}$ maximizes the Rayleigh quotient $(Ag(A)v_1, g(A)v_1)/(g(A)v_1, g(A)v_1)$ but $q_m^{(m)}$ is not available after k steps of the Lanczos process, so we will consider another polynomial of degree $m - 1$. Rewriting (6.5) using (2.2) gives

$$\begin{aligned} \left(\lambda_n - (\theta_k^{(k)} + \|r_k^{(k)}\|)\right) \gamma_n^2 \, g(\lambda_n)^2 \quad &> \quad \left(\theta_k^{(k)} + \|r_k^{(k)}\| - \lambda_{n-1}\right) \gamma_{n-1}^2 \, g(\lambda_{n-1})^2 \\ &+ \quad \sum_{j=1}^{n-2} \left(\theta_k^{(k)} + \|r_k^{(k)}\| - \lambda_j\right) \gamma_j^2 \, g(\lambda_j)^2. \end{aligned} \tag{6.6}$$

In order to satisfy (6.6) with m as small as possible we search for a polynomial g that resembles the Ritz polynomial $q_m^{(m)}$. We have $q_k^{(k)}$ to our disposal, and therefore we take $g(t) = q_k^{(k)}(t)\, h(t)$ with h a suitable polynomial of degree $m - k$. We assume that $|\theta_k^{(k)} - \lambda_{n-1}| \leq \|r_k^{(k)}\|$ (with $\|r_k^{(k)}\|$ small); this assumption is likely to be realistic in case of a misconvergence. In order to amplify the effect of $q_k^{(k)}$ in (6.6) we choose h such that h is large in λ_n and small in $\lambda_1, \ldots, \lambda_{n-2}$. Hence $h(t) = c_{m-k}(t; \lambda_1, \lambda_{n-2})$ would

be a proper choice, but λ_1 and λ_{n-2} are not known, so we replace both quantities. Again let $-\sigma \leq \lambda_1$, and assume that $\lambda_{n-2} \leq \theta_{k-1}^{(k)} + \|r_{k-1}^{(k)}\|$; we now define

$$g(t) \;=\; q_k^{(k)}(t)\, c_{m-k}\big(t; -\sigma, \theta_{k-1}^{(k)} + \|r_{k-1}^{(k)}\|\big).$$

If we replace in the right-hand side of (6.6) the quantity $\theta_k^{(k)} + \|r_k^{(k)}\| - \lambda_{n-1}$ by $2\,\|r_k^{(k)}\|$, γ_{n-1}^2 by 1, $g(\lambda_{n-1})$ by $g(\theta_k^{(k)} + \|r_k^{(k)}\|)$, and $g(\lambda_j)$ by M, where

$$M \;=\; \max\{\, |q_k^{(k)}(t)| \;:\; -\sigma \leq t \leq \theta_{k-1}^{(k)} + \|r_{k-1}^{(k)}\| \,\},$$

then the inequality

$$\begin{aligned} \big(\lambda_n - (\theta_k^{(k)} + \|r_k^{(k)}\|)\big)\, g(\lambda_n)^2 \quad &> \quad 2\,\|r_k^{(k)}\|\, g\big(\theta_k^{(k)} + \|r_k^{(k)}\|\big)^2 / \gamma_n^2 \\ &+ \quad M^2\big(\theta_k^{(k)} + \|r_k^{(k)}\| + \sigma\big) / \gamma_n^2 \end{aligned} \tag{6.7}$$

implies (6.6) (cf. the derivation of (5.5), which is based on the same ideas). We now replace λ_n in (6.7) by the given constant λ and γ_n by δ, where $|\gamma_n| \geq \delta$ holds with probability $1 - \varepsilon$. We determine the smallest integer $m > k$ such that

$$\begin{aligned} \big(\lambda - (\theta_k^{(k)} + \|r_k^{(k)}\|)\big)\, g(\lambda)^2 \quad &> \quad 2\,\|r_k^{(k)}\|\, g\big(\theta_k^{(k)} + \|r_k^{(k)}\|\big)^2 / \delta^2 \\ &+ \quad M^2\big(\theta_k^{(k)} + \|r_k^{(k)}\| + \sigma\big) / \delta^2 \end{aligned} \tag{6.8}$$

is satisfied and perform $m - k$ Lanczos steps to obtain $\theta_m^{(m)}$. If $\theta_m^{(m)} < \theta_k^{(k)} + \|r_k^{(k)}\|$, then (6.5) and (6.6) are violated. This implies that (6.7) does not hold if, e.g., $\lambda_{n-1} \leq \theta_{k-1}^{(k)} + \|r_{k-1}^{(k)}\|$. (This will be satisfied in most cases.) From the fact that (6.7) is violated and (6.8) holds we conclude that $\lambda_n < \lambda$ holds with probability at least $1 - \varepsilon$.

If $\theta_m^{(m)} > \theta_k^{(k)} + \|r_k^{(k)}\|$, we know that a misconvergence has occurred and we do not know whether $\lambda_n < \lambda$ is satisfied or not. In the latter case one may repeat the above construction with k replaced by m.

These ideas can also be used to investigate whether or not the smallest Ritz value has converged to λ_1.

7. Numerical experiments. In this section we compare the different bounds derived in the previous sections. All experiments are carried out with Matlab on a SUN workstation. Without loss of generality we can restrict ourselves to diagonal matrices A (cf. [4, section 6]): this will reduce the influence of rounding errors on our computations. For analysis it is also convenient to know the eigenvalues and eigenvectors of A. The vector v_1 is chosen randomly from the uniform distribution over the unit sphere S^{n-1}; in [4, p. 1116] it is explained how this can be done.

In our first example we take

$$n \;=\; 1000, \quad A \;=\; \mathrm{diag}(1, 2, \ldots, 1000). \tag{7.1}$$

Let $\varepsilon = 0.01$, i.e., we are looking for bounds of the spectrum that are 99% reliable. From (3.2) one obtains $\delta = 3.97 \cdot 10^{-4}$. We checked that our randomly chosen starting vector v_1 satisfied $|\gamma_1| > \delta$ and $|\gamma_n| > \delta$, so the computed probabilistic bounds are true bounds for the spectrum of A. We have performed 100 Lanczos steps. The shifts (see sections 4 and 5) used in our computations are $\sigma = 0$ and $\tau = \lambda_n = 1000$. The results are displayed in Figure 7.1.

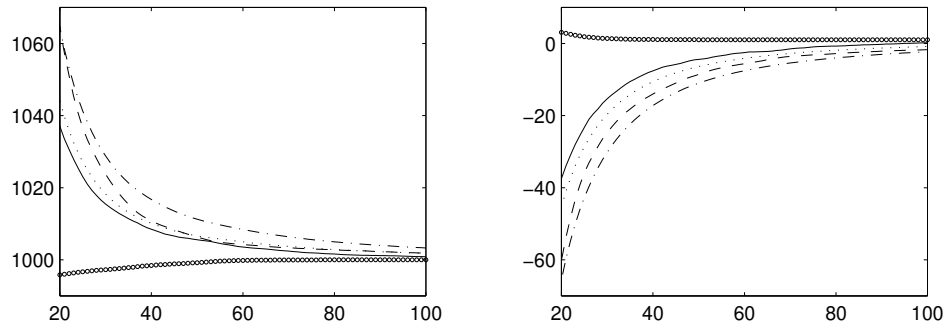

FIG. 7.1. *Probabilistic bounds for the spectrum of A. Solid curves correspond to the bounds based on Lanczos polynomials, the dashed curves correspond to bounds based on Ritz polynomials, the dotted curves correspond to bounds obtained from Theorem* 5.1*, and the dash-dotted curves correspond to* (5.5)*. The left figure shows the upper bounds and the right figure the lower bounds. The largest Ritz values (left picture) and smallest Ritz values (right picture) are indicated by small circles.*

We see that the Lanczos polynomials provide the sharpest bounds and (5.5) yields the worst bounds. In section 4 it has already been explained why the Lanczos polynomials may provide better bounds than the Ritz polynomials. Furthermore, it may not be a surprise that the Lanczos polynomials produce better bounds than the Chebyshev polynomials, because more information regarding the actual Lanczos process is used in the construction of the Lanczos polynomials. The relationship between the different bounds based on Chebyshev polynomials is in agreement with the discussion on this topic in section 5. We repeated the same experiment with other random starting vectors v_1, and the bounds behaved similarly as those displayed in Figure 7.1.

We also investigated how many Lanczos steps are needed to obtain an approximation to λ_n with a relative error less than a prescribed tolerance `tol`. Again we set $\sigma = 0$, so that (6.2) reduces to $t_m \leq 1 + \texttt{tol}$; the upper bound m for the number of Lanczos steps does not depend on the matrix A or the starting vector v_1 and can be computed in advance. The results are displayed in Table 7.1. We see that the upper bound m from (6.2) is much larger than k_1, the actual number of steps needed to obtain a relative error smaller than `tol`; this has already been observed in other examples for the upper bound obtained with (6.3) [4, 5]. We also observe that $m > k_2$, the number of steps needed to obtain $(\lambda^{\mathrm{up}} - \theta_k^{(k)})/\lambda^{\mathrm{up}} \leq \texttt{tol}$ with λ^{up} the upper bound obtained from the Lanczos polynomial of degree k. This is not surprising in view of the results from Figure 7.1, because m is related to the upper bound determined with Theorem 5.1, and these bounds are not as sharp as those based on Lanczos polynomials. Instead of performing m Lanczos steps, it may be useful in practice to compute $(\lambda^{\mathrm{up}} - \theta_k^{(k)})/\lambda^{\mathrm{up}}$ while executing the Lanczos method and check whether this quantity is smaller than `tol` or not.

We have repeated the experiments described above with $\varepsilon = 0.001$ (instead of $\varepsilon = 0.01$). The behavior of the bounds is the same as for $\varepsilon = 0.01$, but of course the bounds are further away from the spectrum of A. In order to compare the different bounds, let λ^{up} be an upper bound corresponding to $\varepsilon = 0.01$ (determined with one of the four techniques discussed here), and let $\widetilde{\lambda}^{\mathrm{up}}$ be the upper bound determined with the same technique but with $\varepsilon = 0.001$. For all four techniques we observed that $1 < (\widetilde{\lambda}^{\mathrm{up}} - \lambda_n)/(\lambda^{\mathrm{up}} - \lambda_n) < 2.2$ for $20 \leq k \leq 100$ (k denotes the number

TABLE 7.1

The second column displays the smallest integer m satisfying (6.2) with $\sigma = 0$. The smallest integer k_1 for which $(\lambda_n - \theta_k^{(k)})/\lambda_n \leq$ `tol` is shown in the third column, and the smallest integer k_2 with $(\lambda^{\mathrm{up}} - \theta_k^{(k)})/\lambda^{\mathrm{up}} \leq$ `tol`, where λ^{up} is the upper bound for λ_n obtained with the Lanczos polynomial of degree k, is listed in the fourth column of the table.

`tol`	m	k_1	k_2
$5.0 \cdot 10^{-2}$	20	5	18
$1.0 \cdot 10^{-2}$	44	11	40
$5.0 \cdot 10^{-3}$	61	17	55
$1.0 \cdot 10^{-3}$	136	48	97

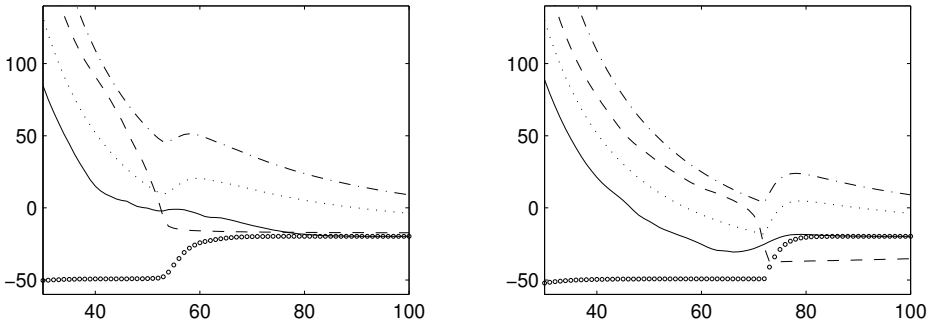

FIG. 7.2. *"Upper bounds" for the spectrum of A, obtained with two different starting vectors; the starting vector for the left picture satisfies $|\gamma_n| > \delta$, while $|\gamma_n| < \delta$ for the starting vector used to produce the right picture. Solid curves correspond to the bounds based on Lanczos polynomials, the dashed curves correspond to bounds based on Ritz polynomials, the dotted curves correspond to bounds obtained from Theorem 5.1, and the dash-dotted curves correspond to (5.5). The largest Ritz values are indicated by small circles.*

of Lanczos steps) and the same holds for $(\lambda_1 - \widetilde{\lambda}^{\mathrm{low}})/(\lambda_1 - \lambda^{\mathrm{low}})$, where the lower bounds λ^{low} and $\widetilde{\lambda}^{\mathrm{low}}$ are defined analogously. Hence the behavior of the bounds for the spectrum of A does not change much when ε is decreased from 0.01 to 0.001, which is reasonable because the polynomials used to derive the bounds grow fast outside the spectrum of A.

The second example comes from the discretization of the Laplace operator on the unit square with homogeneous Dirichlet boundary conditions. When the standard second order finite difference scheme with uniform meshwidth equal to 1/33 (in both directions) is used, one obtains a symmetric matrix of order $n = 32^2 = 1024$ with eigenvalues

$$33^2(-4 + 2\cos(\tfrac{i\pi}{33}) + 2\cos(\tfrac{j\pi}{33})), \qquad i, j = 1, 2, \ldots, 32 \tag{7.2}$$

(see, e.g., [13, section 6.5]). Let A be the diagonal matrix of order 1024 with these eigenvalues on its diagonal in increasing order. Note that A is negative definite.

We have computed bounds for the spectrum of A with $\varepsilon = 0.01$ (which yields $\delta = 3.92 \cdot 10^{-4}$ by (3.2)), $\sigma = -\lambda_1$ and $\tau = 0$, using different randomly chosen starting vectors. For most starting vectors the bounds behave similarly as in the first example and we will not consider this further. Instead we deal with two different starting vectors that provide a different behavior for the upper bounds (similar results can be obtained for lower bounds as well), and the results can be found in Figure 7.2.

In the left picture we see what can happen if $|\gamma_n|$ is small ($|\gamma_n| = 5.46 \cdot 10^{-4}$ for this example), but still greater than δ. The Ritz polynomials provide the sharpest bounds at a certain stage of the Lanczos process. At that stage the misconvergence behavior of the Lanczos process (cf., e.g., [8]) is discovered: for $37 \leq k \leq 49$ one has $|\lambda_{n-1} - \theta_k^{(k)}| \leq 0.15$ ($\lambda_{n-1} = -49.22\cdots$), and the largest Ritz values seem to converge to a number close to the (double) eigenvalue λ_{n-1}. For larger values k the Lanczos process notices the existence of a larger eigenvalue ($\lambda_n = -19.72\cdots$) and starts to converge to this eigenvalue. At the stage of the Lanczos process where the misconvergence behavior is discovered, the norm of the residual usually increases strongly (for example, $\|r_{42}^{(42)}\| = 5.65$ and $\|r_{55}^{(55)}\| = 102$) and a large residual norm may explain why the Ritz polynomials provide sharper bounds than the Lanczos polynomials (see the discussion at the end of section 4). However, for larger k the bounds based on Lanczos polynomials are again the sharpest ones. The misconvergence of the Lanczos process also causes a hump in the upper bounds obtained with the Chebyshev polynomials. Finally we note that the upper bounds obtained with the Lanczos polynomials are much sharper than those obtained with the Chebyshev polynomials.

In the right figure the behavior is shown for a starting vector for which, in contrary to our assumption, $|\gamma_n| < \delta$ ($|\gamma_n| = 3.13 \cdot 10^{-5}$). This means that the probabilistic upper bounds for λ_n need not to be true bounds, and the right picture in Figure 7.2 shows that at certain stages of the Lanczos process the Lanczos and Ritz polynomials provide bounds that are actually smaller than λ_n. The Chebyshev bounds follow the jump of the Ritz values at the discovering of the misconvergence, as in the left picture. At that stage the Lanczos bound corrects its value to give a tight bound, but the Ritz bound fails completely: the upper bound stays far below the largest Ritz value.

In the third example we illustrate the theory of section 6.2. We take

$$n = 1000, \quad A = \operatorname{diag}(1, 2, \ldots, 999, 1020). \tag{7.3}$$

We set $\sigma = -\lambda_1$ and the starting vector v_1 is chosen as follows: $\gamma_1 = \gamma_2 = \gamma_{n-2} = \gamma_{n-1} = c$, $\gamma_j = 10^{-3}c$ ($3 \leq j \leq n-3$), $\gamma_n = 10^{-6}c$, and the constant c is such that $\sum \gamma_j^2 = 1$. For $k = 34$ we have $\theta_k^{(k)} = \lambda_{n-1} - 3.20 \cdot 10^{-5}$, $\|r_k^{(k)}\| = 7.3 \cdot 10^{-2}$ so that $\lambda_n > \theta_k^{(k)} + \|r_k^{(k)}\|$. We now determine the smallest integer m for which (6.8) holds. We take $k = 34$, $\lambda = \lambda_n$, $\delta = \gamma_n = 5.0 \cdot 10^{-7}$ and $M = 2.11$. The smallest m satisfying (6.8) is $m = 69$. The Lanczos process finds the largest eigenvalue λ_n earlier: one has, e.g., $\theta_{50}^{(50)} = \lambda_n - 2.4 \cdot 10^{-2}$, $\theta_{60}^{(60)} = \lambda_n - 5.5 \cdot 10^{-5}$ and $\theta_{69}^{(69)} = \lambda_n - 2.4 \cdot 10^{-7}$. This behavior is not surprising: the Ritz polynomial $q_m^{(m)}$ maximizes the Rayleigh quotient $(Ag(A)v_1, g(A)v_1)/(g(A)v_1, g(A)v_1)$ and several other estimates used in the derivation of (6.8) may not be sharp as well.

8. Conclusion. Using the fact that the Lanczos, Ritz, and Chebyshev polynomials increase rapidly outside the smallest interval containing the Ritz values, we have derived probabilistic bounds for the spectrum of a symmetric matrix. These bounds can be computed while executing the Lanczos process. From theoretical arguments supported by experiments, we conclude that the bounds obtained with the Lanczos polynomials are generally sharper than those derived from Chebyshev polynomials. In most cases the bounds based on Lanczos polynomials are also sharper than the bounds found with Ritz polynomials—unless the norm of the corresponding residual is relatively large (which occurs if the Lanczos method suffers from a misconvergence).

The bounds corresponding to the Lanczos polynomials are cheap to compute, because the Ritz values are not required. When the Ritz values are available, it is

useful to compute the bounds based on these polynomials as well, because they might be sharper; in that case it can indicate a misconvergence of the Lanczos method. The bounds based on Theorem 5.1, using Chebyshev polynomials of the second kind, may be determined as well because they can be computed cheaply when the Ritz values are known. The bounds obtained from Theorem 5.1 are sharper than those derived from (5.5), which are based on Chebyshev polynomials of the first kind, in all cases of practical interest; hence it seems not useful to determine the latter ones.

Chebyshev polynomials may also be used to determine probabilistic bounds for the number of Lanczos steps still to be done to get bounds for the (relative) error which are smaller than the desired tolerance. However, our experiments suggest that these bounds are much larger than the actual number of Lanczos steps still necessary to get an approximation which is sufficiently accurate. From their derivation (6.1) it is clear that one cannot expect a proper estimation of the number of steps required if the bounds from Theorem 5.1 are far from sharp.

A combination of Ritz and Chebyshev polynomials can be used to obtain probabilistic bounds for the number of Lanczos steps needed such that one can decide that either the spectrum lies between certain prescribed bounds or a misconvergence has occurred.

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