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ON SOLVING INDEFINITE SYMMETRIC LINEAR SYSTEMS BY MEANS OF THE LANCZOS METHOD

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A new result on the distribution of Ritz values at two consecutive steps of a simple Lanczos process is proved. It is used in showing why the Lanczos method effectively solves indefinite symmetric linear systems in computer arithmetic. The result of a numerical experiment is presented.

1. INTRODUCTION

The Lanczos algorithm [1. ch. 13] uses a three-term recurrence to construct an orthonormal basis for the Krylov space generated by a symmetric matrix A and a nonzero starting vector φ. Paige made a detailed analysis of the Lanczos algorithm in finite precision arithmetic [2, 3]. A number of subsequent works have dealt with further analysis, on the possible use of the Lanczos vectors for computing eigenvalues, in quadrature formulae and for computing functions of the form $f(A)\varphi$, where f is some smooth function of A (see, e.g., [4–8]). In this paper, we show why the Lanczos vectors produced in finite precision arithmetic can be effectively used for solving indefinite linear systems. The new analysis makes use of the results about the spectra of the tridiagonal matrices produced by the Lanczos algorithm in finite precision arithmetic [3, 7, 9].

Throughout this paper we assume real symmetric matrices, although the results apply to the complex Hermitian case as well.

In Section 2, we list a few known results on the Lanczos method.

In Section 3, we prove that the tridiagonal symmetric matrix T_k, yielded by the simple Lanczos process, has condition number less than about the square of the condition number of A, at least, at every other step k. This enables the Lanczos approximation to the solution of the indefinite linear system to be well-defined.

In Section 4, we give an error bound for the approximate solution of the system valid, at least, at every other step. The proof exploits tridiagonal symmetric extensions of T_k with desirable spectral properties. The bound proved is adaptive to the spectrum of the original matrix.

In Section 5, we present a numerical example showing that the estimate is not necessarily valid at *every* Lanczos step.

The norm symbol $\|\ldots\|$ denotes the Euclidean norm of vectors and the spectral one of matrices. The angular brackets $\langle , \rangle$ stand for the scalar product in the Euclidean space.

2. PRELIMINARIES

Given a symmetric $N \times N$ matrix A, an initial nonzero N-vector φ, and its normalization $q_1 = \varphi/\|\varphi\|$, the Lanczos algorithm constructs successive orthonormal vectors $q_{j+1}, j = 1, 2, \ldots$, using the following formulae:

$$v_j = Aq_j - \alpha_j q_j - \beta_{j-1} q_{j-1}, \quad q_{j+1} = v_j/\beta_j, \tag{2.1}$$

$$\alpha_j = \langle Aq_j - \beta_{j-1} q_{j-1}, q_j \rangle, \quad \beta_j = \|v_j\|, \quad j = 1, 2, \ldots, \quad \beta_0 = 0. \tag{2.2}$$

If this recurrence is run for k steps and Q_k is the N by k matrix whose columns are the Lanczos vectors $q_1, \ldots, q_k$, then the recurrence can be written in matrix form as

$$AQ_k = Q_k T_k + \beta_k q_{k+1} e_k^{\mathrm{T}}, \tag{2.3}$$

where T_k is the k by k tridiagonal matrix of recurrence coefficients

$$T_k = \begin{pmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{k-1} \\ & & \beta_{k-1} & \alpha_k \end{pmatrix} \tag{2.4}$$

and e_k is the k^{th} unit k-vector $(0, \ldots, 0, 1)^{\mathrm{T}}$.

To approximate the matrix function $u = A^{-1}\varphi$, the Lanczos method chooses the approximate solution u_k to be a certain linear combination of the first k Lanczos vectors:

$$u_k = \|\varphi\| Q_k T_k^{-1} e_1. \tag{2.5}$$

We shall refer to this choice of u_k as the *Lanczos approximation*. If T_k is singular, then the Lanczos approximation u_k is undefined.

When the Lanczos algorithm is implemented in finite precision arithmetic, the recurrence (2.1) is slightly perturbed. It is replaced by a recurrence that can be written in matrix form as

$$AQ_k = Q_k T_k + \beta_k q_{k+1} e_k^{\mathrm{T}} + F_k, \tag{2.6}$$

where the columns of F_k represent the rounding errors at each step. Let ε denote the machine precision and define

$$\varepsilon_0 \equiv 2(N+4)\varepsilon, \quad \varepsilon_1 \equiv 2(7 + m\| \, |A| \, \| / \|A\|)\varepsilon, \tag{2.7}$$

where m is the maximum number of nonzeros in any row of A. Under the assumptions

$$\varepsilon_0 < 1/12, \quad k(3\varepsilon_0 + \varepsilon_1) < 1, \tag{2.8}$$

and ignoring higher order terms in ε, Paige [2] showed that the rounding error matrix F_k satisfies

$$\|F_k\| \le \sqrt{k}\varepsilon_1 \|A\|. \tag{2.9}$$

Paige also showed that the coefficient formulas in (2.2) hold to a close approximation so that, in particular,

$$\left|q_j^{\mathrm{T}} q_j - 1\right| \le 2\varepsilon_0, \tag{2.10}$$

$$\beta_j \le \|A\|[1 + (2N+6)\varepsilon + j(3\varepsilon_0 + \varepsilon_1)]. \tag{2.11}$$

We shall assume throughout that the inequalities (2.8) and hence (2.9)–(2.11) hold.

Although the individual roundoff terms are tiny, their effect on the recurrence (2.6) may be great. The Lanczos vectors may lose orthogonality and even become linearly dependent. The recurrence coefficients generated in finite precision arithmetic may be quite different from those that would be generated in exact arithmetic.

Though the computed Lanczos vectors may not be orthogonal, one might still consider using them to approximate $A^{-1}\varphi$, exploiting the formula (2.5). In practice, when solving linear systems, one does not compute the Lanczos vectors and then apply formula (2.5), because this would require saving all of the Lanczos vectors. Other methods of implicitly constructing the Lanczos vectors and updating the approximate solution require far less storage. Still, it is reasonable to try and separate the effects of roundoff on the three-term Lanczos recurrence from that on other aspects of the evaluation of (2.5).

This approach is advocated, for example, in [10], where it is suggested that a standard implementation of the conjugate gradient algorithm for solving symmetric positive definite linear systems will probably be most affected by roundoff in the (implicit) construction of the Lanczos vectors and recurrence coefficients. For indefinite problems with formula (2.5), one must be more careful about the implementation. Since the tridiagonal matrix T_k may be singular or nearly singular at some steps, the iterates produced at those steps will be likely inaccurate. If new iterates are updated from those, then the large errors will propagate, even if subsequent tridiagonal matrices are well-conditioned. Different implementations, such as ones based on the SYMMLQ method of Paige and Saunders [11] and a number of look-ahead type methods [12], appear to overcome this difficulty. At steps where the tridiagonal matrix is well-conditioned, these methods appear to generate iterates that approximately satisfy (2.5), even if an earlier iterate was inaccurate due to a singular or ill-conditioned tridiagonal matrix.

From here on, then, we shall *assume* that the iterate u_k satisfies (2.5) exactly, where Q_k and T_k are the vectors and tridiagonal matrix produced by a finite precision Lanczos computation.

3. THE RITZ VALUES AT CONSECUTIVE LANCZOS STEPS

When the matrix A is nonsingular but indefinite, then it is possible that a tridiagonal matrix T_k generated by the (exact or finite precision) Lanczos algorithm will be singular. We shall show, however, that at least one of two consecutive tridiagonal matrices, T_k or T_{k-1}, must have a spectrum whose distance from the origin (divided by $\|A\|$) is greater than about the *square* of the distance from the spectrum of A to the origin (divided by $\|A\|$). Some related results were established in [13] and by B. Parlett (personal communication).

We shall use a general result about the eigenvalues of a symmetric tridiagonal matrix T_k and its $k-1$ by $k-1$ principal submatrix T_{k-1}, which can be found, for example, in [3]. We then combine this with another result of Paige [3, p. 249] concerning the distance from the spectrum of A to an eigenvalue of the tridiagonal matrix T_k produced by a finite precision Lanczos computation.

Lemma 1. *Let T_k be of the form* (2.4) *with $\beta_j > 0$, $j = 1, 2, \ldots, k-1$. Let θ be an eigenvalue of T_k with normalized eigenvector s and let μ be an eigenvalue of T_{k-1} with normalized eigenvector v. Then*

$$\theta - \mu = \frac{\beta_{k-1}(e_{k-1}^{\mathrm{T}})(e_k^{\mathrm{T}} s)}{s^{\mathrm{T}}\hat{v}}, \tag{3.1}$$

where $\hat{v}$ is the vector v with a 0 appended at the bottom.

Proof. The result follows from equating two expressions for $s^{\mathrm{T}} T_k \hat{v}$:

$$s^{\mathrm{T}} T_k \hat{v} = \theta(s^{\mathrm{T}}\hat{v}) = s^{\mathrm{T}}[\hat{v}\mu + \beta_{k-1}(e_{k-1}^{\mathrm{T}} v)e_k] = \mu(s^{\mathrm{T}}\hat{v}) + \beta_{k-1}(e_{k-1}^{\mathrm{T}} v)(e_k^{\mathrm{T}} s).$$

Since s and $\hat{v}$ each have norm one, it follows from (3.1) that

$$|\theta - \mu| \ge \beta_{k-1}\left|(e_{k-1}^{\mathrm{T}} v)(e_k^{\mathrm{T}} s)\right|. \tag{3.2}$$

Lemma 2 (see [3]). *Let T_k be the tridiagonal matrix produced at step k of a finite precision Lanczos computation satisfying* (2.6)–(2.11). *Let $d(z) \equiv \min_{i=1,2,\ldots,N}|z - \lambda_i|$ denote the distance from a point z to the spectrum of A. Then for any eigenvalue θ of T_k,*

$$d(\theta) \le \max\{2.5(\delta_k + k^{1/2}\|A\|\varepsilon_1),\ [(k+1)^3 + \sqrt{3}k^2]\|A\|\varepsilon_2\}, \tag{3.3}$$

where $\delta_k \equiv \beta_k|e_k^{\mathrm{T}} s|$ and s is a normalized eigenvector of T_k corresponding to θ.

Combining the results of Lemmas 1 and 2, we obtain the following theorem showing that (when A is scaled to have norm 1) at least one of $|\theta|$ and $|\mu|$ must be greater than or equal to a moderate fraction of the *square* of the distance from the spectrum of A to the origin.

Theorem 1. *Using the notation of Lemma 2, assume that the tridiagonal matrix T_k is generated by a finite precision Lanczos computation satisfying* (2.6)–(2.11). *Assume also that $\|A\| = 1$ and that neither θ nor μ is very close to an eigenvalue of A; namely,*

$$\min\{d(\theta), d(\mu)\} > [(k+1)^3 + \sqrt{3}k^2]\varepsilon_2. \tag{3.4}$$

Then

$$\max\{|\theta|, |\mu|\} \ge \frac{d(0)^2 - c\varepsilon_1}{d(0) + 6.25\beta_k + \sqrt{(6.25\beta_k)^2 + 12.5\beta_k d(0) + c\varepsilon_1}}, \tag{3.5}$$

where $c \le 12.5k^{1/2} + O(\varepsilon)$. Under the assumption

$$90.625[(2N+6)\varepsilon + k(3\varepsilon_0 + \varepsilon_1)] + 12.5k^{1/2}\varepsilon_1 \le 8.5, \tag{3.6}$$

and dropping higher order terms in ε, inequality (3.5) *can be replaced by*

$$\max\{|\theta|, |\mu|\} \ge \frac{d(0)^2}{16} - \frac{12.5}{16}k^{1/2}\varepsilon_1. \tag{3.7}$$

Proof. Applying (3.3) at steps k and $k-1$ gives

$$d(\theta)d(\mu) \le 6.25\beta_k|e_k^{\mathrm{T}} s|\ \beta_{k-1}|e_{k-1}^{\mathrm{T}} v| + c\varepsilon_1,$$

where

$$c = 6.25[\beta_{k-1}|e_{k-1}^{\mathrm{T}} v|k^{1/2} + \beta_k|e_k^{\mathrm{T}} s|(k-1)^{1/2} + k^{1/2}(k-1)^{1/2}\varepsilon_1], \tag{3.8}$$

and substituting the bound in (3.2) gives

$$d(\theta)d(\mu) \le 6.25\beta_k|\theta - \mu| + c\varepsilon_1.$$

Let τ denote $\max\{|\theta|, |\mu|\}$. Then $|\theta - \mu| \le 2\tau$ and both $d(\theta)$ and $d(\mu)$ are greater than or equal to $d(0) - \tau$. We therefore have

$$[d(0) - \tau]^2 \le 12.5\beta_k\tau + c\varepsilon_1,$$

from which it follows, upon solving for τ, that

$$\tau \ge d(0) + 6.25\beta_k - \sqrt{(6.25\beta_k)^2 + 12.5\beta_k d(0) + c\varepsilon_1},$$

or, equivalently, (3.5) holds. Using (2.11) to bound β_k in (3.8), it can be seen that $c \le 12.5k^{1/2} + O(\varepsilon)$.

Exploiting (2.11) with $\|A\| = 1$ and the fact that $d(0) \le 1$, it also can be seen that the denominator in (3.5) is less than 16 if inequality (3.6) is satisfied. Utilizing this with the bound on c in the numerator gives (3.7).

Corollary 1. With the notation of Theorem 1, assume that the spectrum of A is not too close to the origin; namely,

$$d(0) \ge \frac{16}{15}[(k+1)^3 + \sqrt{3}k^2]\varepsilon_2. \tag{3.9}$$

Then the conclusion (3.7) holds, whether or not (3.4) is satisfied.

Proof. If (3.4) is not satisfied, then (3.9) implies

$$\max\{|\theta|, |\mu|\} \ge d(0) - [(k+1)^3 + \sqrt{3}k^2]\varepsilon_2 \ge \frac{1}{16}d(0),$$

and this clearly entails (3.7).

While the constants in inequalities (3.5) and (3.7) of Theorem 1 may not be optimal, it is doubtful that one could give a bound on $\max\{|\theta|, |\mu|\}$ that involved, say, a constant multiple of $d(0)$ instead of $d(0)^2$. In fact, an example in [14] shows that not only two but *many* successive tridiagonal matrices generated by the Lanczos algorithm may have eigenvalues that lie considerably closer to the origin than the eigenvalues of A. The example involves a matrix A of order $N = 900$ with eigenvalues $\lambda_1 = 0.0340$, $\lambda_2 = 0.0341$, $\lambda_3 = 0.082$, $\lambda_4 = 0.127$, $\lambda_5 = 0.155$, $\lambda_6 = 0.190$, and $\lambda_7, \ldots, \lambda_{900}$ uniformly distributed in [0.2, 1.2]. It was observed that many successive Ritz values were close to the average $(\lambda_1 + \lambda_2)/2 = 0.03405$, before the Ritz values began to approximate λ_1 and λ_2 individually. If we shift the problem so that the average of λ_1 and λ_2 lies at the origin and normalize so that the shifted matrix has norm one, then the published experimental results show that two successive tridiagonal matrices had eigenvalues μ and θ with absolute values less than 10^{-8}, although the distance from the origin to the spectrum of the shifted and normalized matrix A is $d(0) = 4.3 \times 10^{-5}$. Moreover, the experimental results showed that ten successive tridiagonal matrices (at steps 18–27) had an eigenvalue with absolute value less than $d(0)/16$. As Theorem 1 and Corollary 1 show, however, no two successive tridiagonal matrices could have eigenvalues with absolute values less than $d(0)^2/16 \approx 10^{-10}$.

It is worth noting the exact arithmetic analogue of Theorem 1. In exact arithmetic, Paige's result (3.3) can be replaced by $d(\theta) \le \delta_k$, so it follows from this and (3.2) that $d(\theta)d(\mu) \le \beta_k|\theta - \mu|$. Proceeding as in the proof of Theorem 1, we find that

$$\max\{|\theta|, |\mu|\} \ge \frac{d(0)^2}{d(0) + \beta_k + \sqrt{2d(0)\beta_k + \beta_k^2}} \ge \frac{d(0)^2}{2 + \sqrt{3}}. \tag{3.10}$$

The constant in (3.10) is better than that in (3.7), but this expression still involves the square of the distance from the origin to the spectrum of A.

4. AN ERROR ESTIMATE

We proved in [15] that the norm of the residual $r_k = \varphi - Au_k$ is essentially determined by the *tridiagonal matrix* T_k and the next *recurrence coefficient* β_k produced by the Lanczos algorithm in finite precision arithmetic:

$$\|r_k\|/\|\varphi\| \le \sqrt{1 + 2\varepsilon_0}\left|\beta_k e_k^{\mathrm{T}} T_k^{-1} e_1\right| + \sqrt{k}\varepsilon_1\|A\|\left\|T_k^{-1}\right\|. \tag{4.1}$$

The Lanczos approximation (2.5) is not optimal in any special error norm, when it is used to approximate the solution of an indefinite system of linear equations. However, one can relate the Lanczos approximation to the optimal approximation, of one lower degree, for a problem with coefficient matrix T, where T is any symmetric tridiagonal matrix with T_k as its upper left k by k block.

Denote by $\mathcal{P}_k$ the set of polynomials of degree k or less with value 1 at the origin.

Lemma 3 (see [15]). *Let T be any symmetric tridiagonal matrix whose upper left k by k block is T_k. The expression $|\beta_k e_k^T T_k^{-1} e_1|$ in* (4.1) *satisfies*

$$|\beta_k e_k^T T_k^{-1} e_1| \le \beta_k \|T_k^{-1}\| \min_{p_{k-1} \in \mathcal{P}_{k-1}} \|p_{k-1}(T)e_1\|. \tag{4.2}$$

Proof. (This proof is short, and we duplicate it for convenience of a reader.) Set $p_{k-1}(X) = 1 - Xp_{k-2}(X) \in \mathcal{P}_{k-1}$ with p_{k-2} a real polynomial, $\deg p_{k-2} \le k-2$. Since T_k is tridiagonal, the $(k, 1)$-entry of $p_{k-2}(T_k)$ is zero. Hence, we can write

$$|e_k^T T_k^{-1} e_1| = |e_k^T[T_k^{-1} - p_{k-2}(T_k)]e_1| = |e_k^T T_k^{-1} p_{k-1}(T_k)e_1| \le \|T_k^{-1}\|\|p_{k-1}(T_k)e_1\|.$$

Since $\deg p_{k-1}(T_k) \le k-1$, it follows that for any symmetric tridiagonal matrix T whose upper left k by k block is T_k, the first k entries of the first column of $p_{k-1}(T)$ are the same as those of $p_{k-1}(T_k)$ and the remaining entries are zero. Therefore, we have

$$|e_k^T T_k^{-1} e_1| \le \|T_k^{-1}\|\|p_{k-1}(T)e_1\|.$$

We shall use Theorem 1 and Corollary 1 to bound the quantity $\|T_k^{-1}\|$ in (4.1) and (4.2), at least at every other step.

We could also obtain bounds on the minimum in (4.2), taking T to be either T_k or T_{k+1}, depending on which one has its spectrum bounded away from 0. Using more information about the spectrum of T_k, T_{k+1}, or that of any other symmetric tridiagonal matrix T extending T_k, one can derive sharper bounds on the residual norm in finite precision arithmetic. It is shown in [9], for example, that the eigenvalues of T_k (for any k) lie in clusters of width a modest multiple of the machine precision, with at most one cluster between any pair of consecutive eigenvalues of A.

Stronger[1)] bounds can be obtained, however, by taking $\tilde{T}$ to be the extended tridiagonal matrix derived in [7], whose eigenvalues all lie in *tiny intervals* about the eigenvalues of A. The proven bound on the size δ of these intervals is a large overestimate, however, being of order $\varepsilon^{1/4}$ in the worst case. With such results, one can relate the size of the residual at step k of the finite precision computation to the maximum value of the minimax polynomial on the union of tiny intervals containing the eigenvalues of T.

Let $\lambda_1 \le \ldots \le \lambda_N$ be the eigenvalues of A. Set

$$S = \bigcup_{i=1}^{N} [\lambda_i - \delta, \lambda_i + \delta]. \tag{4.3}$$

We then have the following theorem bounding the norm of the Lanczos residual at every other step in a finite precision computation.

Theorem 2. *Assume that $\|A\| = 1$, that* (3.6) *and* (3.9) *hold, and that the right-hand side of* (3.7) *is greater than zero. Assume also that the origin is not contained in the set S defined in* (4.3), *which contains the eigenvalues of the tridiagonal matrix T defined in* [7]. *Let r_j be the Lanczos residual at step j of a finite precision computation, with Q_j and T_j satisfying* (2.6)–(2.11). *Then*

$$\|r_j\|/\|\varphi\| \le \sqrt{1 + 2\varepsilon_0}(1 + \eta_j)16\tilde{\kappa}^2 \min_{p_{j-1} \in \mathcal{P}_{j-1}} \max_{z \in S} |p_{j-1}(z)| + \varepsilon_1 \sqrt{j} 16\tilde{\kappa}^2 \tag{4.4}$$

holds at least at every other step j, where

$$\tilde{\kappa}^2 = \frac{1}{d(0)^2 - 12.5(j+1)^{1/2}\varepsilon_1},$$

and

$$\eta_j = (2N + 6)\varepsilon + j(3\varepsilon_0 + \varepsilon_1).$$

1) Under the assumption $N^3\varepsilon \ll 1$, which came in [7] from [3, §4].

Proof. From Theorem 1 and Corollary 1 it follows that $\|T_j^{-1}\|$ is bounded, at least at every other step, by $16\tilde{\kappa}^2$. Using this fact in (4.1) gives

$$\|r_j\|/\|\varphi\| \le \sqrt{1+2\varepsilon_0}\left|\beta_j e_j^{\mathrm{T}} T_j^{-1} e_1\right| + \varepsilon_1\sqrt{j}16\tilde{\kappa}^2.$$

Now utilizing (4.2) to bound the quantity $\left|\beta_j e_j^{\mathrm{T}} T_j^{-1} e_1\right|$ and exploiting (2.11) to bound β_j, we have

$$\|r_j\|/\|\varphi\| \le \sqrt{1+2\varepsilon_0}(1+\eta_j)16\tilde{\kappa}^2 \min_{p_{j-1}\in\mathcal{P}_{j-1}} \|p_{j-1}(T)e_1\| + \varepsilon_1\sqrt{j}16\tilde{\kappa}^2,$$

and taking T to be the symmetric tridiagonal matrix defined in [7] gives the desired result (4.4).

The finite precision result of Theorem 2 is somewhat weaker than its exact arithmetic analogue, which can be obtained in some model cases with use of the theorem in [16] relating the residual norms of MINRES and the Lanczos method. Theorem 2 bounds the Lanczos residual at step j in terms of the optimal approximation at step $j-1$ instead of the expected j and involves a factor of about the squared condition number $16\tilde{\kappa}^2$ instead of the condition number for exact arithmetic.

We hope that this is due to the method of proof and that a more natural result might also hold in finite precision arithmetic.

5. A NUMERICAL EXPERIMENT

A simple example illustrating why inequality (4.4) does not necessarily hold at every step is obtained by considering a matrix whose eigenvalues are distributed symmetrically about the origin. If the matrix has many eigenvalues spread throughout the intervals $[-f, -e] \cup [e, f]$, where $f > e > 0$, then the expression

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \max_{z\in S}|p_{j-1}(z)|$$

in (4.4) is approximately equal to

$$2[(\kappa-1)/(\kappa+1)]^{[k/2]}, \tag{5.1}$$

where $\kappa = f/e$ and $[k/2]$ denotes the integer part of $k/2$. Yet if the initial vector in the Lanczos algorithm has eigencomponents distributed symmetrically about the origin, then the tridiagonal matrix at every other step (in exact arithmetic) will be singular and the Lanczos approximation undefined. Even if this is not the case, the Lanczos residual norm may well exceed the estimate (4.4) at every other step.

The figure shows the Lanczos residual norm and the expression (5.1) for a matrix with 100 eigenvalues distributed uniformly in the intervals $[-1, -0.5] \cup [0.5, 1]$. The right-hand side vector was taken to be a

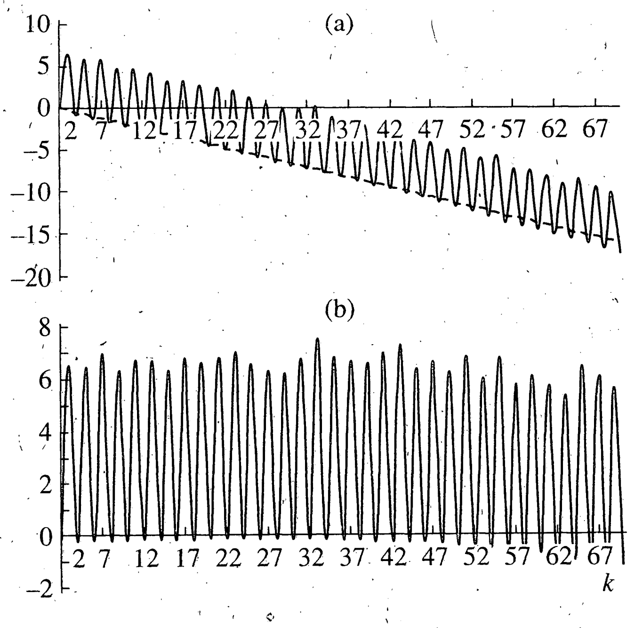

Fig. 1.

small random perturbation of the vector of all ones. The denary logarithms of the Lanczos residual norm (solid) and minimax polynomial value (dashed) are plotted in subfigure (a); the ones of the ratio of Lanczos residual norm to minimax polynomial value are plotted in subfigure (b). According to Theorem 2, the ratio of Lanczos residual norm to expression (5.1) must be less than about $16\kappa^2 = 64$ at every other step. This is indeed the case for the even steps, although the ratio greatly exceeds 64 at some of the odd steps.

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