ランチョス・プロセスに基づく積型反復解法とその一般化 数理計算技術の基礎理論

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ランチョス・プロセスに基づく積型反復解法とその一般化

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Abstract

Recently Bi-CGSTAB as a variant of Bi-CG has been proposed for solving nonsymmetric linear systems, and its attractive convergence behaviour has been confirmed in many numerical experiments. Bi-CGSTAB can be characterized by its residual polynomial which consists of the product of the residual polynomial of Bi-CG with other polynomial of form generated from two-term recurrence relations. In this paper, we propose an unified way to generalize a class of product-type methods whose residual polynomials can be factored by the residual polynomial of Bi-CG and other polynomial of form with standard three-term recurrence relations. Such product-type methods that base on Bi-CG can be regarded as generalizations of Bi-CGSTAB. From the unified way, the well-known variants of the product-type methods, like CGS, Bi-CGSTAB, Bi-CGSTAB2, are reacquired again.

Key words. Bi-CG, Bi-CGSTAB, CGS, nonsymmetric linear systems, product-type methods, reconstructing Bi-CG, residual polynomial, three-term recurrence relations.

AMS(MOS) subject classification. 65F10

1 Introduction

For solving nonsymmetric linear systems, the Bi-Conjugate Gradient (Bi-CG hereafter)[8, 3] was presented as a generalization of the Conjugate Gradient (CG hereafter)[7] for solving symmetric positive definite systems. However, operations of transpose matrix-vector multiplications are needed in Bi-CG because a Krylov subspace generated from the transpose matrix is used. In order to avoid calculating the transpose matrix-vector multiplications and improve the convergence rate in Bi-CG, recently many efforts have been devoted to deriving more efficient methods from reconstructing Bi-CG. A common technique to design a new method by means of reconstructing
Bi-CG is to define its residual polynomial by product of two polynomial factors where one factor is the residual polynomial of Bi-CG and the other one is an undetermined polynomial of form. For example, the Conjugate Gradients-Squared (CGS hereafter)[13] and Bi-CGSTAB[16] were derived from Bi-CG by this technique. In CGS, P. Sonneveld defined the undetermined polynomial of form by the same residual polynomial of Bi-CG, i.e. defined the residual polynomial of CGS by the square of that of Bi-CG. CGS was recognized as a powerful variant of Bi-CG in a lot of numerical experiments[13, 11]. In many situations, however, the property of square may cause the convergence behaviour of CGS to be rather irregular and oscillatory because of the presence of the round-off errors[16, 17, 6]. Therefore, in Bi-CGSTAB, H. A. Van der Vorst selected a polynomial of form with two-term recurrence relations instead of one factor of CGS to design the residual polynomial of Bi-CGSTAB. Since the undetermined parameters with respect to the residual polynomial of Bi-CGSTAB are chosen at least to minimize the residual norm per iteration, Bi-CGSTAB is a rather stable and more efficient variant of Bi-CG. In fact, many numerical experiments also indicated that Bi-CGSTAB can often run faster and its convergence behaviour is more smooth than CGS[16, 5, 1]. Besides, M. H. Gutknecht replaced the two-term recurrent polynomial in Bi-CGSTAB with a three-term recurrent polynomial only at even iterations to solve linear systems with complex spectrum, and implemented the algorithm of Bi-CGSTAB2[4]. Bi-CGSTAB2 is explained as a generalizaton of Bi-CGSTAB, say, the combination Bi-CG with GMRES(2), in the sense that Bi-CGSTAB is the combination of Bi-CG with GMRES(1)[4, 12].

The purpose of this paper is to propose an unified way to extend Bi-CGSATB. In the sense to define the undetermined polynomial of form by standard three-term recurrence relations modelled after the residual polynomial of Bi-CG, we generalize a class of generalizatons of Bi-CGSTAB by means of reconstructing Bi-CG. The well-known CGS, Bi-CGSTAB and Bi-CGSTAB2 are included in the generalized product-type methods based on Bi-CG without the disadvantage to store extra iterates like that in GMRES[12] and GCR[2]. This paper is organized as follows: in the next section, we introduce the background concerned with reconstructing Bi-CG, and characterize the product-type methods based on Bi-CG. In §3, we propose a standard three-term recurrent polynomial of form to construct the residual polynomial of the product-type
methods, and derive the recurrence formulas among the related iterates. In §4, an equivalent approach to reduce the recurrence formulas is presented. Several implementations of variants of the product-type methods are considered, and some well-known variants are recalled in §5.

Throughout this paper, superscripts BCG, CGS, STA, ST2 are used to distinguish iterates generated in the algorithms of Bi-CG, CGS, Bi-CGSTAB and Bi-CGSTAB2 respectively.

2 Reconstructing Bi-CG

To begin with, let us consider the solution of the following linear system

\[(2.1) \quad Ax = b\]

where \(A\) is an \(N \times N\) large and sparse nonsymmetric matrix, and always assumed to be nonsingular.

The algorithm of Bi-CG for solving the system (2.1), described first by C. Lanczos[8], was given by R. Fletcher[3] as follows:

**Algorithm 1 Bi-CG**

Choose an initial guess \(x_0^{BCG}\),

and set \(p_0^{BCG} = r_0^{BCG} = r_0^{BCG} = b - Ax_0^{BCG}\).

For \(n = 0, 1, \ldots\) until \(\|r_n^{BCG}\| \leq \epsilon \|b\|\) do:

\[\alpha_n = \frac{(r_n^{BCG*}, r_n^{BCG})}{(p_n^{BCG}, Ap_n^{BCG})},\]

\[x_{n+1}^{BCG} = x_n^{BCG} + \alpha_n p_n^{BCG},\]

\[r_{n+1}^{BCG} = r_n^{BCG} - \alpha_n Ap_n^{BCG},\]

\[r_{n+1}^{BCG} = r_n^{BCG} - \alpha_n A^T r_n^{BCG*},\]

\[\beta_n = \frac{(r_{n+1}^{BCG*}, r_{n+1}^{BCG})}{(r_n^{BCG*}, r_n^{BCG})},\]

\[p_{n+1}^{BCG} = r_{n+1}^{BCG} + \beta_n p_n^{BCG},\]

\[r_{n+1}^{BCG*} = r_{n+1}^{BCG*} + \beta_n p_n^{BCG*}.\]

Let \(r_0^{BCG}\) and \(r_0^{BCG*}\) be abbreviated as \(r_0\) and \(r_0^{*}\). In the algorithm of Bi-CG, the following two Krylov subspaces

\[(2.2) \quad K_n(A; r_0) := \text{span}\{r_0, Ar_0, \ldots, A^{n-1}r_0\}\]

and

\[(2.3) \quad K_n(A^T; r_0^*) := \text{span}\{r_0^*, A^T r_0^*, \ldots, (A^T)^{n-1}r_0^*\}\]

are generated, and the approximative solution \(x_n^{BCG}\) is given in such way that the residual \(r_n^{BCG} (= b - Ax_n^{BCG}\) theoretically) is made orthogonal with respect to \(K_n(A^T; r_0^{*})\). Therefore, we
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have the following orthogonalities of Bi-CG[3].

\[(2.4) \quad r_n^{\text{BCG}} \perp K_n(A^T; r_0^*), \quad \text{and} \quad A p_n^{\text{BCG}} \perp K_n(A^T; r_0^*).\]

Let $R_n$ and $P_n$ denote the polynomials corresponding to the residual $r_n^{\text{BCG}}$ and the direction $p_n^{\text{BCG}}$, then the iterates $r_n^{\text{BCG}}$, $r_n^{\text{BCG*}}$, and $p_n^{\text{BCG*}}$ can be expressed as follows:

\[(2.5) \quad r_n^{\text{BCG}} = R_n(A)r_0, \quad p_n^{\text{BCG}} = P_n(A)r_0, \quad r_n^{\text{BCG*}} = R_n(A^T)r_0^*, \quad p_n^{\text{BCG*}} = P_n(A^T)r_0^*.\]

$R_n$ is the residual polynomial of Bi-CG, and so-called the Lanczos polynomial. Notice that the basic recurrence relations between $R_n$ and $P_n$ hold as follows:

\[(2.6) \quad R_{n+1}(\lambda) = R_n(\lambda) - \alpha_n \lambda P_n(\lambda), \quad P_{n+1}(\lambda) = R_{n+1}(\lambda) + \beta_n P_n(\lambda), \quad \text{for} \quad n = 1, 2, \ldots,\]

Throughout this paper, it is always assumed that the residual $r_n^{\text{BCG}}$ is convergent towards zero. In the sequel, it is known that two disadvantages appear in the algorithm of Bi-CG:

- to construct the sequence of the residuals $r_0^{\text{BCG}}$, $r_1^{\text{BCG}}$, \ldots, $r_n^{\text{BCG}}$ in the Krylov subspace $K_n(A, r_0)$, one has to use the Krylov subspace $K_n(A^T, r_0^*)$ so that the operations of transpose matrix-vector multiplications appear per iteration;

- although $r_n^{\text{BCG*}}$ also converges towards zero, this convergence property can not be exploited directly for improving the convergence rate of the residual $r_n^{\text{BCG}}$.

Next, an unified way to remedy above disadvantages is proposed. Here, we attempt to use a polynomial $H_n$ to accelerate $r_n^{\text{BCG}}$, say, make $H_n(A)r_n^{\text{BCG}} = H_n(A)r_n(A)r_0$ converge towards zero fast. By doing so, we can derive a class of methods which have product-type residual polynomial from reconstructing Bi-CG. Here, we characterize the product-type methods based on Bi-CG by the following process:

- residual polynomial of a product-type method is defined by product of the following two $n$ degree polynomials of forms

\[(2.7) \quad H_n(\lambda)R_n(\lambda)\]

where $R_n$ is the Lanczos polynomial and $H_n$ is undetermined.
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In the product-type methods, $r_{n}^{BCG}$ would be never formed, nor the transpose matrix-vector multiplications would be needed. According to the description above, we know that CGS, Bi-CGSTAB and Bi-CGSTAB2 all belong to such kind of product-type methods based on Bi-CG.

In general, when one attempts to derive a new product-type method from Bi-CG, one would encounter the following three problems:

(A) by means of establishing new formulas, to compute the first-kind of parameters $\alpha_n$ and $\beta_n$ which are used to determine $R_n$;

(B) to define the construction of $H_n$;

(C) by analyzing the stability of the methods, to compute the second-kind of parameters which are used to determine $H_n$. This aspect is the key-point to design the product-type methods.

In fact, the problem (A) can be solved by a technique depended on the orthogonalities (2.4). This technique is due to P. Sonneveld[13], and developed later by H. A. Van der Vorst[16]. Notice that $r_{n}^{BCG^*}$ and $p_{n}^{BCG^*}$ can be written as

$$r_{n}^{BCG^*} = R_{n}(A^{T})r_{0}^* = \left((-1)^{n} \prod_{i=0}^{n-1}\alpha_{i}\right)(A^{T})^{n}r_{0}^* + z_1;$$

$$p_{n}^{BCG^*} = P_{n}(A^{T})r_{0}^* = \left((-1)^{n} \prod_{i=0}^{n-1}\alpha_{i}\right)(A^{T})^{n}r_{0}^* + z_2.$$ 

with $z_1$ and $z_2 \in K_{n}(A^{T}, r_{0}^*)$. By the orthogonalities (2.4), auxiliary formulas for computing $\alpha_n$ and $\beta_n$ can be recovered:

$$\alpha_n = \frac{(r_{n}^{BCG^*}, r_{n}^{BCG})}{(p_{n}^{BCG^*}, Ap_{n}^{BCG})} = \frac{((A^{T})^{n}r_{0}^*, r_{n}^{BCG})}{((A^{T})^{n}r_{0}^*, Ap_{n}^{BCG})},$$

(2.8)

$$\beta_n = \frac{(r_{n+1}^{BCG^*}, r_{n+1}^{BCG})}{(r_{n}^{BCG^*}, r_{n}^{BCG})} = -\alpha_n \frac{((A^{T})^{n+1}r_{0}^*, r_{n+1}^{BCG})}{((A^{T})^{n}r_{0}^*, r_{n}^{BCG})},$$

(2.9)

The formulas (2.8)~(2.9) imply that we can directly use the basis $(A^{T})^{n}r_{0}^*$ of the Krylov subspace $K_{n+1}(A^{T}; r_{0}^*)$ instead of vectors $r_{n}^{BCG^*}$ and $p_{n}^{BCG^*}$ to determine the first-kind of parameters $\alpha_n$ and $\beta_n$ in the algorithm of Bi-CG. The formulas are fundamental to establish the product-type methods based on Bi-CG.
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In order to deal with the problem (B), i.e. designing the polynomial of form \( H_n \) in (2.7), three different polynomials of forms had been presented[13, 16, 4]:

- in CGS, the polynomial of form \( H_n \) is chosen to be the Lanczos polynomial \( R_n \);
- in Bi-CGSTAB, the polynomial of form \( H_n \) is defined by a factored polynomial of form \( Q_n \) determined by a second-kind of parameter \( \omega_{n-1} \)

\[
Q_n = (1 - \omega_{n-1} \lambda)Q_{n-1};
\]

(2.10)

- in Bi-CGSTAB2, the polynomial of form \( H_n \) is denoted by \( \tau_n \) and chosen to satisfy the following recurrence relations

\[
\tau_{2n+1} = (1 - \chi_n \lambda)\tau_{2n}, \quad \tau_{2n+2} = (\zeta_n + \eta_n \lambda)\tau_{2n+1} + (1 - \zeta_n)\tau_{2n}.
\]

(2.11)

The operations for the second-kind of parameters can be omitted in CGS. For the problem (C), the second-kind of parameter \( \omega_n \) (resp. \( \chi_n, \zeta_n \) and \( \eta_n \)) in Bi-CGSTAB (resp. Bi-CGSTAB2) is determined in the such way that the residual norm per iteration can be minimized locally.

The design of the polynomial of form \( H_n \) in practice is desired as:

(1) to make the polynomial of form \( H_n \) satisfy short-term recurrence relations so that little computational work and low storage costs are required per iteration;

(2) to choose the second-parameter of \( H_n \) reasonably to get rather fast and stable convergence behaviour.

3 Generalized product-type methods based on Bi-CG

In this section, we will describe the basic idea to establish a standard polynomial of form \( H_n \) which leads to generalized product-type methods based on Bi-CG for solving the linear system (2.1).
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3.1 Construction of polynomial of form

By eliminating $P_n$ from (2.6), one would recover the three-term recurrence relations for $R_n$ alone[14]:

\begin{align*}
(3.1) & \quad R_0(\lambda) = 1, \quad R_1(\lambda) = (1 - \alpha_0 \lambda)R_0(\lambda), \\
(3.2) & \quad R_{n+1}(\lambda) = \left(1 + \frac{\beta_{n-1}}{\alpha_{n-1}}\alpha_n - \alpha_n \lambda\right)R_n(\lambda) - \frac{\beta_{n-1}}{\alpha_{n-1}}\alpha_n R_{n-1}(\lambda), \quad n = 1, 2, \cdots.
\end{align*}

The three-term recurrence relations are fundamental for the efficiency of all iterative methods based on the Lanczos process. In fact, the three-term recurrence relations of Bi-CG provide a modest hint that motivate our search for developing generalized product-type methods based on Bi-CG. Here, we introduce two independent parameters $\zeta_n$ and $\eta_n$ and let the polynomial of form $H_n$ model after the three-term recurrence relations (3.1)~(3.2) of $R_n$ as follows:

\begin{align*}
(3.3) & \quad H_0(\lambda) := 1, \quad H_1(\lambda) := (1 - \zeta_0 \lambda)H_0(\lambda), \\
(3.4) & \quad H_{n+1}(\lambda) := (1 + \eta_n - \zeta_n \lambda)H_n(\lambda) - \eta_n H_{n-1}(\lambda),
\end{align*}

where the undetermined parameters $\zeta_n$ and $\eta_n$ belong to the second-kind.

3.2 Recurrence formulas for iterates

Using the basic recurrence relations (2.6), we have the following set of recurrence relations among the products of polynomials $H_n R_n$, $H_n P_n$, $H_{n-1} R_n$, $H_{n-2} R_n$ and $H_{n-1} P_n$:

\begin{align*}
(3.5) & \quad H_{n+1} R_{n+1} = (1 + \eta_n)H_n R_{n+1} - \zeta_n \lambda H_n R_{n+1} - \eta_n H_{n-1} R_{n+1}, \\
(3.6) & \quad H_{n+1} P_{n+1} = H_{n+1} R_{n+1} + \beta_n (1 + \eta_n - \zeta_n \lambda)H_n P_n - \beta_n \eta_n H_{n-1} P_n, \\
(3.7) & \quad H_n R_{n+1} = H_n R_n - \alpha_n \lambda H_n P_n, \\
(3.8) & \quad H_{n-1} R_{n+1} = H_{n-1} R_n - \alpha_n \lambda H_{n-1} P_n, \\
(3.9) & \quad H_n P_{n+1} = H_n R_{n+1} + \beta_n H_n P_n.
\end{align*}

Let us build up the product-type methods with residual:

\begin{equation}
(3.10) \quad r_n := H_n(A)_{n}^{\text{BCG}} = H_n R_n(A)r_0 = b - Az_n
\end{equation}
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which can be obtained with the following iterates:

\[(3.11) \quad p_n := H_n(A)p_n^{BCG}, \quad t_n := H_{n-1}(A)r_n^{BCG}, \quad s_n := H_{n-2}(A)r_n^{BCG}, \quad w_n := H_{n-1}(A)p_n^{BCG}.\]

According to the recurrence relations (3.5)~(3.9), we have the following recurrence formulas among the sequences of the iterates \(r_n, p_n, t_n, s_n\) and \(w_n\):

\[(3.12) \quad r_{n+1} = -\eta_n s_{n+1} + (1 + \eta_n)t_{n+1} - \zeta_n A t_{n+1},\]

\[(3.13) \quad p_{n+1} = r_{n+1} - \beta_n \eta_n w_n + \beta_n (1 + \eta_n)p_n - \beta_n \zeta_n A p_n,\]

\[(3.14) \quad t_{n+1} = r_n - \alpha_n A p_n,\]

\[(3.15) \quad s_{n+1} = t_n - \alpha_n A w_n,\]

\[(3.16) \quad w_{n+1} = t_{n+1} + \beta_n p_n.\]

From the definition (3.10) of the residual \(r_n\) and the recurrence formula (3.12) of the residual \(r_n\), we have the formula to update the approximating solution \(x_{n+1}\):

\[(3.17) \quad x_{n+1} = -\eta_n (x_{n-1} + \alpha_{n-1} p_{n-1} + \alpha_n w_n) + (1 + \eta_n)(x_n + \alpha_n p_n) + \zeta_n t_{n+1}.\]

3.3 Computations for \(\alpha_n\) and \(\beta_n\)

Since the coefficient of the highest order term of \(H_n\) is \((-1)^n \prod_{i=0}^{n-1} \zeta_i\), we have

\[(r_0^*, r_n) = (r_0^*, H_n(A)r_n^{BCG}) = (H_n(A^T)r_0^*, r_n^{BCG}) = \left((-1)^n \prod_{i=0}^{n-1} \zeta_i\right)((A^T)^n r_0^*, r_n^{BCG}),\]

\[(r_0^*, A p_n) = (r_0^*, A H_n(A)p_n^{BCG}) = (H_n(A^T)r_0^*, A p_n^{BCG}) = \left((-1)^n \prod_{i=0}^{n-1} \zeta_i\right)((A^T)^n r_0^*, A p_n^{BCG}).\]

Then, from the formulas (2.8)~(2.9), \(\alpha_n\) and \(\beta_n\) can be recovered from the iterates \(r_{n+1}, r_n\) and \(p_n\):

\[(3.18) \quad \alpha_n = \frac{(r_0^*, r_n)}{(r_0^*, A p_n)}, \quad \beta_n = \frac{\alpha_n}{\zeta_n} \cdot \frac{(r_0^*, r_{n+1})}{(r_0^*, r_n)}.\]

Now, we have accomplished a part of the purpose of this paper, i.e. proposed an unified way to derive generalized product-type methods from the reconstruction of Bi-CG. Due to the lack
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of a criterion for choices of $\zeta_n$ and $\eta_n$, it is very hard in fact to determine the second-kind of parameters $\zeta_n$ and $\eta_n$ that are closely and indissolubly connected with convergence behaviour in practice. Implementations of the second-kind of parameters $\zeta_n$ and $\eta_n$ will be discussed in §5 in detail.

4 Equivalent approach

Notice that the $n$-th iterates $x_{n-1}$ and $p_{n-1}$ are used to update $x_{n+1}$ in the formula (3.17). It is not appreciated in any ideal iterative method. In this section, we propose another approach to establish polynomial of form $H_n(\lambda)$ in (2.7) which is mathematically equivalent to the polynomial of form (3.4). By doing so, we can present new class of product-type methods in which $x_{n+1}$ can be updated without the $n$-th iterates, like $x_{n-1}$ and $p_{n-1}$.

4.1 Equivalent polynomial of form

Let $H_n(\lambda)$ be generated by the three-term recurrence realtions (3.4), we find an important fact that $H_n(0) = 1$ holds for any $n$. Then, we have $H_{n+1}(0) - H_{n}(0) = 0$ for any $n$. Thus, we can find an auxiliary polynomial $G_n(\lambda)$ with degree $n$ so that:

\[(4.1) \quad H_{n+1}(\lambda) - H_n(\lambda) = -\zeta_n \lambda G_n(\lambda).\]

Rewrite the three-term recurrence realtions (3.4) as

\[(4.2) \quad H_{n+1}(\lambda) - H_n(\lambda) = -\zeta_n \lambda H_n(\lambda) + \eta_n (H_n(\lambda) - H_{n-1}(\lambda)),\]

and let $\mu_n = \zeta_n$ and $\nu_n = \frac{\eta_{n+1}}{\zeta_{n+1}}$, then the double sets of polynomials $H_n(\lambda)$ and $G_n(\lambda)$ mutually interlocked by the following recurrence relations can be obtained:

\[(4.3) \quad H_{n+1}(\lambda) = H_n(\lambda) - \mu_n \lambda G_n(\lambda);\]
\[(4.4) \quad G_{n+1}(\lambda) = H_{n+1}(\lambda) + \nu_n G_n(\lambda).\]

Using the recurrence relations (4.3) and (4.4), we can reduce the formula (3.17).
4.2 Equivalent recurrence formulas for iterates

To compute the product of polynomials $H_n R_n$, we make use of a new set of recurrence relations among the products of polynomials $H_n R_n$, $H_n P_n$, $G_n R_n$, $G_n P_n$ and $G_{n-1} R_n$ instead of the set of recurrence relations (3.5)–(3.9):

\begin{align*}
(4.5) & \quad H_{n+1} R_{n+1} = H_n R_n - \alpha_n \lambda H_n P_n - \mu_n \lambda G_n R_{n+1}, \\
(4.6) & \quad H_{n+1} P_{n+1} = H_{n+1} R_{n+1} + \beta_n H_{n+1} P_n, \\
(4.7) & \quad G_n R_{n+1} = G_n R_n - \alpha_n \lambda G_n P_n, \\
(4.8) & \quad G_{n+1} R_{n+1} = H_{n+1} R_{n+1} + \nu_n G_{n} R_{n+1}, \\
(4.9) & \quad G_{n+1} P_{n+1} = H_{n+1} P_{n+1} + \nu_n G_{n} R_{n+1} + \beta_n \nu_n G_{n} P_n.
\end{align*}

To obtain residual $r_n := H_n(A)r_n^{BCG}$, let us define auxiliary iterates as follows:

\begin{align*}
(4.10) & \quad p_n := H_n(A)p_n^{BCG}, \quad u_n := G_n(A)p_n^{BCG}, \quad t_n := G_n(A)t_n^{HCG}, \quad s_n := G_{n-1}(A)r_n^{BCG}.
\end{align*}

Then, we have the following recurrence formulas among the iterates:

\begin{align*}
(4.11) & \quad r_{n+1} = r_n - \alpha_n Ap_n - \mu_n As_{n+1}, \\
(4.12) & \quad p_{n+1} = r_{n+1} + \beta_n p_n - \beta_n \mu_n Au_n, \\
(4.13) & \quad s_{n+1} = t_n - \alpha_n Au_n, \\
(4.14) & \quad t_{n+1} = r_{n+1} + \nu_n s_{n+1}, \\
(4.15) & \quad u_{n+1} = p_{n+1} + \nu_n s_{n+1} + \beta_n \nu_n u_n.
\end{align*}

The formula to update the approximative solution $x_{n+1}$ is written as:

\begin{align*}
(4.16) & \quad x_{n+1} = x_n + \alpha_n p_n + \mu_n s_{n+1}.
\end{align*}

From the equivalence between the three-term recurrence relations (3.4) and (3.3)–(3.4), it is easy to see that the approximative solutions $x_{n+1}$ generated by formula (4.16) is mathematically
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equivalent to the approximative solutions $x_{n+1}$ generated by formula (3.17). The formula (3.17) is reduced to the formula (4.16).

Clearly, the formulas of (3.18) for computing $\alpha_n$ and $\beta_n$ are still valid here:

\begin{equation}
\alpha_n = \frac{(r_0^*, r_n)}{(r_0^*, A p_n)}, \quad \beta_n = \frac{\alpha_n}{\mu_n} \cdot \frac{(r_0^*, r_{n+1})}{(r_0^*, r_n)}.
\end{equation}

5 Implementation details

In accordance with the requirement (2) described at the end of §2, we summarize several possibilities to select $\mu_n$ and $\nu_n$ (resp. $\zeta_n$ and $\eta_n$) for the actual implementation of the product-type methods based on Bi-CG. As well-known variants, the algorithms of CGS, Bi-CGSTAB and Bi-CGSTAB2 will be recalled in terms of special choices.

5.1 The choice for CGS

Suppose that $\mu_n = \alpha_n$ and $\nu_n = \beta_n$ in recurrence relations (4.3)~(4.4), we obtain a significant variant of the product-type methods which only depends on information of Bi-CG. It is easy to see that this variant is mathematically equivalent to CGS.

In this case, we find that $H_n = R_n$ and $G_n = P_n$. This fact leads the relation $p_n = t_n$ in recurrence formulas (4.11)~(4.15) to hold. Letting $r_n^{CGS}, p_n^{CGS}, e_n^{CGS}$ and $h_n^{CGS}$ denote new iterates $R_n(A)r_{n+1}^{BCG}, P_n(A)p_{n+1}^{BCG}, R_n(A)e_{n+1}^{BCG}$ and $P_{n-1}(A)r_{n}^{BCG}$ respectively, and rearranging recurrence formulas (4.11)~(4.15), then the algorithm of CGS[13] is recalled as follows:

ALGORITHM 2 CGS

Choose an initial guess $x_0^{CGS}$, and set $r_0^{CGS} = p_0^{CGS} = e_0^{CGS} = r_0^{CGS} = b - Ax_0^{CGS}$.

For $n = 0, 1, \cdots$ until \( \| r_n^{CGS} \| \leq \epsilon \| b \| \) do:

\begin{align*}
\alpha_n &= \frac{(r_0^{CGS}, r_n^{CGS})}{(r_0^{CGS}, A p_n^{CGS})}, \\
h_{n+1}^{CGS} &= e_n^{CGS} - \alpha_n A p_n^{CGS}, \\
x_{n+1}^{CGS} &= x_n^{CGS} + \alpha_n (r_n^{CGS} + h_{n+1}^{CGS}), \\
r_{n+1}^{CGS} &= r_n^{CGS} - \alpha_n A (e_n^{CGS} + h_{n+1}^{CGS}), \\
\beta_n &= \frac{(r_0^{CGS}, r_{n+1}^{CGS})}{(r_0^{CGS}, r_n^{CGS})}, \\
e_{n+1}^{CGS} &= e_{n+1}^{CGS} + \beta_n h_{n+1}^{CGS}, \\
p_{n+1}^{CGS} &= e_{n+1}^{CGS} + \beta_n (h_{n+1}^{CGS} + \beta_n p_n^{CGS});
\end{align*}
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Note that another version of CGS can be derived from recurrence formulas (3.12)\textasciitilde(3.16) under the assumptions $\zeta_n = \alpha_n$ and $\eta_n = \frac{\beta_{n-1}}{\alpha_n} \alpha_n$, but this version seems to be computationally expensive in practice.

5.2 The choice for Bi-CGSTAB

In the subsection, we attempt to get some variants of the product-type methods with little computational work. Here, suppose that parameter $\eta_n$ (resp. $\nu_n$) in recurrence formulas (3.12)\textasciitilde(3.16) (resp. (4.11)\textasciitilde(4.15)) had been given in advance, the another parameter $\zeta_n$ (resp. $\mu_n$) is selected to minimize the residual norm as function of $\zeta$ (resp. $\mu$)

\[
 f(\zeta) := \| r_{n+1} \| = \| t_{n+1} + \eta_n(t_{n+1} - s_{n+1}) - \zeta A t_{n+1} \| \\
 (\text{resp. } f(\mu) := \| r_{n+1} \| = \| r_n - \alpha_n A p_n - \mu A s_{n+1} \| )
\]

which reaches its minimum value at

\[
 \zeta_n = \frac{(t_{n+1} + \eta_n(t_{n+1} - s_{n+1}), At_{n+1})}{(At_{n+1}, At_{n+1})} \\
 (\text{resp. } \mu_n = \frac{(r_n - \alpha_n A p_n, As_{n+1})}{(As_{n+1}, As_{n+1})} )
\]

Moreover, we consider the following special case that all $\eta_n$ (resp. $\nu_n$) are defined by a quantity $\omega$. $\omega$ is called the relaxation factor. This aspect about how to choose the relaxation factor for solving realistic problems needs further research.

1. According to the recurrence formulas (3.12)\textasciitilde(3.16), we have the following variant of the product-type methods, and name it GPBi-CG($\omega$).

**Algorithm 3** GPBi-CG($\omega$)

Choose an initial guess $x_0$,
and set $r_0^* = p_0 = r_0 = b - Ax_0$, $w_0 = t_0 = 0$, $\eta_0 = 0$.
For $n = 0, 1, \cdots$ until $\| r_n \| \leq \epsilon \| b \|$ do:

\[
 \alpha_n = \frac{(r_0^*, r_n)}{(r_0^*, Ap_n)},
 s_{n+1} = t_n - \alpha_n A w_n,
 t_{n+1} = r_n - \alpha_n A p_n,
 \zeta_n = \frac{(t_{n+1} + \omega(t_{n+1} - s_{n+1}), At_{n+1})}{(At_{n+1}, At_{n+1})},
 x_{n+1} = x_n + \alpha_n p_n + \omega(t_{n+1} - s_{n+1} + \alpha_n p_n - \alpha_{n-1} p_{n-1} - \alpha_n w_n),
 r_{n+1} = t_{n+1} + \omega(t_{n+1} - s_{n+1}) - \zeta_n A t_{n+1},
\]
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\[
\beta_n = \frac{\alpha_n \cdot (r_0^*, r_{n+1})}{(r_0^*, r_0)}, \\
w_{n+1} = \tau_{n+1} + \beta_n p_n, \\
p_{n+1} = r_{n+1} + \beta_n (p_n - \mu_n^A u_n + \omega(p_n - w_n)).
\]

2. According to the recurrence formulas \((4.11)\sim(4.15)\), we have the reduced variant of GPBi-CG(\(\omega\)), and call it RGPBi-CG(\(\omega\)).

**Algorithm 4** \(\text{RGPBi-CG}(\omega)\)

Choose an initial guess \(x_0\), 
and set \(r_0^* = u_0 = I_0 = p_0 = r_0 = b - A x_0\).
For \(n = 0, 1, \ldots\) until \(||r_n|| \leq \epsilon \||b||\) do:
\[
\alpha_n = \frac{(r_0^*, r_n)}{(r_0^*, A p_n)}, \\
\mu_n = \frac{(r_n - \alpha_n A p_n, A s_{n+1})}{(A s_{n+1}, A s_{n+1})}, \\
x_{n+1} = x_n + \alpha_n A u_n, \\
r_{n+1} = r_n - \alpha_n A p_n - \mu_n A s_{n+1}, \\
\beta_n = \frac{\alpha_n}{\mu_n} \frac{(r_0^*, r_{n+1})}{(r_0^*, r_0)}, \\
p_{n+1} = r_{n+1} + \beta_n (p_n - \mu_n A u_n), \\
t_{n+1} = r_{n+1} + \omega s_{n+1}, \\
w_{n+1} = p_{n+1} + \omega (s_{n+1} + \beta_n u_n);
\]

3. It is clear that \(x_{n-1}\) and \(p_{n-1}\) appear in the formula to update \(x_{n+1}\) in GPBi-CG(\(\omega\)) is very awkward. Fortunately, we can remedy this difficulty by letting \(\omega = 0\). Notice that the iterates \(s_n\) and \(w_n\) become worthless in this case. In this way an important and economical variant will be obtained again, recalled Bi-CGSTAB[16]:

**Algorithm 5** \(\text{Bi-CGSTAB}\)

Choose an initial guess \(x_0^{STA}\), 
and set \(r_0^{STA*} = p_0^{STA} = r_0^{STA} = b - A x_0^{STA}\).
For \(n = 0, 1, \ldots\) until \(||r_n^{STA}|| \leq \epsilon \||b||\) do:
\[
\alpha_n = \frac{(r_0^{STA}, r_n^{STA})}{(r_0^{STA}, A p_n^{STA})}, \\
\mu_n^{STA} = \frac{(r_n^{STA} - \alpha_n A p_n^{STA}, A s_{n+1}^{STA})}{(A s_{n+1}^{STA}, A s_{n+1}^{STA})}, \\
x_{n+1}^{STA} = x_n^{STA} + \alpha_n A u_n^{STA}, \\
r_{n+1}^{STA} = r_n^{STA} - \alpha_n A p_n^{STA} - \mu_n^{STA} A s_{n+1}^{STA}, \\
\beta_n^{STA} = \frac{\alpha_n}{\mu_n^{STA}} \frac{(r_0^{STA}, r_{n+1}^{STA})}{(r_0^{STA}, r_0^{STA})}, \\
p_{n+1}^{STA} = r_{n+1}^{STA} + \beta_n^{STA} (p_n^{STA} - \mu_n^{STA} A u_n^{STA}), \\
t_{n+1}^{STA} = r_{n+1}^{STA} + \omega s_{n+1}^{STA}, \\
w_{n+1}^{STA} = p_{n+1}^{STA} + \omega (s_{n+1}^{STA} + \beta_n^{STA} u_n^{STA});
\]
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\[ r_{n+1}^{STA} = t_{n+1}^{STA} - \zeta_n A t_{n+1}^{STA}, \]
\[ \beta_n = \frac{\alpha_n}{\zeta_n} \left( \frac{r_0^{STA*}, r_{n+1}^{STA}}{(r_0^{STA*}, r_{n+1}^{STA})} \right), \]
\[ p_{n+1}^{STA} = r_{n+1}^{STA} + \beta_n (p_n^{STA} - \zeta_n A p_n^{STA}); \]

Similarly, Bi-CGSTAB can be also derived from RGPBi-CG(\( \omega \)) by setting \( \omega = 0 \) where the iterates \( t_n \) and \( u_n \) generated in RGPBi-CG(\( \omega \)) can be omitted.

5.3 The choice for GPBi-CG

It is convenient to determine parameters \( \zeta_n \) and \( \eta_n \) in terms of minimizing the residual norm as the function of \( \zeta \) and \( \eta \):

\[ f(\zeta, \eta) := || r_{n+1} || = || t_{n+1} + \eta (t_{n+1} - s_{n+1}) - \zeta A t_{n+1} ||. \]

It suffices to solve a 2 \times 2 linear equations.

Thus, we have the following variant of the product-type methods, and name it GPBi-CG:

**Algorithm 6** GPBi-CG

Choose an initial guess \( x_0 \),
and set \( r_0^* = p_0 = t_0 = b - A x_0, \ w_0 = t_0, \eta_0 = 0 \).

For \( n = 0, 1, \cdots \) until \( || r_n || \leq \epsilon \ || b \|| \) do:

\[ \alpha_n = \left( \frac{r_0^*, r_n}{r_0^*, A p_n} \right), \]
\[ s_{n+1} = t_n - \alpha_n A w_n, \]
\[ t_{n+1} = r_n - \alpha_n A p_n, \]
\[ \zeta_n = \left( s_{n+1} - t_{n+1}, s_{n+1} - t_{n+1} \right) \left( t_{n+1}, A t_{n+1} \right) - \left( s_{n+1} - t_{n+1}, A t_{n+1} \right) \left( s_{n+1} - t_{n+1}, A t_{n+1} \right)^2, \]
\[ \eta_n = \frac{(A t_{n+1}, A t_{n+1}) (s_{n+1} - t_{n+1}) - (s_{n+1} - t_{n+1}, A t_{n+1}) (s_{n+1} - t_{n+1}) - (s_{n+1} - t_{n+1}, A t_{n+1})^2}{(A t_{n+1}, A t_{n+1}) (s_{n+1} - t_{n+1}) - (s_{n+1} - t_{n+1}, A t_{n+1})^2}, \]
\[ x_{n+1} = x_n + \alpha_n p_n + \zeta_n t_{n+1} + \eta_n (x_n - x_{n-1} + \alpha_n p_n - \alpha_{n-1} p_{n-1} - \alpha_n w_n), \]
\[ t_{n+1} = t_{n+1} + \eta_n (t_{n+1} - s_{n+1}) - \zeta_n A t_{n+1}, \]
\[ \beta_n = \frac{\alpha_n}{\zeta_n} \left( \frac{r_0^*, r_{n+1}}{(r_0^*, r_n)} \right), \]
\[ w_{n+1} = t_{n+1} + \beta_n p_n, \]
\[ p_{n+1} = r_{n+1} + \beta_n (p_n - \zeta_n A p_n + \eta_n (p_n - w_n)); \]

5.4 The choice for RGPBi-CG

In the recurrence formulas (4.11)~(4.15), we select the parameters \( \mu_n \) and \( \nu_{n-1} \) so that the residual norm \( || r_{n+1} || \) with respect to \( \mu_n \) and \( \nu_{n-1} \) reaches its minimum value at \( n \)th iteration.
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Denote $r_n - \alpha_n A p_n$ by $w_n$, and $s_n - \alpha_n A (s_n + \beta_{n-1} u_{n-1})$ by $q_n$. Then, rearranging the recurrence formulas (4.11)~(4.15), we obtain the reduced variant of GPBi-CG, and name it RGPBi-CG.

**Algorithm 7** RGPBi-CG

Choose an initial guess $x_0$, $r_0 = b - Ax_0$, and set $r_0^* = w_0 = p_0 = r_0$, $\alpha_0 = \frac{(r_0^*, r_0)}{(r_0^*, Ap_0)}$, $s_1 = w_0 - r_0 - \alpha_0 A p_0$, $\mu_0 = \frac{(s_1, As_1)}{(As_1, As_1)}$.

For $n = 0, 1, \cdots$ until $\| r_n \| \leq \epsilon \| b \|$ do:

$x_{n+1} = x_n + \alpha_n p_n + \mu_n s_{n+1}$,

$r_{n+1} = w_{n+1} - \mu_n As_{n+1}$,

$\beta_n = \frac{\alpha_n}{\mu_n} \frac{(r_n^*, r_{n+1})}{(r_0^*, r_n)}$,

$p_{n+1} = r_{n+1} + \beta_n (p_n - \mu_n Au_n)$,

$\alpha_{n+1} = \frac{(r_n^*, r_{n+1})}{(r_0^*, r_{n+1})}$,

$w_{n+1} = r_{n+1} - \alpha_{n+1} Ap_{n+1}$,

$q_{n+1} = s_{n+1} - \alpha_{n+1} A(s_{n+1} + \beta_n u_n)$,

$\mu_n = \frac{(Aw_{n+1}, As_{n+1} + \beta_n u_n)}{(Aw_{n+1}, As_{n+1} + \beta_n u_n) - (Aw_{n+1}, Aq_{n+1})^2}$,

$\nu_n = \frac{(Aw_{n+1}, As_{n+1})}{(Aw_{n+1}, As_{n+1}) - (Aw_{n+1}, Aq_{n+1})}$,

$s_{n+2} = w_{n+1} + \nu_n q_{n+1}$,

$u_{n+1} = p_{n+1} + \nu_n (s_{n+1} + \beta_n u_n)$.

5.5 Hybrid variants

Another possibility of implementations is to combine one variant of the product-type methods with other one of the product-type methods without restarting. For example, during the first half of algorithm, we use Bi-CGSTAB, and during the latter half, we use CGS.

Actually, Bi-CGSTAB2 can be explained as a hybrid variant of Bi-CGSTAB and GPBi-CG. In other words, for choice of the second-kind parameters, the minimization of residual norm is defined: as function of two variables $\zeta$ and $\eta$ at even iterations; and as function of one variable $\zeta$ under the assumption $\eta_n = 0$ at odd iterations.

If $n = 2k$, then let $\tilde{\chi}_k = \zeta_n$, else let $\tilde{\zeta}_k = 1 + \eta_n$ and $\tilde{\eta}_k = -\zeta_n$ in the GPBi-CG algorithm, Bi-CGSTAB2 reads as follows[4]:
Algorithm 8  Bi-CGSTAB2

Choose an initial guess $x_0^{ST2}$, and set
$r_0^{ST2*} = p_0^{ST2} = r_0^{ST2} = b - A x_0^{ST2}$,
for $n = 0, 1, \cdots$, until $\| r_n^{ST2} \| \leq \epsilon \| b \|$ do:

when $n = 2k$,

$$\alpha_n = \frac{(r_0^{ST2*}, r_n^{ST2})}{(r_0^{ST2*}, Ap_n^{ST2})},$$
$$t_{n+1}^{ST2} = r_n^{ST2} - \alpha_n Ap_n^{ST2},$$
$$\tilde{\zeta}_k = \frac{(A t_{n+1}^{ST2}, A t_{n+1}^{ST2})}{(A t_{n+1}^{ST2}, A t_{n+1}^{ST2})},$$
$$s_{n+1}^{ST2} = x_n^{ST2} + \alpha_n p_n^{ST2} + \tilde{\zeta}_k t_{n+1}^{ST2},$$
$$\beta_n = \frac{\alpha_n}{\tilde{\zeta}_k} \frac{(r_0^{ST2}, r_{n+1}^{ST2})}{(r_0^{ST2}, r_{n+1}^{ST2})},$$
$$w_{n+1}^{ST2} = t_{n+1}^{ST2} + \beta_n p_n^{ST2},$$
$$p_{n+1}^{ST2} = r_{n+1}^{ST2} + \beta_n p_n^{ST2} - \beta_n \tilde{\zeta}_k Ap_n^{ST2},$$

when $n = 2k + 1$,

$$\alpha_n = \frac{(r_0^{ST2*}, r_n^{ST2})}{(r_0^{ST2}, Ap_n^{ST2})},$$
$$s_{n+1}^{ST2} = t_{n}^{ST2} - \alpha_n Ap_n^{ST2},$$
$$t_{n+1}^{ST2} = r_{n}^{ST2} - \alpha_n Ap_n^{ST2},$$
$$\tilde{\eta}_k = \frac{(t_{n+1}^{ST2}, t_{n+1}^{ST2})}{(t_{n+1}^{ST2}, t_{n+1}^{ST2})},$$
$$x_{n+1}^{ST2} = (1 - \tilde{\eta}_k)(x_n^{ST2} + \alpha_n p_n^{ST2}) + \alpha_n x_{n+1}^{ST2} + \tilde{\eta}_k t_{n+1}^{ST2},$$
$$p_{n+1}^{ST2} = r_{n+1}^{ST2} + \beta_n w_{n}^{ST2} + \beta_n (\tilde{\zeta}_k p_n^{ST2} + \tilde{\eta}_k Ap_n^{ST2});$$

6 Summary

In view of more stable convergence behaviour and little work and low storage, we emphasize
that the polynomial of form $II_n$ generated by the three-term recurrence relation (3.4) is better
than the others which come from such truncated iterative method as GMRES(k)($k > 2$)[12, 4]
for the requirement (1) described at the end of 52,

For solving realistic problems, any variant will be hardly competitive without preconditioning
techniques, however, we did not give any detailed description of preconditioning techniques in this paper. All variants can be combined with the efficient preconditioning techniques, such as incomplete LU factorizations. For more detailed discussion on such studies see, e.g., [9, 10, 15].

References


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