Probabilistic Bounds on the Extremal Eigenvalues and Condition Number by the Lanczos Algorithm

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Abstract

We analyze the Lanczos algorithm with a random start for approximating the extremal eigenvalues of a symmetric positive definite matrix. We present some bounds on the Lebesgue measure (probability) of the sets of these starting vectors for which the Lanczos algorithm gives at the k-th step satisfactory approximations to the largest and smallest eigenvalues. Combining these bounds we get similar estimates for the condition number of a matrix.

1 Introduction

There are many algorithms for approximating the extremal eigenvalues of symmetric positive definite matrices. However, if the size n of the matrix A is large

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then algorithms based on a factorization of A usually require $\Theta(n^3)$ arithmetic operations and therefore are too expensive. On the other hand, large matrices are usually sparse and the matrix-vector multiplication Av can be performed cheaply. This suggests that algorithms based on vectors Av_i for some vectors v_i may be efficient.

The Lanczos algorithm is probably the most popular algorithm that uses a few vectors Av_i for approximating eigenvalues. At the k-th step it gives approximations to the largest eigenvalue λ_1 and to the smallest eigenvalue λ_n of A as the maximal and minimal Rayleigh quotient $(Ax,x)/(x,x)$ over nonzero vectors x from the k-th Krylov subspace $A_k = \mathrm{span}(b, Ab, \ldots, A^{k-1}b)$, where $b \neq 0$. Of course, the quality of such approximations strongly depends both on the matrix A and on the starting vector b. It is intuitively clear that a poor choice of the vector b can cause a bad behaviour of the Lanczos algorithm. The analysis of the Lanczos algorithm for a fixed vector b may be found in many books and papers, in particular, see [2],[5],[7],[8],[10],[11],[12],[14],[15], and [16]. The analysis of the Lanczos algorithm for a random vector b can be found in [9], where average case and probabilistic estimates on the largest eigenvalue are given. These estimates are independent on distribution of eigenvalues of A.

In this paper, see Section 2, we first translate the estimates of [9] for approximating the smallest eigenvalue λ_n of A. We estimate the average relative error of the Lanczos algorithm over all starting vectors b. We also provide an upper bound on the Lebesgue measure (probability) of the set of those b's from the unit ball for which the Lanczos algorithm fails to give an ε-approximation to the smallest eigenvalue at the k-th step.

In the next part of this paper, see Section 3, we present new probabilistic estimates for the Lanczos algorithm for approximating the largest and smallest eigenvalue of A. These estimates depend on distribution of eigenvalues of A.

In Section 4 we apply estimates on the smallest and largest eigenvalue to approximate the condition number, $\mathrm{cond}\, A$, of A in the two norm,

$$\mathrm{cond}\, A = \frac{\lambda_1}{\lambda_n}.$$

An approximation to the condition number of a matrix is often wanted when one deals with matrix calculations, see [1] and [4]. We provide bounds on the probability of the set of these b's for which the Lanczos algorithm gives at the k-th step the approximation κ_k of the condition number of A such that

$$\kappa_k \leq \mathrm{cond}\, A \leq \alpha\, \kappa_k$$

for any $\alpha > 1$. In many cases, only a rough approximation of $\mathrm{cond}\, A$ is needed. Then α may be quite large, say, $\alpha = 10$.

A similar problem of approximating the condition number has been considered by Dixon [3] for arbitrary matrices and by using modified power and inverse power methods. His results are computationally applicable if the vector $A^{-1}z$ can be computed cheaply for any vector z. This is the case when a factorization of A is given. However, if n is large and the matrix A is given only via the subroutine performing a matrix-vector multiplication, the vector $A^{-1}z$ is too expensive to compute. In this case, the Lanczos algorithm is preferable since it does not use the vector $A^{-1}z$.

2 Lanczos algorithm for approximating extremal eigenvalues

Let $A = A^T > 0$ be an $n \times n$ symmetric positive definite matrix with eigenvalues $\lambda_1(A) \geq \lambda_2(A) \geq ... \geq \lambda_n(A) > 0$. The k-th step of the Lanczos algorithm produces approximations to the largest and smallest eigenvalues of A defined as

$$\hat{\xi}_k = \hat{\xi}(A, b, k) = \max \left\{ \frac{(Ax, x)}{(x, x)} : x \in A_k, x \neq 0 \right\}$$

and

$$\xi_k = \xi(A, b, k) = \min \left\{ \frac{(Ax, x)}{(x, x)} : x \in A_k, x \neq 0 \right\},$$

where $A_k = \text{span}(b, Ab, ...A^{k-1}b)$ for some nonzero vector b. Without loss of generality we may assume that $b \in S_n = \{b \in \mathbb{R}^n : ||b|| = 1\}$, where $|| \cdot ||$ is the Euclidean norm of vectors.

First we discuss the error of the Lanczos approximation ξ_k to the smallest eigenvalue λ_n. Probably, the most natural error criterion is the relative error $(\xi_k - \lambda_n)/\lambda_n$. Unfortunately, it can be shown, see Remark 1 of Section 6, that even the average value of

$$\frac{\xi(A, b, k) - \lambda_n(A)}{\lambda_n(A)}$$

with respect to the uniform distribution of b is arbitrary large for some matrices A.

Therefore we have to switch to a different error criterion. One may consider the relative error with respect to the largest eigenvalue $(\xi_k - \lambda_n)/\lambda_1$, or the gap ratio, $(\xi_k - \lambda_n)/(\lambda_1 - \lambda_n)$. It turns out, see Remark 2 of Section 6, that the results both for the average error and probabilistic failure are the same for these two error criteria. Therefore we only consider the relative error with respect to the largest eigenvalue, i.e.,

$$e(A, b, k) = \frac{\xi(A, b, k) - \lambda_n(A)}{\lambda_1(A)}.$$

It is easy to see that there exist vectors b and matrices A for which the error $e(A,b,k)$ can be arbitrary close to 1. Indeed, $\hat{\xi}(A,b,k) \le \lambda_1(A)$ and $\lambda_n(A) \le \xi(A,b,k)$ and therefore

$$e(A,b,k) < \xi(A,b,k)/\hat{\xi}(A,b,k) \le 1.$$

In general, this bound cannot be improved since if b is an eigenvector belonging to the largest eigenvalue $\lambda_1(A)$ then for all k, $\xi(A,b,k) = \hat{\xi}(A,b,k) = \lambda_1(A)$, and yet $\lambda_n(A)$ can be arbitrary close to zero.

Thus, we cannot guarantee that the error of the Lanczos algorithm is smaller than 1 for all matrices A and all vectors b. Moreover, if b is orthogonal to the eigenspace generated by the smallest eigenvalue then the Lanczos error $e(A,b,k) > 0$, for all k. On the other hand, if b is not orthogonal to this subspace then $e(A,b,k) = 0$ for $k \ge m$, where m denotes the number of distinct eigenvalues of A.

It is intuitively clear that if we pick up the vector b randomly according to the uniform distribution over the unit sphere then it is very unlikely that b is orthogonal to the eigenspace of λ_n. This suggests that for any symmetric positive definite matrix, the average relative error of the Lanczos algorithm with respect to vectors b should be small for large k. Also the measure of the set of these b for which the Lanczos algorithm fails to compute a good approximation to the smallest eigenvalue should be small.

Let μ be the uniform distribution over the unit sphere S_n with $\mu(S_n) = 1$. By the average relative error of the k-th step of the Lanczos algorithm we mean

$$e^{avg}(A,k) = \int_{S_n} e(A,b,k)\, \mu(db).$$

Let

$$f^{prob}(A,k,b,\varepsilon) = \mu\left\{b \in S_n : e(A,b,k) > \varepsilon\right\}$$

denote the probability that the k-th step of the Lanczos algorithm fails to approximate the smallest eigenvalue with relative error at most ε. For brevity we call this the probabilistic failure.

We now present an upper bound on the average error of the Lanczos algorithm. It turns out that this bound is the same as this obtained in [9] for the Lanczos algorithm approximating the largest eigenvalue λ_1. For simplicity, as in [9], we assume that $n \ge 8$ and $k \ge 4$.

Theorem 1 *Let A be a symmetric positive definite matrix.*
(a) Let m denote the number of distinct eigenvalues of A. Then for $k \ge m$,

$$e^{avg}(A,k) = 0,$$

for $k \in [4, m-1]$,

$$e^{avg}(A,k) \le 0.103 \left(\frac{\ln\left(n(k-1)^4\right)}{k-1} \right)^2 \le 2.575 \left(\frac{\ln n}{k-1} \right)^2 .$$

(b) Let $p, p < n$, *denote the multiplicity of the smallest eigenvalue* λ_n, *and let* λ_{n-p} *be the second smallest eigenvalue of* A. *Then*

$$e^{avg}(A,k) \le 2.589 \sqrt{n} \left(\frac{1 - \sqrt{(\lambda_{n-p} - \lambda_n)/(\lambda_1 - \lambda_n)}}{1 + \sqrt{(\lambda_{n-p} - \lambda_n)/(\lambda_1 - \lambda_n)}} \right)^{k-1} .$$

Proof: For the proof it is enough to apply Theorem 3.2 of [9] to the matrix $B = \lambda_1 I - A$. $\square$

Theorem 1 states that $e^{avg}(A,k) = 0$ for $k \ge m$, which means that the Lanczos algorithm converges in $m, m \le n$, steps. For $k < m$ the average relative error is bounded by $2.6 \ln^2 n/(k-1)^2$. We do not know if this bound is sharp. Numerical tests suggest that for some matrices A we have

$$e^{avg}(A,k) = \Theta(k^{-2}).$$

Part (b) of Theorem 1 contains nonasymptotic bounds in terms of the gap ratio of the matrix A.

We now turn to the bound on the probabilistic failure of the Lanczos algorithm for the smallest eigenvalue.

Theorem 2 *Let* A *be a symmetric positive definite matrix.*
(a) Let m *denote the number of distinct eigenvalues of* A. *Then for any* $\varepsilon \in (0, 1]$,

$$f^{prob}(A,k,\varepsilon) = 0, \quad for \;\; k \ge m,$$
$$f^{prob}(A,k,\varepsilon) \le 1.648 \sqrt{n}\, e^{-(2k-1)\sqrt{\varepsilon}}, \quad for \;\; any \;\; k .$$

(b) Let $p, p < n$, *denote the multiplicity of the smallest eigenvalue* λ_n *and let* λ_{n-p} *be the second smallest eigenvalue of* A. *Then for* $\varepsilon > 0$,

$$f^{prob}(A,k,\varepsilon) \le 1.648 \sqrt{n/\varepsilon} \left(\frac{1 - \sqrt{(\lambda_{n-p} - \lambda_n)/(\lambda_1 - \lambda_n)}}{1 + \sqrt{(\lambda_{n-p} - \lambda_n)/(\lambda_1 - \lambda_n)}} \right)^{k-1} .$$

Proof: For the proof it is enough to apply Theorem 4.2 of [9] for the matrix $B = \lambda I - A$. $\square$

Theorem 2 gives upper bounds on the probabilistic failure of the Lanczos algorithm for approximating the smallest eigenvalue. For $k \geq m$, $f^{prob}(A, k, \varepsilon) = 0$, which means that the Lanczos algorithm converges in m steps, where $m \leq n$. For $k < m$, the probabilistic failure is bounded by $1.65\sqrt{n}\, e^{-(2k-1)\sqrt{\varepsilon}}$.

Suppose we wish to find an ε-approximation to the smallest eigenvalue with a δ-failure, i.e., $f^{prob}(A, k, \varepsilon) \leq \delta$. Then from Theorem 2 we conclude that we have to perform at most roughly

$$k = \lceil \ln(3n/\delta^2) \,/\, (4\sqrt{\varepsilon}) \rceil$$

steps. Note a weak dependence on δ and the strong dependence on ε.

3 Bounds dependent on distribution of eigenvalues

In this section we provide new probabilistic bounds on extemal eigenvalues which depend on distribution of eigenvalues of the matrix A. For any symmetric positive definite matrix A consider two sets

$$L_k = \{b \in S_n : \hat{\xi}(A, b, k) \leq \lambda_1(A) \leq \theta \hat{\xi}(A, b, k)\} \quad \text{for} \quad \theta > 1$$

and

$$M_k = \{b \in S_n : \eta\, \xi(A, b, k) \leq \lambda_n(A) \leq \xi(A, b, k)\} \quad \text{for} \quad \eta < 1.$$

Obviously, the first inequality in the set L_k and the second one in M_k hold for any vector $b \in S_n$. We now find lower bounds on $\mu(L_k)$ and $\mu(M_k)$. We begin with $\mu(L_k)$.

Theorem 3 *For any symmetric positive definite matrix A let m denote the number of distinct eigenvalues of A. Then*

for $k \geq m$, or $\theta \geq cond\, A$,

$$\mu(L_k) = 1,$$

and

for $k < m$ and $1 < \theta < cond\, A$,

$$\mu(L_k) \geq 1 - \frac{2\,\Gamma((n-j)/2 + 1)}{\sqrt{\pi}\,\Gamma((n-j+1)/2)}\, \frac{1}{\sqrt{\theta - 1}\; U_{2(k-1)}(\sqrt{\theta})} \geq$$

$$1-\frac{2\,\Gamma(n/2)}{\sqrt{\pi}\,\Gamma((n-1)/2)}\,\frac{1}{\sqrt{\theta-1}\;U_{2(k-1)}(\sqrt{\theta})}$$

where the index j is defined by $\lambda_j \le \lambda_1/\theta < \lambda_{j-1}$, $2 \le j \le n$, U_k is the Chebyshev polynomial of the second kind of degree k and Γ is the Euler Γ-function.

Proof: The idea of the proof is similar to the proof of Theorem 4.2 in [9]. Let $b=\sum_{i=1}^n b_i v_i$, where $v_i, i=1,\ldots,n$, are orthonormal eigenvectors of A. Consider the set

$$L_k' = S_n - L_k = \{b \in S_n : \lambda_1(A) > \theta\hat{\xi}(A,b,k)\}.$$

Then we have

$$L_k' = \left\{ b \in S_n : \lambda_1 > \theta \sup_{P\in\mathcal{P}_k} \frac{\sum_{i=1}^n \lambda_i P^2(\lambda_i) b_i^2}{\sum_{i=1}^n b_i^2 P^2(\lambda_i)} \right\},$$

where $\mathcal{P}_k$ denotes the set of nonzero polynomials of degree smaller than k.

Assume that $k \ge m$. Then the set $\{\lambda_1, ..., \lambda_n\}$ contains m distinct elements $\{t_1, ..., t_m\}$, $\lambda_1 = t_1 > ... > t_m$ and for the polynomial $P(x)=\prod_{i=2}^m (x-t_i)$ the supremum takes the value λ_1 for $b_1 \neq 0$. Thus, since $\theta \ge 1$,the set L_k' is empty with probability 1. Thus $\mu(L_k)=1$ as claimed.

Assume now that $k < m$. Then after simple calculations we get

$$L_k' = \left\{ b \in S_n : \sup_{P\in\mathcal{P}_k} \frac{\sum_{i=1}^n b_i^2 P^2(\lambda_i)(\theta\lambda_i - \lambda_1)}{\sum_{i=1}^n b_i^2 P^2(\lambda_i)} < 0 \right\}.$$

Observe that the supremum is negative iff the nominator is negative. Thus

$$L_k' = \{b \in S_n : \sup_{P\in\mathcal{P}_k} \sum_{i=1}^n b_i^2 P^2(\lambda_i)(\theta\lambda_i - \lambda_1) < 0\}.$$

Assume that $\theta \ge \operatorname{cond} A$. Then $\theta\lambda_i - \lambda_1 \ge 0$ for all $i = 1, 2, ..., m$ and the set L_k' is empty. Thus $\mu(L_k) = 1$ as claimed.

Assume now that $\theta < \operatorname{cond} A$. Note that using a continuity argument we may restrict ourselves to polynomials for which $P(\lambda_1) \neq 0$. Let $x_i = \lambda_i/\lambda_1$ and $Q(x) = P(\lambda_1 x)/P(\lambda_1)$. Then $x_i \in (0,1]$ and

$$L_k' = \{b \in S_n : \sup_{Q\in\mathcal{P}_k(1)} \sum_{i=1}^n b_i^2 Q^2(x_i)(\theta x_i - 1) < 0\},$$

where $\mathcal{P}_k(\alpha) = \{w \in \mathcal{P}_k : w(\alpha) = 1\}$.

Clearly, for any polynomial $Q \in \mathcal{P}_k(1)$ we have

$$L'_k \subset \{b \in S_n : \sum_{i=1}^{n} b_i^2 Q^2(x_i)(\theta x_i - 1) < 0\}.$$

From the definition of the index j we have $\theta x_j \leq 1 < \theta x_{j-1}$ and

$$\mu(L'_k) \leq \mu\{b \in S_n : \sum_{i=j}^{n} b_i^2 Q^2(x_i)(1 - \theta x_i) > \sum_{i=1}^{j-1} b_i^2 Q^2(x_i)(\theta x_i - 1)\} \leq$$

$$\mu\{b \in S_n : \sum_{i=j}^{n} b_i^2 Q^2(x_i)(1 - \theta x_i) > b_1^2(\theta - 1)\} \leq$$

$$\mu\{b \in S_n : \sum_{i=j}^{n} b_i^2 \max_{x \in [0, x_j]} [Q^2(x)(1 - \theta x)] > b_1^2(\theta - 1)\}.$$

Let

$$\omega_k(x_j, \theta) = \inf_{Q \in \mathcal{P}_k(1)} \max_{x \in [0, x_j]} Q^2(x)(1 - \theta x).$$

We now find an upper bound on $\omega_k(x_j, \theta)$. It is easy to check that

$$\omega_k(x_j, \theta) = \inf_{Q \in \mathcal{P}_k(\theta)} \max_{x \in [0, \gamma]} Q^2(x)(1 - x),$$

where $\gamma = \theta x_j \leq 1$. Let

$$\hat{Q}(x) = \frac{U_{2(k-1)}(\sqrt{x})}{U_{2(k-1)}(\sqrt{\theta})},$$

where $U_{2(k-1)}$ is the Chebyshev polynomial of the second kind of degree $2(k-1)$. Since $U_{2(k-1)}$ is even, $\hat{Q}$ is a polynomial of degree $k-1$. Obviously $\hat{Q}(\theta) = 1$, so $\hat{Q} \in \mathcal{P}_k(\theta)$. Then

$$\omega_k(x_j, \theta) \leq \max_{x \in [0, \gamma]} \frac{U^2_{2(k-1)}(\sqrt{x})}{U^2_{2(k-1)}(\sqrt{\theta})} (1 - (\sqrt{x})^2) = \frac{1}{U^2_{2(k-1)}(\sqrt{\theta})} =: \sigma,$$

since $U_{2(k-1)}(t)\sqrt{1 - t^2} \leq 1$ and this inequality is sharp, see e.g., [13]. We note in passing that if $\gamma > \cos^2(\pi/(2(2k-1)))$ then $\omega_k(x_j, \theta) = \sigma$, (see the proof of Theorem 4.2 of [9]). Clearly,

$$\mu(L'_k) \leq \mu\{b \in S_n : \sum_{i=j}^{n} b_i^2 > \beta^{-2} b_1^2\},$$

where $\beta^2 = \sigma/(\theta - 1)$.

Let c_i be the Lebesgue measure of the unit ball in $\mathbb{R}^i$, $c_i = \pi^{i/2}/\Gamma(1 + i/2)$. As in [9], see Remark 7.2 of [9], instead of integrating over the unit sphere

S_n we may integrate over the unit ball $||b|| \leq 1$ with respect to normalized Lebesgue measure,

$$\mu\{b \in S_n : \sum_{i=j}^{n} b_i^2 > \beta^{-2}\, b_1^2\} = \frac{1}{c_n} \int_{||b|| \leq 1} \chi(\sum_{i=j}^{n} b_i^2 > \beta^{-2}\, b_1^2) db,$$

where $\chi(Z)$ is the characteristic function of the set Z. Then

$$\mu(L_k') \leq \frac{1}{c_n} \int_{[-1,1]} \int_{\sum_{i=j}^{n} b_i^2 > \beta^{-2} b_1^2} \int_{\sum_{i=2}^{j-1} b_i^2 \leq 1 - b_1^2 - \sum_{i=j}^{n} b_i^2} db\ .$$

The last integral is the measure of the ball in $\mathbb{R}^{j-2}$, and

$$\mu(L_k') \leq \frac{2\, c_{j-2}}{c_n} \int_{[0,1]} \int_{\sum_{i=j}^{n} b_i^2 > \beta^{-2} b_1^2} (1 - b_1^2 - \sum_{i=j}^{n} b_i^2)_+^{(j-2)/2} =$$

$$\frac{2\, c_{j-2}}{c_n} \int_{[0,1]} \int_{\sum_{i=j}^{n} b_i^2 < 1} \chi(\sum_{i=j}^{n} b_i^2 > \beta^{-2}\, b_1^2)(1 - b_1^2 - \sum_{i=j}^{n} b_i^2)_+^{(j-2)/2}\ .$$

Changing variables by $t = \sqrt{\sum_{i=j}^{n} b_i^2}$ and $x = b_1$, the formula 4.642 of [6] yields

$$\mu(L_k') \leq \frac{2\, c_{j-2}\ c_{n-j+1}}{c_n}(n - j + 1)$$

$$\int_0^1 \int_0^1 \chi(t^2 > \beta^{-2} x^2)\,(1 - x^2 - t^2)_+^{(j-2)/2}\, t^{n-j}\, dx\, dt\ \leq$$

$$\frac{2\, c_{j-2}\ c_{n-j+1}}{c_n}(n - j + 1) \int_0^1 \int_0^{\beta t} (1 - x^2 - t^2)_+^{(j-2)/2}\, t^{n-j}\, dx\, dt\ \leq$$

$$\frac{2\, c_{j-2}\ c_{n-j+1}}{c_n}(n - j + 1)\beta \int_0^1 (1 - t^2)^{j/2-1}\, t^{n-j+1}\, dt =$$

$$\frac{c_{j-2}\ c_{n-j+1}}{c_n}(n - j + 1)\beta B((n - j + 2)/2, j/2)\,,$$

where $B(i,j) = \Gamma(i)\Gamma(j)/\Gamma(i+j)$ is the beta function. Finally,

$$\mu(L_k') \leq \frac{\beta\,(n - j + 1)\Gamma((n - j)/2 + 1)}{\sqrt{\pi}\,\Gamma((n - j + 1)/2 + 1)},$$

and

$$\mu(L_k') \leq \frac{2\,\Gamma((n - j)/2 + 1)}{\sqrt{\pi}\,\Gamma((n - j + 1)/2)\,\sqrt{\theta - 1}\ U_{2(k-1)}(\theta)}$$

which completes the first inequality of Theorem 3.

Let

$$s_j = \frac{2\,\Gamma((n - j)/2 + 1)}{\sqrt{\pi}\,\Gamma((n - j + 1)/2)}.$$

Then

$$\mu(L_k) \geq 1 - s_j/\sqrt{\theta - 1}/U_{2(k-1)}(\sqrt{\theta}),$$

and since s_j is a decreasing function of j, the proof is completed. $\square$

We now explain how Theorem 3 is related to Theorem 4.2 of [9]. Observe that using the formula (13) of [9] for $n \geq 8$ we get

$$s_n = 2/\pi < s_{n-1} = 1 < \ldots < s_2 = \frac{2\,\Gamma(n/2)}{\sqrt{\pi}\,\Gamma((n-1)/2)} \leq 0.824\sqrt{n-1}.$$

Take $j = 2$. Then from Theorem 3 it follows that for any $\theta > 1$ we have

$$\mu\{b \in S_n : \lambda_1(A) \leq \theta\,\hat{\xi}(A, b, k)\} \geq 1 - 0.824\,\frac{\sqrt{n-1}}{\sqrt{\theta - 1}\;U_{2(k-1)}(\sqrt{\theta})}.$$

Let $\theta = 1/(1-\varepsilon)$ for some $\varepsilon \in (0, 1)$. Then

$$\mu(L_k) = \mu\{b \in S_n : \frac{\lambda_1(A) - \hat{\xi}(A, b, k)}{\lambda_1(A)} < \varepsilon\} \geq$$

$$1 - 0.824\,\frac{\sqrt{(n-1)\,\varepsilon}}{\sqrt{1-\varepsilon}\,U_{2(k-1)}(1/\sqrt{1-\varepsilon}\,)}.$$

Observe that

$$U_{2(k-1)}(1/\sqrt{1-\varepsilon}) = 0.5\sqrt{(1-\varepsilon)/\varepsilon}\;\left(\left(\frac{1+\sqrt{\varepsilon}}{\sqrt{1-\varepsilon}}\right)^{2k-1} - \left(\frac{1-\sqrt{\varepsilon}}{\sqrt{1-\varepsilon}}\right)^{2k-1}\right),$$

and after some calculations we obtain

$$U_{2(k-1)}(1/\sqrt{1-\varepsilon}) = 0.5\sqrt{(1-\varepsilon)/\varepsilon}\,c^{-1}\,(1 - c^2),$$

where $c = ((1-\sqrt{\varepsilon})/(1+\sqrt{\varepsilon}))^{k-1/2}$. Thus we get

$$\mu\{b \in S_n : \frac{\lambda_1(A) - \hat{\xi}(A, b, k)}{\lambda_1(A)} < \varepsilon\} \geq 1 - 1.648\sqrt{n-1}\,c\,(1-c^2)^{-1}.$$

Recall that Theorem 4.2 of [9] yields

$$\mu\{b \in S_n : \frac{\lambda_1(A) - \hat{\xi}(A, b, k)}{\lambda_1(A)} < \varepsilon\} \geq 1 - 1.648\sqrt{n}\,c \geq 1 - 1.648\sqrt{n}\,e^{-(2k-1)\sqrt{\varepsilon}}.$$

Thus for $j = 2$ Theorem 3 gives essentially the same bound as Theorem 4.2. For $j > 2$ the bound of Theorem 3 is better. Usually we do not know the index j. However, for large θ or for many eigenvalues close to the largest eigenvalue λ_1, the index j is large and s_j becomes independent on n. In this case $\mu(L_k)$ goes quickly to 1 even for very large n.

We now find a lower bound on the probability of the set M_k. Recall that

$$M_k = \{b \in S_n : \eta\, \xi(A,b,k) \le \lambda_n(A) \le \xi(A,b,k)\} \quad \text{for} \quad \eta \le 1.$$

Theorem 4 *For any symmetric positive definite matrix A let m denote the number of distinct eigenvalues. Then we have*

$$\mu(M_k) = 1 \quad \mathit{for} \quad k \ge m \quad \mathit{or} \quad \eta \le 1/\mathit{cond}\, A$$

and

for any $k < m$ and any $1/\mathit{cond}\, A < \eta < 1$,

$$\mu(M_k) \ge 1 - \frac{2\,\Gamma(j/2)}{\sqrt{\pi}\,\Gamma((j-1)/2)}$$

$$\sqrt{\frac{\eta\ \mathit{cond}\, A - 1}{1-\eta}}\ U^{-1}_{2(k-1)}\left(\sqrt{1 + (1-\eta)/(\eta\ \mathit{cond}\, A - 1)}\,\right) \ge$$

$$1 - \frac{2\,\Gamma(n/2)}{\sqrt{\pi}\,\Gamma((n-1)/2)} \sqrt{\frac{\eta\ \mathit{cond}\, A - 1}{1-\eta}}\ U^{-1}_{2(k-1)}\left(\sqrt{1 + (1-\eta)/(\eta\ \mathit{cond}\, A - 1)}\,\right)$$

where the index j is defined by $\lambda_n/\lambda_{j-1} < \eta \le \lambda_n/\lambda_j,\ \ 2 \le j \le n$.

Proof: The proof of Theorem 4 is similar to the proof of Theorem 3. As before we consider the set M'_k,

$$M'_k = S_n - M_k = \{b \in S_n : \lambda_n(A) < \eta\, \xi(A,b,k)\}.$$

Using the same notation and reasoning as in the proof of Theorem 3 we can easily get

$$\mu(M'_k) = \mu\{b \in S_n : \inf_{Q \in \mathcal{P}_k(1)} \sum_{i=1}^{n} b_i^2 Q^2(x_i)(\eta x_i - 1) > 0\},$$

where now $x_i = \lambda_i/\lambda_n$, $1 = x_n \le x_{n-1} \le \ldots \le x_1 = \mathrm{cond}\, A$. Clearly, if $k \ge m$ or if $\eta \le \lambda_n/\lambda_1 = 1/x_1$ then $\mu(M'_k) = 0$ and the first part of Theorem 4 is proved.

Assume now that $k < m$ and $1/x_1 < \eta < 1$. We have $1/x_{j-1} < \eta \le 1/x_j$, and as in Theorem 3 we can show that

$$\mu(M_k') \le \mu\{b \in S_n : \sum_{i=1}^{j-1} b_i^2 Q^2(x_i)(\eta x_i - 1) > b_n^2 Q^2(1)(1-\eta)\},$$

for any $Q \in \mathcal{P}_k(1)$. Hence

$$\mu(M_k') \le \mu\{b \in S_n : \sigma \sum_{i=1}^{j-1} b_i^2 > b_n^2(1-\eta)\},$$

where

$$\sigma = \inf_{Q\in\mathcal{P}_k(1)} \max_{x\in[1/\eta, \mathrm{cond}\, A]} (Q^2(x)(\eta x - 1)).$$

Changing variables by $y = (\mathrm{cond}\, A - x)/(\mathrm{cond}\, A - 1/\eta)$ we get

$$\sigma = (\xi - 1) \inf_{Q\in\mathcal{P}_k(\delta)} \max_{y\in[0,1]} (Q^2(y)(1-y)),$$

where $\xi = \eta \,\mathrm{cond}\, A$ and $\delta = (\xi-\eta)/(\xi-1) > 1$. Using the estimate of $\omega_k(x_j, \theta)$ from the proof of Theorem 3 we obtain

$$\sigma \le \frac{\xi - 1}{U_{2(k-1)}^2(\sqrt{\delta})},$$

and consequently

$$\mu(M_k') \le \mu\{b \in S_n : \sum_{i=1}^{j-1} b_i^2 > U_{2(k-1)}^2(\sqrt{\delta})\,(1-\eta)/(\xi-1)\; b_n^2\}.$$

As in the proof of Theorem 3 we thus conclude that

$$\mu(M_k') \le \frac{2\,\Gamma(j/2)}{\sqrt{\pi}\,\Gamma((j-1)/2)} \sqrt{\frac{\eta\,\mathrm{cond}\, A - 1}{1-\eta}}\, U_{2(k-1)}^{-1}\left(\sqrt{1 + \frac{1-\eta}{\eta\,\mathrm{cond}\, A - 1}}\right),$$

which completes the first inequality of Theorem 4. To get the second one it is enough to observe that

$$s_j' = \frac{2\,\Gamma(j/2)}{\sqrt{\pi}\,\Gamma((j-1)/2)} < \frac{2\,\Gamma(n/2)}{\sqrt{\pi}\,\Gamma((n-1)/2)} = s_n'$$

for $j = 2, 3, ..., n$. Hence the proof is completed. $\square$

We now show how Theorem 4 is related to Theorem 2. Clearly, for $n \ge 8$ we have

$$s_2' = 2/\pi < s_3' = 1 < ... < s_n' = \frac{2\,\Gamma(n/2)}{\sqrt{\pi}\,\Gamma((n-1)/2)} \le 0.824\,\sqrt{n-1}.$$

Take $j = n$. Then from Theorem 4 it follows that for any η: $0 < \eta < 1$ we have

$$\mu\{b \in S_n : \eta\, \xi(A,b,k) \le \lambda_n(A)\} \ge 1 - 0.824\sqrt{(n-1)\,z}\;/U_{2(k-1)}(\sqrt{1+1/z}\;),$$

where $z = (\eta \,\mathrm{cond}\, A - 1)/(1-\eta)$. Let $\eta = 1/(1+\varepsilon\,\mathrm{cond}\,A)$ for some $\varepsilon \in (0,1)$. Then

$$\mu(M_k) = \mu\{b \in S_n : \frac{\xi(A,b,k) - \lambda_n(A)}{\lambda_1(A)} < \varepsilon\} \ge$$

$$1 - 0.824\sqrt{(n-1)(1-\varepsilon-1/\mathrm{cond}\,A)/\varepsilon}\;/U_{2(k-1)}(\sqrt{1+\varepsilon/(1-\varepsilon-1/\mathrm{cond}\,A}\;).$$

Since

$$U_{2(k-1)}(\sqrt{1+1/z}\,) = 0.5\sqrt{z}\,c^{-1}\,(1-c^2),$$

where now $c = (\,(1-\sqrt{\varepsilon/(1-1/\mathrm{cond}\,A)})/(1+\sqrt{\varepsilon/(1-1/\mathrm{cond}\,A)})\,)^{k-1/2}$ (see the proof of Theorem 4), we get

$$\mu\{b \in S_n : \frac{\xi(A,b,k) - \lambda_n(A)}{\lambda_1(A)} < \varepsilon\} \ge 1 - 1.648\sqrt{n-1}\,c\,(1-c^2)^{-1}.$$

Recall that Theorem 2 yields

$$\mu\{b \in S_n : \frac{\xi(A,b,k) - \lambda_n(A)}{\lambda_1(A)} < \varepsilon\} \ge 1 - 1.648\sqrt{n}\left(\frac{1-\sqrt{\varepsilon}}{1+\sqrt{\varepsilon}}\right)^{k-1/2}$$

$$\ge 1 - 1.648\sqrt{n}\,e^{-(2k-1)\sqrt{\varepsilon}}.$$

Thus even for $j = n$ Theorem 4 gives, in general, a better bound than Theorem 2. Let us stress that if we know that j is small, which is the case for small η or cluster eigenvalues, the bound of Theorem 4 is even more attractive than that of Theorem 2.

The bound given in Theorem 4 depends on the condition number of A which is not known. We can avoid this difficulty if we know an upper bound of the condition number of the matrix A. The following corollary holds (the proof is the same as the proof of Theorem 4).

Corollary 1 *Let M be any number, $M > 1$. For any symmetric positive definite matrix A of the size $n \ge 8$ such that cond$A \le M$ let m denote the number of distinct eigenvalues. Then we have*

$$\mu(M_k) = 1 \quad for \quad k \ge m \quad or \quad \eta \le 1/M$$

and

$$\mu(M_k) \ge 1 - \frac{2\,\Gamma(n/2)}{\sqrt{\pi}\,\Gamma((n-1)/2)}\sqrt{\frac{\eta M - 1}{1-\eta}}\,U^{-1}_{2(k-1)}(\sqrt{1+(1-\eta)/(\eta M-1)}\,)$$

$$\geq 1 - 0.824\sqrt{n}\sqrt{\frac{\eta M - 1}{1-\eta}}\, U^{-1}_{2(k-1)}(\sqrt{1+(1-\eta)/(\eta M - 1)}\,)$$

for $k < m$ and $1/M < \eta < 1$.

4 Estimating the condition number λ_1/λ_n

We now apply the results of the previous section and Theorem 4.2 of [9] to estimate the condition number of a matrix. Since $\hat{\xi}_k = \hat{\xi}(A, b, k)$ and $\xi_k = \xi(A, b, k)$ are the Lanczos approximations to the largest and to the smallest eigenvalues of A correspondingly, we estimate the condition number *cond* A by $\kappa_k = \hat{\xi}_k/\xi_k$, $\kappa_k \leq \mathrm{cond}\, A$. Clearly, the quality of this estimation depends on the starting vector b. We now give a lower bound on the measure of the set of vectors b for which $\mathrm{cond}\, A \leq \alpha\kappa_k$ for $\alpha > 1$. Let

$$Z_k = \{b \in S_n : \mathrm{cond}\, A \leq \alpha\kappa_k\}.$$

Then we have

Theorem 5 *Let A be a symmetric positive definite matrix A and let m denote the number of distinct eigenvalues of A. Then*

$$\mu(Z_k) = 1, \quad for \ \ k \geq m,$$

for any k and any $\alpha > 1$

$$\mu(Z_k) \geq 1 - 1.648\sqrt{n} \inf_{0<t<\frac{1-1/\alpha}{\kappa_k}} \phi(t),$$

where

$$\phi(t) = e^{-(2k-1)\sqrt{1-t\kappa_k-1/\alpha}} + e^{-(2k-1)\sqrt{t}}.$$

Proof: The proof for $k \geq m$ follows immediately from the corresponding parts of Theorem 4.2 in [9] and Theorem 2. Assume now that k is any integer. Consider the sets

$$W = \{b \in S_n : \lambda_1 \leq \hat{\xi}_k/(1-\varepsilon_1)\}$$

and

$$\hat{Y} = \{b \in S_n : \lambda_n \geq \xi_k - \varepsilon_2\lambda_1\}$$

for any $\varepsilon_1, \varepsilon_2 \in (0, 1)$. From Theorem 4.2 of [9] it follows that

$$\mu(W) > 1 - \phi_1(\varepsilon_1) = 1 - 1.648\sqrt{n}\, e^{-\sqrt{\varepsilon_1}(2k-1)},$$

while from Theorem 2 we have

$$\mu(\hat{Y}) > 1 - \phi_2(\varepsilon_2) = 1 - 1.648\,\sqrt{n}\,e^{-(2k-1)\sqrt{\varepsilon_2}}.$$

Let

$$Y = \{b \in S_n : \lambda_n \geq \xi_k - \varepsilon_2 \frac{\hat{\xi}_k}{1-\varepsilon_1}\},$$

for ε_1 and ε_2 such that $\xi_k - \varepsilon_2 \frac{\hat{\xi}_k}{1-\varepsilon_1} > 0$. Then $W \cap \hat{Y} \subset Y$ ($W \cap \hat{Y} \subset W \cap Y$) and

$$\mu(W \cap Y) \geq \mu(W \cap \hat{Y}) = \mu(W) + \mu(\hat{Y}) - \mu(W \cup \hat{Y}) >$$
$$1 - \phi_1(\varepsilon_1) + 1 - \phi_2(\varepsilon_2) - 1 = 1 - (\phi_1(\varepsilon_1) + \phi_2(\varepsilon_2)).$$

Thus, since $\xi_k - \varepsilon_2 \frac{\hat{\xi}_k}{1-\varepsilon_1} > 0$, we have

$$\mu\{b \in S_n : \text{cond}\, A \leq \frac{1}{1 - \varepsilon_1 - \varepsilon_2 \kappa_k} \kappa_k\} > 1 - (\phi_1(\varepsilon_1) + \phi_2(\varepsilon_2)).$$

Maximizing the right-hand side of the last inequality under constraints

$$0 < \varepsilon_1 < 1,\ 0 < \varepsilon_2 < 1,\ 0 < \varepsilon_2/(1-\varepsilon_1) < 1/\kappa_k,\ 1 - \varepsilon_1 - \varepsilon_2\kappa_k = 1/\alpha$$

we complete the proof by taking $\varepsilon_2 = t$ and $\varepsilon_1 = 1 - 1/\alpha - t\kappa_k$. $\square$

The first part of Theorem 5 states that the Lanczos algorithm at the m-th step recovers the condition number of a matrix with probability one. This confirms our intuition that for sufficiently large k the Lanczos algorithm may fail only on a set of measure zero.

The second part of Theorem 5 gives a lower bound on the probability that the condition number of a matrix is not greater than $\alpha\,\kappa_k$ for $\alpha > 1$. It may happen that this bound is negative, especially when κ_k grows too rapidly with respect to k (see Table 1 where the approximated minimum of the function ϕ is showed) or for α close to one or n huge. However for $k \geq n$, $\kappa_k = \text{cond}\, A$ with probability one no matter what was happening with κ_k for $k < n$.

It is difficult to calculate the exact value of the infimum of the function ϕ in the interval $(0, \frac{1-1/\alpha}{\kappa_k})$ (note that k, α and κ_k are known), but it is quite easy to find a satisfactory approximation of it numerically. Indeed, having calculated κ_k we can perform a few steps of the bisection method applied to the first derivative ϕ' on the interval $(0, (1-1/\alpha)/\kappa_k)$. Table 1 displays an approximation of the minimum of the function ϕ for $\alpha = 10$ for some values of k and κ_k. The first column contains values of k. The next four columns show an approximation of the minimum of ϕ, $\phi_{min}(k, \kappa_k)$, for $\kappa_k = \sqrt{k},\ \kappa_k = k,\ \kappa_k = k^2$ and $\kappa_k = k^3$ respectively.

k	$\phi_{min}(k,\sqrt{k})$	$\phi_{min}(k,k)$	$\phi_{min}(k,k^2)$	$\phi_{min}(k,k^3)$
10	0.00025	0.00612	0.184	0.585
20	0.0000002	0.00039	0.163	0.667
30	0	0.00005	0.158	0.714
40	0	0.000009	0.156	0.745
50	0	0.000002	0.154	0.768
60	0	0.0000006	0.153	0.785
70	0	0.0000002	0.153	0.799
80	0	0.0000001	0.152	0.810

Table 1

To apply Theorem 5 for $\mu(Z_k)$ we have to compute κ_k. It is possible to estimate $\mu(Z_k)$ without computing κ_k. It can be done by combining Theorem 3 and Theorem 4. Indeed, observe that for $\alpha = \theta/\eta$ we have $L_k \cap M_k \subseteq Z_k$, and

$$\mu(Z_k) \geq \mu(L_k \cap M_k) = \mu(L_k) + \mu(M_k) - \mu(L_k \cup M_k) \geq$$
$$\mu(L_k) + \mu(M_k) - 1.$$

Thus, to find a lower bound on $\mu(Z_k)$, we need to find lower bounds on $\mu(L_k)$ and $\mu(M_k)$. Applying Theorems 3 and 4 we get the following theorem.

Theorem 6 *For any symmetric positive definite matrix A let m denote the number of distinct eigenvalues. Let α be any number, $\alpha > 1$. Then for any numbers θ and η such that $\theta > 1$, $0 < \eta < 1$ and $\alpha = \theta/\eta$ we have*

$$\mu(Z_k) = 1 \quad for \quad k \geq m \quad or \quad (\theta \geq cond A \quad and \quad \eta \leq 1/cond\,A)$$

and

$$\mu(Z_k) \geq 1 - \frac{2\,\Gamma((n-j)/2+1)}{\sqrt{\pi}\,\Gamma((n-j+1)/2)\,\sqrt{\theta-1}\,U_{2(k-1)}(\sqrt{\theta})}$$
$$-\frac{2\,\Gamma(i/2}{\sqrt{\pi}\,\Gamma((i-1)/2)}\sqrt{\frac{\eta\,cond\,A-1}{1-\eta}}U^{-1}_{2(k-1)}(\sqrt{1+(1-\eta)/(\eta\,cond\,A-1)}\,),$$

where $\theta < cond\,A$ or $\eta > 1/cond\,A$ and j and i satisfy:

$$\lambda_j \leq \lambda_1/\theta < \lambda_{j-1}, \quad 2 \leq j \leq n \quad and \quad \lambda_n/\lambda_{i-1} < \eta \leq \lambda_n/\lambda_i, \quad 2 \leq i \leq n.$$

Theorem 6 yields a bound on the measure of the set Z_k which depends on the indices i and j as well as cond A. Usually they are unknown. However, the indices i, j can be replaced by n, and cond A can be replaced by an upper bound M. Using the second inequality of Theorem 3 and Corollary 1, we then get the following theorem.

Theorem 7 *Let A be any symmetric positive definite matrix of the size $n \geq 8$ such that $\operatorname{cond} A \leq M$. Then under assumptions of Theorem 6 we have*

$$\mu(Z_k) = 1 \quad for \quad k \geq m \quad or \quad (\theta \geq M \quad and \quad \eta \leq 1/M\,)$$

and

$$\mu(Z_k) \geq 1 - \frac{2\,\Gamma(n/2)}{\sqrt{\pi}\,\Gamma((n-1)/2)}\,(\,(\theta-1)^{-1/2}\,U^{-1}_{2(k-1)}(\sqrt{\theta}) +$$

$$+\sqrt{\frac{M\eta-1}{1-\eta}}\,U^{-1}_{2(k-1)}(\sqrt{1+(1-\eta)/(M\eta-1)}\,)\,)\ \geq$$

$$1 - 0.824\sqrt{n}\left(\,(\theta-1)^{-1/2}\,U^{-1}_{2(k-1)}(\sqrt{\theta})\,+\sqrt{z}\,U^{-1}_{2(k-1)}(\sqrt{1+1/z}\,)\right),$$

for $1 < \theta < M$ or $1/M < \eta < 1$, where $z = (M\eta-1)/(1-\eta)$.

Note that the better bound M on $\operatorname{cond} A$ is given, the better bound on the measure of the set Z_k is obtained.

Obviously, any number $\alpha > 1$ can be decomposed as $\alpha = \theta/\eta$, $M > \theta > 1$, $1/M < \eta < 1$ in many ways. To get the best probability bound one can maximize it over θ and η under the constrains $\alpha = \theta/\eta$, $M > \theta > 1$, $1/M < \eta < 1$. It can easily be done numerically.

5 Numerical results

We tested several matrices with many pseudo-random starting vectors b. Without loss of generality, see [9], we restricted ourselves only to diagonal matrices. Vectors b were generated in the same way as in [9]. The purpose of the numerical tests was, in particular, to verify the sharpness of the bound of Theorem 1 and to check the quality of the bounds of Theorems 5 and 7. We first report our results for the matrix of dimension $n = 250$ with eigenvalues

$$\lambda_k = 1 + \cos\frac{(2k-1)\pi}{2n},\ k = 1,\ldots,250.$$

Hence, λ_k's are the shifted zeros of the Chebyshev polynomial of the first kind of degree 250. This distribution of eigenvalues seems to be difficult for the Lanczos algorithm. We have selected several values of ε and ten pseudo-random vectors b and for each of them we run the Lanczos algorithm for $k = 1,\ldots,k^*$, where k^* was the minimal k for which the relative error $e(A,b,k)$ was no greater than ε. We compared the relative error with k^{-2}. For each b and k we observed

$$0.20 \leq e(A,b,k)\,k^2 \leq 1.23.$$

In Table 2 we report the average errors achieved after $(k-1)$ steps of the Lanczos algorithm for some values of k displayed in the first column. The second column shows the average errors defined as

$$\varepsilon^{ave} = \frac{1}{10} \sum_{i=1}^{10} e(A, b_i, k),$$

where b_i is the i-th pseudo-random vector. The third column contains upper bounds on the Lanczos errors from Theorem 1 , i.e.,

$$\varepsilon^{up} = 0.103 \left(\frac{\ln (n(k-1)^4)}{k-1} \right)^2 .$$

The fourth column shows the ratio $r_1 = \varepsilon^{up}/\varepsilon^{ave}$, while the last one displays how r_1 is related to the (probably unnecessary) factor $r_2 = r_1/\ln^2(n(k-1)^4)$ in the theoretical bound.

$k-1$	ε^{ave}	ε^{up}	r_1	r_2
10	0.005276	0.2235	42.36	0.195
20	0.001379	0.0789	57.22	0.187
30	0.000688	0.0419	60.87	0.166
40	0.000387	0.0265	68.53	0.167
50	0.000244	0.0185	75.76	0.184
60	0.000165	0.0137	83.23	0.174
70	0.000145	0.0107	73.95	0.146

Table 2

Small changes in the last column of Table 2 may suggest that the error of the Lanczos algorithm for the matrix with Chebyshevian distribution of eigenvalues behaves like k^{-2} and the factor roughly $\ln^2(n(k-1)^4)$ is probably an overestimate in the upper bound.

Table 3 shows for five values of ε how many steps were needed to achieve the relative error no greater than ε. The first row contains the values of ε, the second one the average number k^{ave} of performed steps with $k^{ave} = \sum_{i=1}^{10} k(A, b_i)/10$, where $k(A, b_i)$ was the number of steps needed for the pseudo-random vector b_i. The third row indicates the minimal $k = k^{up}$ such that

$$0.103 \left(\frac{\ln(n(k-1)^4)}{k-1} \right)^2 \ \le \ \varepsilon,$$

which is one of the two theoretical bounds of Theorem 1 for the Lanczos algorithm. The fourth row presents the ratio $r = k^{up}/k^{ave}$.

ε	$1_{10}-3$	$7.5_{10}-4$	$5_{10}-4$	$2.5_{10}-4$	$2.0_{10}-4$
k^{ave}	35.5	41	49.9	65.5	69.2
k^{up}	287	339	429	638	724
r	8.08	8.27	8.6	9.74	10.46

Table 3

Note that the theoretical bound exceeds the actual value by a factor of at most 11. Observe also that all k^{up}'s are greater than $n = 250$ and the second bound of Theorem 1 gives a better estimate.

We also tested matrices of dimension 250 with other distributions of eigenvalues in the interval $(0, 2)$. The following distributions were tested:

- the quadratic, $\lambda_i = 2\,(1 - i/251)^2$ and $\lambda_i = 2\,(1 - (i/251)^2)$,
- the uniform, $\lambda_i = 2\,(1 - i/251)$,
- the logarithmic, $\lambda_i = 2\,\log(252 - i)/\log 252$,
- the expotential, $\lambda_i = 2\,e^{-\sqrt[3]{i}}$, $\lambda_i = 1 + e^{-i}$, $i = 1, \ldots, 250$.

For all these matrices we have observed faster convergence to the smallest eigenvalue than for the matrix with Chebyshevian distribution. For some matrices the difference was significant.

We were also interested in checking the quality of the bound on the condition number presented in Theorems 5 and 7. As before, for each matrix we selected several pseudo-random vectors b and ran the Lanczos algorithm both for the smallest and for the largest eigenvalues with $k = 1, 2, \ldots, k^*$, where k^* was the minimal k for which this algorithm gave approximations with a prescribed accuracy. In all tests, i.e., for all matrices, all starting vectors and all k, the number α was fixed to be equal to 10. We now describe some tests on the bound of Theorem 5. The infimum of the function ϕ from Theorem 5 was computed numerically. The matrices most intensively tested were the matrices which arise as discretizations of a two dimensional Laplace operator. We first report some results for the matrix A of the size 256 (16 points in each direction). The condition number of this matrix is $116.461\ldots$. Table 4 shows some results obtained for ten pseudo-random vectors $b_i, i = 1, 2, \ldots, 10$. The first column contains twelve values of k. The next one indicates the average of the condition numbers obtained for vectors b_i, i.e. ,

$$\mathrm{cond}^{ave} = \frac{1}{10} \sum_{i=1}^{10} \hat{\xi}(A, b_i, k)/\xi(A, b_i, k),$$

while the third one shows the standard deviation $\sigma_{10}^{\mathrm{cond}}$ of the empirical condition number. The last two columns concern the bound on the probability given in Theorem 5, namely the average, $prob^{ave}$, and the standard deviation, σ_{10}^{prob}, of the bound of probability for the vectors b_i.

$k-1$	cond^{ave}	$\sigma_{10}^{\mathrm{cond}}$	$prob^{ave}$	σ_{10}^{prob}
5	21.533	5.997	-2.692	0.913
10	57.481	19.465	-1.178	0.885
15	85.442	21.391	-0.230	0.448
20	102.793	19.770	0.349	0.199
25	111.690	12.074	0.701	0.062
30	116.163	0.782	0.866	0.002
35	116.451	0.018	0.944	0
40	116.457	0.0017	0.977	0
45	116.457	0.0017	0.990	0
50	116.457	0.0017	0.996	0
55	116.457	0.0017	0.998	0
60	116.457	0.0017	0.999	0

Table 4

Observe that the first three elements of the fourth and fifth column should be replaced by zeros but we think it is interesting to see how the bound of Theorem 5 increases with k.

Table 4 shows that the average bound on the probability is close to 1 for k larger than 30. Note that for these k's the average condition number is nearly equal to the exact condition number of this matrix. We stress that the corresponding standard deviations are very small. For k smaller than 20 the average bound of the probability was quite small (or even negative) although for $k \geq 7$ and all pseudo-random vectors b_i the computed condition number, $\hat{\xi}_k/\xi_k$ satisfied: $\hat{\xi}_k/\xi_k \leq \mathrm{cond}\, A \leq 10\,\hat{\xi}_k/\xi_k$.

For the matrix A of the size 1024 (32 points in each direction) the corresponding table is the following one (the condition number of this matrix is 440.6886...):

$k-1$	cond^{ave}	$\sigma_{10}^{\mathrm{cond}}$	$prob^{ave}$	σ_{10}^{prob}
5	24.195	1.625	−7.338	0.496
10	66.358	8.380	−4.223	0.743
15	123.881	30.943	−3.053	1.256
20	181.720	56.008	−2.115	1.312
25	233.467	71.980	−1.347	1.093
30	279.179	80.741	−0.752	0.834
35	321.968	82.043	−0.314	0.588
40	375.354	62.747	−0.049	0.316
45	420.228	32.238	0.191	0.120
50	434.603	11.736	0.452	0.033
55	439.324	2.548	0.643	0.005
60	440.310	0.684	0.771	0.001
65	440.556	0.156	0.854	0
70	440.622	0.042	0.907	0

Table 5

Note that for $k > 8$ and all pseudo-random vectors b_i the computed condition number, $\hat{\xi}_k/\xi_k$ satisfied: $\hat{\xi}_k/\xi_k \leq \mathrm{cond}\, A \leq 10\,\hat{\xi}_k/\xi_k$, while the corresponding probability is positive for $k > 42$. This suggests that the lower bound on the probability given in Theorem 5 is rather poor for this matix.

We have also tested matrices with distributions of eigenvalues described earlier. For instance for Chebyshevian distribution the bound on the probability was negative (usually between -7 and -3). Note that for this matrix the approximations $\hat{\xi}_k/\xi_k$ of the condition number satisfying: $\hat{\xi}_k/\xi_k \leq \mathrm{cond}\, A = 101371 \leq 10\,\hat{\xi}_k/\xi_k$ were observed (on average) for k larger than 70. Let us stress that for all pseudo-random vectors b_i the numbers k^* were smaller than 80. Similar results were observed for the quadratic distribution of eigenvalues $\lambda_i = 2\,(1 - i/251)^2$, $i = 1, \ldots, 250$ (for this matrix the condition number is equal to 62500).

For other distributions we obtained better results. Note that the condition numbers were much smaller than the condition number for the Chebyshevian distribution. For instance for the logarithmic distribution the bound on the probability was on average greater than 0.9 for k larger than 9. The condition number of this matrix is 7.9715 and for each k we got the empirical condition number $\hat{\xi}_k/\xi_k$ satisfying $\hat{\xi}_k/\xi_k \leq \mathrm{cond}\, A = 7.9715 \leq 10\,\hat{\xi}_k/\xi_k$.

We now turn to the bounds for the condition number of a matrix given by Theorem 7. As before, the number α was fixed to 10 and θ and η were chosen to maximize (numerically) the second bound of Theorem 7. Table 6 shows some results for the matrix A of the size 256 which arises as a discretization of a two dimensional Laplace operator got for ten pseudo-random vectors $b_i, i =$

$1, ..., 10$ (compare with Table 4). The first three columns contain values defined in the description of Table 4. The last two columns display the bound on the probability given in Theorem 7 with $M = \text{cond}\, A$ ($prob(1)$) and $M = 100\, \text{cond}\, A$ ($prob(100)$) respectively.

$k-1$	cond^{ave}	$\sigma_{10}^{\text{cond}}$	$prob(1)$	$prob(100)$
5	21.307	6.444	-1.401	-45.042
10	55.979	19.397	0.800	-21.575
15	84.451	20.874	0.984	-13.191
20	103.419	19.902	0.9988	-8.792
25	111.676	12.069	0.99991	-6.057
30	116.162	0.781	0.99999	-4.202
35	116.447	0.020	1	-2.881
40	116.456	0.013	1	-1.915
45	116.456	0.013	1	-1.198
50	116.456	0.013	1	-0.661
55	116.456	0.013	1	-0.256
60	116.456	0.013	1	-0.050
65	116.456	0.013	1	0.2390
70	116.456	0.013	1	0.4236
75	116.456	0.013	1	0.5869
80	116.456	0.013	1	0.6871
85	116.456	0.013	1	0.7627
90	116.456	0.013	1	0.8202
95	116.456	0.013	1	0.8636
100	116.456	0.013	1	0.8968
110	116.456	0.013	1	0.9407
120	116.456	0.013	1	0.9660
130	116.456	0.013	1	0.9804
140	116.456	0.013	1	0.9888
150	116.456	0.013	1	0.9935

Table 6

We observed that the probability bound of Theorem 7 with $M = \text{cond}\, A$ is larger than 0.9 for $k \geq 12$. The fact that relatively early we can be almost sure that the Lanczos algorithm produces a good approximation to the condition number of this matrix is due to the fact that we have used a perfect bound for the condition number, namely the condition number itself. To contrast this we see that the probability bound gets much worse (the fifth column) if we use Theorem 7 with $M = 100\,\mathrm{cond}\,A$. Let us stress that for all $k \geq 7$ the approximations $\kappa_k = \hat{\xi}_k/\xi_k$ to the condition number satisfied

$$\kappa_k \leq \mathrm{cond}\,A \leq 10\kappa_k.$$

For the matrix A of the size 1024 (32 points in each direction) the corresponding table is as follows (compare with Table 5):

$k-1$	cond^{ave}	$\sigma_{10}^{\mathrm{cond}}$	$prob(1)$	$prob(100)$
10	66.358	8.380	−2.695	−88.952
20	181.720	56.008	0.758	−42.527
30	279.179	80.741	0.984	−26.218
40	375.354	62.747	0.999	−17.680
50	434.603	11.736	1	−12.381
60	440.310	0.684	1	−8.801
70	440.622	0.042	1	−6.256
80	440.641	0.023	1	−4.410
90	440.641	0.023	1	−3.047
100	440.641	0.023	1	−2.035
110	440.641	0.023	1	−1.278
120	440.641	0.023	1	−0.710
130	440.641	0.023	1	−0.283
140	440.641	0.023	1	0.035
150	440.641	0.023	1	0.276
160	440.641	0.023	1	0.455
170	440.641	0.023	1	0.591
180	440.641	0.023	1	0.693
190	440.641	0.023	1	0.769
200	440.641	0.023	1	0.827
210	440.641	0.023	1	0.870
220	440.641	0.023	1	0.902
230	440.641	0.023	1	0.926

Table 7

We now briefly report some results for other matrices. The size of the matrices was chosen to be equal to 250. For the quadratic distribution of eigenvalues $\lambda_i = 2(1 - i/251)^2$, $i = 1, ..., 250$ in the interval $(0, 2)$ we obtained much worse probability bounds. For $M = \mathrm{cond}\,A$ the bounds were negative up to the 140-th step and they reached 0.786 at the 201-st step. For $M = 100\,\mathrm{cond}\,A$ the bounds were all negative and at the 201-st step they reached

-25.02. Note that for all $k > 71$, the approximated condition numbers κ_k satisfy

$$\kappa_k \leq \operatorname{cond} A = 62500 \leq 10\kappa_k.$$

Slightly worse results were obtained for the shifted Chebyshev distribution of the eigenvalues. Better results were obtained for matrices with the quadratic distribution of eigenvalues

$$\lambda_i = 2(1-(i/251)^2),\ i = 1, ..., 250.$$

The condition numbers of this matrix is equal to 125.749... . Only 5 steps were needed to get the desired approximations to the condition number of this matrix. The probability bounds for $M = \operatorname{cond} A$ and $M = 100 \operatorname{cond} A$ were positive after 9 and 62 steps. They were greater than 0.5 after 11 and 76 steps, and greater than 0.9 after 15 and 106 steps, respectively.

6 Final Remarks

Remark 1

We now report a result for the average relative error with recpect to the smallest eigenvalue. That is, define

$$e^{avg}_{min}(A,k) = \int_{S_n} \frac{\xi(A,b,k)-\lambda_n}{\lambda_n}\,\mu(db).$$

We will show that this error is unbounded in the class of all symmetric positive definite matrices. Indeed, using the same notation as in the proof of Theorem 3 we get

$$e^{avg}_{min}(A,k) = \frac{1}{c_n\,\lambda_n}\int_{B_n} \inf_{P\in\mathcal{P}_k} \frac{\sum_{i=1}^{n-1}(\lambda_i-\lambda_n)b_i^2P^2(\lambda_i)}{\sum_{i=1}^{n} b_i^2P^2(\lambda_i)}\,db.$$

Assume that the matrix A has n distinct eigenvalues and let $\lambda_i - \lambda_n \geq \delta > 0$ for $i = 1, \ldots, n-1$. Then we have

$$e^{avg}_{min}(A,k) \geq \frac{\delta}{c_n\,\lambda_n}\int_{B_n}\left(1-\sup_{P\in\mathcal{P}_k}\frac{b_n^2P^2(\lambda_n)}{\sum_{i=1}^{n} b_i^2P^2(\lambda_i)}\right)db = \frac{\delta}{c_n\,\lambda_n}\,\phi(A,k),$$

where

$$\phi(A,k) = \int_{B_n}\left(1-\sup_{P\in\mathcal{P}_k}\frac{b_n^2P^2(\lambda_n)}{\sum_{i=1}^{n} b_i^2P^2(\lambda_i)}\right)db.$$

Note that the function ϕ is shift invariant,i.e., $\phi(A+\alpha I, k) = \phi(A, k)$ for all $\alpha \in \mathbb{R}$, and $\phi(A, k) > 0$ for $k \leq n-1$. Take now the matrix $A - \alpha I$, where $\alpha < \lambda_n$. Then for $\alpha \to \lambda_n$ we have

$$e_{min}^{avg}(A - \alpha I, k) \geq \frac{\delta}{c_n(\lambda_n - \alpha)} \phi(A, k) \to +\infty.$$

Thus for any k no greater than $n-1$ and any positive number M there exists a symmetric positive definite matrix A such that

$$e_{min}^{avg}(A, k) > M.$$

Remark 2

We now consider a gap ratio as the error criterion instead of the relative error with respect to the largest eigenvalue, i.e., we want to find ξ such that

$$\frac{\xi - \lambda_n(A)}{\lambda_1(A) - \lambda_n(A)} < \varepsilon.$$

Note that the gap ratio for the Lanczos algorithm approximating the smallest eigengalue is shift invariant, i.e.,

$$\frac{\xi(A+\alpha\, I, b, k) - \lambda_n(A + \alpha\, I)}{\lambda_1(A+\alpha\, I) - \lambda_n(A+\alpha\, I)} = \frac{\xi(A, b, k) - \lambda_n(A)}{\lambda_1(A) - \lambda_n(A)}.$$

Using a continuity argument we can conclude that the bounds given in Theorems 1 and 2 hold, since

$$\frac{\xi(A) - \lambda_n(A)}{\lambda_1(A) - \lambda_n(A)} = \frac{\xi(B) - \lambda_n(B)}{\lambda_1(B) - \lambda_n(B)},$$

where $B = A - \lambda_n\, I,\ B = B^T \geq 0$ with $\lambda_n(B) = 0$).

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