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How to Make the Lanczos Algorithm Converge Slowly

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Abstract. The Paige style Lanczos algorithm is an iterative method for finding a few eigenvalues of large sparse symmetric matrices. Some beautiful relationships among the elements of the eigenvectors of a symmetric tridiagonal matrix are used to derive a perverse starting vector which delays convergence as long as possible. Why such slow convergence is never seen in practice is also examined.

1. Introduction. In 1950 Lanczos [2] presented an algorithm for reducing a symmetric matrix, call it A, to tridiagonal form. The algorithm begins with an arbitrary unit vector q_1. It produces a tridiagonal matrix T and an orthogonal matrix Q such that

$$Q^*AQ = T \quad \text{and} \quad Qe_1 = q_1. \tag{1}$$

In practice the algorithm could not compete in speed or accuracy with later methods based on explicit orthogonal transformations.

In 1971 Paige [3] introduced a modified version of the algorithm which could be used effectively to find a few eigenvalues, and their eigenvectors too if desired, of a large sparse symmetric matrix. Paige suggested terminating the process prematurely at, say, the jth step with T_j the $j \times j$ leading principal minor of T and Q_j the first j columns of Q in hand. In exact arithmetic

$$Q_j^*AQ_j = T_j. \tag{2}$$

Let the spectral decomposition of T_j be

$$T_j = S_j\Theta S_j^* \quad \text{with } \Theta = \operatorname{diag}(\theta_1^j, \theta_2^j, \ldots, \theta_j^j) \text{ and } S_j^*S_j = I_j. \tag{3}$$

Define

$$Y_j = (y_1^j, y_2^j, \ldots, y_j^j) = Q_jS_j.$$

Then $\theta_1^j, \theta_2^j, \ldots, \theta_j^j$ are the Rayleigh-Ritz approximations to the eigenvalues of A (commonly called Ritz values) derivable from the subspace spanned by the columns of Q_j, and $y_1^j, y_2^j, \ldots, y_j^j$ are the corresponding Ritz vectors. The norm of the

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residual of y_i^j, namely $\|Ay_i^j - \theta_i^j y_j^i\|$, is a bound on the accuracy of θ_i^j as an approximation to an eigenvalue of A.

The Kaniel-Paige error estimates [1], [3] lead us to expect that some of the eigenvalues of T_j should converge (have negligible error bound) for $j \ll n$, provided only that the starting vector q_1 is not pathologically deficient in the corresponding eigendirections of A. Numerical tests by Paige and other researchers have confirmed that convergence occurs relatively quickly. Despite this abundance of evidence, Paige was unable to prove that convergence of some Ritz value must occur before $j = n = \dim(A)$ at which point, in exact arithmetic, T is similar to A so that all the "approximations" are exact and all the bounds are zero.

There are several interesting unresolved problems connected with the Lanczos process. Except in its last section, this paper is restricted to the theoretical behavior of the algorithm in the context of exact arithmetic. In the following section we derive some beautiful relationships among the elements of the eigenvectors of a symmetric tridiagonal matrix which may be of interest in their own right. In Section 3 these results are applied to obtain formulas for the Lanczos starting vector. In Section 4 these formulas are used to find a perverse starting vector for matrices with well-separated eigenvalues which delays convergence until $j = n$. Section 5 generalizes the construction to matrices with close or multiple eigenvalues to yield a vector which delays convergence for a long time. The final section will indicate why such slow convergence is never seen in practice.

2. The Eigenvectors of a Symmetric Tridiagonal Matrix.

Definition. Let $\operatorname{adj}(R)$ be the transpose of the matrix of cofactors of R. This is usually called the *adjugate* or *classical adjoint* of R. By the Cauchy-Binet theorem

$$R \operatorname{adj}(R) = \det(R) I. \tag{1}$$

THEOREM 2.1 (THOMPSON AND MCENTEGGERT, 1968). *Let $A = Z\Lambda Z^*$ with $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, $Z = (z_1, z_2, \ldots, z_n)$ and $Z^*Z = I$. Then for $i = 1, 2, 3, \ldots, n$*

$$\operatorname{adj}(\lambda_i I - A) = \prod_{\substack{j=1 \\ j \neq i}}^{n} (\lambda_j - \lambda_i) z_i z_i^* = \chi_A'(\lambda_i) z_i z_i^*,$$

where $\chi_A'(\mu)$ is the derivative of the characteristic polynomial of A.

Note that if λ_i is a multiple eigenvalue of A, then $\chi_A'(\lambda_i) = 0$, so that the ambiguity in the choice of eigenvectors doesn't matter.

Proof. Let $\mu \neq \lambda_i$, for all i, so that $(\mu I - A)^{-1}$ exists. Then

$$\begin{aligned} \operatorname{adj}(\mu I - A) &= \det(\mu I - A)(\mu I - A)^{-1} \\ &= \chi_A(\mu) Z(\mu I - \Lambda)^{-1} Z^* \\ &= Z \Delta Z^*, \end{aligned}$$

where Δ is diagonal and

$$\Delta_{kk} = \frac{\chi_A(\mu)}{\mu - \lambda_k} = \prod_{\substack{j=1 \\ j \neq k}}^{n} (\mu - \lambda_j).$$

Since computing cofactors does not involve division, adj(R) is a continuous function of R. Therefore, the last equation must hold even for $\mu = \lambda_i$. Setting $\mu = \lambda_i$, for $i = 1, 2, 3, \ldots, n$, yields

$$\text{adj}(\lambda_i I - A) = Z \Delta Z^*,$$

where

$$\Delta_{kk} = \prod_{\substack{j=1 \\ j \neq k}}^{n} (\lambda_i - \lambda_j) = 0 \qquad \text{if } k \neq i,$$

$$= \prod_{\substack{j=1 \\ j \neq i}}^{n} (\lambda_i - \lambda_j) \quad \text{if } k = i.$$

Since $\Pi_{j=1; j\neq i}^{n} (\lambda_i - \lambda_j) = \chi'_A(\lambda_i)$, the result follows. □

Thompson and McEnteggert were working with general Hermitian matrices. The application of their theorem to tridiagonal matrices was made by Paige [3].

Notation. Let

$$T_{r,t} \equiv \begin{bmatrix} \alpha_r & \beta_r & & & & \\ \beta_r & \alpha_{r+1} & \beta_{r+1} & & \bigcirc & \\ & \beta_{r+1} & \alpha_{r+2} & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & \bigcirc & & \ddots & \beta_{t-1} & \\ & & & \beta_{t-1} & \alpha_t & \end{bmatrix};$$

let $\chi_{r,t}(\mu) \equiv \det(\mu I - T_{r,t})$, the characteristic polynomial of $T_{r,t}$; and let $\chi_{r,r-1}(t) \equiv 1$ for all r.

THEOREM 2.2 (PAIGE, 1971). *Let $T = T_{1,n} = S\Theta S^*$ with $\Theta = \text{diag}(\theta_1, \theta_2, \ldots, \theta$ and $S^*S = I$. Then for $r \leqslant t$ and all i,*

$$\chi'_{1,n}(\theta_i) s_{ri} s_{ti} = \chi_{1,r-1}(\theta_i) \beta_r \beta_{r+1} \cdots \beta_{t-1} \chi_{t+1,n}(\theta_i).$$

In particular,

$$\chi'_{1,n}(\theta_i) s_{ri}^2 = \chi_{1,r-1}(\theta_i) \chi_{r+1,n}(\theta_i).$$

Proof. By Theorem 2.1

$$\text{adj}(\theta_i I - T) = \chi'_{1,n}(\theta_i) s_i s_i^*. \tag{2}$$

The (r, t) element of the RHS of (2) is $\chi'_{1,n}(\theta_i) s_{ri} s_{ti}$. Because of the tridiagonal form

of T, the (r, t) element of the LHS of (2) is $\chi_{1,r-1}(\theta_i)\beta_r\beta_{r+1}\cdots\beta_{t-1}\chi_{t+1,n}(\theta_i)$. For example,

$$\theta_i I - T_{1,6} = \begin{bmatrix} \theta_i-\alpha_1 & -\beta_1 & & & & \\ -\beta_1 & \theta_i-\alpha_2 & -\beta_2 & & & \\ & -\beta_2 & \theta_i-\alpha_3 & -\beta_3 & & \\ & & -\beta_3 & \theta_i-\alpha_4 & -\beta_4 & \\ & & & -\beta_4 & \theta_i-\alpha_5 & -\beta_5 \\ & & & & -\beta_5 & \theta_i-\alpha_6 \end{bmatrix}$$

The circled elements contribute to the (2, 3) cofactor. Note that the minus signs on the β's cancel with the alternating signs associated with the cofactors. □

3. Formulas for Starting Vectors. The Lanczos algorithm begins with an arbitrary unit vector q_1 and terminates with a tridiagonal matrix T and an orthogonal matrix Q such that q_1 is the first column of Q and $AQ = QT$. The process is geometric, i.e. it is invariant under orthogonal changes in coordinates. The coordinates which give the most insight into the process are the eigenvectors of A.

In these coordinates the operator A is diagonal and the matrix Q becomes the transpose of S, the matrix of eigenvectors of T. The matrix equation $AQ = QT$ becomes

$$\Lambda S^* = S^* T, \tag{1}$$

where $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$.

THEOREM 3.1. *Let $\Lambda S^* = S^* T$ as above. Then for $i = 1, 2, \ldots, n$*

(i) $s_{1i}s_{ni}\chi'_\Lambda(\lambda_i) = \beta_1\beta_2\cdots\beta_{n-1} \equiv \pi_n$ *a constant,*

(ii) $s_{ni}^2\chi'_\Lambda(\lambda_i) = \chi_{1,n-1}(\lambda_i)$.

Proof. Since Λ is similar to T, $\chi_\Lambda(\mu) = \chi_T(\mu) = \chi(\mu)$.

(i) This is Theorem 2.2 with $r = 1$ and $t = n$.

(ii) This is Theorem 2.2 with $r = n$ and $t = n$. □

In order to refer to the Lanczos vectors, we need names for the columns of S^*. For this purpose, when $A = \Lambda$, we define

$$P \equiv (p_1, p_2, \ldots, p_n) \equiv S^*. \tag{2}$$

Theorem 3.1(i) relates the first Lanczos vector p_1 to the last Lanczos vector p_n. Theorem 3.1(ii) relates p_n to the eigenvalues of $T_{1,n-1}$ which are the approximations to eigenvalues of Λ furnished by the $(n-1)$st step of the Lanczos algorithm. Since $T_{1,n}$ is similar to A, the Cauchy Interlace Theorem requires that the eigenvalues of T_{n-1}, call them $\mu_1, \mu_2, \ldots, \mu_{n-1}$, satisfy the inequalities

$$\lambda_1 \leqslant \mu_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \mu_{n-1} \leqslant \lambda_n. \tag{3}$$

Since $T_{1,n}$, the tridiagonal matrix produced by the Lanczos algorithm, will be unreduced, the interlacing must be strict.

THEOREM 3.2. *Let* $A = Z\Lambda Z^*$ *with* $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ *and* $Z^*Z = I$. *Then the Lanczos algorithm run with a starting vector* q_1 *produces a* $T_{1,n-1}$ *with eigenvalues* $\mu_1 < \mu_2 < \cdots < \mu_{n-1}$ *if and only if* $q_1 = Zp_1$, *where*

$$p_{i1}^2 = \pi_n^2 \left[\prod_{\substack{j=1 \\ j \neq i}}^{n} (\lambda_i - \lambda_j) \prod_{j=1}^{n-1} (\lambda_i - \mu_j) \right]^{-1} = \pi_n^2 [\chi'(\lambda_i)\chi_{1,n-1}(\lambda_i)]^{-1}.$$

Strict interlacing is required to make the quantity in the brackets positive for all i.

Proof. The Lanczos algorithm produces the same T whether it runs on the pair (A, q_1) or (Λ, p_1). Combining the two parts of Theorem 3.1 and changing to the P notation yields

$$p_{i1}^2 \chi'(\lambda_i)\chi_{1,n-1}(\lambda_i) = \pi_n^2, \tag{4}$$

for any starting vector p_1.

If p_1 is known, then by interpolation, $\chi_{1,n-1}(\mu)$ can be found from (4), up to a constant factor. Hence, $\mu_1, \mu_2, \ldots, \mu_{n-1}$, the zeros of $\chi_{1,n-1}(\mu)$ can be found.

If $\mu_1, \mu_2, \ldots, \mu_{n-1}$ are given, then p_{i1}^2, for $i = 1, 2, \ldots, n$, can be found from (4) up to the multiplicative factor π_n^2, which can be determined by the required normalization of p_1. The ambiguity in the choice of sign for each component of p_1 merely reflects the choice of sign for each eigenvector of T. All choices yield the same tridiagonal matrix T. □

The required q_1 depends on both the eigenvalues and on the eigenvectors of A. The expression $q_1 = Zp_1$ clarifies their roles; Z is independent of the λ_i, while p_1 is independent of Z.

Example. Let $\Lambda = \operatorname{diag}(1, 3, 5, 7, 9)$ and $\mu_i = 2i$, for $i = 1, 2, 3, 4$.

$$\chi'(1)\chi_\mu(1) = (1-3)(1-5)(1-7)(1-9)(1-2)(1-4)(1-6)(1-8) = 40320$$

$$\chi'(3)\chi_\mu(3) = (3-1)(3-5)(3-7)(3-9)(3-2)(3-4)(3-6)(3-8) = 1440$$

$$\chi'(5)\chi_\mu(5) = (5-1)(5-3)(5-7)(5-9)(5-2)(5-4)(5-6)(5-8) = 576$$

$$\chi'(7)\chi_\mu(7) = (7-1)(7-3)(7-5)(7-9)(7-2)(7-4)(7-6)(7-8) = 1440$$

$$\chi'(9)\chi_\mu(9) = (9-1)(9-3)(9-5)(9-7)(9-2)(9-4)(9-6)(9-8) = 40320,$$

so

$$p_{11} = p_{51} = \pi_5/\sqrt{40320} = .00498\pi_5,$$

$$p_{21} = p_{41} = \pi_5/\sqrt{1440} = .02635\pi_5,$$

$$p_{31} = \pi_5/\sqrt{576} = .04167\pi_5.$$

By normalization $\pi_5 = 17.749$ and

$$p_1 = (.0880, .4677, .7396, .4677, .0880)^*.$$

The Lanczos algorithm run on Λ with p_1 as the starting vector yielded a T_4 with eigenvalues 2, 4, 6, and 8 correct to the precision of the machine used.

Results similar to Theorem 3.2 have been used by D. Boley, C. deBoor, and G. H. Golub [5], [6], in the context of inverse eigenvalue problems for banded matrices.

4. Slow Convergence. Before examining the convergence properties of the Lanczos algorithm in the light of Theorem 3.2, it is useful to describe in more detail the properties of the Rayleigh-Ritz procedure. Let W be any subspace of $\mathbf{R}^n$ and let P_W denote the orthogonal projection of $\mathbf{R}^n$ onto W. Then the Rayleigh-Ritz approximations to eigenpairs of A obtained from W are precisely the eigenpairs of $P_W A$ whose eigenvectors lie in W.

THEOREM 4.1. *If $V \subseteq W$, then the Rayleigh-Ritz approximations for A obtained from V are the same as the Rayleigh-Ritz approximations for $P_W A$ obtained from V. Further, if (y, θ) is a Ritz pair, then $\|(P_W A)y - y\theta\| \leqslant \|Ay - y\theta\|$, with equality holding if and only if the residual vector, $Ay - y\theta$, lies in W.*

Proof. Let P_V be the orthogonal projection onto V. Then, $P_V(P_W A) = (P_V P_W)A = P_V A$, since $V \subseteq W$. Since $y \in V \subseteq W$, $\|(P_W A)y - \theta y\| = \|P_W(Ay - y\theta)\|$. Finally, since P_W is an orthogonal projection, $\|P_W(Ay - y\theta)\| \leqslant \|Ay - y\theta\|$, with equality holding if and only if $Ay - y\theta \in W$. □

COROLLARY. *If V and W are nested Krylov subspaces of different dimensions, then $\|Ay - y\theta\| = \|P_W Ay - y\theta\|$.*

Proof. If $V = K_j(q_1)$ and $W = K_k(q_1)$ for $k > j$, then, since $y \in K_j(q_1)$, $Ay - y\theta \in K_{j+1}(q_1) \subseteq K_k(q_1) = W$.

We now examine the convergence properties of the Lanczos algorithm . The reader is directed to Section 1 for the terminology.

THEOREM 4.2. *Suppose that the Lanczos algorithm when run on (A, q_1) produces $\mu_1, \mu_2, \ldots, \mu_{n-1}$ as Ritz values at the $(n-1)$st step. Let (y, θ) be a Ritz pair from any step except the nth. Then*

$$\gamma \equiv \|Ay - y\theta\| \geqslant \delta_\mu/2,$$

where $\delta_\mu = \min_{i \leqslant n-1;\, k \leqslant n} |\mu_i - \lambda_k|$.

Proof. For any unit vector x and any scalar τ it is well known that

$$\min_{i \leqslant n} |\lambda_i - \tau| \leqslant \|Ax - x\tau\|. \tag{5}$$

In particular,

$$\min_{i \leqslant n} |\lambda_i - \theta| \leqslant \|Ay - y\theta\| = \gamma, \tag{6}$$

and

$$\min |\mu_i - \theta| \leqslant \|P_W Ay - y\theta\| = \gamma, \tag{7}$$

with the last equality following from the Corollary. The smallest γ which can satisfy both (6) and (7) is $\delta_\mu/2$. □

In practice γ cannot be as small as $\delta_\mu/2$. However, no significantly stronger bound can be obtained. In particular, the smallest residual at the $(n-1)$st step can be δ_μ.

The combination of Theorem 3.2 and Theorem 4.2 yields the following.

THEOREM 4.3. *Let A be a symmetric matrix with eigenvalues $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$. Let $\delta_A \equiv \min_{i \neq k} |\lambda_i - \lambda_k|$. Then there exists a starting vector for the Lanczos algorithm such that the residual norm of any Ritz vector at any step $j < n$ will be larger than $\delta_A/4$.*

Proof. If A has multiple eigenvalues, then $\delta_A = 0$ and any vector will do, so we may assume that A has distinct eigenvalues. Let $\mu_i = (\lambda_i + \lambda_{i+1})/2$, for $i = 1, 2, \ldots, n-1$, and let q_1 be any starting vector generated by Theorem 3.2. With this choice of $q_1, \mu_1, \mu_2, \ldots, \mu_{n-1}$ will be the Ritz values at the $(n-1)$st step and $\delta_\mu = \delta_A/2$. The result now follows from Theorem 4.2. □

If the spectrum of A is such that $\delta_A/4$ is larger than some given convergence tolerance, then Theorem 4.3 shows that there exist perverse starting vectors which delay convergence until the nth step. This result does not imply that no earlier Ritz value is accurate enough; it only guarantees that the corresponding bound will not reveal such accuracy. In the previous example of $\Lambda = \text{diag}(1, 3, 5, 7, 9)$ and $\mu_i = 2i$, for $i = 1, 2, 3, 4$, θ_2^3, the middle eigenvalue of $T_{1,3}$ is 5, correct to working accuracy. The corresponding bound is 1.25, which shows that this fortuitous accuracy is due to the symmetry of the example, rather than the accuracy of the Ritz vector.

5. The Problem of Clustered Eigenvalues. If the spectrum of A is such that $\delta_A/4$ is smaller than the given convergence tolerance, Theorem 4.3 does not guarantee slow convergence. However, starting vectors can still be found which delay convergence a long time.

THEOREM 5.1. *Let W be an A-invariant subspace of maximal dimension such that $\bar{A} \equiv A$ restricted to W is such that $\delta_{\bar{A}}/4$ is larger than the given convergence tolerance. Let $m = \dim W$. Then there exists a starting vector for A which delays convergence until the mth step.*

Proof. Apply Theorem 4.3 to $\bar{A}$ to yield a starting vector q_1. Since the Lanczos algorithm run on (A, q_1) yields the same T as the Lanczos algorithm run on $(\bar{A}, q_1)$, this q_1 will do. □

In general, it may be possible to delay convergence even longer.

6. The Beneficial Effects of Rounding Errors. The slow convergence discussed in the previous sections never seems to occur in practice. The reason for this lies in the formula for p_1 given in Theorem 3.2,

$$p_{il}^2 = \pi_n^2 [\chi'(\lambda_i)\chi_{1,n-1}(\lambda_i)]^{-1}. \tag{1}$$

First, we give three examples.

Example 1. Linear distribution.

$$\lambda_i = i \qquad \text{for } i = 1, 2, \ldots, 50,$$

$$\mu_i = \frac{(\lambda_i + \lambda_{i+1})}{2} = i + \frac{1}{2} \qquad \text{for } i = 1, 2, \ldots, 49.$$

p_1 was computed by Theorem 3.2. p_1 is symmetric from top to bottom. The largest elements of p_1 are $p_{25,1} = p_{26,1} = .397$. The smallest elements of p_1 are $p_{1,1} = p_{50,1} = .25 \times 10^{-14}$.

Example 2. Geometric distribution.

$$\lambda_i = (1.1)^i \qquad \text{for } i = 1, 2, \ldots, 50,$$

$$\mu_i = \frac{(\lambda_i + \lambda_{i+1})}{2} \qquad \text{for } i = 1, 2, \ldots, 49.$$

The largest element of p_1 is $p_{8,1} = .495$. The smallest element of p_1 is $p_{50,1} = .162 \times 10^{-52}$.

Example 3. Tchebychev distribution.

$$\lambda_i = \cos\left(\frac{i\pi}{51}\right) \qquad \text{for } i = 1, 2, \ldots, 50,$$

$$\mu_i = \frac{(\lambda_i + \lambda_{i+1})}{2} \qquad \text{for } i = 1, 2, \ldots, 49.$$

The largest elements of p_1 are $p_{25,1} = p_{26,1} = .228$. The smallest elements of p_1 are $p_{1,1} = p_{50,1} = .642 \times 10^{-3}$.

The tiny elements of p_1 in Examples 1 and 2 are due to the large variation in magnitudes of the numbers $\{\chi'(\lambda_k) \mid k = 1, 2, \ldots, n\}$. Most practical examples also show large variations, which leads to a perverse starting vector with some tiny eigencomponents. Such tiny components are unlikely to appear in a randomly chosen vector. More importantly, such tiny components are unstable in the face of rounding errors.

By standard rounding error analysis

$$q_1 = Zp_1 + f, \quad \|f\| \leqslant n^{3/2}\epsilon, \tag{2}$$

where ϵ is the relative machine precision. In exact arithmetic,

$$Z^*q_1 = p_1 + Z^*f. \tag{3}$$

Unless Z has some special symmetry, the term Z^*f will swamp any tiny component of p_1. That is, q_1 is unlikely to have any eigencomponents much smaller than ϵ. Even if q_1 had precisely the eigencomponents desired, the first step of the Lanczos algorithm would obliterate the small components unless the example were specially rigged. The first step of the algorithm computes q_2 as

$$\beta_1 q_2 = (A - \alpha_1 I)q_1 + f, \quad \text{where } \|f\| \leqslant n^{3/2}\epsilon \|A\|. \tag{4}$$

Again, f will be randomly distributed among the various eigendirections and will prevent q_2 from inheriting any tiny components from q_1.

We have been able to observe delayed convergence for large matrices only for two classes. Tchebychev distributions come very close to minimizing the variation in $\chi'_{1,n}(\lambda_i)$. Therefore, Tchebychev distributions (even on fairly large problems) do not have components of p_1 smaller than ϵ. The other class of examples is diagonal matrices in which the rounding errors are uncoupled and tiny elements of p_1 (which is q_1) are not swamped by small multiples of much larger elements.

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