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BiCR variants of the hybrid BiCG methods for solving linear systems with nonsymmetric matrices

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ABSTRACT

We propose Bi-Conjugate Residual (BiCR) variants of the hybrid Bi-Conjugate Gradient (BiCG) methods (referred to as the hybrid BiCR variants) for solving linear systems with nonsymmetric coefficient matrices. The recurrence formulas used to update an approximation and a residual vector are the same as those used in the corresponding hybrid BiCG method, but the recurrence coefficients are different; they are determined so as to compute the coefficients of the residual polynomial of BiCR. From our experience it appears that the hybrid BiCR variants often converge faster than their BiCG counterpart. Numerical experiments show that our proposed hybrid BiCR variants are more effective and less affected by rounding errors. The factor in the loss of convergence speed is analyzed to clarify the difference of the convergence between our proposed hybrid BiCR variants and the hybrid BiCG methods.

1. Introduction

In this paper, we deal with Krylov subspace methods for solving a large sparse linear system

$$A\boldsymbol{x} = \boldsymbol{b}, \qquad (1)$$

where A stands for an n-by-n matrix, and $\boldsymbol{b}$ is an n-vector. The Bi-Conjugate Gradient (BiCG) method [5] is a well-known generic Krylov subspace method for solving this problem, and a number of hybrid BiCG methods such as the Conjugate Gradient Squared method (CGS) [17], the Bi-Conjugate Gradient STABilized method (BiCGSTAB) [19], the BiCGStab2 method [8], the Generalized Product-type method derived from BiCG (GPBiCG) [20] and the BiCGstab(l) method [15] have been developed to improve the convergence.

The Conjugate Residual (CR) [4] method has been known as a Krylov subspace method derived from the minimum residual approach [7] for symmetric matrices. The Bi-Conjugate Residual (BiCR) method [16] has been proposed as a generalization of CR for nonsymmetric matrices. It has been reported that the oscillations in the residual norms of CR and BiCR are smaller than those of BiCG, and that the residual norms of CR and BiCR tend to converge faster than those of BiCG [16]. We expect to see similar advantages in BiCR variants of the hybrid BiCG methods, which have not been previously proposed in an international journal.

Therefore, following [1] we propose BiCR variants of the hybrid BiCG methods (referred to as the hybrid BiCR variants). In other words, the BiCG part, which is a component of the residual polynomials of the hybrid BiCG methods, is replaced with BiCR. The recurrence formulas used to update an approximation and a residual vector are the same as those used in the

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corresponding hybrid BiCG method, but the recurrence coefficients are different; they are determined so as to compute the coefficients of the residual polynomial of BiCR. From our experience it appears that the hybrid BiCR variants often converge faster than their BiCG counterpart. Numerical experiments show that our proposed BiCR variants are more effective and less affected by rounding errors. The factor in the loss of convergence speed is analyzed to clarify the difference of the convergence between our proposed hybrid BiCR variants and the hybrid BiCG methods.

In the following section, the outline of the hybrid BiCG methods is described. In Section 3, the mathematical properties of BiCR and the description of the recurrence coefficients of BiCR are given. In Section 4, the hybrid BiCR variants are proposed. In Section 5, the factor in the loss of convergence speed is analyzed. Numerical experiments on model problems with nonsymmetric matrices demonstrate that the hybrid BiCR variants converge faster and are more effective than the original hybrid BiCG methods.

2. Hybrid BiCG methods

Let $\boldsymbol{x}_0$ and $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$ denote the initial guess and the corresponding initial residual, respectively. Then, the residual vector $\boldsymbol{r}_k^{\mathrm{BCG}}$ generated by BiCG is expressed by $\boldsymbol{r}_k^{\mathrm{BCG}} = R_k(A)\boldsymbol{r}_0$, where $R_k(\lambda)$ is the residual polynomial of BiCG. It is a multiple of the so-called Bi-Lanczos polynomial [18], which satisfies the recurrence relation

$$\begin{cases} R_0(\lambda) = 1, \\ R_1(\lambda) = 1 - \alpha_0\lambda, \\ R_{k+1}(\lambda) = \left(1 + \alpha_k \dfrac{\beta_{k-1}}{\alpha_{k-1}} - \alpha_k\lambda\right) R_k(\lambda) - \alpha_k \dfrac{\beta_{k-1}}{\alpha_{k-1}} R_{k-1}(\lambda), \quad k = 1, 2, \ldots, \end{cases} \tag{2}$$

for certain coefficients α_k and β_{k-1}.

The residual vectors of the hybrid BiCG methods are expressed as

$$S_k(A)\boldsymbol{r}_k^{\mathrm{BCG}}$$

by combining a polynomial $S_k(\lambda)$ of degree k together with BiCG. The polynomial $S_k(\lambda)$ is selected to make the residual of BiCG converge toward zero faster. Although a number of hybrid BiCG methods are known, this paper deals with only the CGS, BiCGSTAB, GPBiCG and BiCGstab(l) methods.

When the relation $S_k(\lambda) = R_k(\lambda)$ is valid for the polynomial $S_k(\lambda)$, the residual vector $R_k(A)\boldsymbol{r}_k^{\mathrm{BCG}}$ of CGS can be derived. The residual vector of BiCGSTAB is expressed by $Q_k(A)\boldsymbol{r}_k^{\mathrm{BCG}}$. Here, the polynomial $Q_k(\lambda)$ is the Generalized Minimal RESidual (1) (GMRES(1)) [13] or Generalized Conjugate Residual (1) (GCR(1)) [4] polynomial. $H_k(A)\boldsymbol{r}_k^{\mathrm{BCG}}$ stands for the residual vector of GPBiCG, where $H_k(\lambda)$ is generated by a three-term recurrence formula similar to one in (2) [20]. Moreover, the residual vector of BiCGstab(l) is equal to $T_k(A)\boldsymbol{r}_k^{\mathrm{BCG}}$, where the polynomial $T_k(\lambda)$ is a product of GMRES(l) polynomials for k, which is a multiple of l.

BiCG and the BiCG part in CGS, BiCGSTAB, GPBiCG and BiCGstab(l) are theoretically equivalent to one another. Therefore, the hybrid BiCR variants can be derived by replacing the recurrence coefficients α_k and β_k of BiCG with the recurrence coefficients α_k and β_k of BiCR. In Section 4, we propose BiCR variants of the hybrid BiCG methods in which the BiCG part $\boldsymbol{r}_k^{\mathrm{BCG}}$ has been replaced by the residual vector of BiCR.

3. BiCR for nonsymmetric matrices

In this section, we introduce BiCR for nonsymmetric matrices. It uses the same recurrence formulas as BiCG for updating the approximation and the residual vector.

The residual vector of BiCR is expressed by

$$\boldsymbol{r}_k = R_k(A)\boldsymbol{r}_0$$

with the polynomial R_k as defined by (2). To update the residual vector $\boldsymbol{r}_k$, we introduce a new auxiliary vector $\boldsymbol{p}_k$, that, for some polynomial P_k of degree k, can be expressed as

$$\boldsymbol{p}_k = P_k(A)\boldsymbol{r}_0.$$

Then, the two sequences of polynomials $R_k(\lambda)$ and $P_k(\lambda)$ are mutually interlocked with the following recurrence relations.

$$R_{k+1}(A) = R_k(A) - \alpha_k A P_k(A),$$
$$P_{k+1}(A) = R_{k+1}(A) + \beta_k P_k(A), \quad k = 1, 2, \ldots.$$

Furthermore, vectors $\boldsymbol{r}_k^*$ and $\boldsymbol{p}_k^*$, which need to be updated in the BiCR algorithm as well as in the BiCG algorithm, are expressed by $\boldsymbol{r}_k^* = R_k(A^{\mathrm{T}})\boldsymbol{r}_0^*$ and $\boldsymbol{p}_k^* = P_k(A^{\mathrm{T}})\boldsymbol{r}_0^*$. Here, $\boldsymbol{r}_0^*$ is called an initial shadow residual, and any vector can be used.

We now will derive expressions for the recurrence coefficients α_k and β_k. We use that the vectors $\boldsymbol{p}_k$ and $\boldsymbol{p}_k^*$ are basis vectors of $K_k(A, \boldsymbol{r}_0)$ and $K_k(A^{\mathrm{T}}, \boldsymbol{r}_0^*)$, respectively, and are derived from the $A^{\mathrm{T}}A$-Lanczos Bi-orthogonalization algorithm [9–11], where $K_k(A, \boldsymbol{r}_0)$ and $K_k(A^{\mathrm{T}}, \boldsymbol{r}_0^*)$ denote the k-th Krylov subspace. From this approach, we learn that $\boldsymbol{p}_k$ and $\boldsymbol{p}_k^*$ satisfy

$$(A\boldsymbol{p}_i, A^{\mathrm{T}}\boldsymbol{p}_j^*) = 0, \quad (i \neq j). \tag{3}$$