

# A study on modified biorthogonalization method for decreasing a breakdown condition<sup>†</sup>

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**요약** 대규모 비대칭 행렬의 특정 고유치들이 많은 중요한 과학, 공학 문제들에서 요구된다. 그 문제를 해결할 수 있는 방법 중의 하나인 biorthogonal 란초스 알고리즘은 심각한 문제점이 있는데, 어떤 특이한 상황에서 알고리즘을 계속할 수 없는 경우가 발생할 수 있다는 것이다. 본 논문에서는 기본적인 biorthogonal 알고리즘이 만드는 축소된 삼중 대각 행렬에 대하여 동일한 고유치를 발견할 수 있는 향상된 biorthogonal 란초스 알고리즘을 소개한다. 이 새로운 알고리즘은 대규모 비대칭 행렬의 특정 고유치들을 구할 수 있으며 기본적인 biorthogonal 란초스 알고리즘에 비해서 안정적인 방법이라는 것을 Cray 컵 컴퓨터를 이용한 실험을 통해서 보여준다.

**Abstract** Many important scientific and engineering problems require the computation of a small number of eigenvalues for large nonsymmetric matrices. The biorthogonal Lanczos method is one of the methods to solve that problem, but it faces serious breakdown problems. In this paper, we introduce a modified biorthogonal Lanczos method to find a few eigenvalues of a large sparse nonsymmetric matrix. The proposed method generates reduction matrices that are similar to those generated by the standard biorthogonal Lanczos method. We prove that the breakdown conditions of our method are less stringent than the standard method. We then implement the modified biorthogonal Lanczos method on the CRAY machine and discuss the decreased breakdown conditions.

## I. Introduction

The most popular way to obtain all the eigenvalues of a  $n \times n$  matrix  $A$  is to use the QR algorithm. As the order  $n$  increases above 100 the QR algorithm becomes less and less attractive, especially if only a few of the eigenvalues must be computed. Many important scientific and engineering problems require the computation of a small number of eigenvalues for large sparse matrices. Earlier work on Krylov methods for nonsymmetric eigenproblems focussed on variants of Arnoldi's method[1].

One difficulty in the use of the Arnoldi's procedure is that it provides only for the computation of the right eigenvectors. Ruhe[4] considered the extension of the one-sided Arnoldi procedure to the 2-sided Arnoldi procedure. This extension generates two orthogonal sets of vectors, essentially independently.

The biorthogonal Lanczos method generates two sets of vectors that are biorthogonal, and a sequence of nonsymmetric but tridiagonal Lanczos matrices [1]. We refer to these tridiagonal matrices as Lanczos reduction matrices. This Lanczos procedure has modest storage requirements and we can therefore use it for very large matrices. In such procedures the eigenvalue and eigenvector computations are performed separately. We find eigenvalues of the

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Lanczos reduction matrices and then use them as approximations to the extreme eigenvalues of  $A$ .

The biorthogonal Lanczos method was neglected for a long time because it faces serious breakdown problems. The problem of building the Lanczos vectors in the nonsymmetric case was addressed by Parlett and Taylor [3], which suggests a Lookahead Lanczos algorithm that can handle possible breakdowns.

In this paper, we introduce a modified biorthogonal Lanczos method. Although the computational work and storage sizes slightly are increased in comparison with the standard one, the modified method has fewer breakdown conditions which needs to be improved for the computations of eigenvalues.

In section 2 we review the biorthogonal Lanczos method. In section 3 we develop the modified biorthogonal Lanczos method, and in section 4, 5 we discuss the decreased breakdown conditions of the modified method.

## II. The Biorthogonal Lanczos method

Let  $A$  be a  $n \times n$  nonsymmetric matrix. There are many tridiagonal matrices similar to  $A$  and  $T_n$  is one of them. Then for some matrix  $Q_n = (q_1, \dots, q_n)$ , we have

$$Q_n^{-1} A Q_n = T_n. \quad (2.1)$$

Let  $P_n = (p_1, \dots, p_n)$  and replace (2.1) by two separate relations,

$$\begin{aligned} P_n^T Q_n &= I \\ P_n^T A Q_n &= T_n. \end{aligned}$$

By equating columns on each side of

$A Q_n = Q_n T_n$  and  $P_n^T A = T_n P_n^T$  in the natural increasing order, we obtain the following equations: For each  $j < n$ ,

$$\begin{aligned} A Q_j &= Q_j T_j + r_j e_j^T \\ P_j^T A &= T_j P_j^T + s_j^T e_j \end{aligned}$$

where  $r_j, s_j$  are residual vectors.  $A$  and two initial vectors  $p_1, q_1$  essentially determine all the other elements of  $P_j, Q_j$  and  $T_j$ .

In this method, the right space  $Q_j$  is a Krylov subspace

$$Q_j = \text{span}[q_1, A q_1, \dots, A^{j-1} q_1]$$

and the left space  $P_j$  is a Krylov subspace

$$P_j = \text{span}[p_1, A^T p_1, \dots, (A^T)^{j-1} p_1]$$

with  $P_j^T Q_j = I_j$ .

The eigenvalues of the biorthogonal Lanczos matrices  $T_j$  are called Ritz values of  $A$ .

For many matrices and for relatively small  $j$ , compared to  $n$ , several of the extreme eigenvalues of  $A$  are well approximated by the corresponding Ritz values. The right Ritz vector  $Q_j y (= z)$  obtained from a right eigenvector  $y$  of a given  $T_j$  is an approximation to a corresponding right eigenvector of  $A$ , and the left Ritz vector  $P_j \hat{y} (= \hat{z})$  obtained from a left eigenvector  $\hat{y}$  of a given  $T_j$  is an approximation to a corresponding left eigenvector of  $A$ . A simpler version of biorthogonal Lanczos algorithm can be formulated as follows:



$s \times s$  upper triangular matrix.

**Remark 3.1**

If  $\widehat{T}_j$  is a tridiagonal matrix generated by the standard block Lanczos algorithm and  $\overline{T}_k = U_k^{-1} \widehat{T}_j U_k$  where  $j = s * k$  and  $U_k = \text{diag}(\overline{U}_1, \overline{U}_2, \dots, \overline{U}_k)$ , then  $\overline{T}_k$  becomes a nonsymmetric matrix similar to  $\widehat{T}_j$  as follows:

$$\overline{T}_k = \begin{bmatrix} G_1 & E_1 & & & & \\ F_1 & G_2 & E_2 & & & \\ & \bullet & \bullet & \bullet & & \\ & & & & E_{k-1} & \\ & & & F_{k-1} & G_k & \end{bmatrix}$$

where  $G_i$  and  $E_i$  are  $s \times s$  matrices. Here  $F_i$  is an  $s \times s$  matrix whose only nonzero element at location  $(1, s)$ .

Also the matrix  $L_k^{-1} \widehat{T}_j L_k$  where  $L_k = \text{diag}(\overline{L}_1, \overline{L}_2, \dots, \overline{L}_k)$  and  $j = s * k$ , becomes the same type of a nonsymmetric matrix  $\overline{T}_k$ .

We demonstrate this for the special case of  $s=3, k=3$ . The general case can be shown in a similar way.

$$U_3^{-1} \widehat{T}_9 U_3 = \begin{bmatrix} * & * & * & & & & & & \\ * & * & * & & & & & & \\ * & & & * & * & * & & & \\ & & & * & * & * & & & \\ & & & & * & * & * & & \\ & & & & & * & * & * & \\ & & & & & & * & * & * \\ & & & & & & & * & * \\ & & & & & & & & * \end{bmatrix}$$

$$\times \begin{bmatrix} * & * & * & & & & & & \\ * & * & * & & & & & & \\ * & * & * & * & * & * & & & \\ * & * & * & * & * & * & * & & \\ * & * & * & * & * & * & * & * & \\ * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * \end{bmatrix}$$

$$\times \begin{bmatrix} * & * & * & & & & & & \\ * & * & * & & & & & & \\ * & & & * & * & * & & & \\ & & & * & * & * & & & \\ & & & & * & * & * & & \\ & & & & & * & * & * & \\ & & & & & & * & * & * \\ & & & & & & & * & * \\ & & & & & & & & * \end{bmatrix}$$

$$= \begin{bmatrix} * & * & * & & & & & & \\ * & * & * & & & & & & \\ * & & & * & * & * & & & \\ & & & * & * & * & & & \\ & & & & * & * & * & & \\ & & & & & * & * & * & \\ & & & & & & * & * & * \\ & & & & & & & * & * \\ & & & & & & & & * \end{bmatrix}$$

$$\times \begin{bmatrix} * & * & * & & & & & & \\ * & * & * & & & & & & \\ * & * & * & * & * & * & & & \\ & & & * & * & * & & & \\ & & & & * & * & * & & \\ & & & & & * & * & * & \\ & & & & & & * & * & * \\ & & & & & & & * & * \\ & & & & & & & & * \end{bmatrix}$$

$$= \begin{bmatrix} * & * & * & | & * & * & * & | & \\ * & * & * & | & * & * & * & | & \\ * & * & & | & * & * & * & | & \\ \hline & & & & * & | & * & * & * & * & * \\ & & & & & | & * & * & * & * & * \\ & & & & & & | & * & * & * & * \\ \hline & & & & & & & * & | & * & * & * \\ & & & & & & & & | & * & * & * \\ & & & & & & & & & | & * & * \end{bmatrix}$$

We now provide the defining equations of the  $s$ -step biorthogonal Lanczos method in the following form.

**Algorithm 3.1** Modified biorthogonal Lanczos algorithm

$$\overline{V}_0 = 0, \quad \overline{W}_0 = 0,$$

$$\overline{V}_1 = [V_1^1, A V_1^1, \dots, A^{s-1} V_1^1]$$

$$\overline{W}_1 = [w_1^1, A^T w_1^1, \dots, (A^T)^{s-1} w_1^1]$$

$$[ \overline{b_{0i}} ] = 0, [ \overline{b_0^i} ] = 0, 1 \leq i \leq s$$

For  $k=1$  until Convergence Do

Select  $[ \overline{a_{ki}} ] = 0, [ \overline{b_{ki}} ] = 0, 1 \leq i \leq s,$

to orthogonalize  $\overline{V_k}$  against  $\overline{W_{k-1}}$ .

Also select  $[ \overline{a_k^i} ] = 0, [ \overline{b_{k-1}^i} ] = 0,$

$$1 \leq i \leq s$$

to orthogonalize  $\overline{W_k}$  against  $\overline{V_{k-1}}$ .

These give

$$v_{k+1}^1 = A v_k^s - \overline{V_{k-1}} b_{k-1}^s - \overline{V_k} a_{k^s}$$

$$w_{k+1}^1 = A^T w_k^s - \overline{W_{k-1}} b_{k-1}^s - \overline{W_k} a_{k^s}$$

Select  $[ \overline{t_{kj}} ], 2 \leq j \leq s,$

to orthogonalize  $\{ A v_{k+1}^1, \dots, A^{s-1} v_{k+1}^1 \}$

against  $\overline{W_k}$ , which gives

$$v_{k+1}^j = A^{j-1} v_{k+1}^1 - \overline{V_k} t_{kj}$$

Select  $[ \overline{t_k^j} ], 2 \leq j \leq s$

to orthogonalize

$$\{ A^T w_{k+1}^1, \dots, (A^T)^{s-1} w_{k+1}^1 \}$$

against  $\overline{V_k}$ , which gives

$$w_{k+1}^j = (A^T)^{j-1} w_{k+1}^1 - \overline{W_k} t_k^j$$

for  $j=2, \dots, s.$

EndFor

Let  $A$  be an  $n \times n$  nonsymmetric matrix and

$$V_k = ( \overline{V_1}, \overline{V_2}, \dots, \overline{V_k} ),$$

$$W_k = ( \overline{W_1}, \overline{W_2}, \dots, \overline{W_k} ).$$

In the  $s$ -step biorthogonal Lanczos method, the Ritz values of  $A$  in  $V_k$  are the eigenvalues

$\lambda_k$  of  $\overline{T_k}$ . The right Ritz vectors are vectors

$V_k x_k (= z_k)$ , where the right eigenvector

$x_k$  of  $\overline{T_k}$  are associated with the  $\lambda_k$  and

the left Ritz vectors are vectors

$W_k \widehat{x}_k (= \widehat{z}_k)$ , where the left eigenvector

$\widehat{x}_k$  of  $\overline{T_k}$  are associated with the  $\lambda_k$ .

#### IV. Decreasing the breakdown condition

It can be easily shown that when algorithm 2.1 does not break down for a null inner product  $(\gamma_j, s_j)$ , then the vectors  $q_{j+1}$  and  $p_{j+1}$  satisfy the biorthonormality property. Although there are various ways of choosing  $\beta_j, \gamma_j$  satisfying  $\beta_j \gamma_j = (\gamma_j, s_j)$ , it is of interest to notice that the product will not depend upon which choice is taken, because

$$\begin{aligned} \|q_{j+1}\| \|p_{j+1}\| &= \frac{\|\gamma_j\| \|s_j\|}{\beta_j \gamma_j} \\ &= \frac{\|\gamma_j\| \|s_j\|}{|(\gamma_j, s_j)|}, \end{aligned}$$

$$\|q_{j+1}\| \|p_{j+1}\| = \frac{1}{\cos} \theta(\gamma_j, s_j),$$

where  $\theta(\gamma_j, s_j)$  denotes the angle between the vectors  $\gamma_j$  and  $s_j$  [5]. This angle  $\theta(\gamma_j, s_j)$  is a function  $A, q_1, p_1$  apart from a normalizing factor. This angle can be equal to  $\pi/2$ , causing the algorithm to stop. It is interesting to note that  $\gamma_j$  and  $s_j$  can be written as  $\gamma_j = \Phi_j(A) q_1,$

$s_j = \Phi_j(A^T) p_1$ , where  $\Phi_j$  denotes polynomial of degree  $j$ . Different choices of the  $\beta_j$  and  $\gamma_j$  correspond to different scaling of the Lanczos vectors. Hence, any resulting tridiagonal matrices  $T_j$  have the same eigenvalues. The biorthogonal Lanczos algorithm can be regarded as the two sided Gram-Schmidt process applied to the column of the special matrices

$$R = R_j = [ q_1, A q_1, A^2 q_1, \dots, A^{j-1} q_1 ]$$

$$L = L_j = [P_1, A^T p_1, \dots, (A^T)^{j-1} p_1].$$

The  $R$  and  $L$  matrices are called Krylov matrices. Note that the  $(i, j)$  element of  $L^T R$  is  $(p_1^T A^{i-1})(A^{j-1} q_1)$ , so

$$L^T R = M = M(p_1, q_1),$$

where  $m_{i+1, j+1} = p_1^T A^{i+j} q_1$ .

The matrix  $M$  is called the moment matrix of  $(p_1, q_1)$  with respect to the matrix  $A$ . The following proposition gives breakdown conditions of the biorthogonal Lanczos method in terms of the nonsingularity of the moment matrices  $M_i$ . This proposition is proven in [3].

**proposition 4.1.** The biorthogonal Lanczos algorithm does not break down in the  $j^{\text{th}}$  iteration if and only if

$$\det(M_i) \neq 0, \quad i = 1, 2, \dots, j.$$

In the modified method the subspace spanned by  $V_k = \{\overline{V}_1, \overline{V}_2, \dots, \overline{V}_k\}$  is the same as the Krylov subspace spanned by the vectors  $\{v_1^1, A v_1^1, A^2 v_1^1, \dots, A^{sk-1} v_1^1\}$ , and the subspace spanned by  $W_k = \{\overline{W}_1, \overline{W}_2, \dots, \overline{W}_k\}$  is the same as the Krylov subspace spanned by the vectors  $\{w_k^1, A^T w_k^1, \dots, A^{sk-1} w_k^1\}$ .

**proposition 4.2.** The modified biorthogonal Lanczos algorithm does not break down in the  $k^{\text{th}}$  iteration if and only if

$$\det(M_i) \neq 0, \quad i = s, 2s, \dots, ks$$

**proof.** Let  $v_k^1$  and  $w_k^1$  be the modified

biorthogonal Lanczos vectors. For each  $k$ ,  $v_k^1$ ,  $1 \leq k \leq s$ , is a linear combination of the first  $(k-1)s+1$  columns of  $R$  while  $w_k^1$  is the same linear combination of the column  $L$ , up to a scaling. This can be expressed compactly in matrix notation as

$$V_k = R \overline{K}^{-T}, \quad W_k = L \overline{K}^{-T} \quad (4.1)$$

where  $\overline{K}$  is the lower triangular whose diagonal elements are 1.

using (4.1) we can rewrite  $M$  as

$$M = L^T R = (\overline{K} W^T)(V \overline{K}^T),$$

that is,

$$M = \overline{K}(W^T V) \overline{K}^T.$$

The matrix  $W^T V$  equals to  $\text{diag}\{W_1^T V_1, \dots, W_k^T V_k\}$ . By a sequence of row operations including exchanging rows, we can reduce  $\overline{W}^T \overline{V}_k$  to an upper triangular matrix  $U_k$  with nonzero diagonal elements and

$$\det(\overline{W}^T) = \pm \det(\overline{U}_k).$$

Let  $U = \text{diag}\{\overline{U}_1, \dots, \overline{U}_k\}$ ;

$$\text{then } \det(W^T V) = \pm \det(U),$$

$$\text{that is } \det(M) = \det(W^T V) =$$

$$\det(\overline{W}_1^T \overline{V}_1) \cdots \det(\overline{W}_k^T \overline{V}_k).$$

This proves the proposition.  $\nabla$

The standard biorthogonal Lanczos algorithm produces a tridiagonal matrix  $T_j$  by the end of step  $j (= ks)$  and the modified method produces a block tridiagonal matrix  $T_k$ .

## V. Numerical Experiments

The test problem was derived from the five-point discretization of the following partial differential equation:

$$-(b u_x)_x - (c u_x)_x + (du)_x + (eu)_y + fu = g$$

on the unit square, where

$$b(x, y) = e^{-xy}, \quad c(x, y) = e^{xy}$$

$$d(x, y) = \beta(x+y), \quad e(x, y) = \gamma(x+y)$$

$$f(x, y) = \frac{1}{1+x+y},$$

subject to the Dirichlet boundary conditions  $u=0$  on the boundary. In the test we took  $\gamma=0.0, \beta=0.0$ , which yielded a symmetric matrix and  $\gamma=50.0, \beta=1.0$ , which yielded a nonsymmetric matrix. Table 5.1 and 5.2 show that matrices generated by the standard and modified biorthogonal Lanczos method have the same largest eigenvalues, but  $s>5$  in the modified method loss of accuracy for eigenvalues has been observed. We tested the methods on the problem of size  $N=4096$ . In the standard and modified biorthogonal Lanczos methods, we find the largest eigenvalues after a reduced matrix of a certain size is generated, so these biorthogonal Lanczos

methods require minimal storage and time. Next we show the reduced breakdown effect of the new biorthogonal Lanczos method compared to the standard one. We borrow the example from [5]:

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

The eigenvalues of  $A$  are the roots of unity, i.e.

$\lambda_j = e^{2N\pi i/j}$  for  $j=0, \dots, N-1$  where  $N$  is the dimension of  $A$ . The biorthogonal Lanczos method starts with initial vectors  $r_1^T = s_1^T = [123456]^T$  on the CRAY machine. At step 4, the standard biorthogonal Lanczos method normalizes  $s_4$  and  $r_4$  by factors of  $\sqrt{10^{-13}}$ , producing elements in the reduced tridiagonal matrix  $T$  of size  $10^{13}$  on the CRAY machine. The 3-step biorthogonal

Table 5.1. Largest eigenvalues using the biorthogonal Lanczos method( $\gamma=0.0, \beta=0.0$ )

$T_j$	standard	2-step	3-step	4-step	5-step
$10 \times 10$	$0.98652673E10$	$0.98652673E10$	—	—	$0.98652673E10$
$20 \times 20$	$0.10202484E10^2$	$0.10202484E10^2$	—	$0.10202484E10^2$	$0.10202491E10^2$
$30 \times 30$	$0.10204000E10^2$	$0.10204000E10^2$	$0.10204000E10^2$	—	$0.10202016E10^2$
$40 \times 40$	$0.10204000E10^2$	$0.10204000E10^2$	—	$0.10204001E10^2$	$0.10202015E10^2$

Table 5.2. Largest eigenvalues using the biorthogonal Lanczos method( $\gamma=50.0, \beta=1.0$ )

$T_j$	standard	2-step	3-step	4-step	5-step
$10 \times 10$	$0.98652673E10$	$0.98652673E10$	—	—	$0.98652673E10$
$20 \times 20$	$0.10202484E10^2$	$0.10202484E10^2$	—	$0.10202484E10^2$	$0.10202491E10^2$
$30 \times 30$	$0.10204000E10^2$	$0.10204000E10^2$	$0.10204000E10^2$	—	$0.10202016E10^2$
$40 \times 40$	$0.10204000E10^2$	$0.10204000E10^2$	—	$0.10204001E10^2$	$0.10202015E10^2$

Lanczos method avoids the large element growth in reduced matrix and can generate a  $3 \times 3$  block tridiagonal matrix which has the sixth root of unity. At the second iteration of the 2-step method we have to solve a linear system with  $2 \times 2$  matrix. This can be explained by proposition 4.2.

## VI. Conclusion

We have showed a modified biorthogonal method to generates reduction matrices which are similar to the reduction matrices generated by the standard biorthogonal Lanczos method. Therefore the new method results in the same eigenvalues as the standard method. We prove that series breakdown conditions are decreased in the resulting algorithm and we show the decreased breakdown condition by the numerical test. For large  $s > 5$  loss of accuracy for eigenvalues has been observed.

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