ISSN 1746-7659, England, UK
Journal of Information and Computing Science
Vol. 1, No. 5, 2006, *pp*. 311-317

New smoothing iterative block methods for linear systems with multiple right-hand sides

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(*Received September 18, 2006 Accepted December. 20, 2006*)

Abstract. In the present paper, we propose new smoothing procedures for iterative block methods for solving nonsymmetric linear systems of equations with multiple right-hand sides. These procedures generalize those known for solving linear systems with one right-hand. We first give some properties of these new algorithms. Then new methods such as the global minimal residual smoothing (GMRS) algorithm and the smoothed global biconjugate gradient (SGL-BCG) algorithm are introduced. Finally, numerical examples are given.

Keywords: Block methods, Smoothing, Iterative methods, Nonsymmetric linear systems, Mutiple right-hand sides, Matrix Krylov subspace, GL-BCG algorithm

1. Introduction

Many applications such as in numerical simulation of wave propagation require the solution of several sparse systems of linear equations with the same coefficient matrix and different right-hand sides.

$$AX = B \tag{1.1}$$

where A is an N×N real nonsymmetric and nonsingular matrix $B = [b_1, \cdots, b_s]$ and $X = [x_1, \cdots, x_s]$ are N×s rectangular matrices with $s << N$.

In the last years, generalizations of the classical Krylov subspace methods have been developed. The first class of these methods contains the block solvers, such as the block biconjugate gradient (BL-BCG) algorithm [6], the block generalized minimal residual (BL-GMRES) algorithm introduced in [9] and studied in [8] , and the block quasi minimal residual (BL-QMR) algorithm[2]. They are generally more efficient as compared to their single right-hand counter parts when the matrix of the linear systems is relatively dense .

Another class of solvers that can handle (1.1) is the seed methods. It consists in selecting a seed system and generating by some method the corresponding Krylov subspace. This procedure is repeated with another seed system until all the systems are solved. This technique is especially attractive when the right-hand sides of (1.1) are not available at the same time; see [7].

Recently, global methods were proposed. These methods were based on the use of a global projection process onto a matrix Krylov subspace. The global full orthogonalization method (GL-FOM) [4], the global generalized minimal residual (GL-GMRES) [4], the global biconjugate gradient (GL-BCG) and the global biconjugate gradient stabilized (GL-BICGSTAB) [5] methods are the most efficient matrix Krylov subspace methods that can solve problem (1.1) .

The BL-BCG algorithm uses a short three-term recurrence formula, but in many situations the algorithm exhibits a very irregular convergence behavior. This problem can be overcome by using a block smoothing technique as defined in [3] or a BL-QMR procedure [2].

In the present paper, we will define new smoothing iterative block methods which improve irregular convergence behavior of the GL-BCG algorithm. The idea of our analysis is originated from [3].

The remainder of the paper is organized as follows. In section 2,we give a brief description of GL-BCG algorithm .The new block generalization of the hybrid procedure is introduced and some properties are given in section 3. In section 4, we propose a global minimal residual smoothing (GMRS) procedure and give some theoretical results. The new smoothed global biconjugate gradient (SGL-BCG) algorithm is presented.

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Section 5 is devoted to some numerical experiments.

Throughout this paper, we use the following notations. For two matrices X and Y in $R^{N\times s}$,we define the following inner product $\left\langle X,Y\right\rangle_F = tr\left(X^TY\right)$,where tr(Z) denotes the trace of the square matrix Z and X^T the transpose of the matrix X.The associated norm is the Forbenius norm which we denote by $\|.\|_F$. $\left\langle .,.\right\rangle_2$ will denote the Euclidean inner product and $\|.\|_2$ the associated norm. For a matrix $V\in R^{N\times s}$, the matrix krylov subspace $\mathcal{K}_k(A,V)$ is the subspace of $R^{N\times s}$ generated by the matrices V, AV, $\cdots, A^{k-1}V$ .A systems of matrices of $R^{N\times s}$ is said to F-orthogonal if it is orthogonal with respect to the inner product $\left\langle .,.\right\rangle_F$.

2. A brief description of GL-BCG algorithm

The GL-BCG algorithm can be derived from the global lanczos algorithm (GL-LANCZOS), see [5] .At step k, the residual R_k generated by this algorithm is such that $R_k - R_0$ lies in the right matrix krylov subspace

$$\mathcal{K}_k(A, AR) = span\{AR_0, A^2R_0, \cdots, A^kR_0\}$$

and R_k is F-orthogonal to the left matrix krylov subspace

$$\mathcal{K}_k(A^T, \tilde{R}_0) = span\{\tilde{R}_0, A^T\tilde{R}_0, \ldots, A^{T^{k-1}}\tilde{R}_0\}$$

where $\tilde{R}_0$ is a given N×s matrix .

The algorithm is defined as follows:

Algorithm 2.1. The global biconjugate gradient (GL-BCG) algorithm

compute $R_0 = B - AX_0$ for a given X_0 ,and choose $\tilde{R}_0$ such that $\left\langle R_0, \tilde{R}_0\right\rangle_F \neq 0$,set $P_0 = R_0$ and $\tilde{P}_0 = \tilde{R}_0$, for j=0,1,… , compute

a. $X_{j+1} = X_j + \alpha_j P_j$, where $\alpha_j = \left\langle R_j, \tilde{R}_j\right\rangle_F \Big/ \left\langle AP_j, \tilde{P}_j\right\rangle_F$,

b. $R_{j+1} = R_j - \alpha_j AP_j$,

c. $\tilde{R}_{j+1} = \tilde{R}_j - \alpha_j A^T\tilde{P}_j$,

d. $P_{j+1} = R_{j+1} + \beta_j P_j$,where $\beta_j = \left\langle R_{j+1}, \tilde{R}_{j+1}\right\rangle_F \Big/ \left\langle R_j, \tilde{R}_j\right\rangle_F$,

e $\tilde{P}_{j+1} = \tilde{R}_{j+1} + \beta_j\tilde{P}_j$.

Proposition 2.1[5]. The matrices produced by the GL-BCG algorithm satisfy the following relation:

(1) $\left\langle R_k, \tilde{R}_l\right\rangle_F = 0$ and $\left\langle AP_k, \tilde{P}_l\right\rangle_F = 0; k \neq l$.

(2) $span\{P_0, \cdots, P_k\} = span\{R_0, \cdots, A^kR_0\}$.

(3) $span\{\tilde{P}_0, \ldots, \tilde{P}_k\} = span\{\tilde{R}_0, \ldots, A^{T^k}\tilde{R}_0\}$.

(4) $R_k - R_0 \in \mathcal{K}_k(A, R_0)$ and R_k is orthogonal to $\mathcal{K}_k(A^T, \tilde{R}_0)$.

3. New generalized smoothing procedure

Consider problem (1.1) and assume that two global iterative methods such as the GL- FOM and the GL-BCG algorithm generate, respectively, at step k, the iterates $X_{k,1}$ and $X_{k,2}$ with the corresponding residuals $R_{k,1}$ and $R_{k,2}$. Similar to linear systems with one right-hand side [1], we define the new approximation of

(1.1) as follows:

$$Y_k = tX_{k,1} + (1-t)X_{k,2} \tag{3.1}$$

and the corresponding residual

$$S_k = tR_{k,1} + (1-t)R_{k,2}.$$

The scalar t is chosen such that

$$\left\langle R_{k,1} - R_{k,2}, S_k \right\rangle_F = 0. \tag{3.2}$$

Setting $E_k = R_{k,1} - R_{k,2}$, the scalar t satisfying (3.2) is given as

$$t = t_k = -\left\langle E_k, R_{k,2} \right\rangle_F \Big/ \left\langle E_k, E_k \right\rangle_F. \tag{3.3}$$

Hence

$$S_k = R_{k,2} + t_k E_k.$$

We assume that the matrix E_k is of full rank. Since $S_k = R_{k,2} + t_k E_k$, then we have

$$\begin{aligned} \|S_k\|_F^2 &= \left\langle S_k, S_k \right\rangle_F \\ &= \|R_{k,2}\|_F^2 + 2t_k \left\langle R_{k,2}, E_k \right\rangle_F + t_k^2 \|E_k\|_F^2. \end{aligned}$$

From (3.3) we can get

$$\|\mathrm{S_k}\|_F^2 = \|R_{k,2}\|_F^2 - \left\langle R_{k,2}, E_k \right\rangle_F^2 \Big/ \|E_k\|_F^2.$$

Thus $\|S_k\|_F \le \|R_{k,2}\|_F$. Similarly, we have $\|S_k\|_F \le \|R_{k,1}\|_F$.

Therefore

$$\|S_k\|_F \le \min(\|R_{k,1}\|_F, \|R_{k,2}\|_F). \tag{3.4}$$

We have the following result.

Proposition 3.1 The residuals defined by the generalized smoothing procedure satisfy the following relations

(1) $\left\langle S_k, S_k \right\rangle_F = \left\langle S_k, R_{k,1} \right\rangle_F$ and $\left\langle S_k, S_k \right\rangle_F = \left\langle S_k, R_{k,2} \right\rangle_F$;

(2) The scalar t_k given by (3.3) solves the minimization problem

$$\|S_k\|_F = \min_{t \in R} \|R_{k,2} + tE_k\|_F.$$

Proof: see [3].

In the following, we will consider a special case of the generalized global smoothing procedure. Instead of combining two different global methods, we consider only one method. At step k, we combine the current approximation X_k with the approximation Y_{k-1} of the generalized smoothing procedure.

4. Smoothed iterative global methods

4.1. A global minimal residual smoothing algorithm

The norm of the residual produced by some block iterative methods such as the GL-BCG algorithm may heavily oscillate. So it would be interesting to apply the global smoothing procedure to such methods to get a norm non-increasing of the new residual.

Let us consider now the following particular case of the generalized global minimal residual smoothing procedure. Suppose that $X_{k,1}$, which will be denoted X_k, is the k-th iterate computed by some iterative global method and take $X_{k,2} = Y_{k-1}$ in expression (3.1). Then we obtain the global minimal residual smoothing (GMRS) procedure as follows:

Algorithm 4.1. Global minimal residual smoothing (GMRS) algorithm

Let $Y_0 = X_0, S_0 = R_0$, compute

$$Y_k = Y_{k-1} + t_k (X_k - Y_{k-1}),$$
$$S_k = S_{k-1} + t_k (R_k - S_{k-1}),$$

Where $t_k = -\left\langle E_k, S_{k-1} \right\rangle_F \Big/ \left\| E_k \right\|_F^2$, $E_k = R_k - S_{k-1}$ is assumed to be of full rank.

Owing to the minimization property (3.4), the norm of residual S_k decreases at each iteration

$$\left\| S_k \right\|_F \le \min(\left\| R_k \right\|_F, \left\| S_{k-1} \right\|_F).$$

Note that for linear systems with one right-hand, the GMRS procedure reduces to the well-known minimal residual smoothing procedure (MRS); see[10].

For the GMRS procedure, we have the following properties.

Proposition 4.1. Let R_k be the residuals generated by some iterative global methods and S_k be the sequence of the residuals produced by the GMRS procedure, then

(1) $\left\langle S_k, R_k \right\rangle_F = \left\langle S_k, S_{k-1} \right\rangle_F$;

(2) $\left\langle S_k, S_k \right\rangle_F = \left\langle S_k, S_{k-1} \right\rangle_F$;

(3) $\left\langle S_k, S_k \right\rangle_F = \left\langle S_k, R_k \right\rangle_F$;

(4) $\left\langle S_k, S_k \right\rangle_F = (1 - t_k) \left\langle S_k, S_k \right\rangle_F + t_k \left\langle S_{k-1}, R_k \right\rangle_F$; Where $t_k = -\left\langle E_k, S_{k-1} \right\rangle_F \Big/ \left\| E_k \right\|_F^2$.

Proof: (1) - (4) may be derived from the results of Proposition 3.1.

Proposition 4.2. Let R_k be the residuals generated by some global iterative methods for solving (1.1) and S_k be the residual defined by the GMRS procedure. Then

(i) $\left\| S_k \right\|_F^2 = \left\| S_{k-1} \right\|_F^2 - \dfrac{\left\langle E_k, S_{k-1} \right\rangle_F^2}{\left\| E_k \right\|_F^2}$;

(ii) $\left\| S_k \right\|_F^2 = \left\| R_k \right\|_F^2 - \dfrac{\left\langle E_k, R_k \right\rangle_F^2}{\left\| E_k \right\|_F^2}$.

Proof: omitted.

When the matrix A is large and sparse, the most important class of iterative global methods for solving linear systems with multiple right-hand sides are matrix Krylov subspace methods. So when applying the GMRS procedure to such methods， it is interesting to know if the obtained methods are also matrix Krylov subspace methods.

If the residuals R_k are generated by a matrix krylov subspace method, then R_k can be expressed as

$$R_k = R_0 + \sum_{i=1}^{k} \alpha_{i,k} A^i R_0 \text{ ,where } \alpha_{i,k} \in R \text{, i=1,…,k.}$$

Let φ_k be the scalar polynomial defined by

$$\varphi_k(t) = \sum_{i=0}^{k} \alpha_{i,k} t^i \text{ and } \varphi_k(0) = 1.$$

Then the residual R_k can be expressed as

$$R_k = \varphi_k(A) R_0 \overset{def}{\equiv} \sum_{i=0}^{k} \alpha_{i,k} A^i R_0 .$$

This is equivalent to the fact that $R_k - R_0 \in \mathcal{K}_k(A, AR_0)$, where $\mathcal{K}_k(A, AR_0)$ is the matrix Krylov subspace generated by the matrices $AR_0, \cdots, A^k R_0$.

When applying the GMRS procedure to matrix Krylov subspace methods we have the following result.

Proposition 4.3. If the approximations X_k are generated by a matrix Krylov subspace method, then the corresponding iterates Y_k produced by the GMRS procedure are also generated by a matrix Krylov subspace method . The residuals S_k are expressed as

$$S_k = S_0 + \sum_{i=1}^{k} \beta_{i,k} A^i R_0, \beta_{i,k} \in R .$$

Proof: We prove the property by induction on the index k.The property is true for k=0.Assume that

$$S_{k-1} = S_0 + \sum_{i=1}^{k-1} \beta_{i,k-1} A^i S_0 \tag{4.1}$$

The kth residual S_k of the GMRS procedure can be written as

$$S_k = (1 - t_k) S_{k-1} + t_k R_k .$$

Hence ,using (4.1) and the last expression of S_k ,we get

$$S_k = (1 - t_k)(S_0 + \sum_{i=1}^{k-1} \beta_{i,k-1} A^i S_0) + t_k (R_0 + \sum_{i=1}^{k} \alpha_{i,k} A^i R_0) .$$

Since $S_0 = R_0$,it follows that

$$S_k = S_0 + \sum_{i=1}^{k-1} [(1 - t_k)\beta_{i,k-1} + t_k \alpha_{i,k}] A^i S_0 + t_k \alpha_{k,k} A^k S_0 .$$

Now setting

$$\beta_{i,k} = (1 - t_k)\beta_{i,k-1} + t_k \alpha_{i,k} \text{ for } i = 1, \cdots, k-1 \text{ and } \beta_{k,k} = t_k \alpha_{k,k} .$$

Finally ,we get the desired result

$$S_k = S_0 + \sum_{i=1}^{k} \beta_{i,k} A^i S_0 .$$

This shows that $S_k - S_0 \in \mathcal{K}_k(A, AS_0)$.

4.2. Smoothing GL-BCG algorithm

One disadvantage of the GL-BCG algorithm is that its residual norm behavior often exhibits very irregular. This problem can be overcome by applying the GMRS procedure to the algorithm. The smoothed GL-BCG algorithm is given as follows:

Algorithm 4.2. Smoothed global biconjugate gradient (SGL-BCG) algorithm.

Let $Y_0 = X_0, S_0 = R_0$, compute

$$Y_k = Y_{k-1} + t_k (X_k - Y_{k-1});$$
$$S_k = S_{k-1} + t_k (R_k - S_{k-1});$$

where X_k is the approximation generated by the GL-BCG algorithm and

$$t_k = -\left\langle E_k, S_{k-1} \right\rangle_F \Big/ \|E_k\|_F^2 \text{ ,with } E_k = R_k - S_{k-1} .$$

Problems of breakdowns and near breakdowns for the GL-BCG algorithm and corresponding smoothed one are not treated in this work.

5. Numerical examples

In this section, we present some numerical examples to illustrate the effectiveness of Algorithm 4.2 for large and sparse matrix equations. All numerical experiments are performed on an AMD 1.4 GHZ PC with main memory 512 MB. We use MATLAB 6.5 with machine precision $\mu = 2.22\times10^{-16}$. The initial guess X_0 is taken to be zero and the right-hand side matrix B is B=rand(N,s) where function rand creates an N×s random matrix with coefficients uniformly distributed in [0 1]. The stopping criterion for two methods is $\frac{\|S_k\|_F}{\|R_0\|_F} \le 1.e-7$.

Example 1. We compared the performances of the GL- BCG and the SGL-BCG algorithms. We used matrices from the Harwell-Boeing collection: A_1 =sherman 1 and A_2 =orsirr_1. In Figure 4.1 and 4.2, we plotted the log10 of the Forbenius norm of the residual versus the iterations. As shown in two figures, SGL-BCG (solide line) returns better results.

Example 2. We compared the performances of the GL- BCG and the SBBCG[3] algorithms. We used matrices from the Harwell-Boeing collection: A_3 =cdde4 . In Figure 4.3, we plotted the log10 of the Forbenius norm of the residual versus the iterations. As can be seen from Figure 4.3, SGL-BCG (solide line) returns better results.The SBBCG algorithm fails to converge .

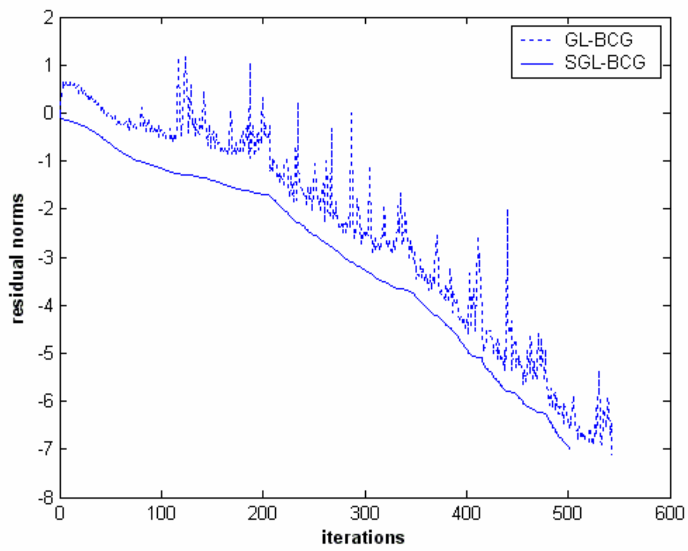

Figure4.1 A_1 =sherman1;N=1000;s=20

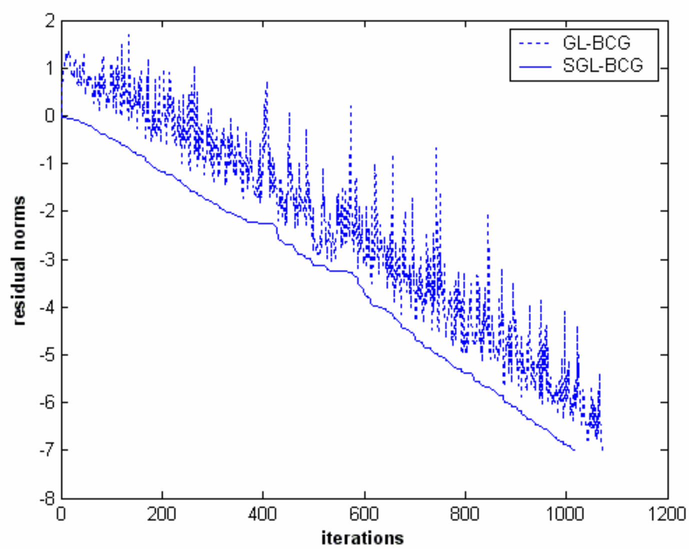

Figure4.2 A_2 =orsirr_1;N=1030;s=10

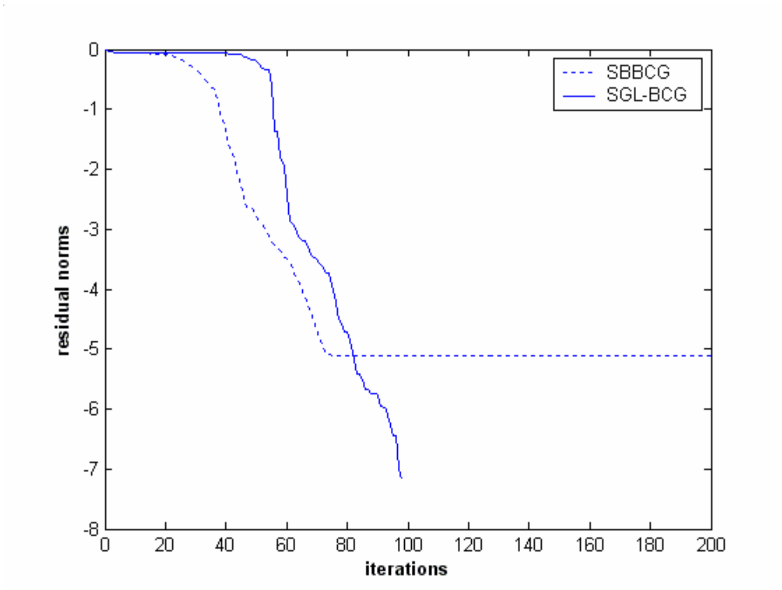

Figure4.3 A_3 =cdde4;N=961;s=10

6. Acknowledgement.

The author wishes to thank Prof. Hua Dai for many helpful comments on this subject.

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