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Adjusting the Rayleigh Quotient in Semiorthogonal Lanczos Methods*

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ABSTRACT

In a semiorthogonal Lanczos algorithm, the orthogonality of the Lanczos vectors is allowed to deteriorate to roughly the square root of the rounding unit, after which the current vectors are reorthogonalized. A theorem of Simon [4] shows that the Rayleigh quotient — i.e., the tridiagonal matrix produced by the Lanczos recursion — contains fully accurate approximations to the Ritz values in spite of the lack of orthogonality. Unfortunately, the same lack of orthogonality can cause the Ritz vectors to fail to converge. It also makes the classical estimate for the residual norm misleadingly small. In this note we show how to adjust the Rayleigh quotient to overcome this problem.

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Adjusting the Rayleigh Quotient in Semiorthogonal Lanczos Methods

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Abstract

In a semiorthogonal Lanczos algorithm, the orthogonality of the Lanczos vectors is allowed to deteriorate to roughly the square root of the rounding unit, after which the current vectors are reorthogonalized. A theorem of Simon [4] shows that the Rayleigh quotient — i.e., the tridiagonal matrix produced by the Lanczos recursion — contains fully accurate approximations to the Ritz values in spite of the lack of orthogonality. Unfortunately, the same lack of orthogonality can cause the Ritz vectors to fail to converge. It also makes the classical estimate for the residual norm misleadingly small. In this note we show how to adjust the Rayleigh quotient to overcome this problem.

1. Introduction and background

Let A be a symmetric matrix of order n and let u_1 be an n-vector of 2-norm one. The Lanczos algorithm generates a sequence of orthonormal vectors by the recurrence

$$\begin{aligned} \beta_1 u_2 &= Au_1 - \alpha_1 u_1 \\ \beta_k u_{k+1} &= Au_k - \alpha_k u_k - \beta_{k-1} u_{k-1}, \qquad k = 1, 2, \ldots, \end{aligned} \tag{1.1}$$

where

$$\alpha_k = u_k^{\mathrm{T}} A u_k \quad \text{and} \quad \beta_k = 1/\|Au_k - \alpha_k u_k - \beta_{k-1} u_{k-1}\|.$$

If we introduce the tridiagonal matrix

$$T_k = \begin{pmatrix} \alpha_1 & \beta_1 & & & & \\ \beta_1 & \alpha_2 & \beta_2 & & & \\ & \beta_2 & \alpha_3 & \beta_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \beta_{k-2} & \alpha_{k-1} & \beta_{k-1} \\ & & & & \beta_{k-1} & \alpha_k \end{pmatrix}$$

and set

$$U_k = (u_1 \ \cdots \ u_k),$$

then we can express the effect of the recurrence (1.1) by the *Lanczos decomposition*

$$AU_k = U_k T_k + \beta_k u_{k+1} \mathbf{e}_k^{\mathrm{T}}, \tag{1.2}$$

where $\mathbf{e}_k$ is the kth unit vector (the kth column of the identity matrix of order k).

It is well known (e.g., see [3]) that as k increases the space spanned by U_k contains increasingly accurate approximations to eigenvectors corresponding to the extreme eigenvalues of A. The approximations can be retrieved by a process known as the Rayliegh–Ritz method. It is based on the observation that if $(\theta, U_k w)$ is an eigenpair of A, then (θ, w) is an eigenpair of T_k. A continuity argument suggests that if U_k contains a good approximation to an eigenvector of A, there should be an eigenvector w of T_k such that $U_k w$ approximates that eigenvector. For a general analysis of this procedure see [2]. In what follows we will call θ a Ritz value, w a primitive Ritz vector, $U_k w$ a Ritz vector, and T_k the Rayleigh quotient.

A difficulty with the Lanczos algorithm is that the Lanczos vectors tend to loose orthogonality. One cure is to reorthogonalize the vectors at each step — a process known as full reorthogonalization. Unfortunately, reorthogonalizing u_{k+1} requires the vectors $u_1, \ldots, u_k$, and for k large enough the cost of moving them in and out of working storage becomes prohibitive. Consequently, it has been proposed to let orthogonality deteriorate up to a point, after which a reorthogonalization step is performed. There are several varieties of this procedure, all going under the common name of semiorthogonal methods. They each require that the elements of $U_k^{\mathrm{T}} U_k - I$ be kept less than some multiple of $\sqrt{\epsilon_{\mathrm{M}}}$, where ϵ_{M} is the rounding unit for the machine in question. In this note we will be concerned with periodic and partial reorthogonalization [1, 5].

Full orthogonalization has the advantage that the Lanczos relation (1.2) continues to be satisfied to working accuracy. In semiorthogonal methods, however, the Lanczos relation must be replaced by the relation

$$AU_k = U_k H_k + \beta_k u_{k+1} \mathbf{e}_k^{\mathrm{T}}, \tag{1.3}$$

where H_k is an upper Hessenberg matrix with elements of up to order $\sqrt{\epsilon_{\mathrm{M}}}$ above the first superdiagonal. We will call (1.3) a Krylov decomposition and H_k the adjusted Rayleigh quotient. The motivating argument given above for the Rayleigh–Ritz procedure applies equally to this Krylov decomposition. Consequently, if the column space of U_k contains a good approximate to an eigenvector of A, we can (under mild restrictions) obtain an approximating eigenpair in the form $(\theta, U_k w)$, where (θ, w) is a suitable eigenpair of H_k.

It seems obvious that the use of T_k in place of H_k will introduce errors into the Ritz pairs. Surprisingly, this is not true of the Ritz values. According to a remarkable theorem of Simon [4], if $U_k = QR$ is the QR factorization of U_k, then $T_k = Q^{\mathrm{T}} A Q + O(\epsilon_{\mathrm{M}})$. Consequently, from the standard perturbation theory for eigenvalues of symmetric matrices, the eigenvalues of T_k are Ritz values to working accuracy.

On the other hand, if a primitive Ritz vector w is computed from T_k, the corresponding Ritz vector is Qw. However, Q is unavailable to us, and the attempt to use the approximation $U_k w$ will introduce errors. These errors cannot be larger than $O(\sqrt{\epsilon_{\mathrm{M}}})$, but, as we shall see, they can cause the convergence of a Ritz vector to stagnate before full working accuracy has been attained. For this reason primitive Ritz vectors should be computed from the adjusted Rayleigh quotient H_k.

A second use for H_k is to compute accurate residual norms. In the classic Lanczos algorithm if $(\theta, z = U_k w)$ is a Ritz pair computed from T_k in (1.2), it is easy to see that in the 2-norm

$$\|Az - \theta z\| = |\beta_k w_k|,$$

where w_k is the last component of w, and it is this quantity that is used to decide when a Ritz vector has converged. In a semiorthogonal method, the formula can be used only if w is computed from the adjusted Rayleigh quotient.

More generally, suppose $(\theta, U_k w)$ is an approximate eigenpair of A, with no assumptions made about the the origin of w. Then from (1.3) it follows that

$$AU_k w - \theta U_k w = U_k r + w_k \beta_k u_{k+1},$$

where

$$r = H_k w - \theta w.$$

By semiorthogonality $U_k r$ and $w_k \beta_k u_{k+1}$ are almost orthogonal, so that

$$\|AU_k w - \theta U_k w\|^2 \cong \|r\|^2 + |w_k \beta_k|^2. \tag{1.4}$$

Thus we can approximate the residual norm of $U_k w$ from the norm of the residual r, the last component of w, and β_k. In general, it is not possible to replace H_k by T_k.

2. Adjusting the Rayleigh quotient

The foregoing discussion suggests that in a semiorthogonal method the adjusted Rayleigh quotient should be computed. For definiteness we will show how this is done in the context of periodic reorthogonalization, in which an orthogonalization is performed against all preceding vectors whenever the semiorthogonality condition is violated. For convenience we have partitioned this algorithm into the main Lanczos loop (Figure 2.1) and an inner reorthogonalization step (Figure 2.2). The reorthogonalization corresponds to statements 12–14 in the main loop.

The main loop is typical of most implementations of the Lanczos method. The vector $v = Au$ is computed via the Lanczos recurrence. Note that the algorithm fills in

```
1.  for k = 1, 2, ...
2.      v = A*u_k
3.      if (k ≠ 1)
4.          v = v − β_{k−1}*u_{k−1}
5.          H[k−1, k] = H[k, k−1] = β_{k−1}
6.      end if
7.      α_k = u_k^T*v
8.      H[k, k] = α_k
9.      v = v − α_k*u_k
10.     if (k ≠ 1) v = v − (u_{k−1}^T v)*u_{k−1} fi
11.     v = v − (u_k^T v)*u_k
12.     if (semiorthogonality is violated)
13.         Reorthogonalize u_k and v. Update H.
14.     end if
15.     β_k = ||v||_2
16.     u_{k+1} = v/β_k
17. end for i
```

Figure 2.1: Lanczos with periodic reorthogonalization: Main loop

the tridiagonal part of H_k, so that if there were no reorthogonalizations H_k would be identical to T_k. Statements 10–11 are a local reorthogonalization step that insures that v is orthogonal to u_k and u_{k-1} to working accuracy.

The reorthogonalization section (Figure 2.2) is entered only if the off-diagonal elements of $U_k^{\mathrm{T}} U_k$ are too large. These elements cannot be computed directly, except by bringing U_k into working storage at each step. Fortunately, there are recurrences that can be used to estimate the components. For details see [5].

It is necessary to reorthogonalize both u_k and v. The reason is that u_{k+2} will depend on both these vectors, and if one fails to be fully orthogonal, its lack of orthogonality will be propagated u_{k+2} and its successors. The reorthogonalization is done by the modified Gram–Schmidt in statements 3–10. The reorthogonalization coefficients for u_k are stored in w; those for v are stored in x and η.

It may be necessary to rereorthogonalize v against the columns of U_k. The reason is not the usual one: namely, that cancellation in the reorthogonalization can magnify nonorthogonal components. Rather the fact that U_k is only semiorthogonal compromises its ability to purge components in the orthogonal complement of its column space. This rereorthogonalization is done in statements 11–19.

The Rayleigh quotient is adjusted in statements 21–23. To derive the formulas, note

```
if (semiorthogonality is violated)
    ρ = ‖v‖_2
    Reorthogonalize u_k and v
    for j = 1 to k−1
        w[j] = u_j^T*u_k
        u_k = u_k − w[j]*u_j
        x[j] = u_j^T*v
        v = v − x[j]*u_j
    end for j
    η = u_k^T*v
    v = v − η*u_k
    If necessary orthogonalize v again
    if ‖x‖_2 ≥ sqrt(nε_M)*ρ
        for j = 1 to k−1
            t = u_j^T*v
            v = v − t*u_j
            x[j] = x[j] + t
        end for j
        t = u_k^T*v
        v = v − t*u_k
        η = η+t
    end if
    Adjust H
    H[1:k−1, k−1] = H[1:k−1, k−1] + H(k−1, k)*w
    H[1:k−1, k] = H[1:k, k] − H[1:k−1, 1:k−1]*w
            (w[k−1] − H[k, k])*w + x
    H[k, k] = H[k, k] − β_{k−1}*w[k−1] + η
end if
```

Figure 2.2: Lanczos with periodic reorthogonalization: Reorthogonalization

that before the reorthogonalization we have the relation

$$AU_k = U_k H_k + v\mathbf{e}_k^{\mathrm{T}}, \tag{2.1}$$

which holds to working accuracy. The results of the reorthogonalization replace u_k with

$$\tilde{u}_k = u_k - U_{k-1} w \tag{2.2}$$

and v with

$$\tilde{v} = v - U_{k-1}x - \eta\tilde{u}_k. \tag{2.3}$$

Solving (2.2) and (2.3) for u_k and v and substituting the results in (2.1), we get

$$\begin{aligned} A(U_{k-1}\ \ \tilde{u}_k) + A(0\ \ U_{k-1}w) = (U_{k-1}\ \ \tilde{u}_k)H_k + (0\ \ U_{k-1}w)H_k \\ + \tilde{v}\mathbf{e}_k^{\mathrm{T}} + (U_k x + \eta\tilde{u}_k)e^{\mathrm{T}}. \end{aligned} \tag{2.4}$$

Now since $AU_{k-1} = UH_{k-1} + \beta_{k-1}u_k\mathbf{e}_k^{\mathrm{T}}$, we have from (2.2)

$$A(0\ \ U_{k-1}w) = U_{k-1}(H_{k-1} + w\mathbf{e}_{k-1}^{\mathrm{T}})w + \beta_{k-1}\tilde{u}_k\mathbf{e}_{k-1}^{\mathrm{T}}w. \tag{2.5}$$

Also

$$(0\ \ U_{k-1}w)H_k = U_{k-1}w\mathbf{e}_{k-1}^{\mathrm{T}}H_k = h_{k-1,k}U_{k-1}w\mathbf{e}_{k-1}^{\mathrm{T}} + h_{kk}U_{k-1}w\mathbf{e}_k^{\mathrm{T}}. \tag{2.6}$$

If we substitute (2.5) and (2.6) into (2.4) and define $\tilde{H}_k$ by

$$\begin{aligned} &1.\quad \tilde{H}[1{:}k{-}1, k{-}1] = H[1{:}k{-}1, k{-}1] + h_{k-1,k}w, \\ &2.\quad \tilde{H}[1{:}k{-}1, k] = H[1{:}k{-}1, k] - H_{k-1}w - w_{k-1}w + h_{kk}w + x, \\ &3.\quad \tilde{H}[k, k] = H[k, k] - \beta_{k-1}w[k{-}1] + \eta, \end{aligned} \tag{2.7}$$

then it is straightforward (but tedious) to verify that

$$A(U_{k-1}\ \ \tilde{u}_k) = (U_{k-1}\ \ \tilde{u}_k)\tilde{H}_k + \tilde{v}\mathbf{e}_k^{\mathrm{T}},$$

which is a Krylov decomposition involving the new vectors $\tilde{u}_k$ and $\tilde{v}$. These are the corrections of statements 21–23.

It is worth noting that the complexity of these corrections is due to the fact that we must orthogonalize both u_k and v. If we omit the orthogonalization of u_k, then $w = 0$, and the corrections reduce to adding the orthogonalization coefficients for v to the kth column of H_k.

3. An example

The following example illustrates how periodic reorthogonalization behaves. Our matrix A is diagonal of order $n = 500$ whose first eigenvalue is $\lambda_1 = 1$ and whose other eigenvalues are given by the recurrence

$$\lambda_i = \frac{\lambda_{i-1}}{1 + 1/i^2}, \qquad i = 2 \ldots n.$$

The periodically reorthogonalized Lanczos algorithm was run on this matrix with a random starting vector and a cutoff for reorthogonalization of $\sqrt{10^{-16}/n}$. Orthogonalizations took place for $k = 11, 17, 22, 28, 33, 38$. Various statistics are summarized in the following table, in which we are concerned with the approximate eigenpairs $(\mu_5^{(k)}, U_k w_5^{(k)})$, where $(\mu_5^{(k)}, w_5^{(k)})$ is the fifth eigenpair of the Lanczos matrix T_k.

k	c1	c2	c3	c4	c5
10	3.9e−15	3.9e−15	1.9e−02	1.9e−02	1.9e−02
20	5.3e−15	3.9e−15	2.5e−07	2.5e−07	2.5e−07
30	6.5e−15	3.9e−15	2.8e−16	1.4e−12	1.4e−12
40	7.0e−15	3.9e−15	8.9e−19	1.4e−12	1.4e−12

The columns of the table contain the following quantities.

c1: $\|T_k - Q^{\mathrm{T}}AQ\|_2$, where Q is the Q factor of U_k.

c2: The global residual norm

$$\|AU_k - U_k H_k - \beta_k u_{k+1} \mathbf{e}_k^{\mathrm{T}}\|_k$$

c3: The classical estimate $|\beta_k \mathbf{e}_k^{\mathrm{T}} w_5^{(k)}|$ for the residual norm.

c4: The true residual norm.

c5: The residual norm estimated by (1.4).

The numbers in the first column illustrate the result of Simon mentioned above. The tridiagonal Lanczos matrix T_k is to working accuracy the Rayleigh quotient formed from the Q-factor of U_k. This means that in spite of the contamination of T_k by the reorthogonalization process, its eigenvalues converge to eigenvalues of A.

The second column shows that the corrections in Algorithm 2.2 produce a Krylov decomposition whose residual is of the order of the rounding unit. Although to the two figures shown this residual is not changing, actually it is increasing very slightly with k.

The third and fourth columns show that the classic estimate for the residual norm deviates from the true residual norm. In particular the latter stagnates at about 10^{-12}, whereas the former continues to decrease. But the two values diverge only after the true residual norm falls below $\sqrt{\epsilon_{\mathrm{M}}}$. The fifth column shows that the approximate residual norm (1.4) is a reliable estimate of the true residual norm.

4. Discussion

The algorithm in Figure 2.2 shows that the running computation of the adjusted Rayleigh H_k quotient is computationally inexpensive. One can also economize on storage, since except for spikes at the reorthogonalization points the elements above the first superdiagonal are zero. These spikes can be squirreled away in a special data structure, so that one does not have to store a full matrix of order k. However, such economies may not be worth the trouble, since it requires an array of order k to store primitive Ritz vectors.

Although H_k must be updated at each orthogonalization step, it does not have to be used until the (suitably scaled) residual norms for the approximate eigenvectors approach $\sqrt{\epsilon_{\mathrm{M}}}$. Thereafter it should be used in residual computations. If a residual stagnates at an unacceptably high value, then one must use primitive Ritz vectors computed from H_k. Since the eigenpairs of T_k are approximations to the eigenpairs of H_k, one can compute the former and use the inverse power method to adjust them — an inexpensive process given the structure of H_k.

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