# THE LANCZOS ALGORITHM WITH SELECTIVE ORTHOGONALIZATION[*]

B.N. Parlett
Mathematics Department, University of California, Berkeley

D.S. Scott
Union Carbide

## ABSTRACT

A new stable and efficient implementation of the Lanczos algorithm is presented.

The Lanczos algorithm is a powerful method for finding a few eigenvalues and eigenvectors at one or both ends of the spectrum of a symmetric matrix A. The algorithm is particularly effective if A is large and sparse in that the only way in which A enters the calculation is through a subroutine which computes Av for any vector v. Thus the user is free to take advantage of any sparsity structure in A and A need not even be represented as a matrix at all.

The simple Lanczos algorithm procedes as follows. Choose $q_1$, an arbitrary unit vector, and define $\beta_0 = 0$ and $q_0 = 0$. Then for $j = 1,2,\ldots$ do 1 to 5.

1. $u_j = Aq_j - q_{j-1}\beta_{j-1}$

2. $\alpha_j = q_j^* u_j$

3. $r_j = u_j - q_j \alpha_j$

4. $\beta_j = \|r_j\|$

5. if $\beta_j = 0$ stop, else $q_{j+1} = r_j / \beta_j$

One cycle through 1-5 is a Lanczos step. Note that only $q_{j-1}$ and $q_j$ are needed to compute $q_{j+1}$ which is another attractive feature of the algorithm.

In exact arithmetic, if $Q_j = (q_1, q_2, \ldots, q_j)$ then it can be shown (cf. ref. 1) that $Q_j$ is an orthonormal matrix, i.e. $1 - Q_j^* Q_j = 0$, and in addition $Q_j^* A Q_j = T_j$ where

---

$$
T_j = \begin{bmatrix}
\alpha_1 & \beta_1 & & & & \\
\beta_1 & \alpha_2 & \beta_2 & & & \\
& \beta_2 & \cdot & & & \\
& & & \cdot & \beta_{j-1} & \\
& & & & \beta_{j-1} & \alpha_j
\end{bmatrix}
$$

is tridiagonal. Furthermore if $T_j = S_j \Theta_j S_j^*$ is the spectral decomposition of $T_j$ with $\Theta_j = \mathrm{diag}(\theta_1^{(j)}, \theta_2^{(j)}, \ldots, \theta_j^{(j)})$ and if $Y_j \equiv (y_1^{(j)}, y_2^{(j)}, \ldots, y_j^{(j)}) = Q_j S_j$ then $(\theta_i^{(j)}, y_i^{(j)})$, $i = 1, 2, \ldots, j$, are the (optimal) Rayleigh-Ritz approximations to eigenpairs of A derivable from $\mathrm{span}(Q_j)$, the subspace spanned by $q_1, q_2, \ldots, q_j$.

Finally and remarkably, the residual norm of $(y_i, \theta_i)$ can be computed without computing the vector $y_i$. Namely

$$
\| Ay_i - y_i \theta_i \| = \beta_{ji}
$$

where $\beta_{ji} = \beta_j |s_{ji}|$ and $s_{ji}$ is the $(j,i)$ element of $S_j$. The quantities $\beta_{ji}$ show how it is possible for _some_ of the Ritz values $(\theta\text{'s})$ to be accurate without the appearance of a small $\beta_j$. If $s_{ji}$ is tiny then $\theta_i^{(j)}$ will be accurate even if $\beta_j$ is not small at all.

By construction $\mathrm{span}(Q_j) = \mathrm{span}(q_1, Aq_1, \ldots, A^{j-1}q_1)$, a Krylov subspace. It can be shown (refs. 2 and 3) that Rayleigh-Ritz approximations converge rapidly as $j$ increases to well separated extreme eigenpairs of A (those near either end of the spectrum).

Unfortunately, as was known to Lanczos when he introduced the algorithm (ref. 4), finite precision causes the computed quantities to diverge completely from their theoretical counterparts. The Lanczos vectors (the q's) inevitably lose their mutual orthogonality and approach linear dependence. This is the infamous "loss of orthogonality" in the Lanczos algorithm.

Lanczos himself recommended that the simple Lanczos algorithm be augmented by a full reorthogonalization of each newly computed $q_{j+1}$. That is, $q_{j+1}$ is explicitly orthogonalized against all preceding Lanczos vectors $(q_i, \text{ for } i \leq j)$. This not only greatly increases the number of computations required to compute $q_{j+1}$, it also requires that all the q's be kept in fast store.

This poses a serious dilemma. For large problems it will be too costly to take more than a few steps using full reorthogonalization but linear independence will surely be lost without some sort of corrective procedure. Selective Orthogonalization (hereafter called SO) interpolates between full reorthogonalization and simple Lanczos to obtain the best of both worlds. Robust linear independence is maintained among the columns of $Q_j$ at a cost which is close to that of simple Lanczos.

SO is based on the analysis of the simple Lanczos algorithm in finite arithmetic given by C. Paige in his doctoral thesis (ref. 3). Paige showed that the loss of orthogonality among the columns of $Q_j$ is highly structured when viewed in the basis of Ritz vectors, the columns of $Y_j = Q_j S_j$, rather than in the basis of $Q_j$ itself.

---

Theorem (Paige). For any step $j$ of the simple Lanczos algorithm and any $i \le j$,

$$|y_i^{(j)*} q_{j+1}| = \epsilon \|A\| \gamma_{ji} / \beta_{ji}$$

where $\gamma_{ji} \doteq 1$ and $\epsilon$ is the working precision.

---

A proof is given in reference 5.[*]

It can also be shown (cf. ref. 5 or 6) that $\beta_{ji}$ is a very good estimate of the residual norm of $y_i^{(j)}$ despite rounding errors. Thus Paige's Theorem shows that $q_{j+1}$ will lose orthogonality only in the direction of Ritz vectors with small $\beta_{ji}$, that is those Ritz vectors which are converging to eigenvectors. This can be stated as

---

loss of orthogonality $\Leftrightarrow$ convergence

---

To maintain orthogonality among the Lanczos vectors below some threshold value $\tau \le 1$ it is only necessary to orthogonalize $q_{j+1}$ against those Ritz vectors which satisfy

$$|y_i^{(j)*} q_{j+1}| > \tau \tag{1}$$

By Paige's Theorem equation (1) holds only if $\beta_{ji} \le \epsilon \|A\| \gamma_{ji} / \tau \doteq \epsilon \|A\| / \tau$. Thus it is possible to determine which Ritz vectors achieve the threshold (1) merely by inspecting the $\beta_{ji}$ which can be computed via a small ($j \times j$) eigenproblem. There are strong theoretical arguments in favor of the choice $\tau = \sqrt{\epsilon}$ (ref. 5 or 6).

Thus SO modifies the simple Lanczos algorithm by explicitly orthogonalizing $q_{j+1}$ against all the Ritz vectors which satisfy

$$\beta_{ji} \le \sqrt{\epsilon} \|A\| \tag{2}$$

We call any Ritz vector which satisfies (2) a good Ritz vector. Good Ritz vectors are already rather well converged and few (if any) of the Ritz vectors at step j will be good, which explains the computational efficiency of the scheme.

In practice it is possible to implement SO even more efficiently. It is not necessary to recompute the good Ritz vectors for orthogonalizing $q_{j+1}$ at each step j as Ritz vectors computed at earlier steps can be used instead.

---

[*] The detailed rounding error analysis needed to complete the proof of Paige's Theorem is given in reference 3.

Furthermore it is not necessary to orthogonalize against a particular good Ritz vector at every step.

In conclusion, SO is an efficient way to maintain robust linear independence among the columns of $Q_j$ and so allow the Lanczos algorithm to be run almost as originally conceived. SO points the way to a high quality subroutine package which can be used off the shelf for large sparse symmetric eigenvalue problems.

## REFERENCES

1. Kahan, W. and Parlett, B.: How Far Should You Go with the Lanczos Algorithm? In Sparse Matrix Computations, J. Bunch and D. Rose, eds. Academic Press, New York, 1976.

2. Kaniel, S.: Estimates for Some Computational Techniques in Linear Algebra. Mathematics of Computation, vol. 20, no. 95, July 1966, pp. 369-378.

3. Paige, C. C.: The Computation of Eigenvalues and Eigenvectors of Very Large Sparse Matrices. Ph.D. Thesis, University of London, 1971.

4. Lanczos, C.: An Iteration Method for the Solution of the Eigenvalue Problem of Linear Differential and Integral Operators. J. Res. Nat. Bur. Stand., vol. 45, 1950, pp. 255-282.

5. Scott, D. S.: Analysis of the Symmetric Lanczos Process. Ph.D. Thesis, Mathematics Department, University of California, Berkeley, 1978.

6. Parlett, B. N.: The Symmetric Eigenvalue Problem. Prentice-Hall, Englewood Cliffs, N.J., 1979.