SIAM J. NUMER. ANAL.
Vol. 17, No. 5, October 1980

0036-1429/80/1705-0010 $01.00/0

ON THE RATES OF CONVERGENCE OF THE LANCZOS AND THE BLOCK-LANCZOS METHODS*

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Abstract. Theoretical error bounds are established, improving those given by S. Kaniel. Similar inequalities are found for the eigenvectors by using bounds on the acute angle between the exact eigenvectors and the Krylov subspace spanned by $x_0, Ax_0, \cdots, A^{n-1}x_0$, where x_0 is the initial vector of the process.

All the results obtained are then extended to the block-Lanczos method, and it is shown that the bounds on the rates of the Block version are superior to those of the single vector process. The difference between the two methods is in many respects similar to the difference between the simultaneous iteration method and the single vector power method. Several numerical experiments are described in order to compare the actual rates of convergence with the theoretical bounds.

1. Introduction. The Lanczos and block-Lanczos methods are widely used for computing a few of the extreme eigenvalues and corresponding eigenvectors of a symmetric sparse matrix A of order N, where N is large.

Let $\lambda_1 > \lambda_2 > \cdots > \lambda_N$ be the eigenvalues of A and $\phi_1, \phi_2, \cdots, \phi_N$ the associated eigenvectors of norm one. Given an initial vector x_0, the method of Lanczos provides a very simple way of realizing the Ritz-Galerkin projection process on the subspace E_n spanned by the Krylov vectors $x_0, Ax_0, \cdots, A^{n-1}x_0$, where $n \leqq N$ [9], [12]. If we call π_n the orthogonal projection on the subspace E_n, then one computes the eigenvalues $\lambda_1^{(n)} > \lambda_2^{(n)} > \cdots > \lambda_n^{(n)}$ of the operator $\pi_n A_{|E_n}: E_n \to E_n$ with their associated eigenvectors $\phi_1^{(n)}, \phi_2^{(n)}, \cdots, \phi_n^{(n)}$ and takes $\lambda_i^{(n)}, \phi_i^{(n)}$ as approximations to λ_i, ϕ_i. Originally, the method was used as a direct method for tridiagonalizing a matrix by carrying on the process until $n = N$.

The numerical behavior of the Lanczos process has been studied by Wilkinson [23], Paige [13], [14], Kahan and Parlett [6], and Scott [20]. They have discussed several versions of the method that can now be effectively used for accurately computing a few of the extreme eigenelements of A.

A block generalization was introduced by Golub and Underwood [5] and Cullum and Donath [3], who replace the single vector x_0 by a system of r independent vectors $(x_1, x_2, \cdots, x_r)$.

Both methods have the attractive feature than when n increases, the computed extreme eigenelements rapidly become good approximations to the exact ones, and are satisfactorily accurate even if n is far less than N. The question which arises quite naturally and on which this paper focuses, is how rapidly would the approximate eigenelements $\lambda_i^{(n)}, \phi_i^{(n)}$ converge to λ_i, ϕ_i, if exact computation were performed? A partial answer was given by Kaniel [7], and completed by Paige [12] and Underwood [21], the latter for the block method. The Kaniel-Paige inequalities are, however, rather complicated (see §§ 2.2 and 2.3) when applied to λ_i with $i > 1$. Instead of concentrating on the eigenvalues as Kaniel did, we take a different approach. We feel that it is of prime importance to estimate first the angle $\theta(\phi_i, E_n)$ between ϕ_i and the subspace E_n. It is well known that $\lambda_i - \lambda_i^{(n)}$ and $\|\phi_i - \phi_i^{(n)}\|$ may be analyzed in terms of $\|(I - \pi_n)\phi_i\|$ [1]. The number $\|(I - \pi_n)\phi_i\|$ is by definition the sine of the angle $\theta(\phi_i, E_n)$. The analysis in terms of $\theta(\phi_i, E_n)$ has many advantages, as will be seen. In particular, it yields good

* Received by the editors August 9, 1978, and in final revised form February 27, 1980.

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estimates of the convergence rates for both eigenvalues and eigenvectors. Furthermore, there will be no difficulty extending this analysis to the block-Lanczos method.

In § 2 we propose a bound for the angle $\theta(\phi_i, E_n)$ and derive theoretical error bounds for the approximate eigenelements. The same analysis is developed in § 3 for the block-Lanczos method. Several numerical experiments are described in § 4 in order to permit a comparison between the actual rates of convergence with their bounds.

2. The Lanczos method, rate of convergence.

2.1. Notation. Since the sequence $\lambda_i^{(n)}$, $n = i, \cdots, n$ is finite, we cannot, strictly speaking, discuss the convergence of $\lambda_i^{(n)}$ when $n \to \infty$. We therefore extend the framework slightly, and deal with a compact operator A on a Hilbert space E. In addition, we will be concerned with *the k largest positive eigenvalues* numbered in a decreasing order $\lambda_1 > \lambda_2, > \cdots > \lambda_k$ (all the other eigenvalues λ_j of A are assumed to satisfy $\lambda_k > \lambda_j$). The same theory may be developed for the negative part of the spectrum with essentially the same results. Obviously, the results apply to the k largest eigenvalues of a finite dimensional operator on a space E of dimension N, numbered in decreasing order, but one must restrict the inequalities to the case where $n \leqq N$.

The acute angle $\theta(x, E_n)$ between a vector $x \neq 0$ and the subspace E_n is defined ([16]) by

$$\theta(x, E_n) = \arcsin \frac{\|(\mathrm{I} - \pi_n)x\|}{\|x\|}.$$

We shall denote by $\lambda_{\inf}$ the infimum of the spectrum of A,

$$\lambda_{\inf} = \inf \{\lambda_j\}.$$

Throughout the paper, P_i will denote the eigenprojection associated with λ_i, that is the orthogonal projection on the eigenspace corresponding to λ_i.

2.2. The basic inequality. Given a starting vector x_0, the Lanczos algorithm will, if exact computation is performed, generate successively an orthonormal basis $v_1, \cdots, v_n$ of the subspace E_n. In this basis the linear operator $\pi_n A_{|E_n}: E_n \to E_n$ is represented by the tridiagonal matrix

$$T_n = \begin{bmatrix} a_1 & b_2 & & & 0 \\ b_2 & a_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b_n \\ 0 & & & b_n & a_n \end{bmatrix}. \tag{2.1}$$

The basis $\{v_i\}_{i=1,\ldots,n}$, and the a_i and b_i can be computed as follows:

- $v_1 = x_0/\|x_0\|, \qquad a_1 = (Av_1, v_1), \qquad b_1 = 0.$
- For $j = 1, 2, \cdots, n-1$ do

$$\begin{cases} \hat{v}_{j+1} = Av_j - a_j v_j - b_j v_{j-1} \\ v_{j+1} = \hat{v}_{j+1}/\|\hat{v}_{j+1}\| \\ b_{j+1} = \|v_{j+1}\|; \qquad a_{j+1} = (Av_{j+1}, v_{j+1}). \end{cases}$$

We now study the behavior of the acute angle between the eigenvector ϕ_i and the subspace E_n by giving a bound for $\tan\theta(\phi_i, E_n)$.

THEOREM 1. [19] *Let $\lambda_1 > \lambda_2 > \cdots > \lambda_k$ be the largest k eigenvalues of A, and P_i the eigenprojection associated with λ_i $(i<k)$. Assume that $P_i x_0 \neq 0$, and consider the eigenvector $\phi_i = P_i x_0/\|P_i x_0\|$ associated with λ_i. Set*

$$\gamma_i = 1 + 2\frac{\lambda_i - \lambda_{i+1}}{\lambda_{i+1} - \lambda_{\inf}} \quad \textit{and} \quad \begin{cases} K_i = \prod_{j=1}^{i-1} \dfrac{\lambda_j - \lambda_{\inf}}{\lambda_j - \lambda_i}, & \text{if } i \neq 1, \\ K_1 = 1. \end{cases}$$

Then

$$\frac{\|(I-\pi_n)\phi_i\|}{\|\pi_n \phi_i\|} \leqq \frac{K_i}{T_{n-i}(\gamma_i)} \frac{\|(I-\pi_1)\phi_i\|}{\|\pi_1 \phi_i\|}, \tag{2.2}$$

where $T_k(x)$ is the Chebyshev polynomial of the first kind of degree k,

$$T_k(x) = \tfrac{1}{2}[(x+\sqrt{x^2-1})^k + (x-\sqrt{x^2-1})^k].$$

Here π_1 is the orthogonal projection on the subspace E_1 spanned by x_0. The inequality (2.2) may also be written

$$\tan\theta(\phi_i, E_n) \leqq \frac{K_i}{T_{n-i}(\gamma_i)} \tan\theta(\phi_i, x_0). \tag{2.3}$$

The theorem is a consequence of the following lemma.

LEMMA 1. [19] *Let $\mathbf{P}_{n-1}$ denote the space of polynomials of degree not exceeding $n-1$. If P_i is the eigenprojection associated with λ_i, and if $P_i x_0 \neq 0$, we set*[1]

$$\hat{x}_0 = \frac{(I-P_i)x_0}{\|(I-P_i)x_0\|} \quad \textit{and} \quad t_{i,n} = \inf_{\substack{p \in \mathbf{P}_{n-1} \\ p(\lambda_i)=1}} \|p(A)\hat{x}_0\|,$$

Then

$$\tan\theta(\phi_i, E_n) = t_{i,n} \tan\theta(\phi_i, x_0). \tag{2.4}$$

Proof of Lemma 1. Since any vector u in E_n is a combination of the vectors $x_0, Ax_0, \cdots, A^{n-1}x_0$, we get $u = q(A)x_0$ where $q \in \mathbf{P}_{n-1}$. Let P_j be the eigenprojection associated with the eigenvalue λ_j. We can decompose x_0 as $x_0 = P_i x_0 + \sum_{j \neq i} P_j x_0$. Hence

$$u = q(A)x_0 = q(\lambda_i)P_i x_0 + \sum_{j \neq i} q(\lambda_j) P_j x_0.$$

The acute angle between u and $P_i x_0$ satisfies

$$\tan^2\theta(P_i x_0, u) = \sum_{j \neq i} \frac{(q(\lambda_j)\|P_j x_0\|)^2}{q^2(\lambda_i)\|P_i x_0\|^2}. \tag{2.5}$$

Using the fact that

$$\sum_{j \neq i} (q(\lambda_j))^2 \|P_j x_0\|^2 = \|q(A)\hat{x}_0\|^2 \cdot \|(I-P_i)x_0\|^2,$$

and setting $p(x) = q(x)/q(\lambda_i)$, we get

$$\tan\theta(P_i x_0, u) = \|p(A)\hat{x}_0\| \cdot \frac{\|(I-P_i)x_0\|}{\|P_i x_0\|}.$$

[1] In the case where $(I-P_i)x_0 = 0$, we may set $\hat{x}_0 = 0$.

Thus

$$\min_{u\in E_n} \tan (P_i x_0, u) = \frac{\|(I-P_i)x_0\|}{\|P_i x_0\|} \cdot \min_{\substack{p\in\mathbf{P}_{n-1}\\ p(\lambda_i)=1}} \|p(A)\hat{x}_0\|.$$

But the left side is just $\tan\theta(P_i x_0, E_n)$ and the right side is equal to the right part of (2.4), which completes the proof.

Proof of Theorem 1.

● *Case* $i=1$. Let us set $\beta_j = \|P_j\hat{x}_0\|$. Note that $\sum_{\substack{j=1\\ j\neq i}}^{\infty} \beta_j^2 = 1$. Therefore

$$t_{1,n} = \min_{\substack{p\in\mathbf{P}_{n-1}\\ p(\lambda_1)=1}} \left(\sum_{j\neq 1} \beta_j^2 p^2(\lambda_j)\right)^{1/2} \leqq \min_{\substack{p\in\mathbf{P}_{n-1}\\ p(\lambda_1)=1}} \left(\max_{\lambda_{\inf}\leqq x\leqq\lambda_2} |p(x)|\right).$$

Now it is well known that the last term of this inequality is $1/T_{n-1}(\gamma_1)$, where $\gamma_1 = 1+2(\lambda_1-\lambda_2)/(\lambda_2-\lambda_{\inf})$, from [2], [8], [11], etc. Thus, $\tan(\phi_i, E_n) \leqq \tan\theta(\phi_i, x_0)/T_{n-1}(\gamma_1)$, which is the required result for $i=1$.

● *Case* $i>1$. The following inequalities are easy to show.

$$t_{i,n}^2 = \min_{\substack{p\in\mathbf{P}_{n-1}\\ p(\lambda_i)=1}} \left(\sum_{j\neq i} \beta_j^2 p^2(\lambda_j)\right) \leqq \min_{\substack{p\in\mathbf{P}_{n-1}\\ p(\lambda_i)=1}} \max_{j\neq i} |p(\lambda_j)|^2$$

$$\leqq \min_{\substack{p\in\mathbf{P}_{n-1}\\ p(\lambda_1)=p(\lambda_2)\cdots=p(\lambda_{i-1})=0\\ p(\lambda_i)=1}} \max_{j\neq i} |p(\lambda_j)|^2.$$

Now since $p(\lambda_k)=0$ for $k=1,2,\cdots,i-1$, and $p(\lambda_i)=1$, $p(x)$ may be decomposed as

$$p(x) = \frac{(x-\lambda_1)\cdots(x-\lambda_{i-1})q(x)}{(\lambda_i-\lambda_1)\cdots(\lambda_i-\lambda_{i-1})q(\lambda_i)},$$

where q is a polynomial of degree $n-i$. Thus

$$\max_{j\neq i} |p(\lambda_j)| = \max_{j\neq i} \left| \frac{(\lambda_1-\lambda_j)\cdots(\lambda_{i-1}-\lambda_j)q(\lambda_j)}{(\lambda_1-\lambda_i)\cdots(\lambda_{i-1}-\lambda_i)q(\lambda_i)} \right|$$

$$\leqq \frac{(\lambda_1-\lambda_{\inf})\cdots(\lambda_{i-1}-\lambda_{\inf})}{(\lambda_1-\lambda_i)\cdots(\lambda_{i-1}-\lambda_i)} \cdot \max_{j\geqq i+1} \frac{|q(\lambda_j)|}{|q(\lambda_i)|}.$$

Therefore

$$t_{i,n} \leqq K_i \min_{\substack{q\in\mathbf{P}_{n-i}\\ q(\lambda_i)=1}} \left(\max_{\lambda_{\inf}\leqq x\leqq\lambda_{i+1}} |q(x)|\right) = \frac{K_i}{T_{n-i}(\gamma_i)}. \tag{2.6}$$

With (2.4), this completes the proof of the theorem.

Remarks.

1. Inequality (2.2) shows that the acute angle between ϕ_i and E_n decreases at least as rapidly as $K_i/T_{n-i}(\gamma_i)$. When n is large, then

$$T_{n-1}(\gamma_i) \simeq \tfrac{1}{2}\left(\gamma_i + \sqrt{\gamma_i^2-1}\right)^{n-i},$$

where

$$\gamma_i = 1 + \frac{2(\lambda_i-\lambda_{i+1})}{(\lambda_{i+1}-\lambda_{\inf})}$$

is greater than 1, and depends on the gap $\lambda_i - \lambda_{i+1}$ and the spread $\lambda_{i+1} - \lambda_{\inf}$. Note here that the first $i-1$ eigenvalues do not interfere in the coefficient $\tau_i = \gamma_i - \sqrt{\gamma_i^2 - 1}$, which estimates the rate of convergence to zero of the bound on $\theta(\phi_i, E_n)$.

2. Theorem 1 indicates that when n increases there is at least one vector in E_n (namely the vector $\pi_n\phi_i$) which converges to the eigenvector ϕ_i (with a rate superior to the τ_i above). This is true even when λ_i is not simple, since the only condition required is that $P_i x_0 \neq 0$. The proof of the theorem reveals that when λ_i is multiple there is only one such vector in E_n which is close to ϕ_i. This shows in particular that a multiple eigenvalue will be approximated by at most *one* eigenvalue of T_n.

3. It is easy to show that the inequality (2.2) is optimal for the case $i = 1$, in that for a given n, A and x_0 can be chosen so this bound can be attained. For this purpose, let us recall that if A is positive definite and if y_0 is any nonzero vector, then the number

$$t_n = \min_{\substack{p \in \mathbf{P}_n \\ p(0) = +1}} \|p(A)y_0\|$$

is estimated by the inequality

$$t_n \leqq \frac{\|y_0\|}{T_{n-1}(\gamma)}, \tag{2.7}$$

where

$$\gamma = \frac{\lambda_1 + \lambda_{\inf}}{\lambda_1 - \lambda_{\inf}}.$$

This inequality is especially useful when one studies the rate of convergence of the conjugate gradient method [7], [8], [11]. Now when $i = 1$, the coefficient $t_{1,n}$ of Lemma 1 can be transformed as follows:

$$t_{1,n} = \inf_{\substack{p \in \mathbf{P}_{n-1} \\ p(\lambda_1) = 1}} \|p(A)\hat{x}_0\| = \inf_{\substack{q \in \mathbf{P}_{n-1} \\ q(0) = 1}} \|q(\lambda_1 I - A)\hat{x}_0\|.$$

Since $\hat{x}_0 \in (\phi_1)^\perp$, if one sets $B = (\lambda_1 I - A)_{|(\phi_1)^\perp}$, it is clear that

$$t_{1,n} = \inf_{\substack{q \in \mathbf{P}_{n-1} \\ q(0) = 1}} \|q(B)\hat{x}_0\|,$$

which, with the above classical inequality, yields

$$t_{1,n} \leqq \frac{\|\hat{x}_0\|}{T_{n-1}(\gamma_1)}.$$

This means that our result (2.2) may be derived, when $i = 1$, from the classical estimation (2.7). It was shown in [7], [11], that the inequality (2.7) cannot be improved. Because of (2.4), it results that when $i = 1$, our inequality (2.4) is optimal as well.

2.3. Theoretical error bounds for the eigenelements. The basic inequality (2.2) (or (2.3)) means that there exists in E_n a vector $(\pi_n\phi_i)$ whose acute angle with ϕ_i decays at least as rapidly as

$$\frac{K_i}{T_{n-i}(\gamma_i)} \simeq \tfrac{1}{2}(\gamma_i + \sqrt{\gamma_i^2 - 1})^{-n+i}.$$

We now study the implications of this inequality for the behavior of the eigenelements. Let us recall a result of Kaniel [7].

COROLLARY 1 (of Theorem 1). *If* $P_1x_0 \neq 0$ *then*

$$0 \leqq \lambda_1 - \lambda_1^{(n)} \leqq (\lambda_1 - \lambda_{\inf}) \frac{\tan^2 \theta(\phi_1, x_0)}{T_{n-1}^2(\gamma_1)}. \tag{2.8}$$

This result can be easily deduced from Theorem 1 by using the minimax principle for $\pi_n A \pi_n$ and the vector $\pi_n\phi_1/\|\pi_n\phi_1\|$. For the other eigenvalues, Kaniel [7] obtained the following bounds,[2]

$$0 \leqq \lambda_i - \lambda_i^{(n)} \leqq \left(\frac{K}{T_{n-i}(\gamma_i)}\right)^2 + \sum_{j=1}^{i-1} (\lambda_j - \lambda_{\inf})\varepsilon_j^2, \tag{2.9}$$

where K is a constant depending on the eigenvalues of A and on x_0, and where ε_j denotes $\|(I-P_j)\phi_j^{(n)}\|$ (which represents the sine of the angle between ϕ_i and $\phi_j^{(n)}$).

The term $\sum_{j=1}^{i-1} (\lambda_j - \lambda_{\inf})\varepsilon_j^2$ is, however, rather complicated to estimate. Moreover, its bound can be nonnegligible, mainly because of the accumulative nature of the inequalities proposed in [7] and [12] for this term (see our example in § 2.4).

Before extending the bound (2.8) to the case $i \neq 1$ we should consider the situation where A has multiple eigenvalues. As pointed out in Remark 2 (§ 2.1), even if λ_i is multiple it is approximated by at most one eigenvalue. Indeed, the method acts, theoretically, exactly as if all the eigenvalues of A were simple. This was noticed by Kaniel [7] and can be shown as follows. The Lanczos method computes the eigenelements of the operator $\pi_n A_{|E_n}$. It is obvious that if E' is the invariant subspace spanned by $P_1x_0, \cdots, P_jx_0, \cdots$, then $E_n \subset E'$, and the process amounts to approximating the eigenelements of $A_{|E'}$, the restriction of A to E', whose eigenvalues are now all simple. From now on we may therefore assume, without loss of generality, that all the eigenvalues of A are simple. (If A admits multiple eigenvalues, then one needs only to replace A by $A_{|E'}$ in the proofs). We recall that the eigenvalues of T_n are all simple under the hypothesis that $b_j \neq 0$, $j = 2, 3, \cdots, n$, and that they are numbered in decreasing order $\lambda_1^{(n)} > \lambda_2^{(n)} > \cdots > \lambda_n^{(n)}$.

THEOREM 2. *Let* λ_i $(i \leqq k)$ *be an eigenvalue of* A *with associated eigenvector* ϕ_i *such that* $(\phi_i, x_0) \neq 0$, *and assume that* $\lambda_{i-1}^{(n)} > \lambda_i$. *Let* γ_i *be defined as in Theorem* 1, *and let*

$$K_i^{(n)} = \prod_{j=1}^{i-1} \frac{\lambda_j^{(n)} - \lambda_{\inf}}{\lambda_j^{(n)} - \lambda_i}, \quad \text{if } i \neq 1,$$

$$K_1^{(n)} = 1.$$

Then

$$0 \leqq \lambda_i - \lambda_i^{(n)} \leqq (\lambda_i - \lambda_{\inf}) \cdot \left(\frac{K_i^{(n)}}{T_{n-i}(\gamma)} \tan \theta(\phi_i, x_0)\right)^2. \tag{2.10}$$

We need two lemmas for the proof.

LEMMA 2. *Let* $\mathbf{P}_n^*$ *be the set of all polynomials of degree n, with leading coefficient equal to* 1, *and* $\bar{p}(x)$ *be the polynomial of* $\mathbf{P}_n^*$ *which minimizes* $\|p(A)x_0\|$ *over all elements of* $\mathbf{P}_n^*$. *Then the approximate eigenvalues* $\lambda_i^{(n)}$ *are the roots of* $\bar{p}$, *and if we set* $q_i(x) = \bar{p}(x)/(x - \lambda_i^{(n)})$, *the vectors* $q_i(A)x_0$ *are associated approximate eigenvectors.*

This is a known result; e.g., see Vandergraft [22], Saad [19].

LEMMA 3. *For* $j = 1, 2, \cdots, i$, *let* $\phi_j^{(n)}$ *be the approximate eigenvectors associated with* $\lambda_j^{(n)}$ *and* $F_i^{(n)}$ *the subspace of* E_n, *orthogonal to* $\phi_1^{(n)}, \phi_2^{(n)}, \cdots, \phi_{i-1}^{(n)}$. *Then* $x \in F_i^{(n)}$ *if and*

[2] The constant K and the ε_j were subject to errors in Kaniel's paper. These were corrected by Paige [12]. (See also [20].)

only if $x=p(A)x_0$, *where* p *is a polynomial of degree* $\leqq n-1$ *such that* $p(\lambda_1^{(n)})=p(\lambda_2^{(n)})=\cdots=p(\lambda_{i-1}^{(n)})=0$.

We omit the proof of this lemma, a part of which is a simple consequence of Lemma 2.

Proof of Theorem 2. By the Courant characterization of the eigenvalues of symmetric operators, we have

$$\lambda_i^{(n)}=\max_{u\in F_i^{(n)}}\frac{(Au,u)}{\|u\|^2}.$$

This gives

$$0\leqq\lambda_i-\lambda_i^{(n)}=\min_{u\in F_i^{(n)}}\frac{((\lambda_i-A)u,u)}{\|u\|^2}.$$

Let $u\in F_i^{(n)}$, $u=p(A)x_0=\sum_{j=1}^{\infty}\alpha_j p(\lambda_j)\phi_j$, where the α_j are the expansion coefficients of x_0 in the eigenbasis $\{\phi_j\}$. Then

$$\frac{((\lambda_i-A)u,u)}{\|u\|^2}=\frac{1}{\|u\|^2}\left(\sum_{j=1}^{i}(\lambda_i-\lambda_j)(p(\lambda_j))^2\alpha_j^2+\sum_{j=i+1}^{\infty}(\lambda_i-\lambda_j)p(\lambda_j)^2\alpha_j^2\right).$$

Since the first term of the right side is negative,

$$\frac{((\lambda_i-A)u,u)}{\|u\|^2}\leqq\frac{\sum_{j=i}^{\infty}(\lambda_i-\lambda_j)(p(\lambda_j))^2\alpha_j^2}{\sum_{j=1}^{\infty}(p(\lambda_j))^2\alpha_j^2}.$$

Thus

$$0\leqq\lambda_i-\lambda_i^{(n)}\leqq(\lambda_i-\lambda_{\inf})\frac{\sum_{j=i+1}^{\infty}p(\lambda_j)^2\alpha_j^2}{p(\lambda_i)^2\alpha_i^2}. \tag{2.11}$$

From Lemma 3, $u\in F_i^{(n)}$ implies that $p(\lambda_1^n)=\cdots=p(\lambda_{i-1}^{(n)})=0$. This means that $p(x)$ can be written as $p(x)=(x-\lambda_1^{(n)})\cdots(x-\lambda_{i-1}^{(n)})q(x)$, with $q(x)$ having degree at most $n-i$. Hence for all $u\in F_1^{(n)}$

$$\begin{aligned}\frac{((\lambda_i I-A)u,u)}{\|u\|^2}&\leqq(\lambda_i-\lambda_{\inf})\cdot\sum_{j=i+1}^{\infty}\frac{(\lambda_j-\lambda_1^{(n)})^2\cdots(\lambda_j-\lambda_{i-1}^{(n)})^2q(\lambda_j)^2\alpha_j^2}{(\lambda_i-\lambda_1^{(n)})^2\cdots(\lambda_i-\lambda_{i-1}^{(n)})^2q(\lambda_i)^2\alpha_i^2}\\&\leqq(\lambda_i-\lambda_{\inf})\cdot\frac{(\lambda_1^{(n)}-\lambda_{\inf})^2\cdots(\lambda_{i-1}^{(n)}-\lambda_{\inf})^2}{(\lambda_1^{(n)}-\lambda_i)^2\cdots(\lambda_{i-1}^{(n)}-\lambda_i)^2}\cdot\sum_{j=i+1}^{\infty}\frac{\alpha_j^2q(\lambda_j)^2}{\alpha_i^2q(\lambda_i)^2}.\end{aligned}$$

Thus

$$\min_{u\in F^{(n)}}\frac{((\lambda_i I-A)u,u)}{\|u\|^2}\leqq(\lambda_i-\lambda_{\inf})(K_i^{(n)})^2\cdot\min_{q\in\mathbf{P}_{n-i}}\sum_{j=i+1}^{\infty}\frac{\alpha_j^2q(\lambda_j)^2}{\alpha_i^2q(\lambda_i)^2}.$$

Operating as in the proof of Theorem 1, we immediately get the inequalities

$$\min_{q\in\mathbf{P}_{n-i}}\sum_{j=i+1}^{\infty}\frac{\alpha_j^2q(\lambda_j)^2}{\alpha_i^2q(\lambda_i)^2}\leqq\left(\sum_{j\geqq i+1}\frac{\alpha_j^2}{\alpha_i^2}\right)\min_{q\in\mathbf{P}_{n-i}}\max_{j\geqq i+1}\left|\frac{q(\lambda_j)}{q(\lambda_i)}\right|^2 \tag{2.12}$$

$$\leqq\sum_{j\geqq i+1}\frac{\alpha_j^2}{\alpha_i^2}\cdot\frac{1}{T_{n-i}^2(\gamma_i)}\leqq\tan^2\theta(\phi_i,X_0)\cdot\frac{1}{T_{n-i}^2(\gamma_i)}. \tag{2.13}$$

Hence, from (2.13) and (2.11) we get (2.10).

Remarks.

1. If P_j is the eigenprojection associated with λ_j, and if we set $y_0 = (I - P_1 - P_2 \cdots - P_{i-1})x_0$, then the quantity $\tan\theta(\phi_i, x_0)$ in (2.10) may be replaced by the smaller one $\tan\theta(\phi_i, y_0)$. This is due to (2.13).

2. The theorem shows the following theoretical result. Let k be fixed, $\lambda_1 > \lambda_2 > \cdots > \lambda_k$ be the largest k eigenvalues of A, and $\lambda_1^{(n)} > \lambda_2^{(n)} > \cdots > \lambda_k^{(n)}$ be the largest k eigenvalues of T_n. Then provided that $P_i x_0 \neq 0$ for $i = 1, 2, \cdots, k$, each $\lambda_i^{(n)}$ (with $1 \leqq i \leqq k$) will converge to λ_i (with a rate of convergence bounded by

$$\tau_i = (\gamma_i + \sqrt{\gamma_i^2 - 1})^2).$$

This can be easily shown by induction as follows.

- When $i = 1$, it results from (2.10) since $K_1^{(n)} = 1$.
- Assume that $\lambda_j^{(n)} \to \lambda_j$ for $j = 1, 2, \cdots, i-1$. Then $K_i^{(n)}$ converges to K_i, and inequality (2.10) shows that $\lambda_i^{(n)} \to \lambda_i$. It is important to notice that the same result can be established for the smallest eigenvalues (i.e., the negative part of the spectrum) numbered in increasing order $\lambda_1^- < \lambda_2^- < \cdots < \lambda_k^-$.

We shall now give an inequality for the eigenvectors.

THEOREM 3. *Let λ_i be the ith eigenvalue of A with associated eigenvector $\phi_i(\|\phi_i\| = 1)$. Let $P_i^{(n)}$ denote the approximate eigenprojection associated with $\lambda_i^{(n)}$, and $d_{i,n} = \min_{j \neq i} |\lambda_i - \lambda_j^{(n)}|$, $r_n = \|(I - \pi_n)A\pi_n\|$. Then*

$$\|(I - P_i^{(n)})\phi_i\| \leqq \left(1 + \frac{r_n^2}{d_{i,n}^2}\right)^{1/2} \|(I - \pi_n)\phi_i\|. \tag{2.14}$$

Equation (2.14) can be written,

$$\sin\theta(\phi_i, \phi_i^{(n)}) \leqq \left(1 + \frac{r_n^2}{d_{i,n}^2}\right)^{1/2} \sin\theta(\phi_i, E_n). \tag{2.15}$$

The angle $\theta(\phi_i, E_n)$ in (2.15) was estimated in Theorem 1, and decreases rapidly to zero.

To show the convergence of $\phi_i^{(n)}$ to ϕ_i, it is important to bound the sequence $(1 + r_n^2/d_{i,n}^2)^{1/2}$ by a constant which does not depend on n. The quantity r_n is the socalled variation of E_n by A [22]. One has $r_n = b_{n+1}$, where b_{n+1} is computed by the Lanczos algorithm (§ 2.2), and $r_n \leqq \|A\|$. Furthermore, if one assumes that the first $i+1$ eigenvectors are such that $(x_0, \phi_j) \neq 0$ for $j = 1, 2, \cdots. i+1$, then $d_{i,n}$ will converge to $d_i = \min_{j \neq i} |\lambda_i - \lambda_j|$ (see Remark 2 above). This shows that for a sufficiently large n, $r_n/d_{i,n}$ is bounded, which implies that $\phi_i^{(n)}$ converges to ϕ_i at a rate bounded by

$$\tau_i = \gamma_i + \sqrt{\gamma_i^2 - 1}.$$

Proof of Theorem 3.

1. We first prove the inequality

$$\|(\pi_n - P_i^{(n)})\phi_i\| \leqq \frac{r_n}{d_{i,n}} \|(I - \pi_n)\phi_i\|. \tag{2.16}$$

Let $\lambda_1^{(n)} \cdots \lambda_s^{(n)}$ be the distinct eigenvalues of $\pi_n A \pi_n$ and $P_j^{(n)}$ the associated eigenprojections. Then it is well known that

$$\begin{aligned} &P_j^{(n)} P_i^{(n)} = \delta_{i,j} P_j^{(n)}, \\ &\sum_{j=1}^{s} P_j^{(n)} = \pi_n. \end{aligned} \tag{2.17}$$

Hence $(\pi_n A - \lambda_i I)\pi_n\phi_i = (\pi_n A - \lambda_i I)\sum_{j=1}^s P_j^{(n)}\phi_i$, and

$$(\pi_n A - \lambda_i I)\pi_n\phi_i = \sum_{j=1}^{s} (\lambda_j^{(n)} - \lambda_i)P_j^{(n)}\phi_i.$$

Multiplying the two sides by $I - P_i^{(n)}$ yields

$$(I - P_i^{(n)})(\pi_n A - \lambda_i I)\pi_n\phi_i = \sum_{j=1}^{s} (\lambda_j^{(n)} - \lambda_i)(I - P_i^{(n)})P_j^{(n)}\phi_i. \tag{2.18}$$

In view of (2.17) this last term is equal to

$$\sum_{j\neq i}^{s} (\lambda_j^{(n)} - \lambda_i)P_j^{(n)}\phi_i.$$

Taking the norms of the two sides of equation (2.18) gives

$$\|(I - P_i^{(n)})(\pi_n A - \lambda_i I)\pi_n\phi_i|^2 = \sum_{j\neq i} (\lambda_j^{(n)} - \lambda_i)^2\|P_j^{(n)}\phi_i\|^2. \tag{2.19}$$

For the right side we get the inequality

$$\sum_{j\neq i} (\lambda_j^{(n)} - \lambda_i)^2\|P_j^{(n)}\phi_i\|^2 \geqq d_{i,n}^2 \sum_{j\neq i} \|P_j^{(n)}\phi_i\|^2, \tag{2.20}$$

where $d_{i,n} = \min_{j\neq i} |\lambda_i - \lambda_j^{(n)}|$. But (2.17) shows that

$$\sum_{j\neq i} \|P_j^{(n)}\phi_i\|^2 = \|(\pi_n - P_i^{(n)})\phi_i\|^2.$$

For the left side of (2.19) we get

$$\begin{aligned}\|(I - P_i^{(n)})(\pi_n A - \lambda_i I)\pi_n\phi_i\|^2 &\leqq \|I - P_i^{(n)}\|^2\|\pi_n(A - \lambda_i I)\pi_n\phi_i\|^2\\ &= \|\pi_n(A - \lambda_i I)[\phi_i - (I - \pi_n)\phi_i]\|^2\\ &= \|\pi_n(A - \lambda_i I)(I - \pi_n)(I - \pi_n)\phi_i\|^2\\ &\leqq \|\pi_n(A - \lambda_i I)(I - \pi_n)\|^2 \cdot \|(I - \pi_n)\phi_i\|^2.\end{aligned}$$

Thus

$$\|(I - P_i^{(n)})(\pi_n A - \lambda_i I)\pi_n\phi_i\|^2 \leqq r_n^2\|(I - \pi_n)\phi_i\|^2. \tag{2.21}$$

Now using (2.19), (2.20) and (2.21) yields easily the desired inequality (2.16).

2. Inequality (2.14) is obtained from the decomposition

$$(I - P_i^{(n)})\phi_i = (I - \pi_n)\phi_i + (\pi_n - P_i^{(n)})\phi_i,$$

where the two vectors in the right side are orthogonal. Thus

$$\|(I - P_i^{(n)})\phi_i\|^2 = \|(I - \pi_n)\phi_i\|^2 + \|(\pi_n - P_i^{(n)})\phi_i\|^2, \tag{2.22}$$

which by (2.16) gives (2.14) and completes the proof.

The theorem can be completed as follows.

COROLLARY 2. *Under the assumptions of Theorem* 3, *the angle* $\theta(\phi_i, \phi_i^{(n)})$ *satisfies*

$$\sin\theta(\phi_i, E_n) \leqq \sin\theta(\phi_i, \phi_i^{(n)}) \leqq \sqrt{1 + \frac{r_n^2}{d_{i,n}^2}} \cdot \frac{K_i}{T_{n-i(\gamma_i)}} \cdot \tan\theta(\phi_i, x_0). \tag{2.23}$$

Proof. The second part of (2.23) follows from (2.15), (2.3), and the fact that $\sin\theta \leqq \tan\theta$. The first part is obvious, since, as is seen from (2.22),

$$\|(I - \pi_n)\phi_i\| \leqq \|(I - P_i^{(n)})\phi_i\|,$$

2.4. Refined error bounds. A look at the bounds (2.10) and (2.23) reveals that they may be weak in the case where λ_i is close to λ_{i+1}, for λ_i is then close to 1 and the right sides of (2.10), (2.23) can decrease too slowly to 0. Therefore, one needs to improve the previous results by generalizing them so that they allow to take advantage of a particular structure of the spectrum. This may be achieved by choosing more appropriate polynomials than those used in the proofs of Theorems 1 and 2.

In the following, p is any integer such that $0 \leqq p \leqq n-i$. We shall call L the set of the p integers $i+1, i+2, \cdots, i+p$. (If $p=0$, then L is the empty set).

THEOREM 4. *Let λ_i be an eigenvalue of A with associated eigenvector ϕ_i. Let x_0 satisfy $P_i x_0 \neq 0$ and assume that $\lambda_i < \lambda_{i-1}^{(n)}$. Let $K_i^{(n)}$ be defined as in Theorem* 2, *and*

$$x_L = \prod_{j \in L} (A-\lambda_j)x_0, \qquad y_L = (I-P_1-P_2-\cdots-P_{i-1})x_L,$$

$$\gamma_L = 1+2\frac{\lambda_i-\lambda_{i+p+1}}{\lambda_{i+p+1}-\lambda_{\inf}}.$$

Then

$$0 \leqq \lambda_i - \lambda_i^{(n)} \leqq (\lambda_i-\lambda_{\inf}) \cdot \left[\frac{K_i^{(n)}}{T_{n-i-p}(\gamma_L)} \cdot \tan(\phi_i, y_L)\right]^2. \tag{2.24}$$

Proof. It is obvious that the set $\hat{E}_n$ which contains all elements of the form $u=p(A)x_L$, where p is any polynomial of degree at most $n-p-1$, is a subspace of E_n orthogonal to $\phi_{i+1}, \phi_{i+2}, \cdots, \phi_{i+p}$. Let $\hat{F}_i^{(n)}$ be the subspace of E_n orthogonal to the subspace spanned by $\phi_1^{(n)}, \phi_2^{(n)}, \cdots, \phi_{i-1}^{(n)}$. Then $\hat{F}_i^{(n)} \subset F_i^{(n)}$ and we can perform again the proof of Theorem 2, with $\hat{F}_i^{(n)}$ instead of $F_i^{(n)}$, x_L instead of x_0, and $\mathbf{P}_{n-p-i}$ instead of $\mathbf{P}_{n-i}$. This leads to the following inequality (see 2.12 and 2.13):

$$0 \leqq \lambda_i - \lambda_i^{(n)} \leqq (\lambda_i-\lambda_{\inf}) \sum_{j=i+p+1}^{\infty} \frac{\hat{\alpha}_j^2}{\hat{\alpha}_i^2} \min_{\substack{q \in \mathbf{P}_{n-p-i} \\ q(\lambda_i)=1}} \max_{j \geqq i+P+1} \left|\frac{q(\lambda_j)}{q(\lambda_i)}\right|^2, \tag{2.25}$$

where the $\hat{\alpha}_j$ are the expansion coefficients of x_L in the eigenbasis. Now the term $\sum_{j>i+p} \hat{\alpha}_j^2/\hat{\alpha}_i^2$ is just $\tan^2(\phi_i, y_L)$ and the use of Chebyshev polynomials in (2.25) easily gives the inequality (2.24) sought for. By majorizing $\tan(\phi_i, y_L)$ one obtains the following weakening of the bound (2.24).

COROLLARY 3. *Let*

$$K_L = \begin{cases} 1 & \text{if } p=0, \\ \prod_{j \in L} \dfrac{\lambda_j-\lambda_{\inf}}{\lambda_i-\lambda_j} & \text{if } p \neq 0. \end{cases}$$

Then, under the assumptions of Theorem 4, *we have*

$$0 \leqq \lambda_i - \lambda_i^{(n)} \leqq (\lambda_i-\lambda_{\inf})\left[\frac{K_i^{(n)} \cdot L_L}{T_{n-i-p}(\gamma_L)} \cdot \tan(\phi_i, x_0)\right]^2. \tag{2.26}$$

Proof. $x_0 = \sum_{k=1}^{\infty} \alpha_k \phi_k$; then we have $\hat{\alpha}_k = \prod_{j \in L} (\lambda_k-\lambda_j)\alpha_k$, so that the term $\sum_{j>p+i} \hat{\alpha}_j^2/\hat{\alpha}_i^2$ can be bounded by

$$K_L^2 \cdot \sum_{j=i+p+1}^{\infty} \frac{\alpha_j^2}{\alpha_i^2}. \tag{2.27}$$

Noticing that (2.27) is smaller than $K_L^2 \tan^2(\phi_i, x_0)$ gives the result (2.26).

For the eigenvectors, one can easily obtain the following generalization of Corollary 2:

$$\sin\theta(\phi_i, E_n) \leqq \sin\theta(\phi_i, \phi_i^{(n)}) \leqq \sqrt{1+\frac{r_n^2}{d_{i,n}^2}} \cdot \frac{K_i \cdot K_L}{T_{n-p-i}(\gamma_L)} \tan\theta(\phi_i, x_0). \tag{2.28}$$

Remark. We emphasize that the bounds (2.26) and (2.28) appear as generalizations of their analogues of § 2.3, since choosing $p=0$ would merely give (2.10) and (2.23). Moreover, one can select p optimally, i.e., so that the right-hand side of (2.26) is minimal over all possible p. This gives the "optimal" bound,

$$0 \leqq \lambda_i - \lambda_i^{(n)} \leqq (\lambda_i - \lambda_{\inf})\left[K_i^{(n)} \tan(\phi_i, x_0) \times \min_{0\leqq p\leqq n-i} \frac{K_L}{T_{n-p-i}(\gamma_L)}\right]^2. \tag{2.29}$$

Obviously, a similar optimal error bound can be derived from inequality (2.28) for the eigenvectors.

Example. Let us illustrate these results with the following example which was considered in Kaniel's original paper [7].

Eigenvalues of A.

$$\lambda_1 = 1; \quad \lambda_2 = 0.99; \quad \lambda_3 = 0.96; \quad \text{and} \quad 0 \leqq \lambda_j \leqq 0.9 \text{ for } j \geqq 4.$$

Initial vector x_0. We assume that $\tan(\phi_i, x_0) = 10^2$ for $i = 1, 2, 3$. If the Lanczos algorithm is interrupted at $n = 53$, we shall have

- For the 1st eigenvalue, with $p=2$, ($L_1 = \{2, 3\}$) one gets

$$K_1^{(n)} = 1; \quad K_{L_1} = \frac{0.99 \times 0.96}{0.01 \times 0.04} \simeq 2.4 \times 10^{-3},$$

$$\gamma_{L_i} = 1 + 2 \cdot \left(\frac{0.1}{0.9}\right) \simeq 1.22 \cdots; \quad (T_{n-p-1}(\gamma_{L_1}))^{-1} = (T_{50}(1.22))^{-1} \simeq 1.2 \times 10^{-14};$$

so that

$$0 \leqq \lambda_1 - \lambda_1^{(n)} \leqq 1 \times (2.4 \times 10^3 \times 1.2 \times 10^{-14} \times 10^2)^2 \simeq 8.4 \times 10^{-18}.$$

- For the 2nd eigenvalue, when $p=1$, $L_2 = \{2\}$,

$$K_2^{(n)} \simeq 1/10^{-2} = 10^2; \qquad K_{L_2} = \frac{0.96}{0.03} \simeq 32;$$

$$\gamma_{L_2} = 1 + 2\left(\frac{0.09}{0.9}\right) = 1.2; \qquad T_{n-p-2}(\gamma_{L_2})^{-1} = (T_{50}(1.2))^{-1} \simeq 6.1 \times 10^{-14}.$$

Therefore

$$0 \leqq \lambda_2 - \lambda_2^{(n)} \leqq 0.99 \times [10^2 \times 32 \times 6.1 \times 10^{-14} \times 10^2]^2 \simeq 3.1 \times 10^{-16}.$$

- For the 3rd eigenvalue, we take $L_3 = \phi$, $p = 0$;

$$K_3^{(n)} = \frac{1 \times 0.99}{0.04 \times 0.03} \simeq 8.25 \times 10^2; \quad K_{L_3} = 1;$$

$$\gamma_3 = 1 + 2\left(\frac{0.06}{0.9}\right) = 1.13 \cdots; \quad T_{n-p-3}(\gamma_3)^{-1} = (T_{50}(1.13))^{-1} \simeq 1.6 \times 10^{-11};$$

and

$$0 \leqq \lambda_3 - \lambda_3^{(n)} \leqq (0.96)(8.25 \times 10^2 \times 10^2 \times 1.6 \times 10^{-11})^2 \simeq 1.7 \times 10^{-12}.$$

For this example the Kaniel-Paige refined bounds yield the same result as above for the 1st eigenvalue. For $\lambda_2-\lambda_2^{(n)}$ they give

$$0 \leqq \lambda_2-\lambda_2^{(n)} \leqq 3\times 10^{-16}+(\lambda_1-\lambda_{\inf})\varepsilon_1^2,$$

where ε_1^2 can be bounded by using Paige's result,

$$\varepsilon_j^2 \leqq \frac{\lambda_j-\lambda_j^{(n)}+\sum_{k=1}^{j-1}(\lambda_k-\lambda_{j+1})\varepsilon_k^2}{\lambda_j-\lambda_{j+1}}, \qquad j=1,\cdots,i. \tag{2.30}$$

This gives $\varepsilon_1^2 \leqq 8\times 10^{-16}$, and therefore $0\leqq \lambda_2-\lambda_2^{(n)} \leqq 1.1\times 10^{-15}$. By (2.30) $\varepsilon_2^2 \leqq 3\times 10^{-3}$, and for the 3rd eigenvalue one gets

$$0\leqq \lambda_3-\lambda_3^{(n)} \leqq 1.7\times 10^{-12}+3\times 10^{-13}.$$

We note that the term $\sum_{j=1}^{i-1}(\lambda_k-\lambda_{\inf})\varepsilon_k^2$ in (2.9) can be nonnegligible and, as i increases, it becomes rather complicated to bound it by the inequality (2.30).

3. The block-Lanczos method, rate of convergence.

3.1. The block generalization of the Lanczos method uses a system U_0 of r vectors $U_0=(x_1, x_2, \cdots, x_r)$ instead of a single vector x_0 [3], [5], [17]. If π_n is the orthogonal projection on the subspace E_n spanned by U_0, $AU_0, \cdots, A^{n-1}U_0$, it amounts to computing the eigenelements of $\pi_n A_{|E_n}$. Underwood [21] has studied the convergence of the process and obtained theoretical error bounds, generalizing Kaniel's results, for the r largest eigenvalues. In this section we shall extend our previous a priori error bounds, and we will show that the rate of convergence is now bounded by $\hat{\tau}_i = \hat{\gamma}_i+\sqrt{\hat{\gamma}_i^2-1}$, where

$$\hat{\gamma}_i = 1+2\frac{\lambda_i-\lambda_{i+r}}{\lambda_{i+r}-\lambda_{\inf}}.$$

In addition to the new definition of E_n given above, the notation remains essentially the same as before. We shall, however, alter the numbering of the eigenvalues. Indeed, a remark similar to that which preceded Theorem 2 would show that there is no loss of generality in assuming that all the eigenvalues of A are of multiplicity not exceeding r. The largest k positive eigenvalues of A under consideration will therefore be numbered in decreasing order $\lambda_1 \geqq \lambda_2 \geqq \cdots \geqq \lambda_k \geqq \lambda_{k+1}$, and $\lambda_j \leqq \lambda_{k+1}$ if $j>k+1$. In the above sequence each eigenvalue of A appears at most r times. The same numbering is assumed for the approximate eigenvalues $\lambda_i^{(n)}$.

3.2. The basic inequality.

3.2.1. The simplest block-Lanczos algorithm can be described as follows.

ALGORITHM ([3], [5]).

1. Choose U_0 such that $U_0U_0=I_r$.
   Set $A_1=U_0^TAU_0$; $B_1=0$; $U_{-1}=0$.
2. For $j=1, 2, \cdots, n-1$ do
   $D_j=AU_{j-1}-U_{j-1}A_j-U_{j-2}B_j^T$.
   Perform the orthonormalization of D_j to obtain
   $D_j=Q_jR_j$, where Q_j is orthonormal and where R_j is an $r\times r$ matrix.
   Take $B_{j+1}=R_j$, $U_j=Q_j$, and $A_{j+1}=U_j^TAU_j$.

If $\dim(E_n)=$ n.r., the realization of this algorithm will be possible and the linear operator $\pi_n A_{|E_n}: E_n \to E_n$ will be represented in the (orthonormal) basis $[U_0, \cdots, U_{n-1}]$ by the block-triadiagonal matrix

$$\begin{bmatrix} A_1 & B_2^T & & & 0 \\ B_2 & A_2 & B_3^T & & \\ & B_3 & \ddots & \ddots & \\ & & \ddots & \ddots & B_n^T \\ 0 & & & B_n & A_n \end{bmatrix}.$$

3.2.2. The rate of convergence can be studied in terms of the number $\|(I-\pi_n)\phi_i\|/\|\pi_n\phi_i\|$ which we now want to estimate. An approach similar to that of Theorem 1 would be difficult, and we prefer to give a natural extension of the inequality (2.2). We shall see that the results obtained are optimal in a certain sense, and that when U_0 reduces to a single vector, the formulas correspond to those of Theorem 1.

In order to state the main inequality we need the following lemma.

LEMMA 4. *Let E_1 be the subspace spanned by the initial system of vectors U_0 and π_1, the orthogonal projection on E_1. Let us assume that the initial system U_0 is such that the vectors $\pi_1\phi_i, \pi_1\phi_{i+1}, \cdots, \pi_1\phi_{i+r-1}$ are independent. Then there exists in E_1 a unique vector $\hat{x}_i$ such that*

$$(\hat{x}_i, \phi_j) = \delta_{ij} \qquad \text{for } j = i, \quad i+1, \cdots, i+r-1. \tag{3.1}$$

The vector $\hat{x}_i$ defined by this lemma is *the vector of E_1* whose orthogonal projection on the (invariant) subspace spanned by $\{\phi_i, \phi_{i+1}, \cdots, \phi_{i+r-1}\}$ is exactly ϕ_i.

Proof of Lemma 4. Since $\{\pi_1\phi_j\}_{j=i,i+r-1}$ forms a basis of E_1, let us write any element x of E_1 as $x = \sum_{j=i}^{i+r-1} t_j \pi_1 \phi_j$. The equations $(x, \phi_k) = \delta_{ik}$, $k = i, i+r-1$, yield the

$$r \times r \text{ linear system } \sum_{j=i}^{i+r-1} (\pi_1\phi_j, \phi_k) t_j = \delta_{ik}. \tag{3.2}$$

Consider the element $(\pi_1\phi_j, \phi_k)$ of the matrix of the system (3.2),

$$(\pi_1\phi_j, \phi_k) = (\pi_1\phi_j, \pi_1\phi_k + (I-\pi_1)\phi_k) = (\pi_1\phi_j, \pi_1\phi_k),$$

since π_1 is an orthogonal projection. This means that the matrix of the linear system (3.2) is the Gram matrix of the system of vectors $\pi_1\phi_i, \pi_1\phi_{i+1}, \cdots, \pi_1\phi_{i+r-1}$ which we assumed independent. It follows that (3.2) admits a unique solution $\{t_j\}$, and (3.1) is satisfied with

$$\hat{x}_i = \sum_{j=1}^{i+r-1} t_j \pi_i \phi_j.$$

The following theorem generalizes the inequalities of Theorem 1 to the block-Lanczos method.

THEOREM 5. *Let λ_i be an eigenvalue of A and ϕ_i an associated eigenvector of norm one. Let us assume that the vectors $\pi_1\phi_j$, $j = i, \cdots, i+r-1$, are linearly independent. Let $\hat{x}_i$ be the vector defined by Lemma 4, that is the vector of E_1 whose orthogonal projection on the subspace spanned by $\{\phi_i, \cdots, \phi_{i+r-1}\}$ is the vector ϕ_i. Let us set*

$$\hat{\gamma}_i = 1 + 2\frac{\lambda_i - \lambda_{i+r}}{\lambda_{i+r} - \lambda_{\inf}} \quad \textit{and} \quad \begin{cases} K_i = \prod_{\lambda_j \in \sigma_i} \dfrac{\lambda_j - \lambda_{\inf}}{\lambda_j - \lambda_i} & \text{if } i \neq 1, \\ K_1 = 1, \end{cases}$$

where σ_i is the set of the first $i-1$ distinct eigenvalues.

Then

$$\frac{\|(I-\pi_n)\phi_i\|}{\|\pi_n\phi_i\|} \leqq \frac{K_i}{T_{n-i}(\hat{\gamma}_i)} \cdot \|\phi_i - \hat{x}_i\|. \tag{3.3}$$

Since $\phi_i - \hat{x}_i$ is orthogonal to ϕ_i, and $\|\phi_i\| = 1$ we note that

$$\|\phi_i - \hat{x}_i\| = \frac{\|\phi_i - \hat{x}_i\|}{\|\phi_i\|} = \tan\theta(\phi_i, \hat{x}_i).$$

Thus (3.3) is equivalent to

$$\tan\theta(\phi_i, E_n) \leqq \frac{K_i}{T_{n-i}(\hat{\gamma}_i)} \cdot \tan\theta(\phi_i, \hat{x}_i). \tag{3.4}$$

Proof of Theorem 5. The vector $\hat{x}_i$ may be written as $\hat{x}_i = \sum_{j=1}^{\infty} \alpha_j\phi_j$. Since $(\hat{x}_i, \phi_j) = \delta_{ij}$ for $j = i, \cdots, i+r-1$, we have $\alpha_j = 1$ and $\alpha_j = 0$ if $i+1 \leqq j \leqq i+r-1$. Thus

$$\hat{x}_i = \alpha_1\phi_1 + \cdots + \alpha_{i-1}\phi_{i-1} + \sum_{j \geqq i+r} \alpha_j\phi_j + \phi_i.$$

Let us consider an element u of E_n of the form $u = p(A)\hat{x}_i$, where p is a polynomial of degree not exceeding $n-1$. Then

$$u = \sum_{j \leqq i-1} p(\lambda_j)\alpha_j\phi_j + p(\lambda_i)\phi_i + \sum_{j \geqq i+r} p(\lambda_j)\alpha_j\phi_j.$$

Let P_i denote the eigenprojection associated with λ_i.

Case $i = 1$. If $i = 1$, then

$$\frac{\|(I-P_1)u\|^2}{\|P_1u\|^2} = \sum_{j \geqq i+r} \frac{(p(\lambda_j)\alpha_j)^2}{p(\lambda_1)^2}. \tag{3.5}$$

Let $\bar{p}$ be the polynomial of degree not exceeding $n-1$, for which the right side of (3.5) is least, and $\bar{u}$ the corresponding vector of E_n; that is, $\bar{u} = \bar{p}(A)\hat{x}_1$. Then, as in Theorem 1, an interesting way of bounding the minimal value of (3.5) is to use the polynomial $t_1(x) = T_{n-1}(\alpha_1 x - \beta_1)$, where $\alpha_1 = 2/(\lambda_{i+r} - \lambda_{\inf})$ and $\beta_1 = (\lambda_{1+r} + \lambda_{\inf})/(\lambda_{1+r} - \lambda_{\inf})$, for which $|T_{n-1}(\alpha_1\lambda_j - \beta_j)| \leqq 1$ for $j \geqq 1+r$. We get

$$\frac{\sum_{j \geqq 1+r} \bar{p}(\lambda_j)^2\alpha_j^2}{\bar{p}(\lambda_1)^2} \leqq \frac{\sum_{j \geqq 1+r} T_{n-1}^2(\alpha_1\lambda_j - \beta_1)\alpha_j^2}{T_{n-1}^2(\alpha_1\lambda_1 - \beta_1)}. \tag{3.6}$$

In (3.6) the numerator is less than $\sum_{j \geqq 1+r} \alpha_j^2$, which is equal to $\|\hat{x}_1 - \phi_1\|^2$, whereas the denominator is exactly $T_{n-1}^2(\hat{\gamma}_1)$. This yields

$$\frac{\|(I-P_1)\bar{u}\|}{\|P_1\bar{u}\|} \leqq \frac{1}{T_{n-1}(\hat{\gamma}_1)} \|\hat{x}_1 - \phi_1\|. \tag{3.7}$$

Now $\hat{x}_1$ is orthogonal to $\phi_2, \cdots, \phi_r$, and this is also true for $\bar{u} = \bar{p}(A)\hat{x}_1$, showing that the orthogonal projection $P_1\bar{u}$ of $\bar{u}$ on the eigenspace associated with λ_1 reduces to its orthogonal projection on the eigenvector ϕ_1. So (3.7) means that there exists in E_n a vector $\bar{u}$ whose acute angle with ϕ_1 satisfies

$$\tan\theta(\phi_1, \bar{u}) \leqq \frac{\|\hat{x}_1 - \phi_1\|}{T_{n-1}(\gamma_1)},$$

so that

$$\tan\theta(\phi_1, E_n) \leqq \frac{\|\hat{x}_1 - \phi_1\|}{T_{n-1}(\hat{\gamma}_i)}.$$

Case $i \neq 1$. If $i \neq 1$, then we get instead of (3.5)

$$\frac{\|(I-P_i)u\|^2}{\|P_i u\|^2}=\frac{1}{p(\lambda_i)^2}\left[\sum_{j=1}^{i-1} p(\lambda_j)^2\alpha_j^2+\sum_{j\geqq i+r} p(\lambda_j)^2\alpha_j^2\right]$$

Here the use of the polynomial

$$t_i(x)=\prod_{\lambda_j\in\sigma_i}(x-\lambda_j)T_{n-i}(\alpha_i x-\beta_i),$$

where $\alpha_i=2/(\lambda_{i+r}-\lambda_{\inf})$ and $\beta_i=(\lambda_{i+r}+\lambda_{\inf})/(\lambda_{i+r}-\lambda_{\inf})$, is suggested by the proof of Theorem 1.

If $\bar{p}$ is the polynomial of degree not exceeding $n-1$ for which $\|(I-P_1)u\|/\|P_1u\|$ is minimal over all elements of the form $u=p(A)\hat{x}_i$, where degree $(p)\leqq n-1$, then

$$\frac{\|(I-P_i)\bar{u}\|^2}{\|P_i\bar{u}\|^2}\leqq\frac{\sum_{j\geqq i+1} t_i^2(\alpha_i\lambda_j-\beta_j)\alpha_j^2}{t_i^2(\alpha_i\lambda_i-\beta_i)}\leqq\frac{K_i^2}{T_{n-i}^2(\gamma_i)}\sum_{j\geqq i+r}\alpha_j^2,$$

where $\sum_{j\geqq i+r}\alpha_j^2$ is smaller than[3]

$$\|\phi_i-\hat{x}_i\|^2=\sum_{j\leqq i-1}\alpha_j^2+\sum_{j\geqq i+r}\alpha_j^2.$$

The proof ends in the same way as for the case $i=1$.

Remarks.

1. Theorem 4 generalizes Theorem 1. Indeed when U_0 reduces to a single vector, that is when $r=1$, then the inequality (3.3) gives back its analogue (2.2) of paragraph 2.

2. In order to show that Theorem 5 is in a certain sense an optimal extension of Theorem 1, let us consider the case where $r=2$, $x_1=\sum_{j\neq 2}\alpha_j\phi_j$, $x_2=\phi_2$. Then it is clear that if one wants to compute the first eigenvalue and its associated eigenvector, the block-Lanczos method will provide the same approximation as with the simple Lanczos method because the second vector x_2 does not contain any more information with that contained in x_1. More precisely, any vector x in E_n can be written $x=p_1(A)x_1+P_2(A)x_2$, where p_1 and p_2 are two polynomials of degree not exceeding $n-1$, and its angle with ϕ_1 will satisfy

$$\tan^2\theta(\phi_1,x)=\frac{1}{\alpha_1^2 p_1(\lambda_1)^2}\left[p_2^2(\lambda_2)+\sum_{j\geqq 3}p_1^2(\lambda_j)\alpha_j^2\right]. \tag{3.8}$$

The minimum of (3.8) is realized when $p_2=0$ (that is when $x=p_1(A)x_1$) and when

$$\sum_{j\geqq 3}\frac{\alpha_j^2}{\alpha_1^2}\frac{p_1^2(\lambda_j)}{p_1^2(\lambda_1)}, \tag{3.9}$$

is minimum over all polynomials p_1 of degree less than n. Now to minimize the expression (3.8) it is sufficient to remark that we need to minimize the angle between the vector ϕ_1 and all vectors of the form $p(A)x_1$, $p\in\mathbf{P}_{n-1}$. This shows that in this case the process reduces to the simple Lanczos process, except that the eigenvalue λ_2 is skipped. Then the equality in (3.3) may be achieved by choosing a suitable sequence of λ_k and α_k (see Remark 3 following Theorem 1 in § 2). This allows us to say that when $i=1$, the result of Theorem 5 is optimal in a certain sense.

[3] This remark shows that the term $\|\phi_i-\hat{x}_i\|$ in (3.3) can be replaced by the smaller one $\|(I-P_1-P_2-\cdots-P_{i-1})(\phi_i-\hat{x}_i)\|$.

3.3. Theoretical error bounds for the eigenelements. In the following theorem, we propose a bound for the theoretical errors on the eigenvalues, similar to that of § 2.

THEOREM 6. *Let us make the same assumptions as for Theorem 5, and set*

$$\hat{\gamma}_i = 1 + 2\frac{\lambda_i - \lambda_{i+r}}{\lambda_{i+r} - \lambda_{\inf}} \quad \text{and} \quad \begin{cases} K_i^{(n)} = \prod_{\lambda_j^{(n)} \in \sigma_i^{(n)}} \dfrac{\lambda_j^{(n)} - \lambda_{\inf}}{\lambda_j^{(n)} - \lambda_i}, & \text{if } i \neq 1, \\ K_1^{(n)} = 1, \end{cases}$$

where $\sigma_i^{(n)}$ is the set of the first $i-1$ approximate eigenvalues.
Then

$$0 \leqq \lambda_i - \lambda_i^{(n)} \leqq (\lambda_i - \lambda_{\inf}) \left[\frac{K_i^{(n)} \|\phi_i - \hat{x}_i\|}{T_{n-i}(\hat{\gamma}_i)} \right]^2. \tag{3.10}$$

Proof. Let $t_i(x)$ be the polynomial defined by

$$t_i(x) = \prod_{\lambda_j^{(n)} \in \sigma_i^{(n)}} (x - \lambda_j^{(n)}) T_{n-i}(\hat{\alpha}_i x - \hat{\beta}_i), \tag{3.11}$$

(if $i = 1$ take $\prod_{j=1}^{i-1} (x - \lambda_j^{(n)}) = 1$), with

$$\hat{\alpha}_i = \frac{2}{\lambda_{i+r} - \lambda_{\inf}}; \qquad \hat{\beta}_i = \frac{\lambda_{i+r} + \lambda_{\inf}}{\lambda_{i+r} - \lambda_{\inf}}. \tag{3.12}$$

Then consider the vector $\psi_i = t_i(A)\hat{x}_i$, where $\hat{x}_i$ is the vector defined by Lemma 4.

- $\psi_i \in E_n$ since degree $(t_i) \leqq n-1$ and $\hat{x}_i \in E_1$.
- ψ_i is orthogonal to each approximate eigenvector $\phi_j^{(n)}$ for $j \leqq i-1$. Indeed, (3.11) and (3.12) show that for each j ($j \leqq i-1$), ψ_i can be written as $\psi_i = (A - \lambda_j^{(n)})u$, where u is a vector of E_n. Thus

$$(\psi_i, \phi_j^{(n)}) = ((A - \lambda_j^{(n)})u, \phi_j^{(n)}) = (u, (A - \lambda_j^{(n)} I)\phi_j^{(n)}) = 0.$$

Here we make use of the fact that $A - \lambda_j^{(n)} I$ is selfadjoint, and that $(A - \lambda_i^{(n)} I)\phi_j^{(n)}$ is orthonormal to the subspace E_n.

- Hence

$$\lambda_i^{(n)} \geqq \frac{(A\psi_i, \psi_i)}{\|\psi_i\|^2} \tag{3.13}$$

because

$$\lambda_i^{(n)} = \max_{u \perp \phi_j^{(n)}, j = 1, \cdots, i-1} \frac{(Au, u)}{\|u\|^2}.$$

Writing $\hat{x}_i = \sum_{j=1}^{\infty} \alpha_j \phi_j$, we may develop (3.13) to obtain

$$0 \leqq \lambda_i - \lambda_i^{(n)} \leqq \frac{\sum_{j=1}^{\infty} (\lambda_i - \lambda_j) t_i^2(\lambda_j) \alpha_j^2}{\sum_{j=1}^{\infty} t_i^2(\lambda_j) \alpha_j^2}.$$

The first i terms of the numerator are nonpositive, and the denominator satisfies

$$\sum_{j=1}^{\infty} t_i^2(\lambda_j) \alpha_j^2 \geqq t_i^2(\lambda_i) \alpha_i^2.$$

(In fact the right-hand side of the inequality is just the dominant term of the left side when n is large). Therefore

$$0 \leqq \lambda_i - \lambda_i^{(n)} \leqq \sum_{j=i+1}^{\infty} (\lambda_i - \lambda_j) \frac{t_i^2(\lambda_j) \alpha_j^2}{t_i^2(\lambda_i) \alpha_i^2}.$$

To complete the proof it is sufficient to notice that

$$\forall j \geqq i+1, \qquad (\lambda_i-\lambda_j)\frac{t_i^2(\lambda_j)}{t_i^2(\lambda_i)} \leqq (\lambda_i-\lambda_{\inf})\left(\frac{K_i^{(n)}}{T_{n-i}(\hat{\gamma}_i)}\right)^2,$$

and that

$$\sum_{j\leqq i+1} \frac{\alpha_i^2}{\alpha_i^2} \leqq \|\phi_i-\hat{x}_i\|^2 = \tan^2\theta(\phi_i,\hat{x}_i).$$

For the eigenvectors, and when λ_i is simple, it is clear that the proof of Theorem 3 is still valid for the block-method, providing the bound

$$\sin\theta(\phi_i,\phi_i^{(n)}) \leqq \left(1+\frac{r_n^2}{d_{i,n}^2}\right)^{1/2} \|(I-\pi_n)\phi_i\|,$$

where

$$r_n = \|(I-\pi_n)A\pi_n\| \quad \text{and} \quad d_{i,n} = \min_{j\neq i} |\lambda_i - \lambda_j^{(n)}|.$$

Now if λ_i is of multiplicity m, which does not exceed r, then that proof can be carried out with the projection $P_i^{(n)}+P_{i+1}^{(n)}+\cdots+P_{i+m-1}^{(n)}$ instead of $P_i^{(n)}$, to yield

$$\left\|\left(I-\sum_i^{i+n-1} P_j^{(n)}\right)\phi_i\right\| \leqq \left(1+\frac{r_n^2}{d_{i,n}^2}\right)^{1/2} \|(I-\pi_n)\phi_i\|,$$

where $d_{i,n} = \min_{j\neq i,\cdots,i+r-1} |\lambda_i-\lambda_j^{(n)}|$ and ϕ_i is any eigenvector associated with λ_i.

4. Numerical experiments.

4.1. The Lanczos method. We now compare, with the help of a few numerical examples, the effective quantities $\theta(\phi_i, E_n)$, $\lambda_i-\lambda_i^{(n)}$, $\theta(\phi_i,\phi_i^{(n)})$, with their theoretical bounds. All the computations were performed on the IBM 360/67 computer of the Grenoble University Computing Center, using a double-precision length of 64 bits with a mantissa of 56 bits.

Only diagonal matrices are considered. As a first example, we select a diagonal matrix A of order $N=50$, with the following distribution for the eigenvalues:

$$\lambda_1 = 1.8;\quad \lambda_2 = 1/4;\quad \lambda_k = \cos[(2k-5)\pi/2(N-2)], \quad \text{for } k=3,\cdots,N.$$

The initial vector x_0 is the vector $e=(1,1,1,\cdots,1)^T$, which forms the same acute angle with each eigenvector of A. The eigenvector ϕ_i is the ith vector of the canonical basis, and therefore $\tan(\phi_i, x_0) = \sqrt{N-1} = 7)$. The Lanczos algorithm with full reorthogonalization was run, and stopped at $n=15$ and at $n=18$. The particular distribution of the spectrum suggests using the refined bound with $p=1$ for the first eigenvalue and the nonrefined one ($p=0$) for the second eigenvalue. This gives the following table.

TABLE 1

$n=15$

i	observed $\tan\theta(\phi_i,E_n)$	bound for $\tan\theta(\phi_i,E_n)$	observed $\lambda_i-\lambda_i^{(n)}$	bound for $\lambda_i-\lambda_i^{(n)}$	observed $\sin\theta(\phi_i,\phi_i^{(n)})$	bound for $\sin\theta(\phi_i,\phi_i^{(n)})$
1	3.9×10^{-6}	1.5×10^{-5}	2.06×10^{-11}	6.5×10^{-10}	4.07×10^{-6}	2.45×10^{-5}
2	3.5×10^{-4}	1.2×10^{-3}	1.02×10^{-7}	3.7×10^{-6}	3.08×10^{-4}	1.9×10^{-3}

$n=18$

i	observed $\tan\theta(\phi_i,E_n)$	bound for $\tan\theta(\phi_i,E_n)$	observed $\lambda_i-\lambda_i^{(n)}$	bound for $\lambda_i-\lambda_i^{(n)}$	observed $\sin\theta(\phi_i,\phi_i^{(n)})$	bound for $\sin\theta(\phi_i,\phi_i^{(n)})$
1	1.06×10^{-7}	4.3×10^{-7}	1.97×10^{-14}	5.10×10^{-13}	9.3×10^{-8}	6.8×10^{-7}
2	2.63×10^{-5}	9.15×10^{-5}	5.60×10^{-10}	2.01×10^{-8}	2.85×10^{-5}	1.4×10^{-4}

In our second example we test the refined bounds of § 2.4 with an *optimal choice* of the parameter p (inequality (2.29)), for the case where A is a 50×50 diagonal matrix with diagonal elements

$$\lambda_1=1.8;\quad \lambda_2=1.6;\quad \lambda_3=1.4;\quad \lambda_4=1.2;\quad \text{and}\quad \lambda_k=1-(k-1)/N,\qquad k=5,\cdots,N;$$

x_0 is again the vector e.

When $n=15$, we obtain the following table for $i=1,2,3$.

TABLE 2

i	p	observed $\tan\theta(\phi_i, E_n)$	bound for $\tan\theta(\phi_i, E_n)$	observed $\lambda_i-\lambda_i^{(n)}$	bound for $\lambda_i-\lambda_i^{(n)}$	observed $\lambda_i-\lambda_i^{(n)}$	bound for $\sin\theta(\phi_i, \phi_i^{(n)})$
1	3	4.0×10^{-7}	3.39×10^{-6}	1.2×10^{-13}	2.04×10^{-11}	4.06×10^{-7}	5.08×10^{-6}
2	2	9.35×10^{-6}	7.87×10^{-5}	8.64×10^{-11}	9.79×10^{-6}	9.55×10^{-6}	1.18×10^{-4}
3	1	1.17×10^{-4}	9.81×10^{-4}	1.04×10^{-8}	1.33×10^{-6}	1.21×10^{-4}	1.47×10^{-3}

In order to show that the bound on $\lambda_i-\lambda_i^{(n)}$ can become very close to the actual errors $\lambda_i-\lambda_i^{(n)}$, we plot in Fig. 1 the values of $\tan\theta(\phi_1, E_n)$ and $\lambda_1-\lambda_1^{(n)}$, as well as their bounds with n taking the values $n=4, 6, 8, \cdots, 16$. This is done for the following choice of A:

$$\text{Dimension } N=50;\quad \lambda_1=1.4;\quad \lambda_k=1-k/N,\qquad k=2,\cdots,50.$$

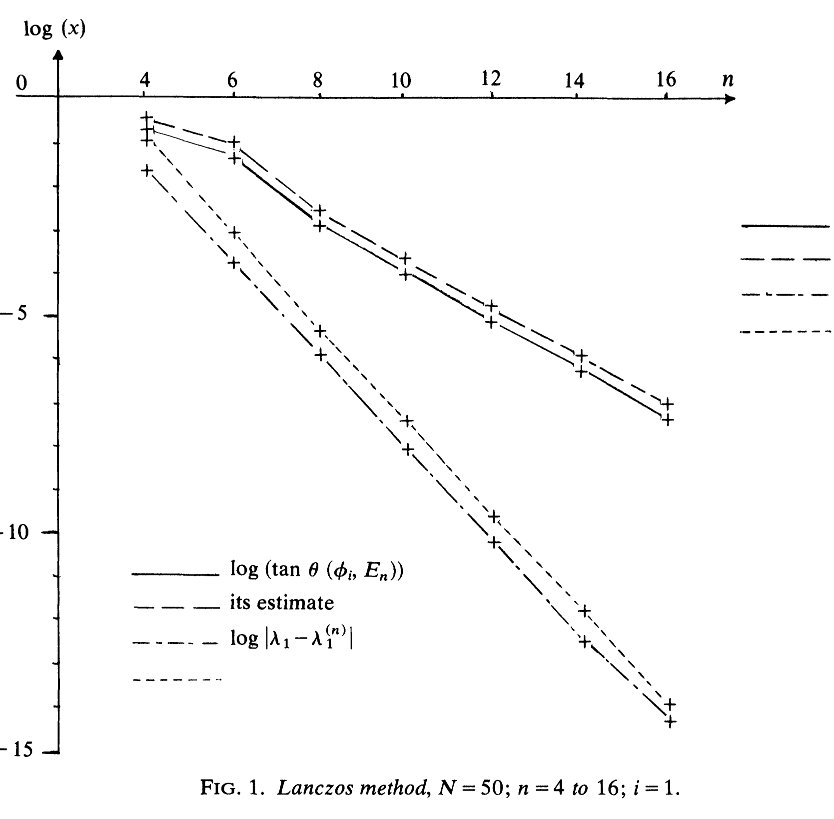

FIG. 1. *Lanczos method, $N=50$; $n=4$ to 16; $i=1$.*

4.2. The block-Lanczos method. For the block-Lanczos method we illustrate the bounds on $\lambda_i - \lambda_i^{(n)}$ and on $\tan \theta(\phi_i, E_n)$ with two examples. In our first example A is a (diagonal) matrix of order 70 with the eigenvalues $\lambda_1 = 2$; $\lambda_2 = 1.5$; $\lambda_k = \cos((2k-2)/(2N-2)$, $k = 3, \cdots, N$. We used two-dimensional blocks ($r = 2$). The starting system $U_0 = (x_1, x_2)$ was chosen as follows. Let

$$e = (1, 1, \cdots, 1)^T; \qquad g = (1, -1, 1, -1, \cdots, 1, -1)^T.$$

Then

$$x_1 = \frac{e}{\|e\|}; \qquad x_2 = \frac{g}{\|g\|}.$$

At $n = 15$, and for $i = 1, 2$, we obtain the results in Table 3.

TABLE 3

i	observed $\tan \theta(\phi_i, E_n)$	bound for $\tan \theta(\phi_i, E_n)$	observed $\lambda_i - \lambda_i^{(n)}$	bound for $\lambda_i - \lambda_i^{(n)}$
1	7.31×10^{-8}	1.14×10^{-7}	1.91×10^{-14}	3.94×10^{-14}
2	9.44×10^{-6}	2.2×10^{-4}	8.60×10^{-11}	1.27×10^{-7}

The second example describes an experiment with three-dimensional blocks. A is of order $N = 60$, with eigenvalues

$$\lambda_1 = 2; \quad \lambda_2 = 1.6; \quad \lambda_3 = 1.4; \quad \lambda_k = 1 - (k-3)/N, \qquad \text{for } k > 3.$$

The starting system has vectors as follows.

$$x_1 = \frac{e}{\|e\|}; \quad x_2 = \frac{f}{\|f\|}; \quad x_3 = \frac{g}{\|g\|},$$

where $f = (1, 0, -1, 1, 0, -1, \cdots, 1, 0, -1)^T$ and $g = (1, -2, 1, 1, -2, 1, \cdots, 1, -2, 1)^T$.

Table 4 gives the results obtained when $n = 12$ and $i = 1, 2, 3$.

TABLE 4

i	observed $\tan \theta(\phi_i, E_n)$	bound for $\tan \theta(\phi_i, E_n)$	observed $\lambda_i - \lambda_i^{(n)}$	bound for $\lambda_i - \lambda_i^{(n)}$
1	4.66×10^{-7}	7.40×10^{-7}	3.14×10^{-13}	1.06×10^{-12}
2	4.11×10^{-6}	4.11×10^{-4}	1.60×10^{-11}	2.62×10^{-7}
3	2.74×10^{-5}	2.33×10^{-2}	5.54×10^{-10}	7.38×10^{-4}

5. Conclusion. In conclusion it should be noted that the theoretical error bounds are often large overestimates of the actual theoretical errors, but that there are cases where the actual errors and their bounds become close to each other when n increases. The principal interest of those a priori error bounds is that they show the convergence of the first k approximate eigenelements towards the first k eigenelements of A, where k is any fixed integer, and when the eigenvalues are ordered in decreasing (or increasing) order. For the block-Lanczos method there are many other possibilities of obtaining a priori error bounds by using vectors of E_n of the form $p_n(A)\hat{x}$, where p_n is a polynomial of degree at most $n-1$, and where $\hat{x}$ is a vector of E_1 (i.e., $x \in \text{span}(U_0)$), which is the best in a certain sense (see e.g. Underwood's bounds [21]). However one cannot say that a certain kind of error bound is the sharpest *in all cases*. Our aim has been to give error bounds which yield sharp estimates of the *asymptotic rates* of convergence (even if the initial constants are large). We mention also that it is possible to derive refined error bounds for the block method, similar to those of § 2.4.

Acknowledgments. The author would like to express his thanks to Professor B. Parlett for a helpful discussion on the present paper. The author is very indebted to the referees for their corrections and suggestions.

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