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The Lanczos Algorithm With Selective Orthogonalization*

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Abstract. The simple Lanczos process is very effective for finding a few extreme eigenvalues of a large symmetric matrix along with the associated eigenvectors. Unfortunately, the process computes redundant copies of the outermost eigenvectors and has to be used with some skill. In this paper it is shown how a modification called selective orthogonalization stifles the formation of duplicate eigenvectors without increasing the cost of a Lanczos step significantly. The degree of linear independence among the Lanczos vectors is controlled without the costly process of reorthogonalization.

1. Introduction. The Lanczos method is well suited to the task of computing a few (p) eigenvalues and eigenvectors of a large ($n \times n$) symmetric matrix A. The wanted eigenvalues may be at either, or both, ends of the spectrum. Typical values are $p = 4$ and $n = 1000$; in a typical application the smallest eigenvalues of A will correspond to the natural frequencies which can be excited in some structure after it is perturbed away from equilibrium.

It seems appropriate to give a brief review of the history of the method. Simple processes, like the Power Method, require, in principle, an infinite number of matrix-vector products to converge to an eigenvector. On the other hand, the method of Minimized Iterations, which Lanczos announced in 1950, expands each eigenvector in a convergent series with at most n terms.** However, Lanczos' method was promptly switched to a different channel. It was used as a process for computing a tridiagonal matrix T orthogonally congruent to A; $T = Q^*AQ$, $Q = (q_1, q_2, \ldots, q_n)$, $Q^* = Q^{-1}$.

Despite its theoretical attractions the Lanczos process was soon displaced by the Givens [1954] and Householder [1958] methods which employ explicit similarity transformations on A. To compete in accuracy the Lanczos process has to be supplemented with the explicit orthogonalization of the Lanczos vectors $\{q_i\}$ which, in exact arithmetic, would be orthogonal automatically.

In 1971 C. Paige showed that the simple Lanczos procedure, without orthogonalization, was very effective for finding a few of the extreme eigenvalues and their matching eigenvectors.

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**Convergence is usually very quick for eigenvectors belonging to extreme eigenvalues.

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In part this is because the only way A enters the Lanczos algorithm is through a subprogram which computes Ax for any given vector x. The user is free to exploit sparseness and compact storage of A in the coding of this subprogram. Equally important is the fact that the algorithm need not go the whole way. It builds up $Q_j = (q_1, \ldots, q_j)$ and $T_j = Q_j^* A Q_j$ by step j and can often be stopped at values of j as small as $2\sqrt{n}$. Paige [1971] showed that loss of orthogonality among the Lanczos vectors $\{q_1, q_2, \ldots\}$ was a necessary and sufficient condition, in finite precision arithmetic, for convergence of at least one of T_j's eigenvalues to one of A's eigenvalues.

This left the Lanczos algorithm as a very powerful tool in the hands of an experienced user. However, it did not provide a black box program which could be used "off the shelf" in the same way as eigenvalue programs for small matrices. There are several rather technical reasons for this. For one thing suitable criteria for accepting good approximations, rejecting spurious approximations, or stopping were all rather elusive. Left to itself a simple Lanczos program will run forever, doggedly finding more and more copies of the outer eigenvalues for each new inner eigenvalue it discovers. This uncertainty about the amount of storage which is needed prompted the suggestion, by Golub and others, that the Lanczos method be used iteratively. That is, after k steps the best approximation to an eigenvector is computed and it, or some modification of it, is used as a new starting vector. With this approach the old difficulties take on new forms: how to choose k and how to select the new starting vector.

Another variation which has been used with success is the block form of the Lanczos method. Each step becomes more costly but fewer are needed, and this seemed to be the only way to find small clusters of close or multiple eigenvalues. However, the user has to make the difficult choice of the block size.

The remainder of this article describes an inexpensive modification of the simple algorithm (we call it Lanczos with *selective orthogonalization*) which permits the simple Lanczos process to be used as a black box. Moreover,

1. No redundant copies of eigenvectors are computed.

2. A posteriori error bounds and estimates cost almost nothing and are used in order to stop the program as soon as possible.

3. Multiple eigenvalues, and their eigenvectors, are found naturally, thanks to roundoff error.

Not surprisingly, the idea of purifying Lanczos vectors did not come out of the blue. Cullum and Donath [1974] found it necessary to deflate converged Ritz vectors from their blocks, Lewis [1977] found that some deflation helped in a difficult calculation of interior eigenvalues, and Underwood [1975] removed such vectors from his blocks when restarting the iterative version of Lanczos. However, we do not regard deflation as an aid in adversity but as a tool for producing orthogonal Ritz vectors; and thus, our orthogonalization is independent of convergence and will occur beforehand, especially when the user wants high accuracy.

2. Notational Conventions.

Integers–i, j, k, l, m, n, p.

Scalars–small Greek letters $\alpha, \beta, \ldots$.

(Column) Vectors–small roman letters $x, y, \ldots$ (except for the integers).

Matrices–capital roman letters.

Identity matrix–$I = (e_1, e_2, \ldots, e_n)$.

Diagonal matrices–capital Greek letters.

SYMMETRIC (nondiagonal) MATRICES–SYMMETRIC LETTERS A, H, M, U, V, W, X.

Tridiagonal matrices–

$$T_j = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \alpha_{j-1} & \beta_{j-1} \\ & & & \beta_{j-1} & \alpha_j \end{bmatrix}.$$

All vectors are n-dimensional unless the contrary is stated. All square matrices are $n \times n$ unless the contrary is stated.

$A - \xi$ is written for $A - \xi I$.

Span$(b_1, \ldots, b_j)$ denotes the subspace generated by $b_1, \ldots, b_j$.

x^* is the transpose of x.

$\|x\| = \sqrt{x^*x}$, the Euclidean norm.

$\lambda_i[M]$–the ith eigenvalue of M (from the left).

$$\text{Eigenvalue Ordering:} \begin{cases} \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n, \\ \lambda_{-n} \leqslant \cdots \leqslant \lambda_{-2} \leqslant \lambda_{-1}. \end{cases}$$

$\|M\| = \max_i |\lambda_i[M]| = \max \|Mv\|/\|v\|, v \neq 0$.

(j)–a formula in the current section.

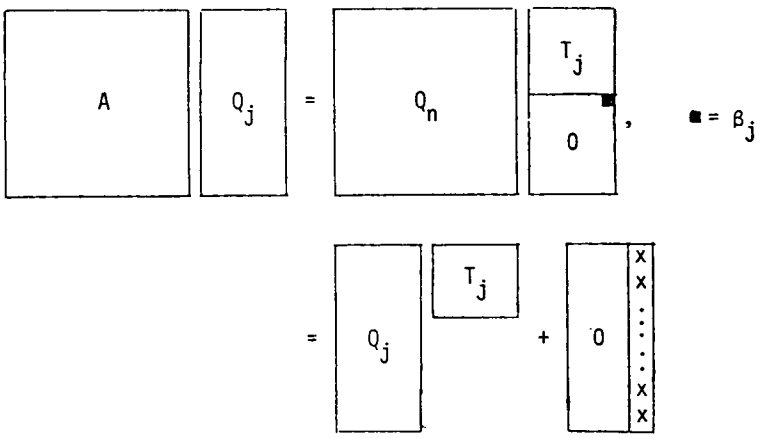
(k, j)–a formula in section k.

3. Lanczos in Exact Arithmetic. A can be reduced to tridiagonal form T_n in many different ways. Let

$$Q_n^* A Q_n = T_n \tag{1}$$

be one such reduction, where $\mathbf{Q}_n = (q_1, \ldots, q_n)$ is orthogonal. If the off-diagonal elements β_i, $i = 1, \ldots, n-1$, of T_n are positive then, in fact, T_n and Q_n are completely determined by q_1 or by q_n. Let us write (1) in the form $AQ_n = Q_n T_n$ and see what it says about the $n \times j$ submatrix $Q_j = (q_1, \ldots, q_j)$, $j < n$.

(2)



The last column on the right is $r_j \equiv q_{j+1}\beta_j$. Now (2) can be written compactly as

$$AQ_j = Q_jT_j + r_je_j^*, \qquad j = 1, \ldots, n, \tag{3}$$

where $e_j^* = (0, \ldots, 0, 1)$ has j elements and $\beta_n = 0$. From the orthogonality of Q_n follows

$$Q_j^*Q_j = 1, \tag{4}$$

whereas $Q_jQ_j^*$ is an orthogonal projector onto span Q_j.

Note that if β_j $(= \|\mathbf{r}_j\|) = 0$, then span Q_j is an invariant subspace and T_j is the restriction of A to it. In genuine applications $\beta_j = 0$ never happens, even for $j > n$!

The Lanczos algorithm builds up Q_j and T_j one column per step. Some important relations follow from (3) and (4) and are independent of the specific implementation of the algorithm.

Orthogonality. Since r_j is a multiple of q_{j+1} it must be orthogonal to all previous q_i, $i = 1, \ldots, j$. In fact, this property can be deduced from (3) and (4) without invoking (1).

LEMMA 1. *Let Q_j be any matrix satisfying* (3) *and* (4). *Then $Q_{j-1}^*r_j = 0$ and, if $\alpha_j = q_j^*Aq_j$, then $Q_j^*r_j = 0$ too.*

A proof is given in Kahan and Parlett [1974].

The Lanczos algorithm proceeds from Q_j to Q_{j+1} by forcing $q_j^*r_j = 0$ via the choice of α_j and then normalizing r_j to get β_j and q_{j+1}. What could be simpler? Note that $Q_{j-1}^*r_j$ is not forced to vanish because, *in exact arithmetic,* the lemma guarantees it. From (3)

$$r_j = r_je_j^*e_j = (AQ_j - Q_jT_j)e_j = Aq_j - q_{j-1}\beta_{j-1} - q_j\alpha_j. \tag{5}$$

Observe that $q_1, \ldots, q_{j-2}$ are not needed for the computation of α_j, r_j, β_j, q_{j+1} (i.e. the jth step) and so may be put out to a secondary storage medium. This is a very attractive feature of the method.

Suppose that the Lanczos algorithm pauses at the jth step and makes a subsidiary computation of some, or all, of the eigenvalues and eigenvectors of T_j. Let

$$T_j = S_j \Theta_j S_j^*, \tag{6}$$

where $S_j = (s_1, \ldots, s_j)$ is $j \times j$ and orthogonal and $\Theta_j = \operatorname{diag}(\theta_1, \ldots, \theta_j)$ has the eigenvalues of T_j. Since $T_j = Q_j^* A Q_j$, the values θ_i and the vectors $y_i = Q_j s_i$ are the (optimal) Rayleigh-Ritz approximations to A from the information on hand, i.e. from $\operatorname{span}(Q_j)$. Note that

$$\|AQ_j - Q_j T_j\| = \|r_j e_j^*\| = \beta_j. \tag{7}$$

How good are these optimal approximations?

THEOREM 1. *There are j eigenvalues of A, call them $\lambda_{1'}, \ldots, \lambda_{j'}$, such that $|\lambda_{i'} - \theta_i| \leqslant \beta_j$, $i = 1, \ldots, j$.*

A proof is given in Kahan [1967]. See also Kahan and Parlett [1976]. The bound covers all the θ_i and does not discriminate between them. We can do better. Let s_{ji} denote the bottom (jth) element of T_j's eigenvector s_i.

THEOREM 2. *To each i there is a corresponding eigenvalue of A, call it $\lambda_{i'}$, such that*

$$|\lambda_{i'} - \theta_i| \leqslant \beta_j |s_{ji}| \equiv \beta_{ji}, \quad i = 1, \ldots, j.$$

A proof is given in Kahan and Parlett [1976]. The quantity $\beta_{ji} = \|(A - \theta_i)\mathbf{y}_i\|$, the ith residual.

THEOREM 3. *Let $Az_{i'} = z_{i'}\lambda_{i'}$, let ψ_i be the angle between $z_{i'}$ and its Ritz vector $y_i \equiv Q_j s_i$, and let the gap $\gamma_i \equiv \min_{k \neq i'} |\lambda_k - \theta_i|$. Then, for $i = 1, \ldots, j$,*

$$|\lambda_{i'} - \theta_i| \leqslant \beta_{ji}^2/\gamma_i, \qquad \tan \psi_i \leqslant \beta_{ji}/\gamma_i.$$

Proofs are given in Davis and Kahan [1970].

In principle γ_i is unknown and these bounds are not computable. However, $\delta_i = \min_{k \neq i} |\theta_k \pm \beta_{jk} - \theta_i|$ can be used in place of γ_i to give an estimate.

The following result, proved in Kahan [1967], shows that the previous bounds fail gracefully when Q_j is not orthonormal. Specifically, the bounds must be multiplied by $\sqrt{2}/\sigma_1$, where σ_1^2 is the smallest eigenvalue of $Q_j^* Q_j$.

THEOREM 4. *Given $A, n \times n$, $Q, n \times m$, $H, m \times m$, with $\lambda_i[H] = \theta_i$, $i = 1, \ldots, m$, there are m of A's eigenvalues, call them $\lambda_{i'}$, so that for $i = 1, \ldots, m$,*

$$|\lambda_{i'} - \theta_i| \leqslant \sqrt{2}\,\|AQ - QH\|/\sigma_1(Q),$$

where $\sigma_1^2 = \lambda_1[Q^*Q]$.

The Kaniel-Paige theory (Kaniel [1966]) shows that it is the extreme (leftmost and rightmost) eigenvalues which are most likely to be approximated by some of the θ_i. Moreover, the rapidity of convergence, as j increases, depends on the (unknown)

gaps between A's eigenvalues. Cases have occurred in which an unusual distribution of eigenvalues coupled with special q_1's have caused interior eigenvalues to come out first. See Cline, Golub and Platzman [1976].

In principle, then, the Lanczos algorithm should be continued, with periodic pauses, until, and only until, adequate approximations to the wanted eigenvalues and eigenvectors are in hand. This sometimes happens for values of j as small as $2\sqrt{n}$, another attraction of the method.

In practice, things are not this simple. With finite precision computation convergence goes hand in hand with loss of linear independence among the q_i, and so the error bounds cease to be valid by the time the first of the θ_i converges.

Before leaving the context of exact arithmetic we want to emphasize the value of the bounds β_{ji}. They show why the absence of small β_j does not impede convergence of *some* of the θ_i to eigenvalues and the computable numbers s_{ji} show *which* of the θ_i are converging. There are extensions of Theorem 3, which allow a bunch of close θ's and their y's to be treated simultaneously; the gap then becomes the distance of the cluster from eigenvalues not associated with the cluster.

4. Orthogonality Versus Convergence. The use of finite precision arithmetic provokes significant departures from the exact version of the Lanczos algorithm described above. In order to examine these effects we turn our backs on the quantities which would be produced by use of exact arithmetic and make a standard change of notation. The symbols Q_j, T_j, α_j, β_j from now on denote the computed quantities stored in the computer under these names. We shall not try to compare them with their Platonic counterparts but instead we will seek the (more complicated) relations which do hold between the objects on hand.

The fundamental equation (3.3) becomes

$$AQ_j = Q_jT_j + r_je_j^* - \bar{F}_j, \tag{1}$$

where $\bar{F}_j$ accounts for local round-off effects. Paige has shown that if the algorithm is implemented correctly, $\bar{F}_j$ is harmless, satisfying an inequality of the form $\|\bar{F}_j\| \leqslant \phi(n)\epsilon\|A\|$ for some almost linear function ϕ (Paige [1972], [1976]). The orthogonality relation (3.4) fails and in its place we write

$$\|1 - Q_j^*Q_j\| \leqslant \kappa_j. \tag{2}$$

In the last section we given an expression for κ_j; but here we focus on the more special and more important issue of orthogonality loss among the vectors $y_i = Q_js_i$, $i = 1, \ldots, j$, which we continue to call Ritz vectors despite the fact that the optimality with which they approximate eigenvectors of A departs hand in hand with Q_j's orthogonality.

In Paige [1971] can be found the following remarkable results in which the bottom elements s_{ji} $(= e_j^* s_i)$ of T_j's eigenvectors s_i appear again.

THEOREM 5. *Consider the jth step of the simple Lanczos algorithm, and drop the index j on which all the quantities depend. The computed approximate eigenpairs* (θ_i, y_i), $i = 1, \ldots, j$, *satisfy*

$$y_i^* y_k = [g_{ii}(s_{jk}/s_{ji}) - g_{kk}(s_{ji}/s_{jk}) + f_{ik}]/(\theta_i - \theta_k), \qquad i \neq k,$$

where G and F are round-off matrices; $\|G\| \doteq \|F\| \doteq \epsilon\sqrt{n}\,\|T\|$, *where* ϵ *is the relative precision of the arithmetic. Moreover,*

$$y_i^* q_{j+1} = g_{ii}/\beta_{ji} = g_{ii}/(\beta_j |s_{ji}|), \qquad i = 1, \ldots, j.$$

The bottom elements of the s_i appear in a special way. With any good program, S will be orthonormal (to working accuracy) so that $\Sigma_{i=1}^{j} s_{ji}^2 = 1$. If

$$|s_{jk}| \doteq |s_{ji}| \doteq j^{-1/2}, \qquad |\theta_i - \theta_k| > \|T\|/100, \tag{3}$$

then the error bounds (Theorems 3 and 4) on θ_i and θ_k indicate that they are poor eigenvalue approximations while Theorem 5 shows that y_i and y_k are orthogonal to working accuracy. Conversely, if $|s_{ji}| < 10^{-3}$, say, then θ_i (if isolated) is a good eigenvalue approximation, y_i is good too, and y_i will *not* be orthogonal to any *unconverged* y_k (indicated by $s_{jk} \doteq j^{-1/2}$). Since S is orthogonal to working accuracy, it is Q_j which must have lost orthonormality. The better the approximations θ_i and y_i the greater the departure of Q_j from orthogonality.

A further analysis (Paige [1971]) shows that $\frac{1}{2} \leqslant \|y_i\| \leqslant 2$ provided that the θ's are not too close. What this means in practice is that Ritz vectors y_i cannot shrink alarmingly unless there are two or more θ's approximating a *single* eigenvalue λ. Our orthogonalization forestalls this calamity.

As the Lanczos algorithm proceeds with increasing j, the loss of orthogonality among the Lanczos vectors $\{q_i\}$ is widespread but has no apparent structure. It is the Ritz vectors $\{y_i\}$ which display the pattern of the loss of orthogonality. Unconverged Ritz vectors will be mutually orthogonal while both the unconverged Ritz vectors and q_{j+1} will have strong components in the direction of Ritz vectors which have nearly converged.

Example of Loss of Orthogonality.
$n = 6$.
$A = \text{diag}(0., .00025, .0005, .00075, .001, 10.)$.
$q_1 = 6^{-1/2}(1., 1., 1., 1., 1., 1.)^T$.
Unit round off $\doteq 10^{-14}$.
Simple Lanczos was run for six steps. $Y_6 = Q_6 S_6$.

$Q_6^*Q_6$

.10E+01	.75E-14	-.30E-10	.25E-06	.97E-02	.41E+00
.75E-14	.10E+01	.33E-10	.55E-06	.22E-01	.91E+00
-.30E-10	.33E-10	.10E+01	-.97E-10	.19E-05	.79E-04
.25E-06	.55E-06	-.97E-10	.10E+01	.11E-09	.23E-08
.97E-02	.22E-01	.19E-05	.11E-09	.10E+01	-.12E-12
.41E+00	.91E+00	.79E-04	.23E-08	-.12E-12	.10E+01

$\theta_i \longrightarrow$ .62E-05 .32E-03 .68E-03 .99E-03 .10E+02 .10E+02

$\downarrow$ $Y_6^*Y_6$

.62E-05	.10E+01	.53E-10	.18E-10	.16E-13	-.12E-12	-.41E-08
.32E-03	.53E-10	.10E+01	-.39E-14	-.18E-10	-.93E-13	-.98E-08
.68E-03	.18E-10	.39E-14	.10E+01	-.53E-10	-.78E-13	-.98E-08
.99E-03	.16E-13	-.18E-10	-.53E-10	.10E+01	-.13E-12	-.41E-08
.10E+02	-.12E-12	-.93E-13	-.78E-13	-.13E-12	.10E+01	.10E+01
.10E+02	-.41E-08	-.98E-08	-.98E-08	-.41E-08	.10E+01	.10E+01

Note that the general loss of orthogonality seen in $Q_6^*Q_6$ is represented in $Y_6^*Y_6$ as the second copy of the eigenvector associated with the eigenvalue 10.

5. Selective Orthogonalization. One way to restore orthogonality to Q_j is to use the modified Gram-Schmidt process in order to force q_{j+1} to be orthogonal to all previous q's. Besides the ever increasing expense in arithmetic operations, this reorthogonalization process requires the presence of all the q_i at each step. Paige's result suggests that linear independence of the q's can be maintained by merely orthogonalizing the q's against a few selected vectors, namely the Ritz vectors which have nearly converged. Hence, the name of the algorithm.

The modification of the simple Lanczos process is as follows. At each pause T_j is diagonalized and the bounds on the not-yet-computed Ritz vectors are inspected. Those Ritz vectors with error bounds less than $\sqrt{\epsilon}\|A\|$ are declared good, are computed, orthonormalized, and then stored in the fast memory. From that point until the next pause all future q's are kept nearly orthogonal to these directions.

It might appear to be necessary to orthogonalize only q_{j+1} and q_{j+2} against these good y's. It follows from (3.5) that all subsequent q's would remain orthogonal to them. In finite precision, however, the error vector in each computation of Aq_k will bring back small multiples of *all* A's eigenvectors. Fortunately, it is not necessary

to orthogonalize r_j against the y's at every step as Section 7 reveals.

The purpose of selective orthogonalization is to prevent the computation of many unwanted copies of all the well-separated outer eigenvectors. This reduces the number of Lanczos steps required to compute the wanted eigenvalues and eigenvectors and so keeps the number of calls on the large matrix A as low as possible. The algorithm must compute and store good Ritz vectors even if some of them are not wanted by the user. For example, if the three eigenvectors at the left end of the spectrum are wanted, the algorithm may well have computed three or more eigenvectors at the right end as well, should they happen to be better separated from the rest of the spectrum than are the ones we want.

Example of Selective Orthogonalization.

$n = 6$.

A = diag(0., .00025, .0005, .00075, .001, 10.).

$q_1 = 6^{-1/2}(1., 1., 1., 1., 1., 1.)^T$.

Unit round off $\doteq 10^{-14}$.

The Lanczos algorithm with selective orthogonalization was run for six steps. It paused after four steps and computed a good Ritz vector for the eigenvalue 10. It then took two more steps orthogonalizing against this vector.

$Q_6^*Q_6$ for Selective Orthogonalization

.10E+01	.75E-14	-.30E-10	.25E-06	-.11E-09	.92E-10
.75E-14	.10E+01	.33E-10	.55E-06	.51E-10	-.36E-10
-.30E-10	.33E-10	.10E+01	-.97E-10	-.44E-10	-.37E-07
.25E-06	.55E-06	-.97E-10	.10E+01	.24E-07	-.64E-08
-.11E-09	.51E-10	-.44E-10	.24E-07	.10E+01	.10E-13
.92E-10	-.36E-10	-.37E-07	-.64E-08	.10E-13	.10E+01

Note that the leading 4×4 principal minor is the same as in the earlier example. Robust linear independence has been maintained by selective orthogonalization.

6. When to Pause. There are five possible strategies for deciding when to pause. The simplest (and cheapest) is to pause every m steps, where m is some constant, possibly depending on $n = \dim(A)$, but independent of all other characteristics of A. Such a plan is completely insensitive to the loss of orthogonality in Q_j and is unsatisfactory in practice.

Paige and others have suggested keeping q_1 in fast store and computing $q_1^* q_j$ as a measure of the loss of orthogonality. This is not cheap since it requires the storage of an n-vector as well as the computation of a vector inner product at each step. This scheme usually works quite well. However, this estimate is a lower bound rather than an upper bound on $\|I - Q_j^*Q_j\|$. Therefore, on occasion, the pause may come too late and disastrous failures of this kind are possible in practice. Furthermore, it is

not clear how to apply this scheme, after the first pause, for deciding when to pause again.

Kahan and Parlett [1974], [1976] have described two different schemes for bounding $\|I - Q_j^* Q_j\|$. The scoreboard majorizes the matrix $I - Q_j^* Q_j$, which requires j^2 storage locations. Since the orthogonalizations will permit the Lanczos process to continue well beyond $j = \sqrt{n}$ steps, this storage cost becomes excessive. The other scheme is a scalar bound κ_j on $\|I - Q_j^* Q_j\|$. Only a few arithmetic operations are needed to update κ at each step, independent of both j and n.

Rather than monitoring the loss of orthogonality, it is also possible to monitor convergence of the Ritz vectors instead. If the β_{ji} are calculated at each step (or even a few of them from each end of the spectrum), the moment to pause can be determined exactly. One way of doing this would be to calculate *all* the Ritz values at each step and use a formula from Paige [1971] that states that

$$s_{ji}^2 = \chi_{j-1}(\theta_i)/\chi_j'(\theta_i), \tag{1}$$

where $\chi_j(\mu)$ is the characteristic polynomial of T_j. Another way would be to calculate a few eigenvalues of T_j at each end of the spectrum, and then use inverse iteration to find the bottom elements of the corresponding eigenvectors.

The program described in the rest of this paper uses the kappa bound exclusively to determine when to pause. The details of the implementation are given in Section 14.

On the other hand the possibility of directly monitoring convergence is quite appealing. This approach, used on its own or in conjunction with the kappa bound, is being actively investigated.

7. Monitoring the Return of Banished Ritz Vectors. Let y be a good normalized Ritz vector, and let τ_j be a bound on $|y^* q_j|$, the unwanted component of y in q_j. There is a simple three term recurrence governing the τ's. We have

$$Ay = \theta y + r \quad (r \text{ is not to be confused with } r_j). \tag{1}$$

The quantities computed in the jth step of the Lanczos algorithm satisfy

$$q_{j+1}\beta_j = Aq_j - q_j\alpha_j - q_{j-1}\beta_{j-1} + f_j, \tag{2}$$

where f_j accounts for the round off and $\|f_j\| \leqslant \nu\epsilon\|A\|$ for some constant ν which depends on A but not on j. Hence,

$$y^* q_{j+1}\beta_j = y^* Aq_j - y^* q_j\alpha_j - y^* q_{j-1}\beta_{j-1} + y^* f_j. \tag{3}$$

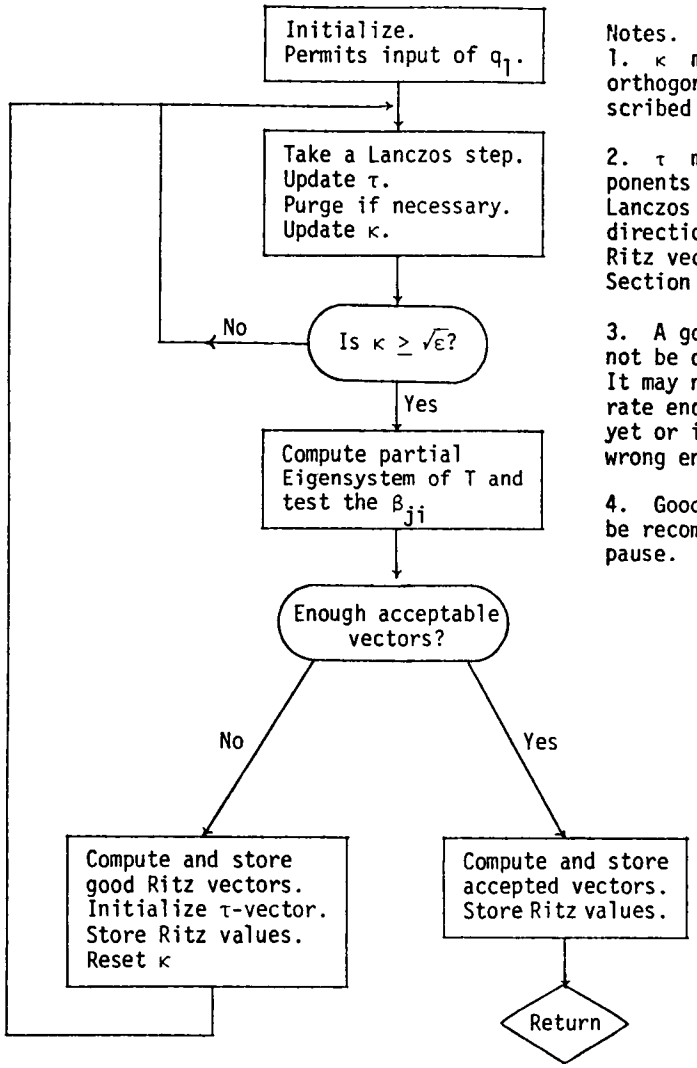
Because $|y^* q_j| \leqslant \tau_j$, (1) and (2) yield

$$(4) \qquad |y^*q_{j+1}| \leqslant [|\theta - \alpha_j|\tau_j + \beta_{j-1}\tau_{j-1} + |r^*q_j| + \nu\epsilon\|A\|]/\beta_j \equiv \tau_{j+1}.$$

Moreover, $r = q_{k+1}\beta_{ki}$ for some $k < j$, so $|r^*q_j| \leqslant \beta_{ki}|q_k^*q_j| \leqslant \beta_{ki}\sqrt{\epsilon} = O(\epsilon\|A\|)$. Since ν and $\|A\|$ are not readily available, the program simply drops the last two terms in (4). Each time that a pair of q's are explicitly orthogonalized against y the corresponding τ's are set to ϵ. Then the recurrence is updated by (4) at each step and tested. As soon as τ_j again exceeds the tolerance, y is explicitly deflated out of q_j and q_{j+1}. The tolerance is not critical ($\sqrt{\epsilon}$ seems to be an appropriate value).

Along with each computed Ritz vector is stored the associated eigenvalue θ_i, the residual norm estimate β_{ji}, and cells for the current and previous τ-values. The cost of updating this information is negligible. Thus, τ may be thought of as a two-rowed array of length equal to the number of good Ritz vectors.

8. Flowchart I. Lanczos with selective orthogonalization, ample storage and no multiple eigenvalues.



Notes.

1. κ monitors loss of orthogonality and is described in Section 14.

2. τ monitors the components of the current Lanczos vector in the directions of the good Ritz vectors. See Section 7.

3. A good Ritz vector need not be one which is wanted. It may not be quite accurate enough to be accepted yet or it may belong to the wrong end of the spectrum.

4. Good Ritz vectors will be recomputed at each pause.

9. Running Out of Storage. Information is always lost when the Lanczos process is restarted. Since our algorithm maintains semiorthogonality among the q-vectors at a modest cost, the usual reason for restarting is not present. However, since the available storage may be quite limited on some computer systems, the program must be capable of restarting when necessary and as much information as possible should be retained.

Every time that storage has been exhausted, the program calculates and permanently stores all acceptable wanted R-vectors and all good vectors not among those desired. It also stores the corresponding Ritz values and sorts all the permanently stored Ritz vectors by increasing Ritz value.

There remains the question of what the starting vector should be. The new q_1 is currently taken to be a linear combination of some of the Ritz vectors which are not acceptable. The one with smallest residual β_{ji} is always used as well as any others which have converged to half the acceptable accuracy. The weights for the linear combination are the reciprocals of the β_{ji}. Other choices for the restart vector could be made. Before restarting q_1 is orthogonalized against all the permanent vectors, and the τ-vector (see Section 7) is initialized.

10. Multiple Eigenvalues. Since the Lanczos algorithm only examines the subspace spanned by the vectors $(q_1, Aq_1, A^2q_1, \ldots, A^jq_1)$, it is unable to detect any eigenvector which is orthogonal to q_1. In particular, it is incapable of finding multiple eigenvalues. If V is the eigenspace of a multiple eigenvalue λ, then the Lanczos algorithm will find only the single eigenvector in the direction of the projection of q_1 onto V.

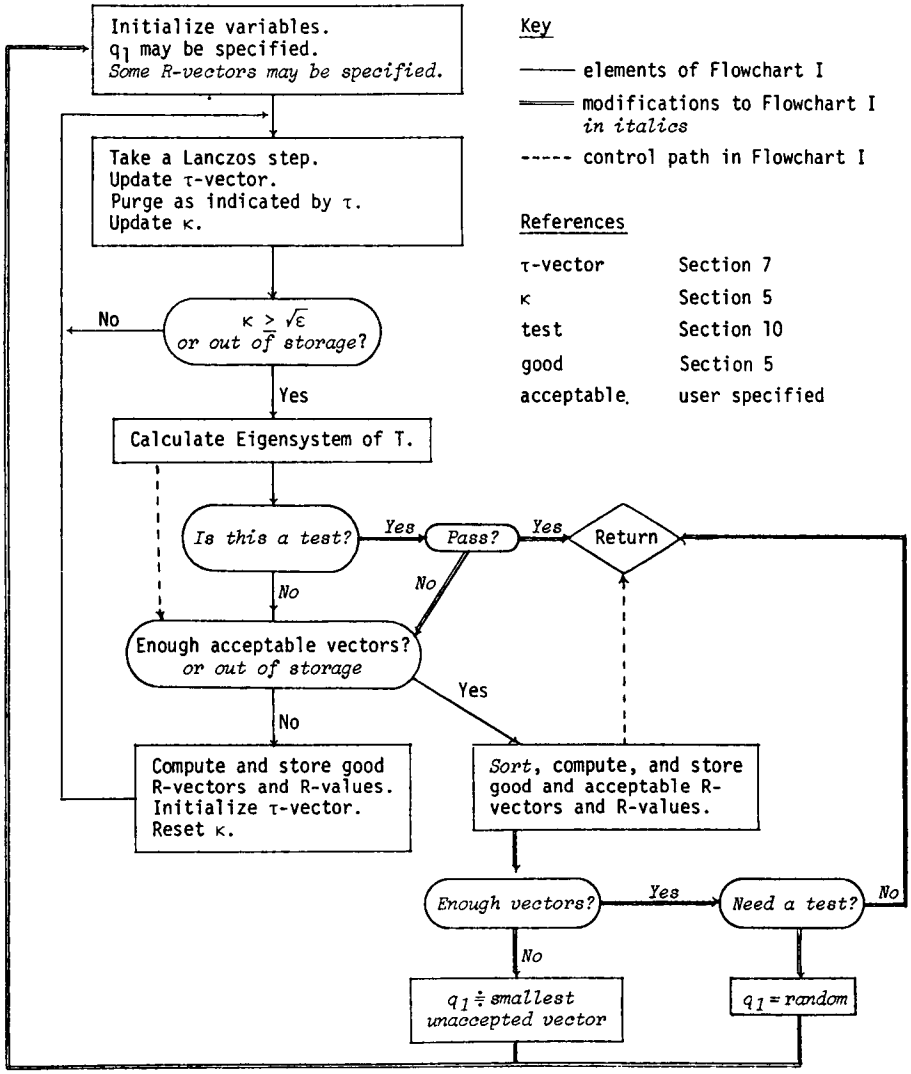
Despite this, the program finds multiple eigenvalues quite naturally. Rounding errors introduce components in all directions. After one eigendirection of a multiple eigenvalue has been found the components in orthogonal directions will persist after purification. These components will grow as the algorithm continues until a second eigenvector, orthogonal to the first, has been found.

Since multiple eigenvalues are found sequentially instead of simultaneously, a more sophisticated termination criterion is needed. For example, if A has a double eigenvalue at zero, a simple eigenvalue at 1, and the rest of the spectrum larger than 2, then the program will find an eigenvector of 0 and the eigenvector of 1 at about the same time. Therefore, if the program finds enough acceptable vectors it must decide whether to start over again to test for undisclosed multiplicities. Currently, the program makes a test run if, at the last pause, more than one acceptable eigenvalue is found, or if the only one found is in the convex hull of the rest of the acceptable eigenvalues found so far. This strategy is rather conservative and will often make test runs which are unnecessary. However, with this criterion multiple eigenvalues will always be correctly unearthed.

11. Can Low Accuracy Be Achieved Safely? Yes. The user desired accuracy is used only in determining which of the desired vectors should be saved permanently

when the process is started. A simple perturbation argument shows that any eigenvalue found after a restart is perturbed by no more than the maximum of the norms of the residuals of the permanent vectors. Consequently, eigenvalues found on later passes will be of the same order of accuracy as those found earlier.

12. **Flowchart II.** Modifications of Flowchart I to cope with limited storage and multiple eigenvalues.



13. **Some Numerical Comparison for Lanso.** We present some comparisons of LANSO (Lanczos Algorithm with Selective Orthogonalization) with published examples of block Lanczos programs written by R. Underwood and by J. Cullum and W. E. Donath. We have numbered the examples as they appear in the references. Unfortunately, the number of vector inner products needed by the Cullum and Donath program is not available. After the comparison we also trace the history of LANSO as it solved the problem. In all but the last example, significant effort was spent on the final multiple

eigenvalue check. A modification is planned which would reduce the length of the check run significantly.

Underwood Examples. (Example 2 omitted.)

Example 1. This example has a cluster of three eigenvalues well separated from the rest. Three eigenvalues were requested (nval = 3).

$n = 453$, nval = 3, ifig = 8 = no. of correct decimal digits desired

$\lambda_1 = -10., \lambda_2 = -9.99, \lambda_3 = -9.98, \lambda_i = -9. + .02 \times (i-4), i = 4, 5, \ldots, 454$

	matrix-vector products	vector inner products	max error in eigenvalues	max residual norm
Block Lanczos	165	1265	10^{-13}	3×10^{-6}
LANSO	70	191	10^{-11}	3×10^{-6}

History of LANSO (mxstep = 50. = maximum no. of Lanczos steps permitted in a run)

	pause at j =	κ	new κ	comments
	26	2.4	1.6×10^{-12}	
	44	3.4		3 vectors found
restart (check)	26	1.1		terminate

Example 3. This example is a purely linear distribution. It is the most difficult of the Underwood examples since the eigenvalues desired are not well separated from the rest.

$n = 101$, nval = 6, ifig = 5

$\lambda_i = -(101 - i)/100$

	matrix-vector products	vector inner products	max error in eigenvalues	max residual norm
Block Lanczos	350	1974	10^{-9}	2×10^{-5}
LANSO	112	383	10^{-7}	1×10^{-4}

History of LANSO (mxstep = 50.)

	pause at j =	κ	new κ	comments
	27	2.8	1×10^{-12}	
	46	2.4	6×10^{-10}	
	50	3×10^{-7}		3 vectors found
restart				
	20	3.1	4×10^{-11}	
	36	.92		3 more vectors found
restart (check)	26	2.2		terminate

Example 4. This example has two double eigenvalues separated from the rest of the spectrum. Note that LANSO finds the eigenpairs to higher precision than desired. This is very common when low accuracy is desired for *well-separated* multiplicities.

$n = 180$, nval = 4, ifig = 4

$\lambda_1 = \lambda_2 = 0, \lambda_3 = \lambda_4 = .1, \lambda_i = .25 + .01 \times (i - 5)$, for $i = 5, 6, \ldots, 180$

	matrix-vector products	vector inner products	max error in eigenvalues	max residual norm
block size = 1	158	997		
block size = 2	125	725	2×10^{-9}	1.5×10^{-4}
block size = 3	140	699		
block size = 4	317	1330		
LANSO	120	361	3×10^{-13}	5×10^{-7}

History of LANSO (mxstep = 50.)

	pause at j =	κ	new κ	comments
	25	1.8	3×10^{-9}	
	38	3.5	6×10^{-5}	
	44	1.0	1×10^{-5}	
	50	.12		2 vectors found (one of each)
restart				
	19	2.7	1×10^{-10}	
	34	2.5	2×10^{-7}	
	44	2.2		2 more found
restart (check)	j = 26	1.6		terminate

Example 5. This example has a triple eigenvalue between a single and the rest. Note that the rest of the spectrum is *not* linear which improves convergence. Note that LANSO finds five vectors, all with better accuracy than desired. The new multiplicity check will make the most difference on this example.

$n = 300$, nval = 3, ifig = 3

$\lambda_1 = 0, \lambda_2 = \lambda_3 = \lambda_4 = .1, \lambda_i = 1 - 3/(i - 1)$, for $i = 5, 6, \ldots, 300$

block sizes of 1, 2, and 3 were tried but only the best, block size = 3, was reported

	matrix-vector products	vector inner products	max error in eigenvalue	max residual norm
Block Lanczos	36	288	2×10^{-9}	3.3×10^{-4}
LANSO	67	249	2×10^{-13}	5×10^{-9}

History of LANSO (mxstep = 50)

	pause at j =	κ	new κ	comments
	17	2.9		0, .1, and .25 found
restart (check)	16	9.1		another .1 found
restart (check)	16	1.6		another .1 found
restart (check)	18	5.1		terminate with 5 vectors

Example 6. This is just the previous example with the triple eigenvalue slightly perturbed.

$n = 300$, nval = 4, ifig = 3

$\lambda_1 = 0$, $\lambda_2 = .0999999$, $\lambda_3 = .1$, $\lambda_4 = .1000001$, $\lambda_i = 1 - 3/(i-1)$, $i = 5, 6, \ldots, 300$

	matrix-vector products	vector inner products	max error in eigenvalues	max residual norm
Block Lanczos	54	408	2×10^{-8}	9×10^{-4}
LANSO	58	204	2×10^{-7}	6×10^{-8}

History of LANSO:

	pause at j =	κ	new κ	comments
	18	5.5	5×10^{-7}	
	24	2.4		4 vectors found: 0, .1, .1, and .25
restart (check)	16	1.5		another .1 found
restart (check)	18	8.0		terminate

Cullum and Donath Examples.

Example 7.1B. This example has two eigenvalues with a good separation from the rest.

$n = 316$, nval = 2, ifig = 9

$\lambda_n = 0$, $\lambda_{n-1} = -.1$, $\lambda_{n-i} = -.6 - .03 \times (i-2)$, $i = 2, 3, \ldots, n-1$

	matrix-vector products	vector inner products	max error in eigenvalue	max residual norm
BLAN	94	*	6×10^{-10}	2×10^{-5}
LANSO	69	179	6×10^{-12}	3×10^{-6}

History of LANSO:

	pause at j =	κ	new κ	comments
	26	1.2	8×10^{-12}	
	43	1.2		2 vectors found
restart (check)	26	2.7		terminate

Example 7.4A, A. This example has two eigenvalues with less separation than the previous one. A higher value for mxstep (say 100 instead of 50) would improve the convergence rate for LANSO. Note again that LANSO produces more accuracy.

$n = 201$, nval = 2, ifig = 11

$\lambda_n = 0$, $\lambda_{n-1} = -.01$, $\lambda_{n-i} = -.1 - .05 \times (i-2)$, for $i = 2, 3, \ldots, n-1$

	matrix-vector products	vector inner products	max error in eigenvalues	max residual norm
BLAN	184	*	3×10^{-9}	5×10^{-6}
LANSO	142	346	5×10^{-14}	2×10^{-7}

History of LANSO (mxstep = 50)

	pause at j =	κ	new κ	comments
	27	2.5	9×10^{-13}	
	46	1.2	6×10^{-12}	
	50	3×10^{-9}		mxstep
restart				
	21	1.8	1×10^{-10}	
	37	2.0	2×10^{-9}	
	50	.57		mxstep, 1 vector found
restart				
	15	1.2		second vector found
restart (check)	27	3.1		terminate

Example 7.4A, B. The two eigenvalues are much closer together this time. This slows the convergence rate for LANSO somewhat.

Same as 7.4A, A except $\lambda_{n-1} = -.0001$

	matrix-vector products	vector inner products	max error in eigenvalues	max residual norm
BLAN	184	*	7×10^{-12}	2×10^{-6}
LANSO	156	353	3×10^{-14}	2×10^{-7}

History of LANSO (mxstep = 50)

pause at j =	κ	new κ	comments
27	2.7	1×10^{-12}	
46	1.6	7×10^{-11}	
50	3×10^{-8}		mxstep
restart			
20	1.0	1×10^{-11}	
37	.98	1×10^{-10}	
50	3.2×10^{-2}		mxstep
restart			
20	2.3	4×10^{-7}	
30	1.0		2 vectors found
restart (check)			
26	2.5		terminate

Example 7.4A, C. With the two eigenvalues equal the convergence is about the same as for BLAN. Setting mxstep = 100 would improve LANSO.

Same as 7.4A, A except $\lambda_{n-1} = 0$.

	matrix-vector products	vector inner products	max error in eigenvalues	max residual norm
BLAN	184	*	2×10^{-12}	2×10^{-6}
LANSO	186	490	1×10^{-14}	2×10^{-7}

History of LANSO (mxstep = 50)

pause at j =	κ	new κ	comments
27	2.7	1×10^{-12}	
46	1.7	7×10^{-11}	
50	3×10^{-8}		mxstep
restart			
20	1.5	2×10^{-8}	
33	3.9	3×10^{-7}	
43	1.1	7×10^{-6}	
50	.26		mxstep, 1 vector found
restart			
15	2.5		.1 found
restart			
27	3.0	1×10^{-12}	
45	1.3	1×10^{-10}	
50	3×10^{-7}		mxstep
restart			
20	1.9		other 0 found, terminate

14. The Kappa Bound.* Let κ_1 be an upper bound on the error committed in normalizing an n-vector, so

$$|1 - \|q_j\|^2| \leqslant \kappa_1, \quad \text{for all } j. \tag{1}$$

κ_1 will depend on the arithmetic unit, the square root routine and other details of the program. Suppose that numbers ζ_i are known such that

$$\|Q_j^* q_{j+1}\| \leqslant \zeta_j, \quad \text{for all } j. \tag{2}$$

Then define κ_{j+1} by

$$\kappa_{j+1} \equiv \left\| \begin{bmatrix} \kappa_j & \zeta_j \\ \zeta_j & \kappa_1 \end{bmatrix} \right\| = [\kappa_j + \kappa_1 + \sqrt{(\kappa_j - \kappa_1)^2 + 4\zeta_j^2}]/2. \tag{3}$$

LEMMA 1. *If* $\|1 - Q_j^* Q_j\| \leqslant \kappa_j$ *then* $\|1 - Q_{j+1}^* Q_{j+1}\| \leqslant \kappa_{j+1}$.

Proof.

$$\|1 - Q_{j+1}^* Q_{j+1}\| \leqslant \left\| \begin{matrix} \|1 - Q_j^* Q_j\| & \|-Q_j^* q_{j+1}\| \\ \|-q_{j-1}^* Q_j\| & \|1 - q_{j+1}^* q_{j+1}\| \end{matrix} \right\|. \qquad \square$$

In order to compute κ_j we must first compute ζ_j. The vector q_{j+1} is obtained by dividing r_j of (4.1) by β_j. Hence,

$$\|Q_j^* q_{j+1}\| \leqslant \|Q_j^* r_j\|/\beta_j + \|Q_j^* g_j\|, \tag{4}$$

where g_j accounts for the error introduced by the division by β_j. g_j is always small and satisfies $\|g_j\| < \epsilon$, where ϵ is the relative machine precision. To bound $\|Q_j^* r_j\|$ we first prove the following result.

LEMMA 2.

$$Q_j^* r_j = [(1 - Q_j^* Q_j) T_j - (1 - e_j e_j^*) T_j (1 - Q_j^* Q_j)] e_j - \bar{F}^* q_{j+1}$$
$$+ (q_j^* A g_j - \alpha_j) e_j + Q_j^* \bar{f}_j.$$

Proof. Recall Eq. (4.1), namely

$$AQ_j = Q_j T_j + r_j e_j^* - \bar{F}_j. \tag{5}$$

*** The three lemmas are taken from the unpublished report (Kahan and Parlett [1974]).

Then we have

$$\begin{aligned} Q_j^* r_j &= Q_j^*(AQ_j - Q_j T_j + \bar{F}_j)e_j, \quad \text{using (5)}, \\ &= (Q_j^* A Q_j - Q_j^* Q_j T_j)e_j + Q^* \bar{f}_j, \quad \text{where } \bar{f}_j = \bar{F}_j e_j, \\ &= [(AQ_j)^* Q_j - Q_j^* Q_j T_j]e_j + Q^* \bar{f}_j, \quad \text{using } A^* = A, \\ &= [T_j Q_j^* Q_j - \bar{F}_j^* Q_j + e_j r_j^* Q_j - Q_j^* Q_j T_j]e_j + Q_j^* \bar{f}_j, \quad \text{using (5) again}, \\ &= [-T_j(1 - Q_j^* Q_j) + (1 - Q_j^* Q_j)T_j - F_j^* Q_j]e_j + e_j r_j^* Q_j e_j + Q_j^* \bar{f}_j, \\ &\qquad\qquad \text{adding and subtracting } T_j. \end{aligned}$$

Finally, using the second line above,

$$\begin{aligned} e_j^* Q_j^* r_j &= e_j^*(Q_j^* A Q_j - Q_j^* Q_j T_j)e_j \\ &= q_j^* A q_j - e_j^* Q_j^* Q_j T_j e_j \\ &= q_j^* A q_j - \alpha_j + e_j^*(1 - Q_j^* Q_j)T_j e_j. \end{aligned}$$

After transposing, substituting, and rearranging terms the lemma's assertion is obtained. □

The expansion for $Q_j^* r_j$ falls into two parts $Q_j^* r_j = c_j + d_j$, where

$$\begin{aligned} c_j &\equiv [(1 - Q_j^* Q_j)T_j - (1 - e_j e_j^*)T_j(1 - Q_j^* Q_j)]e_j, \\ d_j &\equiv -\bar{F}_j^* q_{j+1} + (q_j^* A q_j - \alpha_j)e_j + Q_j^* \bar{f}_j. \end{aligned} \tag{6}$$

Using the stable implementation of the algorithm analyzed by Paige [1976], d_j is always tiny. In practice, it has been found that the contribution of d_j to $Q_j^* r_j$ can be ignored completely in computing the bound ζ_j.

LEMMA 3. *Let* $\|Q_i^* q_{i+1}\| \leqslant \zeta_i$, *for* $i < j$. *Then*

$$\|c_j\| \leqslant \|(T_{j-1} - \alpha_j)\|\xi_{j-1} + \beta_{j-1}(\zeta_{j-1} + \zeta_{j-2} + 2\kappa_1) + |\alpha_j|\kappa_1.$$

Proof. Partition T_j and $1 - Q_j^* Q_j$ to find

$$(1 - Q_j^* Q_j)T_j e_j = \begin{bmatrix} -Q_{j-1}^* q_1 \\ \\ 1 - \|q_j\|^2 \end{bmatrix} \alpha_j + \begin{bmatrix} -Q_{j-2}^* q_{j-1} \\ 1 - \|q_{j-1}\|^2 \\ -q_j^* q_{j-1} \end{bmatrix} \beta_{j-1},$$

$$T_j(1 - Q_j^* Q_j)e_j = \begin{bmatrix} -T_{j-1} Q_{j-1}^* q_j + e_{j-1}\beta_{j-1}(1 - \|q_j\|^2) \\ \\ \alpha_j(1 - \|q_j\|^2) - \beta_{j-1} q_{j-1}^* q_j \end{bmatrix}.$$

The factor $(1 - e_j e_j^*)$ simply annihilates the bottom element. Moreover, by (1),

$$|1 - \|q_i\|^2| \leqslant \kappa_1, \quad \text{and} \quad |q_j^* q_{j-1}| = |q_{j-1}^* q_j| \leqslant \zeta_{j-1}.$$

The bound is obtained by collecting terms. □

Finally, to compute numbers we need a value for κ_1. It can be shown that $\kappa_1 = (n + 6)\epsilon$ will do. We also use $\|T_{j-1} - \alpha_j\|_\infty$ as an upper bound on $\|T_{j-1} - \alpha_j\|$.

After the program has made a pause, it is necessary to reset the kappa recurrence in order to use it to determine the next pause. To do this we make use of Theorem 5 (Section 4) which states

$$y_i^* q_{j+1} = g_{ii}/\beta_{ji}. \tag{7}$$

The quantities β_{ji} are available at a pause. A current estimate of $\|A\|$ (= $\max|\theta|$) is also available. An estimate of ζ_j is obtained from the formula

$$\zeta_j \cong \epsilon \|A\|/\hat{\beta}_{ji}, \tag{8}$$

where $\hat{\beta}_{ji}$ is the minimum of the β_{ji} above the tolerance. To restart the recurrence ζ_{j-1} and κ_j are set to this value as well.

To avoid a search over all of T_{j-1} to compute $\|T_{j-1} - \alpha_j\|_\infty$, the program maintains values for AMAX, AMIN, and BMAX which are, respectively, the largest α, the smallest α, and the largest beta from T_{j-1}. These values permit the program to compute the right-hand side of

$$\|T_{j-1} - \alpha_j\| \leqslant \max\{\text{AMAX} - \alpha_j, \alpha_j - \text{AMIN}\} + 2 * \text{BMAX}. \tag{9}$$

Further, if the program pauses at step j, the eigenvalues of T_j must be computed. If TLARGE and TSMALL are the largest and smallest eigenvalues of T_j, respectively, then

$$\|T_{k-1} - \alpha_k\| \leqslant \max\{\max(\text{TLARGE} - \alpha_k, \alpha_k - \text{TSMALL}), \|T_{k-1}^j - \alpha_k\|\} + \beta_j, \tag{10}$$

where

$$T_{k-1}^j = \begin{bmatrix} \alpha_{j+1} & \beta_{j+1} & & \\ \beta_{j+1} & \cdot & & \\ & \cdot & & \beta_{k-2} \\ & & \cdot & \\ & \beta_{k-2} & & \alpha_{k-1} \end{bmatrix};$$

and $\|T_{k-1}^j - \alpha_k\|$ is estimated as in (9).

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