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Hybrid Bi-CG methods with a Bi-CG formulation closer to the IDR approach

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ABSTRACT

The Induced Dimension Reduction(s) (IDR(s)) method has recently been developed. Sleijpen et al. have reformulated the Bi-Conjugate Gradient STABilized (BiCGSTAB) method to clarify the relationship between BiCGSTAB and IDR(s). The formulation of Bi-Conjugate Gradient (Bi-CG) part used in the reformulated BiCGSTAB is different from that of the original Bi-CG method; the Bi-CG coefficients are computed by a formulation that is closer to the IDR approach. In this paper, we will redesign variants of the Conjugate Gradient Squared method (CGS) method, BiCGSTAB and the Generalized Product-type method derived from Bi-CG (GPBiCG)/BiCG×MR2 by using the Bi-CG formulation that is closer to the IDR approach. Although our proposed variants are mathematically equivalent to their counterparts, the computation of one of the Bi-CG coefficients differs, and the recurrences of the variants are also partly different from those of the original hybrid Bi-CG methods. Numerical experiments show that the variants of BiCGSTAB and GPBiCG/BiCG×MR2 are more stable and lead to faster convergence typically for linear systems for which the methods converge slowly (long stagnation phase), and that the variants of CGS attain more accurate approximate solutions.

1. Introduction

We treat Krylov subspace method for solving a large sparse linear system

$$\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$$

for $\boldsymbol{x}$, where $\mathbf{A}$ is a given n-by-n matrix, and $\boldsymbol{b}$ is a given n-vector. The Bi-Conjugate Gradient (Bi-CG) method [4] is well-known for solving the linear system. A number of hybrid Bi-CG methods such as Conjugate Gradient Squared (CGS) [16], Bi-CG STABilized (BiCGSTAB) [19], BiCGStab2 [7], BiCGstab(ℓ) [12], Generalized Product-type Bi-CG (GPBiCG) [20], BiCG×MR2 [8,2], and Generalized CGS (GCGS) [5] have been developed to improve the convergence of Bi-CG and to avoid multiplication by the conjugate transpose $\mathbf{A}^*$ of $\mathbf{A}$. The residuals of the hybrid Bi-CG method are expressed as the product of the residual of Bi-CG and a stabilization polynomial ([14]). The Induced Dimension Reduction(s) (IDR(s)) method [17] has recently been proposed, and it has been reported that IDR(s) is often more effective than the hybrid Bi-CG methods. IDR(s) can be considered as a block version of BiCGSTAB, and IDR(s) for $s = 1$ is equivalent to BiCGSTAB [14,13]. Sleijpen et al. have reformulated BiCGSTAB to clarify the relationship between BiCGSTAB and IDR(s) in [14,13]. The formulation of Bi-CG part used in the reformulated BiCGSTAB is different from the standard Bi-CG; the Bi-CG coefficients are computed by using the formulation that is closer to the IDR approach, which is referred to as a *Bi-CG*$_{(IDR)}$ formulation.

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In this paper, therefore, we will redesign variants of CGS, BiCGSTAB and GPBiCG/BiCG$\times$MR2 by using the *Bi-CG*$_{(IDR)}$ formulation, i.e., the formulation of Bi-CG described in [14,13]. Following [1], we derive four variants of GPBiCG/BiCG$\times$MR2 by combining the *Bi-CG*$_{(IDR)}$ formulation and a three-term recurrence or coupled two-term recurrences for the stabilization polynomial since it has not been remarked in [1] that GPBiCG/BiCG$\times$MR2 can profit from inside IDR. Two variants of BiCGSTAB are given by combining the *Bi-CG*$_{(IDR)}$ formulation and a two-term recurrence for the stabilization polynomial. One of our variants of BiCGSTAB coincides with the reformulated BiCGSTAB described in [14,13], but its advantage has not previously been described. We design two variants of CGS by combining the *Bi-CG*$_{(IDR)}$ formulation and the coupled two-term recurrences for Lanczos polynomials [18] with the same analogy as was used in GCGS. Although these variants are mathematically equivalent to their counterparts, the computation of one of the Bi-CG coefficients differs, and the recurrences of the variants are also partly different from those of the original hybrid Bi-CG methods. This modification leads to slightly more accurate Bi-CG coefficients and faster convergence for the variants of BiCGSTAB and GPBiCG/BiCG$\times$MR2, and more accurate approximate solutions for the variants of CGS.

We compare the convergence between the original CGS, BiCGSTAB, GPBiCG and BiCG$\times$MR2 methods, and our proposed variants. Numerical experiments show that the variants of BiCGSTAB and GPBiCG/BiCG$\times$MR2 are more stable and lead to faster convergence typically for linear systems for which the methods converge slowly (long stagnation phase), and that the approximate solutions solved by the variants of CGS are more accurate. Following [15], we also examine the accuracy for the computation of an inner product computed in the Bi-CG coefficients.

We first outline the standard Bi-CG method and the *Bi-CG*$_{(IDR)}$ formulation in Section 2. In Section 3, we derive alternative implementations of the original CGS, BiCGSTAB and GPBiCG/BiCG$\times$MR2. Numerical experiments in Section 4 show that the variants are more effective. The results imply that the hybrid Bi-CG methods profit from inside IDR.

2. Standard Bi-CG and an alternative Bi-CG

In this section, we describe the formulation of the standard Bi-CG method and the *Bi-CG*$_{(IDR)}$ formulation used in the reformulated BiCGSTAB.

The residuals $\boldsymbol{r}_k^{\rm bcg}$ of the standard Bi-CG method are generated by the coupled two-term recurrences

$$\boldsymbol{r}_{k+1}^{\rm bcg} = \boldsymbol{r}_k^{\rm bcg} - \alpha_k \mathbf{A}\boldsymbol{u}_k^{\rm bcg}, \tag{1}$$
$$\boldsymbol{u}_{k+1}^{\rm bcg} = \boldsymbol{r}_{k+1}^{\rm bcg} - \beta_k \boldsymbol{u}_k^{\rm bcg}, \tag{2}$$

where, for each k, the Bi-CG coefficients α_k and β_k are determined such that

$$\boldsymbol{r}_{k+1}^{\rm bcg}, \mathbf{A}\boldsymbol{u}_{k+1}^{\rm bcg} \perp \tilde{\boldsymbol{r}}_k. \tag{3}$$

The n-vector $\tilde{\boldsymbol{r}}_0$ is selected at the initialization of Bi-CG, and the n-vectors $\tilde{\boldsymbol{r}}_0, \tilde{\boldsymbol{r}}_1, \ldots, \tilde{\mathrm{r}}_{k-1}$ are such that they span the kth Krylov subspace $\mathscr{K}_k(\boldsymbol{A}^*; \tilde{\boldsymbol{r}}_0)$ for each k. An induction argument shows that $\boldsymbol{r}_k^{\rm bcg} \perp \mathscr{K}_k(\boldsymbol{A}^*; \tilde{\boldsymbol{r}}_0)$.

The residuals $\boldsymbol{r}_k$ of the hybrid Bi-CG method can be expressed as

$$\boldsymbol{r}_k \equiv P_k(\mathbf{A})\boldsymbol{r}_k^{\rm bcg}$$

by combining a polynomial $P_k(\lambda)$ of degree k together with the residual of Bi-CG. The hybrid Bi-CG method finds the residuals in the kth Sonnoveld space $\{P_k(\mathbf{A})\boldsymbol{r}_k^{\rm bcg} | \boldsymbol{r}_k^{\rm bcg} \perp \mathscr{K}_k(A^*; \tilde{\boldsymbol{r}}_0)\}$ [14]. When the relation $P_k(\lambda)$ is valid for the Lanczos polynomials $R_k(\lambda)$, the residuals $R_k(\mathbf{A})\boldsymbol{r}_k^{\rm bcg}$ of CGS can be obtained. The residuals of BiCGSTAB are expressed by $Q_k(\mathbf{A})\boldsymbol{r}_k^{\rm bcg}$. Here, the polynomial $Q_k(\lambda)$ is the Generalized Minimal RESidual (1) (GMRES (1)) [11] or Generalized Conjugate Residual (1) (GCR (1)) [3] polynomial. $H_k(\mathbf{A})\boldsymbol{r}_k^{\rm bcg}$ stands for the residuals of GPBiCG/BiCG$\times$MR2, where the polynomials $H_k(\lambda)$ satisfy a three-term recurrence formula similar to the one for the Lanczos polynomials ([20]).

Sleijpen et al. have reformulated BiCGSTAB to clarify the relationship between BiCGSTAB and IDR(s) in [14,13]. The formulation of *Bi-CG*$_{(IDR)}$ described in [14,13] is different from that of the standard Bi-CG, i.e., (1) and (2), and the orthogonality (3) have been rewritten by alternative recurrences

$$\boldsymbol{r}_{k+1}^{\rm bcg} = \boldsymbol{r}_k^{\rm bcg} - \alpha_k \mathbf{A}\boldsymbol{u}_k^{\rm bcg} \perp \tilde{\boldsymbol{r}}_k, \tag{4}$$
$$\mathbf{A}\boldsymbol{u}_{k+1}^{\rm bcg} = \mathbf{A}\boldsymbol{r}_{k+1}^{\rm bcg} - \beta_k \mathbf{A}\boldsymbol{u}_k^{\rm bcg} \perp \tilde{\boldsymbol{r}}_k, \tag{5}$$
$$\boldsymbol{u}_{k+1}^{\rm bcg} = \boldsymbol{r}_{k+1}^{\rm bcg} - \beta_k \boldsymbol{u}_k^{\rm bcg}. \tag{6}$$

Note that $\mathbf{A}\boldsymbol{u}_{k+1}^{\rm bcg}$ is obtained here by a vector update, whereas in the standard Bi-CG (6) is used to compute and then $\mathbf{A}\boldsymbol{u}_{k+1}^{\rm bcg}$ is obtained by explicitly multiplying $\boldsymbol{u}_{k+1}^{\rm bcg}$ by $\mathbf{A}$. We will redesign the algorithms of the hybrid Bi-CG method using the formulas (4)–(6).

3. Alternative implementations of the hybrid Bi-CG methods

In this section, we derive alternative implementations of the CGS, BiCGSTAB and GPBiCG/BiCG$\times$MR2 methods.