ML(N)BICGSTAB: REFORMULATION, ANALYSIS AND IMPLEMENTATION

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Abstract. With the aid of index functions, we re-derive the ML(N)BiCGStab algorithm in [39] more systematically. There are \( n \) ways to define the ML(N)BiCGStab residual vector. Each definition leads to a different ML(N)BiCGStab algorithm. We demonstrate this by presenting a second algorithm which requires less storage. In theory, this second algorithm serves as a bridge that connects the Lanczos-based BiCGStab and the Arnoldi-based FOM while ML(N)BiCG is a bridge connecting BiCG and FOM. We also analyze the breakdown situation from the probabilistic point of view and summarize some useful properties of ML(N)BiCGStab. Implementation issues are also addressed.

Key words. CGS, BiCGStab, ML(N)BiCGStab, multiple starting Lanczos, Krylov subspace, iterative methods, linear systems

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1. Introduction. Consider the solution of the linear system

\[ Ax = b \]  

where \( A \in \mathbb{C}^{N \times N} \) and \( b \in \mathbb{C}^N \). If we express the BiCG[4, 15] residual as \( r_{BiCG}^k = p_k(A)r_0 \) in terms of a polynomial \( p_k(\lambda) \) of degree \( k \) and the initial residual \( r_0 \), the residual vector \( r_k \) of a Lanczos-type product method\(^2\) based on BiCG is defined to be \( r_k = \phi_k(A)p_k(A)r_0 \) where \( \phi_k(\lambda) \) is some polynomial of degree \( k \) with \( \phi_k(0) = 1 \). In CGS[28], \( \phi_k = p_k \). Since, in every iteration, CGS searches for an approximate solution in a larger Krylov subspace, it often converges much faster than BiCG. However, CGS usually behaves irregularly due to a lack of a smoothing mechanism. In BiCGStab[31], the \( \phi_k \) is

\[ \phi_k(\lambda) = \begin{cases} 1 & \text{if } k = 0 \\ (1 - \omega_k \lambda)\phi_{k-1}(\lambda) & \text{if } k > 0. \end{cases} \]  

(1.2)

Here \( \omega_k \) is a free parameter selected to minimize the 2-norm of \( r_{BiCGStab}^k \) in the \( k \)th iteration. As a result, BiCGStab is generally more stable and robust than CGS. BiCGStab has been extended to BiCGStab2[7] and BiCGStab(l)[23, 27] through the use of minimizing polynomials of higher degree. In BiCGStab2, the \( \phi_k \) is defined by the recursion

\[ \phi_k(\lambda) = \begin{cases} 1 & \text{if } k = 0 \\ (1 - \omega_k \lambda)\phi_{k-1}(\lambda) & \text{if } k \text{ is odd} \\ ((\alpha_k \lambda + \beta_k)(1 - \omega_k - 1 \lambda) + 1 - \beta_k)\phi_{k-2}(\lambda) & \text{if } k \text{ is even}. \end{cases} \]  

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\(^2\)For this type of Krylov subspace methods, one can consult [9]. They are called hybrid BiCG methods in [27].
The parameters are again chosen to minimize BiCGStab2 residuals. Likewise, BiCGStab(l) defines its $\phi_k$ as

$$
\phi_k(\lambda) = \begin{cases} 
1 & \text{if } k = 0 \\
(1 + \sum_{j=1}^{l} \alpha_j \lambda^j) \phi_{k-l}(\lambda) & \text{if } k \text{ is a multiple of } l 
\end{cases}
$$

where the parameters in the factor $1 + \sum_{j=1}^{l} \alpha_j \lambda^j$ yields an $l$-dimensional minimization in every $l$th step. BiCGStab2 and BiCGStab(l) usually converge faster than BiCGStab because of smaller residuals in magnitude while avoiding near-breakdowns caused by a possibly too small $\omega_k$. CGS, BiCGStab and BiCGStab2 have been summarized and generalized by GPBi-CG\[40\] where $\phi_k$ is

$$
\phi_k(\lambda) = \begin{cases} 
1 & \text{if } k = 0 \\
1 - \omega_1 \lambda & \text{if } k = 1 \\
(1 + \beta_k - \omega_k \lambda) \phi_{k-1}(\lambda) - \beta_k \phi_{k-2}(\lambda) & \text{if } k > 1.
\end{cases}
$$

GPBi-CG will become CGS, BiCGStab or BiCGStab2 when the $\alpha, \beta, \omega$ are appropriately chosen. For detailed descriptions of these and other product-type methods, one is referred to \[6, 8, 20, 22, 32\] and the references therein. Moreover, a history of product-type methods can be found in \[10\]. The history starts three decades ago with IDR\[36\] method which can be considered as the predecessor of CGS and BiCGStab\[24\]. Recently, IDR has been generalized to IDR(s) with a shadow space of higher dimension, see \[24, 30, 34\]. IDR(s) has close relations with ML(s)BiCGStab.

Generalizations of BiCGStab to methods based on the generalizations of BiCG have been made. For example, BL-BiCGStab\[3\] is a BiCGStab variant built on the BL-BiCG\[16\] for the solution of systems with multiple right-hand sides. ML(n)BiCGStab\[39\] is another BiCGStab variant built on ML(n)BiCG, a BiCG-like method derived from a variant of the band Lanczos process described in \[1\] with $n$ left-starting vectors and a single right-starting vector.

The derivation of the ML(n)BiCGStab algorithm in \[39\] was complicated. In this paper, we exploit the concept of index functions to re-derive the algorithm in a more systematic way, step by step. Index functions were introduced in \[38\] by Boley for the purpose of simplifying the development of the transpose-free multiple starting Lanczos process or the Sonneveld-van der Vorst-Lanczos process (SVLP)\[^3\], and they proved to be very helpful.

Motivated from the study of SVLP in \[38\], we recognized that the definition of the ML(n)BiCGStab residual $r_k$ in \[39\] is not unique. There are $n$ different ways to define $r_k$. Let $\tilde{r}_k$ be the residual of ML(n)BiCG and $\phi_k(\lambda)$ as in (1.2). Then, the ML(n)BiCGStab residual $r_k$ in \[39\] is

\[
(1.3) \quad r_k = \phi_{j+1}(A) \tilde{r}_k
\]

where $k = jn + i$, $1 \leq i \leq n$, $j = 0, 1, 2, \cdots$. Starting from $k = 1$, let us call every $k$ consecutive $k$-iterations an iteration “cycle”. For example, iterations $k = 1, 2, \cdots, n$ form the first cycle, iterations $k = n+1, n+2, \cdots, 2n$ the second cycle and so on. Then definition (1.3) increases the degree of $\phi$ by 1 at the beginning of a cycle. One actually can define $r_k$ by increasing the degree of $\phi$ by 1 anywhere within an iteration cycle.

\[^3\]We rename the process to remember the contributions of the two pioneers in this field of transpose-free Lanczos. In \[38\], it was shown that the Arnoldi process is an extreme case of SVLP.
Each definition will lead to a different ML\((n)\)BiCGStab algorithm. As an illustration, we shall derive a second ML\((n)\)BiCGStab algorithm associated with the definition
\[
(1.4) \quad r_{jn+i} = \begin{cases} 
\phi_j(A) \overline{r}_{jn+i} & \text{if } 1 \leq i \leq n-1 \\
\phi_{j+1}(A) \overline{r}_{jn+i} & \text{if } i = n.
\end{cases}
\]

(1.4) increases the degree of \(\phi\) by 1 at the end of a cycle. The resulting algorithm requires about 25\% less storage (not counting the storage of the coefficient matrix and the preconditioner) than the algorithm associated with definition (1.3). However, one drawback with this storage-saving algorithm is that, in some experiments, its computed residual \(r_k\) can easily diverge from the corresponding exact residual when \(n\) is moderately large.

ML\((n)\)BiCG and ML\((n)\)BiCGStab possess a set of left starting vectors (or, shadow vectors) \(q_1, \ldots, q_n\) that can be chosen freely. This freedom appears to be an advantage of the methods. It helps stabilize the performance of the algorithms (see [39, p.1] for an explanation) and allows us to see a connection between the Lanczos-based BiCG/BiCGStab and the Arnoldi-based FOM.

One question of interest about ML\((n)\)BiCG and ML\((n)\)BiCGStab is: can they solve (1.1) when \(A\) is singular? Since both methods search for a solution of (1.1) in the affine Krylov subspace
\[
(1.5) \quad x_0 + \mathcal{K}(A, r_0) \equiv x_0 + \{ \sum_{i=0}^{k} c_i A^i r_0 \mid c_i \in \mathbb{C}, k \in \mathbb{N}_0 \}
\]
where \(\mathbb{N}_0\) is the set of nonnegative integers, they must fail to converge if (1.5) contains no solution of the linear system. Notice that (1.5) contains a solution of (1.1) if and only if GMRES converges to a solution of (1.1) that lies in (1.5) — this can be derived from [2, Lemma 2.1]. It then follows from [2, Th. 2.6] and [5, Th. 4.1] that (1.5) contains a solution of (1.1) for any initial guess \(x_0\) if and only if (1.1) is consistent and \(\ker(A) \cap \text{Im}(A) = \{0\}\).

In the case when (1.1) is consistent but \(\ker(A) \cap \text{Im}(A) \neq \{0\}\), the selection of \(x_0\) should be a careful step\(^4\). The other thing that hampers the convergence of ML\((n)\)BiCG and ML\((n)\)BiCGStab is breakdown by zero division. We shall show that the two methods will almost surely converge without breakdown by zero division to a solution of (1.1) if the shadow vectors are chosen randomly and the initial guess \(x_0\) is selected such that (1.5) contains a solution of (1.1).

The outline of the paper is as follows. In §2, we introduce index functions. In §3, we present the ML\((n)\)BiCG algorithm introduced in [39], from which ML\((n)\)BiCGStab algorithms are derived. In §4, we rederive the ML\((n)\)BiCGStab algorithm in [39] by index functions. In §5, we derive a storage-saving ML\((n)\)BiCGStab algorithm from a different definition of the residual vector. In §6, we discuss relationships of ML\((n)\)BiCGStab with some other methods. In §7, implementation issues are addressed. Conclusions are made in §8.

2. Index Functions. Let be given a positive integer \(n\). For all integers \(k\), we define
\[
g_n(k) = \lfloor (k - 1)/n \rfloor \quad \text{and} \quad r_n(k) = k - ng_n(k)
\]
\(^4\)For an example where the affine space contains no solution, consider \(A = [0, 1; 0, 0], b = [1, 0]^T\) and select \(x_0 = [1, 0]^T\). Note that this linear system is consistent. This example comes from [2].
where $\lfloor \cdot \rfloor$ rounds its argument to the nearest integer towards minus infinity. We call $g_n$ and $r_n$ index functions; they are defined on $\mathbb{Z}$, the set of all integers, with ranges $\mathbb{Z}$ and $\{1, 2, \cdots, n\}$, respectively.

If we write
\begin{equation}
  k = jn + i
\end{equation}
with $1 \leq i \leq n$ and $j \in \mathbb{Z}$, then
\begin{equation}
  g_n(jn + i) = j \quad \text{and} \quad r_n(jn + i) = i.
\end{equation}

Table 2.1 illustrates the behavior of $g_n$ and $r_n$ with $n = 3$. It can be seen that $g_n(k)$ has a jump when $k$, moved from left to right, passes a multiple of $n$.

The following properties can be easily verified by using (2.2).

\textbf{Proposition 2.1.} Let $k \in \mathbb{N}$, the set of all positive integers, and $s \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$.

(a) $g_n(k + n) = g_n(k) + 1$ and $r_n(k + n) = r_n(k)$.
(b) $g_n(s + 1) = g_n(k + 1)$ if $\max(k - n, 0) \leq s \leq g_n(k)n - 1$.
(c) $g_n(s + 1) = g_n(g_n(k)n + 1) = g_n(k)$ if $g_n(k)n \leq s \leq k - 1$.
(d) $g_n(k + 1) = g_n(k) + 1$ if $r_n(k) = n$.
\begin{equation}
  g_n(k + 1) = g_n(k) \quad \text{if} \quad r_n(k) < n.
\end{equation}
\begin{equation}
  \max(k - n, 0) > g_n(k)n - 1 \quad \text{if} \quad r_n(k) = n \quad \text{or} \quad g_n(k) = 0.
\end{equation}

3. A ML($n$)BiCG Algorithm. Analogously to the derivation of BiCGStab from BiCG, ML($n$)BiCGStab in [39] was derived from a BiCG-like method named ML($n$)BiCG, which was built upon a band Lanczos process with $n$ left starting vectors and a single right starting vector. In this section, we present the algorithm of ML($n$)BiCG from [39] and summarize some of its properties.

\textbf{3.1. The Algorithm.} Consider the solution of (1.1). Throughout the paper we do not assume that the coefficient matrix $A$ is nonsingular. The iterative solution of singular systems has been extensively studied, see, for instance, [2, 5, 14, 18, 35] and the references therein.

Let be given $n$ vectors $q_1, \ldots, q_n \in \mathbb{C}^N$, which we call left starting vectors or shadow vectors. Define
\begin{equation}
  p_k = (A^H)^{g_n(k)} q_{r_n(k)}
\end{equation}
for $k = 1, 2, 3, \cdots$. The following algorithm for the solution of (1.1) is from [39].

\textbf{Algorithm 3.1. ML($n$)BiCG} \footnote{Algorithm 3.1 consists of exact mathematical formulas for $\alpha_k, \beta_k^{(k)}, \xi_k, \tilde{r}_k$ and $\tilde{g}_k$ obtained in}
1. Choose an initial guess \( \hat{x}_0 \) and \( n \) vectors \( q_1, q_2, \ldots, q_n \).
2. Compute \( \bar{r}_0 = b - A\hat{x}_0 \) and set \( p_1 = q_1 \), \( g_0 = r_0 \).
3. For \( k = 1, 2, 3, \ldots \), until convergence:
   4. \( \alpha_k = p_k^H r_{k-1} / p_k^H A g_{k-1} \);
   5. \( \hat{x}_k = \hat{x}_{k-1} + \alpha_k g_{k-1} \);
   6. \( \bar{r}_k = \bar{r}_{k-1} - \alpha_k A g_{k-1} \);
   7. For \( s = \max(k-n, 0), \ldots, k-1 \):
      \( \beta_s^{(k)} = -p_{s+1}^H A (\bar{r}_k + \sum_{t=\max(k-n, 0)}^{s-1} \beta_t^{(k)} g_t) / p_{s+1}^H A g_s \);
   8. \( g_s = \bar{r}_k + \sum_{s=\max(k-n, 0)}^{k-1} \beta_s^{(k)} g_s \);
   9. \( \beta_s^{(k)} \) with respect to \( b \) and \( c \) of \( M \). For \( q \):
   10. \( q = \max(b, c) \) of minimum degree \( n \) and \( t \) in \( A \). Moreover, in \( ML(n)BiCG \), the basis used for \( B_k \) is not chosen to be bi-orthogonal, but simply the set \( \{ p_1, p_2, \ldots, p_k \} \). Therefore, the \( ML(n)BiCG \) algorithm can be viewed as a generalization of a one-sided Lanczos algorithm (see [9, 19]). The likely ill-conditioning of this basis does not matter, as the algorithm is only a technical tool for deriving \( ML(n)BiCGStab \) and this basis disappears in \( ML(n)BiCGStab \) because \( A^H \) will be absorbed by the residuals and direction vectors of \( ML(n)BiCGStab \). For constructing the right-hand side basis consisting of residuals \( \bar{r}_k \), we used recurrences that generalize the coupled two-term recurrences of BiCG, that is, direction vectors \( g_k \) are also constructed.

3.2. Properties. Let \( \nu \) be the degree of the minimal polynomial \( p_{\min}(\lambda; A, \bar{r}_0) \) of \( \bar{r}_0 \) with respect to \( A \), namely, the unique monic polynomial \( p(\lambda) \) of minimum degree such that \( p(A)\bar{r}_0 = 0 \), and let

\[
\mathbf{S}_\nu = [p_1, p_2, \ldots, p_\nu]^H A [\bar{r}_0, A\bar{r}_0, \ldots, A^{\nu-1}\bar{r}_0] \]

and

\[
\mathbf{W}_\nu = [p_1, p_2, \ldots, p_\nu]^H [\bar{r}_0, A\bar{r}_0, \ldots, A^{\nu-1}\bar{r}_0].
\]

Denote by \( \mathbf{S}_l \) and \( \mathbf{W}_l \) the \( l \times l \) leading principal submatrices of \( \mathbf{S}_\nu \) and \( \mathbf{W}_\nu \) respectively. We now summarize some useful facts about Algorithm 3.1. They can be derived from §3 of [39]. Even though the algorithm has not been tested, it is believed to be numerically unstable because of Line 11 in which the shadow vectors are repeatedly multiplied by \( A^H \), a type of operation which is highly sensitive to round-off errors. The algorithm is introduced only for the purpose of developing \( ML(n)BiCGStab \) algorithms.
the construction procedure of the algorithm.

**Proposition 3.2.** In infinite precision arithmetic, if \( \prod_{i=1}^{\nu} \det(\mathbf{S}_i) \det(\mathbf{W}_i) \neq 0 \), then Algorithm 3.1 does not break down by zero division for \( k = 1, 2, \cdots, \nu \), and \( x_\nu \) is an exact solution of (1.1). Moreover, the computed quantities satisfy

(a) \( \mathbf{x}_k \in \mathbf{x}_0 + \kappa_k(\mathbf{A}, \mathbf{r}_0) \) and \( \mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k \in \mathbf{r}_0 + \mathbf{A}\kappa_k(\mathbf{A}, \mathbf{r}_0) \) for \( 1 \leq k \leq \nu \).

(b) \( \operatorname{span}\{\mathbf{r}_0, \mathbf{r}_1, \cdots, \mathbf{r}_{k-1}\} = \kappa_k(\mathbf{A}, \mathbf{r}_0) \) for \( 1 \leq k \leq \nu \).

(c) \( \operatorname{span}\{\mathbf{A}\mathbf{r}_0, \mathbf{A}\mathbf{r}_1, \cdots, \mathbf{A}\mathbf{r}_{\nu-1}\} = \kappa_\nu(\mathbf{A}, \mathbf{r}_0) \).

(d) \( \mathbf{r}_k \perp \operatorname{span}\{\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_k\} \) and \( \mathbf{r}_k \notin \mathbf{p}_{k+1} \) for \( 0 \leq k \leq \nu - 1 \).

(e) \( \operatorname{span}\{\mathbf{g}_0, \mathbf{g}_1, \cdots, \mathbf{g}_{k-1}\} = \kappa_k(\mathbf{A}, \mathbf{r}_0) \) for \( 1 \leq k \leq \nu \).

(f) \( \operatorname{span}\{\mathbf{A}\mathbf{g}_0, \mathbf{A}\mathbf{g}_1, \cdots, \mathbf{A}\mathbf{g}_{\nu-1}\} = \kappa_\nu(\mathbf{A}, \mathbf{r}_0) \).

(g) \( \mathbf{A}\mathbf{g}_k \perp \operatorname{span}\{\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_k\} \) and \( \mathbf{A}\mathbf{g}_k \notin \mathbf{p}_{k+1} \) for \( 0 \leq k \leq \nu - 1 \).

Because of Proposition 3.2(a) and (d), ML\((n)\)BiCG is an oblique projection Krylov subspace method\([20]\).

**Remarks 3.3.**

(i) The matrices \( \mathbf{S}_i \) and \( \mathbf{W}_i \) have already appeared in \([12, 13]\) where they were called moment matrices. Proposition 3.2 can be regarded as a generalization of Theorem 2 in \([13]\) from \( n = 1 \) to \( n > 1 \).

(ii) Just like BiCG, ML\((n)\)BiCG also has two types of breakdown caused, respectively, by the failure of the underlying Lanczos process and the nonexistence of the LU factorizations of the Hessenberg matrix of the recurrence coefficients. Both types of breakdown are reflected in Algorithm 3.1 by \( \mathbf{p}_k^H \mathbf{A}\mathbf{g}_{k-1} = 0 \). The condition \( \prod_{i=1}^{\nu} \det(\mathbf{W}_i) \neq 0 \) guarantees that the underlying Lanczos process works without breakdown by zero division, and the condition \( \prod_{i=1}^{\nu} \det(\mathbf{S}_i) \neq 0 \) ensures that the LU factorizations exist.

(iii) \( \det(\mathbf{S}_s) \neq 0 \) implies that \( p_{\min}(0; \mathbf{A}, \mathbf{r}_0) \neq 0 \) which, in turn, implies that (1.1) has a solution lying in \( \mathbf{x}_0 + \kappa_\nu(\mathbf{A}, \mathbf{r}_0) \).

The derivation of a ML\((n)\)BiCGStab algorithm will require the following result which, in the case when \( n = 1 \), has been used in CGS and BiCGStab.

**Corollary 3.4.** Let \( s \in \mathcal{N} \) and

\[
\psi_{g_n}(s)(\lambda) = c_{g_n}(s)\lambda^{g_n(s)} + c_{g_n(s)-1}\lambda^{g_n(s)-1} + \cdots + c_0
\]

be any polynomial of exact degree \( g_n(s) \). Then, under the assumptions of Proposition 3.2,

\[
\mathbf{p}_s^H \mathbf{r}_k = \frac{1}{c_{g_n(s)}} \mathbf{q}_n^H \psi_{g_n}(\mathbf{A}) \mathbf{r}_k \quad \text{and} \quad \mathbf{p}_s^H \mathbf{A}\mathbf{g}_k = \frac{1}{c_{g_n(s)}} \mathbf{q}_n^H \mathbf{A} \psi_{g_n}(\mathbf{A}) \mathbf{g}_k
\]

if \( 0 \leq k \leq \nu - 1 \) and \( s \leq k + n \).

**Proof.** It is easy to verify that

\[
\mathbf{p}_s = \frac{1}{c_{g_n(s)}} \psi_{g_n}(s)(\mathbf{A}^H) \mathbf{q}_n(s) \in \mathcal{B}_k
\]

by Proposition 2.1(a) and (3.1), where the overbar denotes complex conjugation. The corollary then follows from Proposition 3.2(d) and (g).

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\(^6\)We say that \( \mathbf{u} \perp \mathbf{v} \) if \( \mathbf{u}^H \mathbf{v} = 0 \).
Corollary 3.4 essentially says that adding to $p_k$ a vector from $B_k$ does not change the inner products $p_k^H r_k$ and $p_k^H A_k r_k$.

The condition $\prod_{i=1}^n \det(W_i) \neq 0$ in Proposition 3.2 holds in all but very exceptional examples. In fact, it is a generic property in the following sense.

**Lemma 3.5.** [13, Prop. 4] If $p$ is a nonzero polynomial in the variables $x_1, x_2, \ldots, x_k \in C$, then $\{(x_1, x_2, \ldots, x_k) \in C^k | p(x_1, x_2, \ldots, x_k) = 0\}$ is a measure-zero set in $C^k$.

We apply Lemma 3.5 to $\det(W_i)$ and $\det(S_i)$, which are polynomials in the elements of $q_1, \ldots, q_n$, to obtain

**Lemma 3.6.** Let $\bar{r}_0 \in C^N$, $\bar{r}_0 \neq 0^T$ and $A \in C^{N \times N}$. Then

(a) $\{(q_1, \ldots, q_n) \in C^{nN} | \det(W_i) = 0\}$ is measure-zero for $1 \leq l \leq \nu$.

(b) $\{(q_1, \ldots, q_n) \in C^{nN} | \det(S_i) = 0\}$ is measure-zero for $1 \leq l \leq \nu - 1$.

(c) $\{(q_1, \ldots, q_n) \in C^{nN} | \det(S_\nu) = 0\}$ is measure-zero if $p_{min}(0; A, \bar{r}_0) \neq 0$.

Proof. We only prove Part (c) since the arguments for Parts (a) and (b) are similar. If $p_{min}(0; A, \bar{r}_0) = 0$, then $A^T \bar{r}_0$ is a linear combination of $A_0^T \bar{r}_0, \ldots, A^T_{\nu-1} \bar{r}_0$ or $A^T \bar{r}_0 = 0$ in the case when $\nu = 1$. Hence $\det(S_\nu) = 0$ no matter what $q_1, \ldots, q_n$ are. Thus, we assume $p_{min}(0; A, \bar{r}_0) \neq 0$ in the following.

Case $n = 1$. In this case, $p_k = (A^H)_{q_{\nu}(k)} q_{\nu(k)} = (A^H)^{k-1} q_1$ and $\hat{S}_\nu$ is a Hankel matrix

$$\hat{S}_\nu = \begin{bmatrix} \hat{s}_1 & \hat{s}_2 & \cdots & \hat{s}_\nu \\ \hat{s}_2 & \hat{s}_3 & \cdots & \hat{s}_{\nu+1} \\ \vdots & \vdots & \ddots & \vdots \\ \hat{s}_{\nu} & \hat{s}_{\nu+1} & \cdots & \hat{s}_{2\nu-1} \end{bmatrix}$$

where $\hat{s}_t = q_1^H A^T \bar{r}_0$ for $t = 1, 2, \ldots, 2\nu - 1$. Since $p_{min}(0; A, \bar{r}_0) \neq 0$, $\{A_0^T \bar{r}_0, A^T_1 \bar{r}_0, \ldots, A^T_{\nu-1} \bar{r}_0\}$ is a linearly independent set. Perform a $QR$ factorization on the $N \times \nu$ matrix

$$[A_0^T \bar{r}_0, A^T_1 \bar{r}_0, \ldots, A^T_{\nu-1} \bar{r}_0] = QR$$

where $Q \in C^{N \times \nu}$ is unitary and $R \in C^{\nu \times \nu}$ is upper triangular with positive main diagonal elements $r_{11}, r_{22}, \ldots, r_{\nu \nu}$. Write

$$[\hat{s}_1, \hat{s}_2, \cdots, \hat{s}_{\nu}, \hat{s}_{\nu+1}, \cdots, \hat{s}_{2\nu-1}] = q_1^H [A_0^T \bar{r}_0, A^T_1 \bar{r}_0, \ldots, A^T_{\nu-1} \bar{r}_0] = q_1^H [QR, A^T_{\nu+1} \bar{r}_0, \ldots, A^T_{2\nu-1} \bar{r}_0]$$

$$= \theta^H [R, Q^H [A^T_{\nu+1} \bar{r}_0, \ldots, A^T_{2\nu-1} \bar{r}_0]]$$

where $\theta = [\theta_1, \ldots, \theta_{\nu}]^T \equiv Q^H q_1$. If we set $\theta_\nu = 1$ and all other elements of $\theta$ to zero, then (3.3) has the form

$$[\hat{s}_1, \cdots, \hat{s}_{\nu-1}, \hat{s}_{\nu+1}, \cdots, \hat{s}_{2\nu-1}] = [0, \ldots, 0, r_{\nu \nu}, \ldots, \nu_1, \cdots, \nu_\nu]$$
For this special choice of $\theta$, we have $|\det(\mathbf{S}_v)| = r^\nu_{\nu} \neq 0$. Thus $\det(\mathbf{S}_t)$ is a nonzero polynomial and Part (c) follows from Lemma 3.5.

Case $n > 1$. The proof of this case can be reduced to that of the case $n = 1$ by setting $\mathbf{q}_1 = (A^H)^{k_i}\mathbf{q}_1$ for some appropriate integers $k_i > 0$ where $2 \leq i \leq n$. As an illustration, assume that the affine subspace contains a solution of (1.1).

The following theorem then follows from Proposition 3.2 and Corollary 3.7.

**Theorem 3.9.** If $\mathbf{q}_1, \cdots, \mathbf{q}_n$ are vectors with independent and continuous random elements, Algorithm 3.1 will almost surely work without breakdown by zero division to find a solution from the affine subspace $\mathbf{X}_0 + \mathcal{K}(A, \mathbf{r}_0)$ provided that $\mathbf{X}_0$ is chosen such that the affine subspace contains a solution of (1.1).

**Remarks 3.10.**

(i) If we randomly pick the initial guess $\mathbf{X}_0$ and set $\mathbf{q}_1 = \mathbf{b} - A\mathbf{X}_0$, then Algorithm 3.1 with $n = 1$, or equivalently in mathematics, the standard BiCG (see §6), will almost surely solve (1.1) without breakdown by zero division for all, but a certain small class of, nonsingular $A$. For details, see [13]. In Theorem 3.9, the vectors $\mathbf{q}_1, \cdots, \mathbf{q}_n$ are independent of $\mathbf{X}_0$.

(ii) The $\mathbf{X}_0$ in Theorem 3.9 is a user-provided vector. It may not be a random vector in some applications. For example, in cases where a sequence of similar linear systems is solved, the solution from the previous system may be used as the $\mathbf{X}_0$ for the new system.

4. A ML(n)BiCGStab Algorithm. A ML(n)BiCGStab algorithm was derived from ML(2)BiCG in [39] (Algorithm 2 without preconditioning and Algorithm 3 with preconditioning in [39]), but the derivation there is complicated and less inspiring. In this section, we re-derive the algorithm in a more systematic fashion with the help of index functions.
4.1. Notation and Definitions. Let \( \phi_k(\lambda) \) be defined by (1.2). If expressed in terms of the power basis

\[
\phi_k(\lambda) = c_k^{(k)} \lambda^k + \cdots + c_1^{(k)} \lambda + c_0^{(k)},
\]

it is clear that \( c_k^{(k)} = (-1)^k \omega_1 \omega_2 \cdots \omega_k \) and \( c_0^{(k)} = 1 \). Thus,

\[
c_k^{(k)} = -\omega_k c_{k-1}^{(k-1)}.
\]

In \( \text{ML}(n)\text{BiCGStab} \), we construct the following vectors: for \( k \in \mathbb{N} \),

\[
\begin{align*}
\mathbf{r}_k &= \phi_{g_n(k)+1}(\mathbf{A}) \tilde{\mathbf{r}}_k, & \mathbf{u}_k &= \phi_{g_n(k)}(\mathbf{A}) \tilde{\mathbf{r}}_k, \\
\mathbf{g}_k &= \phi_{g_n(k)+1}(\mathbf{A}) \tilde{\mathbf{g}}_k, & \mathbf{d}_k &= -\omega_{g_n(k)+1} \mathbf{A} \phi_{g_n(k)}(\mathbf{A}) \tilde{\mathbf{g}}_k,
\end{align*}
\]

and for \( k = 0 \), set

\[
\begin{align*}
\mathbf{r}_0 &= \tilde{\mathbf{r}}_0 & \mathbf{g}_0 &= \tilde{\mathbf{g}}_0.
\end{align*}
\]

The vector \( \mathbf{r}_k \) will be the residual vector of the approximate solution \( \mathbf{x}_k \) computed by \( \text{ML}(n)\text{BiCGStab} \).

4.2. Algorithm Derivation. The derivation parallels the one of BiCGStab from BiCG. We first replace all the inner products \( \mathbf{p}_H^H \tilde{\mathbf{r}} \) and \( \mathbf{p}_H^H \tilde{\mathbf{g}} \) in \( \text{ML}(n)\text{BiCG} \) respectively by the inner products of the forms \( \mathbf{q}_H^H \phi(\mathbf{A}) \tilde{\mathbf{r}} \) and \( \mathbf{q}_H^H A \phi(\mathbf{A}) \tilde{\mathbf{g}} \), where \( \phi \) is the polynomial (1.2). Corollary 3.4 guarantees that the inner products remain unchanged with such replacements. Then we compile the recurrences for the new residuals \( \mathbf{r}_k \) and the corresponding iterates. The overall derivation is best described and verified in stages, and depends on Proposition 2.1 and Corollary 3.4.

The derivation is complicated by the fact that the recurrences in the \( k \)-th iteration of \( \text{ML}(n)\text{BiCG} \) involve \( n \) terms which stretch from \( k - n \) to \( k - 1 \). Note that \( k - n \leq g_n(k)n \leq k - 1 \). The degrees of the \( \phi_{g_n(s)} \) and \( \phi_{g_n(s)+1} \) in (4.3) are increased at \( g_n(k)n+1 \) as \( s \) runs from \( k - n \) to \( k - 1 \) (see, for example, Table 2.1). Therefore, our first task is to split up in \( \text{ML}(n)\text{BiCG} \) the loops and the sums of length \( n \) into two parts, one from \( k - n \) to \( g_n(k)n-1 \) and the other from \( g_n(k)n+1 \) to \( k-1 \). The following Derivation Stage (DS) \#1 is computationally equivalent to Algorithm 3.1 (forgetting Lines 1, 2, 5 and 11).

**Derivation Stage \#1.**

1. For \( k = 1, 2, \ldots \), until convergence:
   2. If \( r_n(k) = 1 \)
      3. \( \alpha_k = \mathbf{p}_H^H \tilde{\mathbf{r}}_{k-1} / \mathbf{p}_k^H \tilde{\mathbf{A}} \tilde{\mathbf{g}}_{k-1}; \)
      4. \( \tilde{\mathbf{r}}_k = \tilde{\mathbf{r}}_{k-1} - \alpha_k \tilde{\mathbf{A}} \tilde{\mathbf{g}}_{k-1}; \)
   5. Else
      6. \( \alpha_k = \mathbf{p}_H^H \tilde{\mathbf{r}}_{k-1} / \mathbf{p}_k^H \tilde{\mathbf{A}} \tilde{\mathbf{g}}_{k-1}; \)
      7. \( \tilde{\mathbf{r}}_k = \tilde{\mathbf{r}}_{k-1} - \alpha_k \tilde{\mathbf{A}} \tilde{\mathbf{g}}_{k-1}; \)
   8. End
   9. If \( r_n(k) < n \)
      10. For \( s = \max(k-n,0), \ldots , g_n(k)n-1 \)
       11. \( \beta_s^{(k)} = -\mathbf{p}^H_{s+1} \mathbf{A} \left( \tilde{\mathbf{r}}_k + \sum_{t=\max(k-n,0)}^{s-1} \beta_t^{(k)} \tilde{\mathbf{g}}_t \right) / \mathbf{p}^H_{s+1} \tilde{\mathbf{A}} \tilde{\mathbf{g}}_s; \)
      12. End
We have adopted the conventions: empty loops are skipped and empty sums are zero. These conventions will also be applied in the sequel.

In the next stage of the derivation, we replace inner products $\mathbf{p}_k^H \mathbf{r}$ and $\mathbf{p}_k^H \mathbf{g}$ by inner products of the forms $\mathbf{q}_k^H \phi(\mathbf{A}) \mathbf{r}$ and $\mathbf{q}_k^H \phi(\mathbf{A}) \mathbf{g}$ respectively. That is, the factor $(\mathbf{A}^H \mathbf{g})^{(k)}$ that is hidden in the left basis vector $\mathbf{p}_k$ is moved to the right-hand side space and replaced by the factor $\phi(\mathbf{g})^{(k)}$. Formally, by Corollary 3.4 together with (3.1), (4.2) and Proposition 2.1(a), DS#1 can be further transformed into the version below. Explanations are given after listing.

**Derivation Stage #2.**

1. For $k = 1, 2, \ldots$, until convergence:
   2. If $r_n(k) = 1$
   3. $\alpha_k = \mathbf{q}_k^H (\phi(\mathbf{g})^{(k)} \mathbf{A}) \mathbf{r}_{k-1}/\mathbf{q}_n^{(k)} \mathbf{A} \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{g}_{k-1};$
   4. $\phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{r}_{k-1} = \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{r}_{k-1} - \alpha_k \mathbf{A} \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{g}_{k-1};$
   5. $\phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{r}_{k} = (\mathbf{I} - \omega^{n(k)+1} \mathbf{A}) \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{r}_{k};$
   6. Else
   7. $\alpha_k = \mathbf{q}_n^{(k)} \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{r}_{k-1}/\mathbf{q}_n^{(k)} \mathbf{A} \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{g}_{k-1};$
   8. $\phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{r}_{k-1} = \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{r}_{k-1} - \alpha_k \mathbf{A} \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{g}_{k-1};$
   9. $\phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{r}_{k} = \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{r}_{k-1} - \alpha_k \mathbf{A} \phi(\mathbf{g})^{(k)} \mathbf{A} \mathbf{g}_{k-1};$
   10. End
   11. If $r_n(k) < n$
   12. For $s = \max(k - n, 0), \ldots, \max(k - n, 0) + 1$
   13. $\beta^{(k)} = \mathbf{q}_s^{(k+1)} (\phi(\mathbf{g})^{(k+1)} \mathbf{A}) \mathbf{r}_{k} - \sum_{t=\max(k-n,0)}^{s-1} \omega^{(k+1)\mathbf{g}_{s+1}} + 1 \mathbf{A} \phi(\mathbf{g})^{(k+1)} \mathbf{A} \mathbf{g}_{s};$
   14. End
   15. $\beta^{(k)} = \mathbf{q}_s^{(k+1)} (\phi(\mathbf{g})^{(k+1)} \mathbf{A}) \mathbf{r}_{k} - \sum_{t=\max(k-n,0)}^{s-1} \omega^{(k+1)\mathbf{g}_{s+1}} + 1 \mathbf{A} \phi(\mathbf{g})^{(k+1)} \mathbf{A} \mathbf{g}_{s};$
   16. For $s = \max(k-n, 0), \ldots, k - 1$
   17. $\beta^{(k)} = \mathbf{q}_s^{(k+1)} (\phi(\mathbf{g})^{(k+1)} \mathbf{A}) \mathbf{r}_{k} - \sum_{t=\max(k-n,0)}^{s-1} \omega^{(k+1)\mathbf{g}_{s+1}} + 1 \mathbf{A} \phi(\mathbf{g})^{(k+1)} \mathbf{A} \mathbf{g}_{s};$
   18. End
By Corollary 3.4, the term transformation of Line 3, DS#1, into Line 3, DS#2 and (ii) the transformation of DS#1, through a multiplication by $\phi$, as follows.

$$\omega_{g_n}(k+1)A\phi_{g_n}(k)(A)\bar{g}_k = \omega_{g_n}(k+1)A\phi_{g_n}(k)(A)\bar{r}_k + \sum_{s=\max(k-n,0)}^{g_n(k)n} \beta_s^{(k)} \omega_{g_n}(k+1)A\phi_{g_n}(k)(A)\bar{g}_s + \sum_{s=g_n(k)n+1}^{\omega_{g_n}(k+1)A\phi_{g_n}(k)(A)\bar{g}_k;}
$$

$\phi_{g_n}(k+1)(A)\bar{g}_k = \phi_{g_n}(k+1)(A)\bar{r}_k + \sum_{s=\max(k-n,0)}^{g_n(k)n} \beta_s^{(k)} \phi_{g_n}(k+1)(A)\bar{g}_s + \sum_{s=g_n(k)n+1}^{\omega_{g_n}(k+1)A\phi_{g_n}(k)(A)\bar{g}_k;}
$.

(ii) Lines 4, 8, 9, 19, 20 and 26, DS#2, were obtained from Lines 4, 7, 17 and 23, from the denominator. missed from Line 15, DS#2, because it was canceled out by the coefficient $/c$.

Hence application of Corollary 3.4 to $p$, $k$, $g$, $n$, $s$ is the leading coefficient of $g_{b}(k)(\lambda)$ (see (4.1)).

(i) By Corollary 3.4,

$$\alpha_k = \frac{p_{g_n(k)n+1}^{H}A\bar{r}_k}{p_{g_n(k)n+1}^{H}A\bar{g}_k} = \frac{1}{c_{g_n(k)(k)}} q_{g_n(k)(k)}^{H}A\phi_{g_n(k)(k)}(A)\bar{r}_k - \frac{1}{c_{g_n(k)(k)}} q_{g_n(k)(k)}^{H}A\phi_{g_n(k)(k)}(A)\bar{g}_k = \frac{q_{g_n(k)(k)}^{H}A\phi_{g_n(k)(k)}(A)\bar{r}_k - q_{g_n(k)(k)}^{H}A\phi_{g_n(k)(k)}(A)\bar{g}_k}{q_{g_n(k)(k)}^{H}A\phi_{g_n(k)(k)}(A)\bar{g}_k-1}
$$

where $c_{g_n(k)(k)}$ is the leading coefficient of $\phi_{g_n(k)(k)}(\lambda)$ (see (4.1)).

(ii) By (3.1) and Proposition 2.1(a), we have

$$A^{H}p_{g_n(k)n+1} = (A^{H})_{g_n(k)(k)+1}^{g_n(k)(k)+1}q_{g_n(k)(k)+1} = (A^{H})_{g_n((k+1)n+1)}^{g_n((k+1)n+1)}q_{g_n((k+1)n+1)} = p_{g_n(k)n+1}^{(g_n(k)+1)n+1}.
$$

Hence $p_{g_n(k)n+1}^{(g_n(k)+1)n+1}A\bar{r}_k = p_{g_n(k)n+1}^{(g_n(k)+1)n+1}A\bar{r}_k$. Since $(g_n(k) + 1)n + 1 \leq k + n$, an application of Corollary 3.4 to $p_{g_n(k)n+1}^{(g_n(k)+1)n+1}A\bar{r}_k$ thus yields

$$p_{g_n(k)n+1}^{(g_n(k)+1)n+1}A\bar{r}_k = \frac{1}{c_{g_n(k)(k)+1}^{(g_n(k)+1)n+1}} q_{g_n(k)(k)+1}^{(g_n(k)+1)n+1} A\phi_{g_n(k)(k)+1}(A)\bar{r}_k
$$

The second equation above follows from (2.2). The coefficient $1/c_{g_n(k)+1}$ is missed from Line 15, DS#2, because it was canceled out by the coefficient from the denominator.
Our goal is to establish updating relations for the quantities introduced in (4.3). To this end, we further transform DS\#2 into the following version. This time, we work on the index function $g_n$ with the aid of Proposition 2.1 so that the definitions in (4.3) can be applied. Again, further explanations are given after the listing.

**Derivation Stage \#3.**

1. For $k = 1, 2, \ldots$, until convergence:
   2. If $r_n(k) = 1$
      3. $\alpha_k = q^{n\ell}(k)\phi_{g_n(k)}(k+1)A\bar{r}_k-1/q_{n\ell}(k)A\phi_{g_n(k)}(k+1)A\bar{g}_k-1; \omega$
      4. $\phi_{g_n(k)}(k)\bar{r}_k = \phi_{g_n(k)}(k+1)A\bar{r}_k-1 - \alpha_k A\phi_{g_n(k)}(k+1)A\bar{g}_k-1; \omega$
      5. $\phi_{g_n(k)+1}(A)\bar{r}_k = (I - \omega_{g_n(k)+1}A)\phi_{g_n(k)}(A)\bar{r}_k; \omega$
      6. Else
      7. $\alpha_k = q^{n\ell}(k)\phi_{g_n(k)}(k)A\bar{r}_k-1/q_{n\ell}(k)A\phi_{g_n(k)}(k)A\bar{g}_k-1; \omega$
      8. $\phi_{g_n(k)}(k)\bar{r}_k = \phi_{g_n(k)}(k+1)A\bar{r}_k-1 - \alpha_k A\phi_{g_n(k)}(k)A\bar{g}_k-1; \omega$
      9. $\phi_{g_n(k)+1}(A)\bar{r}_k = \phi_{g_n(k)+1}A\bar{r}_k-1 - \alpha_k A\phi_{g_n(k)+1}A\bar{g}_k-1; \omega$
      10. End
   11. If $r_n(k) < n$
   12. For $s = \max(k - n, 0), \ldots, g_n(k) - 1$
      13. $\beta_k = q^{n\ell}(s+1)\phi_{g_n(k)}(A)\bar{r}_k-1 + \sum_{t=\max(k-n,0)}^{k-1} q^{n\ell}(s+1)A\phi_{g_n(k)}(A)\bar{g}_t; \omega$
      14. End
   15. $\beta_{g_n(k)}(k) = q^{n\ell}(g_n(k)+1)A\bar{r}_k-1 + \sum_{t=\max(k-n,0)}^{g_n(k)-1} q^{n\ell}(g_n(k)+1)A\phi_{g_n(k)}(g_n(k)+1)A\bar{g}_t; \omega$
   16. For $s = g_n(k)n + 1, \ldots, k - 1$
      17. $\beta_k = q^{n\ell}(s+1)\phi_{g_n(k)+1}(A)\bar{r}_k-1 + \sum_{t=\max(k-n,0)}^{g_n(k)n} q^{n\ell}(s+1)A\phi_{g_n(k)+1}(A)\bar{g}_t-1 + \sum_{t=\max(k-n,0)}^{g_n(k)n-1} q^{n\ell}(s+1)A\phi_{g_n(k)+1}A\bar{g}_t; \omega$
      18. End
   19. $\omega_{g_n(k)+1}A\phi_{g_n(k)}(A)\bar{g}_k = \omega_{g_n(k)+1}A\phi_{g_n(k)}(A)\bar{r}_k-1 + \sum_{s=\max(k-n,0)}^{g_n(k)n} q^{n\ell}(s+1)A\phi_{g_n(k)}(A)\bar{g}_t; \omega$
   20. Else
      21. $\beta_{g_n(k)}(k) = q^{n\ell}(g_n(k)+1)A\bar{r}_k-1 + \sum_{t=\max(k-n,0)}^{g_n(k)n} q^{n\ell}(g_n(k)+1)A\phi_{g_n(k)}(g_n(k)n+1)A\bar{g}_t; \omega$
      22. For $s = g_n(k)n + 1, \ldots, k - 1$
      23. $\beta_k = q^{n\ell}(s+1)\phi_{g_n(k)+1}(A)\bar{r}_k-1 - \sum_{t=\max(k-n,0)}^{k-1} q^{n\ell}(s+1)A\phi_{g_n(k)}(s+1)A\bar{g}_t; \omega$
      24. End
      25. $\phi_{g_n(k)+1}(A)\bar{g}_k = \phi_{g_n(k)+1}(A)\bar{r}_k-1 + \sum_{s=\max(k-n,0)}^{k-1} q^{n\ell}(s+1)A\phi_{g_n(k)}(s+1)A\bar{g}_t; \omega$
      26. End
      27. End
      28. End

As an example, let us show how the $g_n(s + 1)$ inside the sum $\sum_{t=\max(k-n,0)}^{k-1}$
in Line 13, DS#2, was written as the $g_n(t)$ in Line 13, DS#3.

If $g_n(k) = 0$, Line 13 of DS#2 is not implemented because of the conventions immediately following DS#1. So, we assume that $g_n(k) > 0$. Since

$$\max(k-n,0) \leq s, \ t \leq g_n(k)n - 1,$$

we have

$$g_n(s+1) = g_n(k+1) - 1 = g_n(t+1)$$

by Proposition 2.1(b). Now that $g_n(k) > 0$, $\max(k-n,0) = k - n$. Hence

$$k - n \leq t \leq g_n(k)n - 1$$

by (4.5). Let $k = jn + i$ as in (2.1). Then (4.7) is

$$(j-1)n + i \leq t \leq (j-1)n + n - 1$$

which implies that $r_n(t) < n$. Now, Proposition 2.1(d) yields $g_n(t+1) = g_n(t)$ and therefore we have $g_n(s+1) = g_n(t)$ by (4.6).

We are now ready to apply the vectors defined in (4.3) and (4.4). Substituting them into DS#3 leads to the following stage.

**Derivation Stage #4.**

1. For $k = 1, 2, \ldots$, until convergence:
   2. If $r_n(k) = 1$
      3. $\alpha_k = q_{n,k}^H r_{k-1}/q_{n,k}^H A g_{k-1}$;
      4. $u_k = r_{k-1} - \alpha_k A g_{k-1}$;
      5. $r_k = -\omega g_{n}(k+1) u_k + u_k$;
      6. Else
      7. $\alpha_k = -\omega g_{n}(k)+1 q_{n,k}^H u_{k-1}/q_{n,k}^H d_{k-1}$;
      8. $u_k = u_{k-1} + (\alpha_k/\omega g_{n}(k)+1) d_{k-1}$;
      9. $r_k = r_{k-1} - \alpha_k A g_{k-1}$;
     10. End
    11. If $r_n(k) < n$
    12. For $s = \max(k-n,0), \ldots, g_n(k)n - 1$
    13. $\beta_s^{(k)} = -q_{n,k}^H (u_k + \sum_{t=\max(k-n,0)}^{s-1} \beta_t^{(k)} d_t) / q_{n,k}^H (s+1) d_s$;
    14. End
    15. $\tilde{\beta}_{g_n(k),n}^{(k)} = q_{n,k}^H (r_k - \omega g_{n}(k)+1 \sum_{t=\max(k-n,0)}^{g_n(k)n-1} \beta_t^{(k)} A g_t - \sum_{t=\max(k-n,0)}^{g_n(k)n} \beta_t^{(k)} d_t) / q_{n,k}^H (s+1) d_s$;
    16. For $s = g_n(k)n + 1, \ldots, k - 1$
    17. $\beta_s^{(k)} = -q_{n,k}^H (r_k - \omega g_{n}(k)+1 \sum_{t=\max(k-n,0)}^{g_n(k)n} \beta_t^{(k)} A g_t + \sum_{t=\max(k-n,0)}^{g_n(k)n} \beta_t^{(k)} d_t) / q_{n,k}^H (s+1) d_s$;
    18. End
    19. $d_k = r_k - u_k - \omega g_{n}(k)+1 \sum_{t=\max(k-n,0)}^{g_n(k)n} \beta_t^{(k)} A g_t + \sum_{s=g_n(k)n+1}^{k-1} \beta_s^{(k)} d_s$;
    20. $g_s = r_k + \sum_{t=\max(k-n,0)}^{g_n(k)n} \beta_t^{(k)} (I - \omega g_{n}(k)+1 A) g_t + \sum_{s=g_n(k)n+1}^{k-1} \beta_s^{(k)} g_s$;
    21. Else
    22. $\tilde{\beta}_{g_n(k),n}^{(k)} = q_{n,k}^H r_k / \omega g_{n}(k)+1 q_{n,k}^H A g_{g_n(k)n}$;
    23. For $s = g_n(k)n + 1, \ldots, k - 1$
\[ \beta_s^{(k)} = -q_{n(n+1)}^H \left( r_k - \omega_{g_n(k)+1}\beta_{g_n(k)} A g_{g_n(k)}^n + \sum_{s=g_n(k)}^{n-1} \beta_s^{(k)} d_s \right) / q_{n(n+1)}^H d_s; \]

```
24. End
26. \( g_k = r_k + \beta_{g_n(k)}^n (I - \omega_{g_n(k)+1} A) g_{g_n(k)}^n + \sum_{s=g_n(k)+1}^{k-1} \beta_s^{(k)} g_s; \)
28. End
```

We consider \( r_k \) to be the residual of the \( k \)th approximate solution \( x_k \). Updating relations for \( x_k \) can be obtained from Lines 4, 5 and 9 respectively:

\[ x_k = \begin{cases} 
  x_{k-1} + \omega_{g_n(k)+1} u_k + \alpha_k g_{k-1}, & \text{if } r_n(k) = 1 \\
  x_{k-1} + \alpha_k g_{k-1}, & \text{if } r_n(k) > 1. 
\end{cases} \]

After adding (4.8) to DS#4 and simplifying the operations appropriately, we arrive at the following ML(\( n \))BiCGStab algorithm. Just like BiCGStab, the free parameter \( \omega_{g_n(k)+1} \) in Line 5, DS#4, is chosen to minimize the 2-norm of \( r_k \).

**Algorithm 4.1. ML(\( n \))BiCGStab without preconditioning associated with definition (4.3)**

1. Choose an initial guess \( x_0 \) and \( n \) vectors \( q_1, q_2, \ldots, q_n \).
2. Compute \( r_0 = b - Ax_0 \) and set \( g_0 = r_0 \). Compute \( w_0 = Ag_0 \); \( c_0 = q_1^H w_0 \).
3. For \( k = 1, 2, \ldots, \) until convergence:
   4. If \( r_n(k) = 1 \)
      5. \( \alpha_k = q_{n(n)}^H r_{k-1}/c_{k-1}; \)
      6. \( u_k = r_{k-1} - \alpha_k w_{k-1}; \)
      7. \( x_k = x_{k-1} + \alpha_k g_{k-1}; \)
      8. \( \omega_{g_n(k)+1} = (A u_k)^H u_k / \|A u_k\|^2; \)
      9. \( x_k = x_k + \omega_{g_n(k)+1} u_k; \)
     10. \( r_k = -\omega_{g_n(k)+1} A u_k + u_k; \)
   11. Else
      12. \( \tilde{\alpha}_k = -q_{n(n)}^{H+1} u_{k-1}/c_{k-1}; \) \( \% \) \( \tilde{\alpha}_k = \alpha_k/\omega_{g_n(k)+1} \)
     13. If \( r_n(k) < n \)
        14. \( u_k = u_{k-1} + \tilde{\alpha}_k d_{k-1}; \)
     15. End
     16. \( x_k = x_{k-1} + \omega_{g_n(k)+1} \tilde{\alpha}_k g_{k-1}; \)
     17. \( r_k = r_{k-1} - \omega_{g_n(k)+1} \tilde{\alpha}_k w_{k-1}; \)
   18. End
   19. If \( r_n(k) < n \)
      20. \( z_d = u_k; \) \( g_k = 0; \) \( z_w = 0; \)
     21. For \( s = k - n, \ldots, g_n(k)n - 1 \) \( \) and \( g_n(k) \geq 1 \)
        22. \( \beta_s^{(k)} = -q_{n(n+1)}^H z_d/c_s; \)
        23. \( z_d = z_d + \beta_s^{(k)} d_s; \)
        24. \( g_k = g_k + \beta_s^{(k)} g_s; \)
        25. \( z_w = z_w + \beta_s^{(k)} w_s; \)
     26. End
     27. \( z_w = r_k - \omega_{g_n(k)+1} z_w; \)
     28. \( \beta_{g_n(k)}^n = q_1^H z_w / (\omega_{g_n(k)+1} c_{g_n(k)n}) ; \)
     29. \( z_w = z_w - \omega_{g_n(k)+1} \beta_{g_n(k)}^n w_{g_n(k)n}; \)
     30. \( g_k = g_k + z_w + \beta_{g_n(k)}^n g_{g_n(k)n}; \)
Table 4.1
Average cost per $k$-iteration of Algorithm 9.1 and its storage requirement. This table does not count the costs in Lines 1-2 of the algorithm.

<table>
<thead>
<tr>
<th>Operation</th>
<th>Cost 1</th>
<th>Cost 2</th>
<th>Storage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preconditioning $M^{-1}v$</td>
<td>$1 + \frac{1}{n}$</td>
<td>$u \pm v, \alpha v$</td>
<td>$\max(4 - \frac{\beta}{n}, 0)$</td>
</tr>
<tr>
<td>Matvec $Av$</td>
<td>$1 + \frac{1}{n}$</td>
<td>Saxpy $u + \alpha v$</td>
<td>$\max(2.5n + 0.5 + \frac{1}{n}, 0)$</td>
</tr>
<tr>
<td>dot product $u^Tv$</td>
<td>$n + 1 + \frac{2}{n}$</td>
<td>Storage</td>
<td>$A + M + (4n + 4)N + O(n)$</td>
</tr>
</tbody>
</table>

31. For $s = g_n(k)n + 1, \ldots, k - 1$
32. $\beta_s^{(k)} = -q_{s+1}^H r_k / (\omega_{g_n(k)n} + 1)c_{s+1}$;
33. $g_k = g_k + \beta^{(k)} g_s$;
34. $z_w = z_w + \beta^{(k)} d_s$;
35. End
36. $d_k = z_w - u_k; c_k = q_{s+1}^H d_k$;
37. $w_k = Ag_k$;
38. Else
39. $\beta^{(k)} = q_{s+1}^H r_k / (\omega_{g_n(k)n} + 1)c_{s+1}$;
40. $z_w = r_k - \omega_{g_n(k)n} + 1\beta^{(k)} g_n(k)n w_{g_n(k)n}$;
41. $g_k = z_w + \beta^{(k)} g_s$;
42. For $s = g_n(k)n + 1, \ldots, k - 1$
43. $\beta_s^{(k)} = -q_{s+1}^H z_w / c_s$;
44. $g_k = g_k + \beta^{(k)} g_s$;
45. $z_w = z_w + \beta^{(k)} d_s$;
46. End
47. $w_k = Ag_k; c_k = q_{s+1}^H w_k$;
48. End
49. End

Remarks 4.2.
(i) Algorithm 4.1 does not compute the quantities $u_k$ and $d_k$ when $r_n(k) = n$ (see Lines 13-15 and Lines 39-47).
(ii) If the $u_k$ in Line 6 happens to be zero, then the $\omega_{g_n(k)n}$ in Line 8 and therefore the $x_k$ and $r_k$ in Lines 9 and 10 will not be computable. In this case, however, the $x_k$ in Line 7 will be an exact solution to system (1.1) and Algorithm 4.1 stops there.

We now compare Algorithm 4.1 with the ML(n)BiCGStab algorithm in [39]. First, the definitions of $r_k, u_k$ and $g_k$ are the same in both algorithms, but $d_k$ is defined differently. In [39], $d_k = \phi_{g_n(k)}(A)g_k$. In exact arithmetic, however, both algorithms compute the same $r_k$ and $x_k$. Second, the derivation of Algorithm 4.1 has been made simpler by using index functions. As a result, some redundant operations in Algorithm 2 of [39] can be seen and removed and some arithmetics are simplified. For example, the vectors $d_k, u_k$ are computed in every $k$-iteration in Algorithm 2 of [39]. They are now computed only when $r_n(k) < n$. Also, the expression of $\beta^{(k)}_{g_n(k)n}$ in Line 39 of Algorithm 4.1 is simpler. Some other minor changes were also made so that the algorithm becomes more efficient.
Computational cost and storage requirement of Algorithm 4.1, obtained based on its preconditioned version, Algorithm 9.1 in §9, are summarized in Table 4.1. Since the vectors \(\{q_1, \ldots, q_n\}, \{d_{k-n}, \ldots, d_{g_{2}(k)-1}, d_{g_{2}(k)+1}, \ldots, d_{k-1}\}, \{g_{k-1}, \ldots, g_{2}(k)-1\}\) are required in iteration \(k\), they must be stored. When \(n\) is large, this storage is dominant. So, the storage requirement of the algorithm is about \(4nN\).

### 4.3. Properties

We summarize the properties of Algorithm 4.1 in the following proposition. Since \(r_0 = \tilde{r}_0\) by (4.4), \(\nu\) (see §3.2) is also the degree of \(p_{\text{min}}(\lambda; A, r_0)\).

**Proposition 4.3.** Under the assumptions of Proposition 3.2, if \(\omega_{g_{2}(k)+1} \neq 0\) and \(1/\omega_{g_{2}(k)+1} \notin \sigma(A)\) for \(1 \leq k \leq \nu - 1\), where \(\sigma(A)\) is the spectrum of \(A\), then Algorithm 4.1 does not break down by zero division for \(k = 1, 2, \ldots, \nu\), and \(x_\nu\) is an exact solution of (1.1). Moreover, the computed quantities satisfy

\[ \begin{align*}
(a) & \quad x_k \in x_0 + K_{g_{2}(k)+1}(A, r_0) \text{ and } r_k = b - Ax_k \in r_0 + AK_{g_{2}(k)+1}(A, r_0) \\
(b) & \quad r_k \neq 0 \text{ for } 1 \leq k \leq \nu - 1 \text{ and } r_0 = 0. \\
(c) & \quad r_k \nmid q_1, \text{ for } 1 \leq k \leq \nu - 1 \text{ with } r_n(k) = n. \\
(d) & \quad u_k \nmid \text{span}\{q_1, q_2, \ldots, q_{r_n(k)}\} \text{ and } u_k \nmid q_{r_n(k)+1} \text{ for } 1 \leq k \leq \nu - 1 \text{ with } r_n(k) < n. \\
(e) & \quad d_k \nmid \text{span}\{q_1, q_2, \ldots, q_{r_n(k)}\} \text{ and } d_k \nmid q_{r_n(k)+1} \text{ for } 1 \leq k \leq \nu - 1 \text{ with } r_n(k) < n. 
\end{align*} \]

**Proof.** The divisors in Algorithm 4.1 are \(c_k, \|Au_k\|_2^2\) and \(\omega_{g_{2}(k)+1}\) respectively, where the \(\omega\)'s have not been assumed to be nonzero. By Proposition 3.2(c), we have \(A\tilde{r}_k \neq 0\) for \(1 \leq k \leq \nu - 1\). Since \(1/\omega \notin \sigma(A)\) by assumption, \(\phi_{g_{2}(k)}(A)\) is nonsingular. Hence \(Au_k = \phi_{g_{2}(k)}(A) A\tilde{r}_k \neq 0\) (see (4.3) for the first equation). Therefore, \(\|Au_k\|_2 \neq 0\) for \(1 \leq k \leq \nu - 1\).

\(c_k\) is defined respectively in Lines 36 and 47 in the algorithm. When \(r_n(k) < n\), we have \(c_k = q_{r_n(k)+1} \in D_k\). In this case, \(c_k = -\omega_{g_{2}(k)+1} q_{r_n(k)+1} \phi_{g_{2}(k)}(A) \tilde{g}_k = -\omega_{g_{2}(k)+1} q_{r_n(k)+1} \phi_{g_{2}(k)}(A) \tilde{g}_k = -\omega_{g_{2}(k)+1} c_{g_{2}(k)+1} H_{g_{2}(k)+1} \tilde{g}_k = -\omega_{g_{2}(k)+1} c_{g_{2}(k)+1} H_{g_{2}(k)+1} \tilde{g}_k = c_{g_{2}(k)+1} H_{g_{2}(k)+1} \tilde{g}_k\)

\(= c_{g_{2}(k)+1} H_{g_{2}(k)+1} \tilde{g}_k\) by (4.3), Proposition 2.1(d), Corollary 3.4, (4.1) and (4.2). Since the \(\omega\)'s are nonzero by assumption and \(\|p_{g_{2}(k)+1} \tilde{g}_k\|_2 \neq 0\) by Proposition 3.2(g), we have \(c_{g_{2}(k)+1} H_{g_{2}(k)+1} \neq 0\) by (4.2) and hence \(c_k \neq 0\). When \(r_n(k) = n\), on the other hand, \(c_k = q_{r_n(k)+1} \in D_k\). In this case, \(c_k = q_{r_n(k)+1} \phi_{g_{2}(k)+1}(A) \tilde{g}_k = q_{r_n(k)+1} \phi_{g_{2}(k)+1}(A) \tilde{g}_k = c_{g_{2}(k)+1} H_{g_{2}(k)+1} \tilde{g}_k = c_{g_{2}(k)+1} H_{g_{2}(k)+1} \tilde{g}_k \neq 0\). Therefore, in either case, we always have \(c_k \neq 0\) for \(1 \leq k \leq \nu - 1\). Moreover, \(c_0 = q_{g_{2}(k)+1} \in D_k\) according to Line 2 of the algorithm. Since \(p_1 = q_1\) by (3.1) and \(g_0 = \tilde{g}_0\) by (4.4), \(c_0 \neq 0\) by Proposition 3.2(g).

Now that \(\|Au_k\|_2 \neq 0\), \(\omega_{g_{2}(k)+1} \neq 0\) for \(1 \leq k \leq \nu - 1\) and \(c_k \neq 0\) for \(0 \leq k \leq \nu - 1\), Algorithm 4.1 does not break down by zero division in the first \(\nu - 1\) iterations. When \(k = \nu\), \(u_\nu = u_\nu = \phi_{g_{2}(\nu)}(A) \tilde{r}_\nu = 0\) and \(r_\nu = r_\nu = \phi_{g_{2}(\nu)+1}(A) \tilde{r}_\nu = 0\) due to \(\tilde{r}_\nu = 0\) by Proposition 3.2. If it happens that \(r_\nu(\nu) = 1\), then the \(x_\nu(= x_\nu)\) in Line 7 is an exact solution to system (1.1) because its residual \(u_\nu\) is zero. So, the algorithm stops there. Otherwise, the \(x_\nu(= x_\nu)\) in Line 16 will be exact with residual \(r_\nu = 0\) and where the algorithm stops.

Part (a) follows from the definition of \(r_k\) in (4.3) and Proposition 3.2(a).

Since \(\tilde{r}_k \neq 0\) for \(1 \leq k \leq \nu - 1\) by Proposition 3.2(b) and \(\phi_{g_{2}(k)+1}(A)\) is non-
singular due to 1/ω ∉ σ(A), we have \( r_k = \phi_{g_n(k)+1}(A)\tilde{r}_k \neq 0 \). Therefore, Part (b) holds.

For Part (c), write \( k = jn + i \) with \( 0 \leq j \). By (4.3), (4.1) and Corollary 3.4, we have \( q_H^H r_k = q_H^H \phi_{g_n(k)+1}(A)\tilde{r}_k = q_H^H \phi_{g_n((j+1)n+1)}\phi_{g_n((j+1)n+1)+1}(A)\tilde{r}_k = q_H^H c_{g_n(k+1)}(g_{n+1}k+1)(A)\tilde{r}_k = c_{g_n(k+1)}(g_{n+1}k+1) p_H^k + 1 r_k \). Now Part (c) follows from Proposition 3.2(d) and \( c_{g_n(k)+1} \neq 0 \).

For the proof of Part (d), we first note that Algorithm 4.1 does not compute \( u_k \) when \( r_n(k) = n \) (see Lines 13 - 15). Write \( k = jn + i \) as in (2.1) and let \( 1 \leq t \leq i < n \). Then \( r_n(k) = i, g_n(k) = j = g_n(jn + t) \) and \( r_n(jn + t) = t \). Now, by (4.3) and Corollary 3.4, we have \( q_H^H u_k = q_H^H \phi_{g_n(k)}(A)\tilde{r}_k = q_H^H r_n(jn+t)\phi_{g_n(jn+t)}(A)\tilde{r}_k = c_{g_n(jn+t)} p_H^{jn+t+1} r_k \). Since \( p_H^{jn+t+1} r_k = 0 \) by Proposition 3.2(d), \( q_H^H u_k = 0 \) for \( 1 \leq t \leq i \). Similarly, \( q_H^H u_k = c_{g_n(k)}(g_{n+1}k+1) p_H^{jn+i+1} r_k = c_{g_n(k)} p_H^{jn+i+1} r_k \) (the validity of the first equation requires \( i < n \)). Because of Proposition 3.2(d) and \( c_{g_n(k)} \neq 0 \), \( q_H^H u_k \neq 0 \).

Similar to the quantity \( u_k \), Algorithm 4.1 does not compute \( d_k \) when \( r_n(k) = n \) (see Lines 39 - 47). By (4.3), \( d_k = -\omega_{g_n(k)+1} A \phi_{g_n(k)}(A) g_k \) and the proof of Part (e) is parallel to that of Part (d).

The conditions of \( \omega_{g_n(k)+1} \neq 0 \) and \( 1/\omega_{g_n(k)+1} \notin \sigma(A) \) can be easily made satisfied. For example, one can add some small random noise to \( \omega_{g_n(k)+1} \) after it is computed. The following theorem then holds from Proposition 4.3, Corollary 3.7 and Remark 3.8(ii).

**THEOREM 4.4.** If \( q_1, \ldots, q_n \) are vectors with independent and continuous random elements and if some small and continuous random number is added to \( \omega_{g_n(k)+1} \) after it is computed, then Algorithm 4.1 will work almost surely without breakdown by zero division to find a solution of (1.1) from the affine subspace \( x_0 + K(A, r_0) \) provided that \( x_0 \) is chosen such that the affine subspace contains a solution to (1.1).

Proposition 4.3 indicates that exact solution can only be found at iteration \( k = \nu \). It is possible, however, that \( \| r_k \|_2 \) can become very small for some \( k < \nu \). In practice, we terminate the algorithm when \( \| r_k \|_2 \) falls within a given tolerance.

Theorem 4.4 guarantees that an exact breakdown is almost impossible. However, ML(n)BiCGStab can encounter a near breakdown in its implementation. Besides the two types of breakdown of ML(n)BiCG, ML(n)BiCGStab has one more type of breakdown caused by \( \omega_{g_n(k)+1} \). In more details, the divisors in Algorithm 4.1 are \( c_k, \| A u_k \|_2^2 \) and \( \omega_{g_n(k)+1} \). If \( \| A u_k \|_2 \approx 0 \), then \( \omega_{g_n(k)+1} \approx \infty \) and a breakdown due to the overflow of \( \omega_{g_n(k)+1} \) occurs. It can be shown (see the proof of Proposition 4.3) that \( c_k = c_{g_n(k)+1}^H p_{k+1}^H A g_k \), where \( c_{g_n(k)+1}^H p_{k+1}^H A g_k \) is the leading coefficient of \( \phi_{g_n(k)+1}(A) \) (see (4.1)). So, \( c_k \) is a quantity that relates to \( \omega_{g_n(k)+1} \) and the ML(n)BiCG divisor \( p_{k+1}^H A g_k \). Thus, either \( \omega_{g_n(k)+1} \approx 0 \) or \( p_{k+1}^H A g_k \approx 0 \) can cause \( c_k \approx 0 \).

A breakdown-free ML(n)BiCGStab algorithm was derived in [17].

**5. A Second ML(n)BiCGStab Algorithm.** If we write \( k = jn + i \) as in (2.1), then the \( r_k \) defined by (4.3) become

\[
(5.1) \quad r_{jn+i} = \phi_{j+i}(A) \tilde{r}_{jn+i}
\]

where \( i = 1, 2, \ldots, n \) and \( j = 0, 1, 2, \ldots \). (5.1) increases the degree of the polynomial \( \phi \) by 1 at the beginning of every cycle (see §1 for the definition of a cycle). For example,
consider $n = 3$. Then (5.1) implies that
\[
\begin{align*}
    r_1 &= \phi_1(A) \hat{r}_1, \quad r_4 = \phi_2(A) \hat{r}_4, \quad r_7 = \phi_3(A) \hat{r}_7, \\
    r_2 &= \phi_1(A) \hat{r}_2, \quad r_5 = \phi_2(A) \hat{r}_5, \quad r_8 = \phi_3(A) \hat{r}_8, \\
    r_3 &= \phi_1(A) \hat{r}_3, \quad r_6 = \phi_2(A) \hat{r}_6, \quad r_9 = \phi_3(A) \hat{r}_9.
\end{align*}
\]
Iteration $k = 4$ is the first iteration of the second cycle and the degree of $\phi$ is increased from 1 to 2 there.

One can define $r_k$ by increasing the degree of $\phi$ by one anywhere within a cycle. Increasing the degree of $\phi$ at a different moment in a cycle gives a different value for $\omega$ and hence a different polynomial $\phi$ So the resulting algorithms are different. As an illustration, let us increase the degree at the end of a cycle and derive the algorithm associated with it.

5.1. Notation and Definitions. Let $\phi_k(\lambda)$ be defined as in (1.2). For $k \in N$, define
\[
\begin{align*}
    r_k &= \phi_{g_s(k+1)}(A) \hat{r}_k, \quad g_k = \phi_{g_s(k+1)}(A) \hat{g}_k, \\
    u_k &= \phi_{g_s(k)}(A) \hat{r}_k, \quad w_k = A \hat{g}_k
\end{align*}
\]
and set
\[
\begin{align*}
    r_0 &= \hat{r}_0 \quad \text{and} \quad g_0 = \hat{g}_0.
\end{align*}
\]
We remark that $r_k = u_k$ when $r_n(k) < n$ since $g_n(k+1) = g_n(k)$ in this case.

Definition (5.2) increases the degree of $\phi$ at the end of a cycle. To see this, let $n = 3$. Then (5.2) yields
\[
\begin{align*}
    r_1 &= \phi_0(A) \hat{r}_1, \quad r_4 = \phi_1(A) \hat{r}_4, \quad r_7 = \phi_2(A) \hat{r}_7, \\
    r_2 &= \phi_0(A) \hat{r}_2, \quad r_5 = \phi_1(A) \hat{r}_5, \quad r_8 = \phi_2(A) \hat{r}_8, \\
    r_3 &= \phi_1(A) \hat{r}_3, \quad r_6 = \phi_2(A) \hat{r}_6, \quad r_9 = \phi_3(A) \hat{r}_9.
\end{align*}
\]

5.2. Algorithm Derivation. To derive the algorithm associated with (5.2), we first transform Algorithm 3.1 (forgetting Lines 1, 2, 5 and 11) into the following version which is computationally equivalent to Algorithm 3.1, but is more convenient for us to apply Proposition 2.1.

Derivation Stage #5.
\begin{enumerate}
    \item For $k = 1, 2, \ldots$, until convergence:
    \item $\alpha_k = p_k^H \hat{r}_{k-1} / p_{k+1}^H A \hat{g}_{k-1}$;
    \item If $r_n(k) < n$
    \item $\tilde{r}_k = \tilde{r}_{k-1} - \alpha_k A \hat{g}_{k-1}$;
    \item For $s = \max(k - n, 0), \ldots, g_n(k) n - 1$
    \item \[ \beta_{s}^{(k)} = -p_{s+1}^H A \left( \hat{r}_k + \sum_{t=\max(k-n,0)}^{s-1} \beta_{t}^{(k)} \hat{g}_t + \sum_{t=g_n(k) n}^{s-1} \beta_{t}^{(k)} \hat{g}_t \right) / p_{s+1}^H A \hat{g}_s; \]
    \item End
    \item For $s = g_n(k) n, \ldots, k - 1$
    \item \[ \beta_{s}^{(k)} = -p_{s+1}^H A \left( \hat{r}_k + \sum_{t=\max(k-n,0)}^{g_n(k) n - 1} \beta_{t}^{(k)} \hat{g}_t + \sum_{t=g_n(k) n}^{s-1} \beta_{t}^{(k)} \hat{g}_t \right) / p_{s+1}^H A \hat{g}_s; \]
    \item End
    \item $\hat{g}_s = \hat{r}_k + \sum_{s=\max(k-n,0)}^{g_n(k) n-1} \beta_{s}^{(k)} \hat{g}_s + \sum_{s=g_n(k) n}^{k-1} \beta_{s}^{(k)} \hat{g}_s$;
    \itemElse
\end{enumerate}
Then we transform DS#5 as follows by Corollary 3.4.

### Derivation Stage #6.

1. For \( k = 1, 2, \ldots, \) until convergence:
   \[ \alpha_k = q_{r_n(k)}^H \phi_{g_n(k)}(A) \tilde{r}_k - \frac{q_{r_n(k)}^H A \phi_{g_n(k)}(A) \bar{g}_{k-1}}{q_{r_n(k)}^H A \phi_{g_n(k)}(A) \bar{g}_{k-1}}; \]
   \[ \text{If } r_n(k) < n \]
   \[ \phi_{g_n(k)}(A) \tilde{r}_k = \phi_{g_n(k)}(A) \tilde{r}_k - \alpha_k A \phi_{g_n(k)}(A) \bar{g}_{k-1}; \]
   \[ \text{For } s = \max(k-n,0), \ldots, g_n(k)n - 1 \]
   \[ \beta_s^{(k)} = q_{r_n(s+1)}^H \phi_{g_n(s+1)}(A) \tilde{r}_k - \omega_{g_n(s+1)+1} \sum_{t=\max(k-n,0)}^{s-1} \beta_t^{(k)} A \phi_{g_n(s+1)}(A) \bar{g}_t / q_{r_n(s+1)}^H A \phi_{g_n(s+1)}(A) \bar{g}_s; \]
   \[ \text{End} \]
   \[ \phi_{g_n(k+1)}(A) \bar{g}_k = \phi_{g_n(k+1)}(A) \tilde{r}_k + (I - \omega_{g_n(k+1)} A) \sum_{s=\max(k-n,0)}^{g_n(k)n-1} \beta_s^{(k)} \phi_{g_n(k+1)-1} \bar{A} \bar{g}_s + \sum_{s=g_n(k)n}^{k-1} \beta_s^{(k)} \phi_{g_n(k+1)}(A) \bar{g}_s; \]
   \[ \text{End} \]

12. Else
   \[ \phi_{g_n(k)}(A) \tilde{r}_k = \phi_{g_n(k)}(A) \tilde{r}_k - \alpha_k A \phi_{g_n(k)}(A) \bar{g}_{k-1}; \]
   \[ \phi_{g_n(k+1)}(A) \tilde{r}_k = (I - \omega_{g_n(k+1)} A) \phi_{g_n(k+1)-1}(A) \tilde{r}_k; \]
   \[ \text{For } s = g_n(k)n, \ldots, k - 1 \]
   \[ \beta_s^{(k)} = q_{r_n(s+1)}^H \phi_{g_n(s+1)+1}(A) \tilde{r}_k - \omega_{g_n(s+1)+1} \sum_{t=g_n(k)n}^{s-1} \beta_t^{(k)} A \phi_{g_n(s+1)+1}(A) \bar{g}_t / q_{r_n(s+1)}^H A \phi_{g_n(s+1)+1}(A) \bar{g}_s; \]
   \[ \text{End} \]

18. \[ \phi_{g_n(k+1)}(A) \bar{g}_k = \phi_{g_n(k+1)}(A) \tilde{r}_k + (I - \omega_{g_n(k+1)} A) \sum_{s=g_n(k)n}^{k-1} \beta_s^{(k)} \phi_{g_n(k+1)-1} \bar{A} \bar{g}_s; \]

### Derivation Stage #7.

1. For \( k = 1, 2, \ldots, \) until convergence:
   \[ \alpha_k = q_{r_n(k)}^H \phi_{g_n(k)}(A) \tilde{r}_k - \frac{q_{r_n(k)}^H A \phi_{g_n(k)}(A) \bar{g}_{k-1}}{q_{r_n(k)}^H A \phi_{g_n(k)}(A) \bar{g}_{k-1}}; \]
   \[ \text{If } r_n(k) < n \]
   \[ \text{End} \]

Lines 4, 11, 13 and 18, DS#6, were obtained from Lines 4, 11, 13 and 17, DS#5, by multiplying them with \( \phi_{g_n(k)}(A) \) and \( \phi_{g_n(k+1)}(A) \) respectively. Line 14, DS#6, is a direct result of the definition (1.2) of \( \phi \).

Now we use Proposition 2.1 to write DS#6 as

### Derivation Stage #7.
\[ \phi_{g_n(k+1)}(A) \bar{r}_k = \phi_{g_n(k)}(A) \bar{r}_k - \alpha_k \phi_{g_n(k)}(A) \bar{g}_k; \]
For \( s = \max(k - n, 0) \), \( \cdots \), \( g_n(k)n - 1 \)
\[ \beta^{(k)}_s = q_{r_s(n+1)}^H \left( \phi_{g_n(k+1)}(A) \bar{r}_k \right) - \omega_{g_n(k+1)} \sum_{t=\max(k-n,0)}^{s-1} \beta^{(k)}_t \phi_{g_n(t+1)}(A) \bar{g}_t / \omega_{g_n(k+1)} q_{r_s(n+1)}^H \phi_{g_n(s+1)}(A) \bar{g}_s; \]
End
For \( s = g_n(k)n, \cdots, k - 1 \)
\[ \beta^{(k)}_s = -q_{r_s(n+1)}^H A \left( \phi_{g_n(k+1)}(A) \bar{r}_k + \sum_{t=\max(k-n,0)}^{g_n(k)n-1} \beta^{(k)}_t \phi_{g_n(t+1)}(A) \bar{g}_t \right) + \sum_{t=g_n(k)n}^{s-1} \beta^{(k)}_t \phi_{g_n(t+1)}(A) \bar{g}_t / q_{r_s(n+1)}^H \phi_{g_n(s+1)}(A) \bar{g}_s; \]
End
\[ \phi_{g_n(k+1)}(A) \bar{g}_k = \phi_{g_n(k+1)}(A) \bar{r}_k + (I - \omega_{g_n(k+1)} A) \sum_{s=\max(k-n,0)}^{g_n(k)n-1} \beta^{(k)}_s \phi_{g_n(s+1)}(A) \bar{g}_s; \]
End
Else
\[ \phi_{g_n(k)}(A) \bar{r}_k = \phi_{g_n(k)}(A) \bar{r}_k - \alpha_k \phi_{g_n(k)}(A) \bar{g}_k; \]
End
End

We remark that the term \( \phi_{g_n(t+1)+1}(A) \bar{g}_t \) in the first sum in Line 9 can be further written as
\[
\phi_{g_n(t+1)+1}(A) \bar{g}_t = \left( I - \omega_{g_n(t+1)+1} A \right) \phi_{g_n(t+1)}(A) \bar{g}_t = \left( I - \omega_{g_n(k+1)} A \right) \phi_{g_n(t+1)}(A) \bar{g}_t.
\]

Substituting (5.4) and (5.2) into DS#7 then yields a set of updating relations of the vectors defined by (5.2).

Derivation Stage #8.
1. For \( k = 1, 2, \cdots \), until convergence:
2. \( \alpha_k = q_{r_k(n)}^H r_{k-1} / q_{r_k(n)}^H w_{k-1}; \)
3. If \( r_{n}(k) \) is not
4. \( r_k = r_{k-1} - \alpha_k w_{k-1}; \)
5. For \( s = \max(k - n, 0) \), \( \cdots \), \( g_n(k)n - 1 \)
6. \[ \beta^{(k)}_s = q_{r_s(n+1)}^H \left( A r_k + \sum_{t=\max(k-n,0)}^{g_n(k)n-1} \beta^{(k)}_t w_t \right) / \omega_{g_n(k+1)} q_{r_s(n+1)}^H w_s; \]
End
For \( s = g_n(k)n, \cdots, k - 1 \)
\[ \beta^{(k)}_s = -q_{r_s(n+1)}^H A r_k + \sum_{t=\max(k-n,0)}^{g_n(k)n-1} \beta^{(k)}_t (I - \omega_{g_n(k+1)} A) w_t + \sum_{t=\max(k-n,0)}^{g_n(k)n-1} \beta^{(k)}_t w_t / q_{r_s(n+1)}^H w_s; \]
End
\[ g_k = r_k - \omega_{g_n(k+1)} \sum_{s=\max(k-n,0)}^{g_n(k)n-1} \beta^{(k)}_s w_s + \sum_{s=\max(k-n,0)}^{g_n(k)n-1} \beta^{(k)}_s g_s + \sum_{s=g_n(k)n}^{k-1} \beta^{(k)}_s g_s; \]
Else
13. \( \mathbf{u}_k = \mathbf{r}_{k-1} - \alpha_k \mathbf{w}_{k-1}; \)
14. \( \mathbf{r}_k = (I - \omega g_n(k+1) \mathbf{A}) \mathbf{u}_k; \)
15. For \( s = g_n(k)n, \ldots, k - 1 \)
16. \[ \beta^{(k)}_s = q^H_{\mathbf{r}_k(s+1)} \left( \mathbf{r}_k - \omega g_n(k+1) \sum_{t=g_n(k)n}^{s-1} \beta^{(k)}_t \mathbf{w}_t \right) \left/ \omega g_n(k+1) q^H_{\mathbf{r}_n(s+1)} \mathbf{w}_s; \right. \]
17. End
18. \( \mathbf{g}_k = \mathbf{r}_k - \omega g_n(k+1) \sum_{s=g_n(k)n}^{k-1} \beta^{(k)}_s \mathbf{w}_s + \sum_{s=g_n(k)n}^{k-1} \beta^{(k)}_s \mathbf{w}_s; \)
19. End
20. End

DS#8 does not contain any update about \( \mathbf{w}_k \). For the updates, we multiply the equations in Lines 11 and 18 by \( \mathbf{A} \) to get

\[
\begin{align*}
(5.5) \quad \mathbf{w}_k &= \mathbf{A}(\mathbf{r}_k - \omega g_n(k+1) \sum_{s=\max(k-n,0)}^{g_n(k)n-1} \beta^{(k)}_s \mathbf{w}_s + \sum_{s=\max(k-n,0)}^{g_n(k)n-1} \beta^{(k)}_s \mathbf{w}_s) \\
&+ \sum_{s=g_n(k)n}^{k-1} \beta^{(k)}_s \mathbf{w}_s
\end{align*}
\]

if \( r_n(k) < n \), and

\[
(5.6) \quad \mathbf{w}_k = \mathbf{A}(\mathbf{r}_k - \omega g_n(k+1) \sum_{s=g_n(k)n}^{k-1} \beta^{(k)}_s \mathbf{w}_s + \sum_{s=g_n(k)n}^{k-1} \beta^{(k)}_s \mathbf{w}_s)
\]

if \( r_n(k) = n \).

Again, we consider \( \mathbf{r}_k \) to be a residual. To be consistent with Lines 4, 13 and 14, we update the approximate solution \( \mathbf{x}_k \) as

\[
(5.7) \quad \mathbf{x}_k = \begin{cases} 
\mathbf{x}_{k-1} + \alpha_k \mathbf{g}_{k-1}, & \text{if } r_n(k) < n \\
\omega_g (k+1) \mathbf{u}_k + \mathbf{x}_{k-1} + \alpha_k \mathbf{g}_{k-1}, & \text{if } r_n(k) = n.
\end{cases}
\]

Now adding (5.5), (5.6) and (5.7) to DS#8 and simplifying the operations appropriately, we then arrive at the following algorithm. The free parameter \( \omega g_n(k+1) \) is chosen to minimize the 2-norm of \( \mathbf{r}_k \).

**Algorithm 5.1.** ML\((n)\)BiCGStab without preconditioning associated with definition (5.2)

1. Choose an initial guess \( \mathbf{x}_0 \) and \( n \) vectors \( \mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_n \). Set \( \omega_0 = 1 \).
2. Compute \( \mathbf{r}_0 = \mathbf{b} - \mathbf{A} \mathbf{x}_0 \) and \( \mathbf{g}_0 = \mathbf{r}_0 \), \( \mathbf{w}_0 = \mathbf{A} \mathbf{g}_0 \), \( c_0 = q^H_1 \mathbf{w}_0 \).
3. For \( k = 1, 2, \cdots \), until convergence:
4. \( \alpha_k = q^H_{\mathbf{r}_n(k)} \mathbf{r}_{k-1}/c_{k-1}; \)
5. \( \text{If } r_n(k) < n \)
6. \( \mathbf{x}_k = \mathbf{x}_{k-1} + \alpha_k \mathbf{g}_{k-1}; \)
7. \( \mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_k \mathbf{w}_{k-1}; \)
8. \( \mathbf{z}_w = \mathbf{r}_k, \; \mathbf{g}_k = \mathbf{0}; \)
9. For \( s = \max(k-n,0), \cdots, g_n(k)n - 1 \)
10. \( \beta^{(k)}_s = -q^H_{\mathbf{r}_n(s+1)} \mathbf{z}_w/c_s; \) \( \% \beta^{(k)}_s = -\beta^{(k)}_s \omega g_n(k+1) \)
11. \( \mathbf{z}_w = \mathbf{z}_w + \beta^{(k)}_s \mathbf{w}_s; \)
12. \( \mathbf{g}_k = \mathbf{g}_k + \beta^{(k)}_s \mathbf{g}_s; \)
13. End
14. \( \mathbf{g}_w = \mathbf{z}_w = \frac{1}{\omega g_n(k+1)} \mathbf{g}_k; \) \( \mathbf{w}_k = \mathbf{A} \mathbf{g}_k; \)
15. For \( s = g_n(k)n, \cdots, k - 1 \)
16. \( \beta^{(k)}_s = -q^H_{\mathbf{r}_n(s+1)} \mathbf{w}_k/c_s; \)
We summarize the properties about Algorithm 5.1 below. Saxpy
\[ u + v, \ \alpha v \]
\[ 1 + \frac{1}{n} \]
\[ 1 + \frac{1}{n} \]
\[ \text{Storage} \]
\[ A + M + (3n + 5)N + O(n) \]
\[ n + 1 + \frac{2}{n} \]
\[ \text{Matvec} \]
\[ Av \]
\[ \text{dot product} \]
\[ u^H v \]

17. \[ w_k = w_k + \beta_1^{(k)} w_s; \]
18. \[ g_k = g_k + \beta_2^{(k)} g_s; \]
19. \[ \text{End} \]
20. \[ \text{Else} \]
21. \[ x_k = x_{k-1} + \alpha_k g_{k-1}; \]
22. \[ u_k = r_{k-1} - \alpha_k w_{k-1}; \]
23. \[ \omega_{g_n(k+1)} = (Au_k)^H u_k / \|Au_k\|_2^2; \]
24. \[ x_k = x_k + \omega_{g_n(k+1)} u_k; \]
25. \[ r_k = -\omega_{g_n(k+1)} Au_k + u_k; \]
26. \[ z_w = r_k, \ g_k = 0; \]
27. \[ \text{For} \ s = g_n(k)n, \ldots, k - 1 \]
28. \[ \beta_2^{(k)} = -q_{1(s+1)} z_w / c_s; \]
29. \[ z_w = z_w + \beta_2^{(k)} w_s; \]
30. \[ g_k = g_k + \beta_2^{(k)} g_s; \]
31. \[ \text{End} \]
32. \[ g_k = z_w - \frac{1}{\omega_{g_n(k+1)}} g_k; \]
33. \[ \text{End} \]
34. \[ c_k = q_{1(s+1)}^H w_k; \]
35. \[ \text{End} \]

We remark that (i) the algorithm does not compute \( u_k \) when \( r_n(k) < n \). In fact, \( u_k = r_k \) when \( r_n(k) < n \) (see the remark right after (5.3)); (ii) if the \( u_k \) in Line 22 happens to be zero, then the \( x_k \) in Line 21 will be the exact solution to system (1.1) and the algorithm stops there.

The cost and storage requirement, obtained from its preconditioned version, Algorithm 9.2 in §9, are listed in Table 5.1. Compared to Algorithm 4.1, Algorithm 5.1 saves about 20% in saxpy. Since only three sets of vectors \( \{q_1, \ldots, q_n\} \), \( \{g_n - n, \ldots, g_k\} \) and \( \{w_k - n, \ldots, w_k - 1\} \) are needed in iteration \( k \), the storage is about \( 3nN \) besides storing \( A \) and \( M \).

### 5.3. Properties

We summarize the properties about Algorithm 5.1 below. Their proofs are similar to those in Proposition 4.3. Since \( r_0 = r_0 \) by (5.3), \( \nu \) is also the degree of \( p_{\min}(\lambda; A, r_0) \).

**Proposition 5.2.** Under the assumptions of Proposition 3.2, if \( \omega_{g_n(k+1)} \neq 0 \) and \( 1/\omega_{g_n(k+1)} \notin \sigma(A) \) for \( 1 \leq k \leq \nu - 1 \), then Algorithm 5.1 does not break down by zero division for \( k = 1, 2, \ldots, \nu \), and the approximate solution \( x_\nu \) at step \( k = \nu \) is exact to the system (1.1). Moreover, the computed quantities satisfy

(a) \( x_k \in x_0 + \text{span}\{r_0, A r_0, \ldots, A^{g_n(k+1)+k-1} r_0\} \) and \( r_k = b - A x_k \in r_0 + \text{span}\{A r_0, A^2 r_0, \ldots, A^{g_n(k+1)+k} r_0\} \) for \( 1 \leq k \leq \nu - 1 \).
(b) \( r_k \neq 0 \) for \( 1 \leq k \leq \nu - 1 \); \( r_\nu = 0 \).

(c) \( r_k \perp \text{span}\{q_1, q_2, \ldots, q_{r_n(k)}\} \) and \( r_k \perp q_{r_n(k)+1} \) for \( 1 \leq k \leq \nu - 1 \) with \( r_n(k) < n \); \( r_k \perp q_1 \) for \( 1 \leq k \leq \nu - 1 \) with \( r_n(k) = n \).

(d) \( \hat{u}_k \perp \text{span}\{q_1, q_2, \ldots, q_n\} \) for \( 1 \leq k \leq \nu \) with \( r_n(k) = n \).

(e) \( \hat{A}_k \perp \text{span}\{q_1, q_2, \ldots, q_{r_n(k)}\} \) and \( \hat{A}_k \perp q_{r_n(k)+1} \) for \( 1 \leq k \leq \nu - 1 \) with \( r_n(k) < n \); \( \hat{A}_k \perp q_1 \) for \( 1 \leq k \leq \nu - 1 \) with \( r_n(k) = n \).

6. Relations to Some Existing Methods. In this section, we discuss the relations of ML\((n)\)BiCGStab with the FOM, BiCGStab and IDR\((s)\) methods under the assumptions of Proposition 3.2.


1. Relation with FOM[31]. Consider the case where \( n \geq \nu \). In this case, \( g_n(k) = 0 \) and \( r_n(k) = k \) for \( k = 1, 2, \ldots, \nu \). Hence \( p_k = q_k \) by (3.1). If we choose \( q_k = \hat{r}_{k-1} \) in Algorithm 3.1 (it is possible since \( \hat{r}_{k-1} \) is computed before \( q_k \) is used), then the \( \hat{x}_k \) and \( \hat{r}_k \) computed by the algorithm satisfy

\[
\begin{align*}
\hat{x}_k &\in \hat{x}_0 + \text{span}\{\hat{r}_0, A\hat{r}_0, \ldots, A^{k-1}\hat{r}_0\}, \\
\hat{r}_k &\perp \text{span}\{\hat{r}_0, \hat{r}_1, \ldots, \hat{r}_{k-1}\}
\end{align*}
\]

for \( 1 \leq k \leq \nu \) by Proposition 3.2(a),(d). (6.1) is what the FOM approximate solution \( x^{\text{FOM}}_k \) needs to satisfy. Therefore, when \( n \geq \nu \) and with the choice \( q_k = \hat{r}_{k-1} \), Algorithm 3.1 is mathematically equivalent to FOM.

Now, from (4.3), the \( r_k \) computed by Algorithm 4.1 satisfies

\[ r_k = \phi_{g_n(k)+1}(A)\hat{r}_k = \phi_1(A)\hat{r}_k = (I - \omega_1 A)\hat{r}_k. \]

Note that \( u_k = \phi_{g_n(k)}(A)\hat{r}_k = \phi_0(A)\hat{r}_k = \hat{r}_k \). Thus, for \( 1 \leq k \leq \nu \), \( r_k \) is the factor \( I - \omega_1 A \) times the FOM residual \( u_k \) if we set \( q_1 = r_0 \) and \( q_{k+1} = u_k \) in Algorithm 4.1.\(^8\)

2. Relation with BiCGStab[31]. When \( n = 1 \), we have \( g_n(k) = k - 1 \) and \( r_n(k) = 1 \) for \( k \in \mathbb{N} \). Hence \( p_k = (A^H)^{k-1}q_1 \) by (3.1). By Proposition 3.2(a) and (d), the \( \hat{x}_k \) and \( \hat{r}_k \) computed by Algorithm 3.1 satisfy

\[
\begin{align*}
\hat{x}_k &\in \hat{x}_0 + \text{span}\{\hat{r}_0, A\hat{r}_0, \ldots, A^{k-1}\hat{r}_0\} \\
\hat{r}_k &\perp \text{span}\{q_1, A^Hq_1, \ldots, (A^H)^{k-1}q_1\}
\end{align*}
\]

for \( 1 \leq k \leq \nu \). (6.2) is what the BiCG approximate solution \( x^{\text{BiCG}}_k \) needs to satisfy. Therefore, when \( n = 1 \), Algorithm 3.1 is mathematically equivalent to BiCG.

Now, from (4.3), the \( r_k \) computed by Algorithm 4.1 satisfies

\[ r_k = \phi_{g_n(k)+1}(A)\hat{r}_k = \phi_k(A)\hat{r}_k \]

\(^8\)We are only concerned about the first \( \nu \) iterations since ML\((n)\)BiCG and ML\((n)\)BiCGStab converge at the \( \nu \)-th iteration.

\(^9\)In [39], a remark immediately following Theorem 4.1 states that, when \( n \geq \nu \) and with the choice that \( q_1 = \phi_1(A^H)\hat{r}_0 \) and \( q_k = \phi_k(A^H)\hat{r}_{k-1} \) for \( k \geq 2 \), the \( \hat{x}_k \) and \( \hat{r}_k \) computed by Algorithm 2 (which is mathematically equivalent to Algorithm 4.1 of this paper) will satisfy (6.1) and therefore Algorithm 2 is a FOM. The argument there about the remark is not correct. The author remembers that the referees of [39] were skeptical about that argument.
which is the definition of the BiCGStab residuals. Thus Algorithm 4.1 is mathematically equivalent to BiCGStab when \( n = 1 \).

3. **Relation with IDR(s)**\(^{[30]}\). Write \( k = jn + i \) as in (2.1) with \( 1 \leq i \leq n, 0 \leq j \). Let \( G_0 = \mathcal{K}(A, r_0) \) be the complete Krylov subspace and let \( S = \text{span}\{q_1, q_2, \ldots, q_n\}^\perp \). Define the Sonneveld spaces

\[
G_{j+1} = (I - \omega_{j+1}A)(G_j \cap S) = (I - \omega_{g_n(k)+1}A)(G_j \cap S)
\]

for \( j = 0, 1, 2, \ldots \). By (4.3), we have

\[
r_{jn+i} = \phi_{j+1}(A)\tilde{r}_{jn+i} = (I - \omega_{j+1}A)\phi_j(A)\tilde{r}_{jn+i} = (I - \omega_{j+1}A)u_{jn+i}.
\]

From Proposition 4.3(d), \( u_{jn+i} \notin q_{i+1} \) if \( i < n \). Hence \( u_{jn+i} \notin G_j \cap S \) and therefore \( r_{jn+i} \notin G_{j+1} \) when \( i < n \). From this point of view, Algorithm 4.1 is not an IDR(s) algorithm.

However, if we regard \( r_{jn+i} \) with \( 1 \leq i < n \) as auxiliary vectors and instead, consider the followings as residuals

\[
\begin{align*}
\phi_t(A)\tilde{r}_{jn+i} &\in S & \text{if } 1 \leq i < n, 0 \leq t < j, \\
\phi_t(A)\tilde{r}_{jn+n} &\in S & \text{if } 0 \leq t \leq j.
\end{align*}
\]

Thus, by induction on \( t \),

\[
\begin{align*}
\phi_t(A)\tilde{r}_{jn+i} &\in G_t \cap S & \text{if } 1 \leq i < n, 0 \leq t < j, \\
\phi_t(A)\tilde{r}_{jn+n} &\in G_t \cap S & \text{if } 0 \leq t \leq j.
\end{align*}
\]

Therefore, by (4.3),

\[
\begin{align*}
u_{jn+i} = \tilde{r}_i &\in G_0 & \text{if } 1 \leq i < n, j = 0, \\
u_{jn+i} = (I - \omega_jA)\phi_{j-1}(A)\tilde{r}_{jn+i} &\in G_j & \text{if } 1 \leq i < n, 1 \leq j, \\
r_{jn+n} = (I - \omega_{j+1}A)\phi_j(A)\tilde{r}_{jn+n} &\in G_{j+1}.
\end{align*}
\]

So, the residuals in (6.3) lie in the Sonneveld spaces \( G_j \).

That (6.4) holds becomes obvious if one applies the following result from \([24]\) and Proposition 3.2(d),

\[
G_j = \{ \phi_j(A)v | v \perp \text{span}\{p_1, p_2, \ldots, p_n\} \}. \tag{6.5}
\]

An early discussion of the relation between ML(n)BiCGStab and IDR(s) was made in \([30]\).  

\(^{10}\)The parameter \( \omega \), however, is different from the \( \omega \) of the IDR algorithm in \([30]\) since they are selected to minimize the norm of different residuals.
6.2. Algorithm 5.1.

1. Relation with FOM. When \( n \geq \nu \), \( g_n(k) = 0 \) and \( r_n(k) = k \) for \( 1 \leq k \leq \nu \) and Algorithm 3.1, with the choice \( q_k = \hat{r}_{k-1} \), is a FOM algorithm as seen in §6.1. Now, from (5.2), the \( r_k \) computed by Algorithm 5.1 satisfies
\[
r_k = \phi_{g_n(k+1)}(A) \hat{r}_k = \phi_0(A) \hat{r}_k = \hat{r}_k.
\]
Thus Algorithm 5.1 is a FOM algorithm when we set \( q_k = r_{k-1} \).

2. Relation with BiCGStab. When \( n = 1 \), we have \( g_n(k) = k - 1 \) and \( r_n(k) = 1 \) for \( k \in \mathbb{N} \) and Algorithm 3.1 is a BiCG algorithm. From (5.2), the \( r_k \) computed by Algorithm 5.1 satisfies
\[
r_k = \phi_{g_n(k+1)}(A) \hat{r}_k = \phi_k(A) \hat{r}_k
\]
which is the definition of the BiCGStab residuals. Thus Algorithm 5.1 is mathematically equivalent to BiCGStab.

3. Relation with IDR. Write \( k = jn + i \) as in (2.1) with \( 1 \leq i \leq n, 0 \leq j \). By (5.2), we have
\[
r_{jn+i} = \phi_{g_n(jn+i+1)}(A) \hat{r}_{jn+i} = \left\{ \begin{array}{ll}
\phi_j(A) \hat{r}_{jn+i} & \text{if } 1 \leq i < n, \\
\phi_{j+1}(A) \hat{r}_{jn+i} & \text{if } i = n.
\end{array} \right.
\]
Thus, (6.5) and Proposition 3.2(d) yield
\[
r_{jn+i} \in \left\{ \begin{array}{ll}
\mathcal{G}_j & \text{if } 1 \leq i < n, \\
\mathcal{G}_{j+1} & \text{if } i = n.
\end{array} \right.
\]
So, the residuals computed by Algorithm 5.1 lie in the \( \mathcal{G} \) spaces and therefore it is an IDR(\( n \)) algorithm.

7. Implementation Issues. A preconditioned ML(\( n \))BiCGStab algorithm can be obtained by applying either Algorithm 4.1 or Algorithm 5.1 to the system
\[
AM^{-1}y = b
\]
where \( M \) is nonsingular, then recovering \( x \) through \( x = M^{-1}y \). The resulting algorithms, Algorithm 9.1 and Algorithm 9.2, together with their Matlab codes are presented in §9. To avoid calling the index functions \( r_n(k) \) and \( g_n(k) \) every \( k \)-iteration, we have split the \( k \)-loop into an \( i \)-loop and a \( j \)-loop where \( i,j,k \) are related by (2.1) with \( 1 \leq i \leq n, 0 \leq j \). Moreover, we have optimized the operations as much as possible in the resulting preconditioned algorithms.

Since we have compared ML(\( n \))BiCGStab with some existing methods in [39], we will only concentrate on the performance of ML(\( n \))BiCGStab itself. The following test data were downloaded from Matrix Market at http://math.nist.gov/MatrixMarket/.

1. \( e20r0100 \), DRIVCAV Fluid Dynamics. \( e20r0100 \) contains a \( 4241 \times 4241 \) real unsymmetric matrix \( A \) with 131,556 nonzero entries and a real right-hand side \( b \).

2. \( qc2534 \), H2PLUS Quantum Chemistry, NEP Collection. \( qc2534 \) contains a \( 2534 \times 2534 \) complex symmetric indefinite matrix with 463,360 nonzero entries, but does not provide the right-hand side \( b \). Following [24], we set \( b = A1 \) with \( 1 = [1,1,\ldots,1]^T \).
3. *utm5940*, TOKAMAK Nuclear Physics (Plasmas). *utm5940* contains a 5940×5940 real unsymmetric matrix *A* with 83,842 nonzero entries and a real right-hand side *b*.

All computing was done in Matlab Version 7.1 on a Windows XP machine with a Pentium 4 processor. *ILU*(0) preconditioner (p.294, [20]) was used in all the experiments. For *e20r0100*, the *U*-factor of the *ILU*(0) decomposition of *A* has some zeros along its main diagonal. In that experiment, we replaced those zeros by 1 so that the *U*-factor was invertible.

In all the experiments, initial guess was *x*₀ = 0 with the stopping criterion \( \frac{\| r_k \|_2}{\| b \|_2} < 10^{-7} \) where *rₖ* was the computed residual. Except where specified, shadow vectors \( Q = [q_1, q_2, \ldots, q_n] \) were chosen to be \( Q = [r_0, \text{randn}(N, n-1)] \) for *e20r0100* and *utm5940* and \( Q = [r_0, \text{randn}(N, n-1) + \sqrt{-1} \ast \text{randn}(N, n-1)] \) for *qc2534*.

Moreover, for the convenience of our presentation, we introduce the following functions:

(a) \( T_{\text{conv}}(n) \) is the time that a ML\((n)\)BiCGStab algorithm takes to converge.

(b) \( I_{\text{conv}}(n) \) is the number of *k*-iterations (not iteration cycles) that a ML\((n)\)BiCGStab algorithm takes to converge.

(c) \( E(n) \equiv \frac{\| b - A x_k \|_2}{\| b \|_2} \) is the true relative error of *x* where *x* is the computed solution output by a ML\((n)\)BiCGStab algorithm when it converges.

**7.1. Stability.** We plot the graphs of \( I_{\text{conv}}(n) \) in Figures 7.1(a), 7.2(a) and 7.3(a). For *e20r0100* and *qc2534*, \( I_{\text{conv}}(n) \) decreases as *n* increases. However, the \( I_{\text{conv}}(n) \) for *utm5940* behaves very irregularly due to some of the \( \omega \)'s are too small.

![Fig. 7.1](image_url)

The graphs of \( E(n) \) are plotted in Figures 7.1(b), 7.2(b) and 7.3(b). It can be seen that the computed relative errors \( \| r_k \|_2/\| b \|_2 \) by Algorithm 9.2 can significantly diverge from its exact counterpart \( \| b - A x_k \|_2/\| b \|_2 \). By contrast, the computed \( \| r_k \|_2/\| b \|_2 \) by Algorithm 9.1 well approximate their corresponding true ones. Thus, from this point of view, we consider that Algorithm 9.1 is numerically more stable than Algorithm 9.2. One explanation about this difference in stability is the following.
Recall that \( w_k = A g_k \) by definition (see (4.3) and (5.2)). In Algorithm 4.1, \( w_k \) is updated by \( w_k = A g_k \) (see Lines 37 and 47) for all \( k \). In Algorithm 5.1, however, \( w_k \) is updated by \( w_k = A g_k \) only when \( r_n(k) = n \) (see Line 32). As a result, the \( r_k \)'s computed by Algorithm 4.1 (see Lines 6, 10 and 17) are closer to the true residuals \( b - A x_k \) than those computed by Algorithm 5.1. This observation has led to a ML(\( n \))BiCGStab algorithm which updates \( w_k \) by \( w_k = A g_k \) for all \( k \), has less computational cost than Algorithm 5.1, but involves \( A^H \) in its implementation. See [37] for details.

We remark that the issues of divergence of computed residuals and corresponding remedy techniques were discussed in details in [26, 33].

### 7.2. Choice of \( n \)

In this and the following subsections, we will focus on Algorithm 9.1.

From the experiments in [39] and this paper, we have observed that ML(\( n \))BiCGStab

![Fig. 7.2. qc2534: (a) Graphs of \( I_{conv}(n) \) against \( n \). BiCGStab took 329 iterations/658 MVs to converge. Full GMRES converged with 439 MVs. (b) Graphs of \( E(n) \) against \( n \).](image1)

![Fig. 7.3. utm5940: (a) Graphs of \( I_{conv}(n) \) against \( n \). BiCGStab took 228 iterations/455 MVs to converge. Full GMRES converged with 176 MVs. (b) Graphs of \( E(n) \) against \( n \).](image2)
behaves more and more robust as \( n \) is increased. So, for an ill-conditioned system, we would tend to suggest a large \( n \) for ML(\( n \))BiCGStab. On the other hand, ML(\( n \))BiCGStab minimizes \( \| r_k \|_2 \) once every \( n \) \( k \)-iterations. Notice that the convergence of a well-conditioned system is usually accelerated by the minimization steps. So, when a problem is well-conditioned, we would suggest a small \( n \).

In [30, 34], it is suggested to fix \( s \) at 4 or 8 for the general use of IDR(\( s \)). This idea also applies to ML(\( n \))BiCGStab.

In the case where a sequence of linear systems is solved, one can fix the parameter \( n \) for the overall solution process or alternatively one can choose \( n \) dynamically based on the information obtained from the solution of previous systems. We once tested the Matlab code of Algorithm 9.1 in §9.1, translated into Fortran and with \( n = 9 \), \( \kappa = 0 \) (see §7.3 for \( \kappa \)) and ILU(0) preconditioners, on the standard oil reservoir simulation test data called SPE9 at University of Calgary. We found that ML(\( n \))BiCGStab reduced the total computational time by over 70% when compared to BiCGStab. A later test on SPE9 with Code #4 in §9.3, at Jinan University, showed that a 60% reduction in time could be reached. Code #4 is a design of an automatic selection of \( n \) during the solution process of a sequence of linear systems. It tries to minimize the time per \( k \)-iteration of ML(\( n \))BiCGStab.

We also plot the graphs of \( T_{conv}(n) \) in Figures 7.4 and 7.5(a) to provide more information on how \( n \) affects the performance of ML(\( n \))BiCGStab.

![Graphs of T_{conv}(n) of Algorithm 9.1 against n. (a) e20r0100: T_{conv}(n) reaches its minimum at n = 22. (b) qc2534: T_{conv}(n) reaches its minimum at n = 8.](image)

**7.3. Choice of \( \omega \).** The standard choice for \( \omega_{j+1} \) in Algorithm 9.1 (see Line 8) is

\[
\omega_{j+1} = (A\tilde{u}_{jn+1})^H u_{jn+1}/\|A\tilde{u}_{jn+1}\|^2.
\]

This choice of \( \omega_{j+1} \) minimizes the 2-norm of \( r_{jn+1} = -\omega_{j+1}A\tilde{u}_{jn+1} + u_{jn+1} \) (see Line 10), but sometimes can cause instability due to that it can be very small during an execution. The following remedy to guard \( \omega_{j+1} \) away from zero has been proposed in
\[ \omega_{j+1} = \left( A \tilde{u}_{jn+1} \right)^H u_{jn+1} / \| A \tilde{u}_{jn+1} \|_2^2; \]
\[ \rho = \left( A \tilde{u}_{jn+1} \right)^H u_{jn+1} / \| A \tilde{u}_{jn+1} \|_2 \| u_{jn+1} \|_2; \]
\[ \text{if } |\rho| < \kappa, \quad \omega_{j+1} = \kappa \omega_{j+1} / |\rho|; \quad \text{end} \]

(7.2)

where \( \kappa \) is a user-defined parameter. In Figures 7.5(b) and 7.6(a), we compare the performances of Algorithm 9.1 with (7.1) and (7.2) respectively (we only plot the results of \( \text{qc2534} \) and \( \text{utm5940} \). The result of \( \text{e20r0100} \) with \( \kappa = 0.1 \) is analogous to Figure 7.5(b)). Also, see the numerical experiments in [30] for more information about (7.2).
7.4. Choice of \( q \)'s. We usually pick
\[
Q = [r_0, \text{randn}(N, n-1)]
\]
for a real problem and
\[
Q = [r_0, \text{randn}(N, n-1) + \text{sqrt}(-1) \ast \text{randn}(N, n-1)]
\]
for a complex problem. In our experiments, however, we observed a comparable performance when we chose
\[
Q = [r_0, \text{sign} \ast \text{randn}(N, n-1)]
\]
or
\[
Q = [r_0, \text{sign} \ast \text{randn}(N, n-1) + \text{sqrt}(-1) \ast \text{sign} \ast \text{randn}(N, n-1)].
\]
See Figure 7.6(b) (we only plot the result of \text{utm5940} for saving space).

The advantages of (7.5) and (7.6) over (7.3) and (7.4) are that (i) the storage of \( Q \) is substantially reduced. In fact, we just need to store the random signs (except its first column); (ii) an inner product with \( q_i, 2 \leq i \leq n \), is now reduced to a sum without involving scalar multiplications.

For other choices for \( Q \), one is referred to [30].

8. Conclusions. With the help of index functions, we re-derived the ML\((n)\)BiCGStab algorithm in [39] in a more systematic way. This time, we have been able to find out and remove some redundant operations so that the algorithm becomes more efficient. We also recognized that there were \( n \) ways to define the ML\((n)\)BiCGStab residual \( r_k \). Each of the definitions leads to a different algorithm. We presented two definitions together with their associated algorithms, namely, (i) definition (4.3), increasing the degree of \( \phi \) at the beginning of an iteration cycle, and the associated Algorithm 4.1; (ii) definition (5.2), increasing the degree of \( \phi \) at the end of an iteration cycle, and the associated Algorithm 5.1. By comparison, Algorithm 5.1 is cheaper in storage and computational cost, faster to converge, but less stable. For other definitions of \( r_k \) that increase the degree of \( \phi \) somewhere within a cycle, we expect that the associated algorithms would lie between Algorithms 4.1 and 5.1 in computational cost, storage and performance.

We showed that the Lanczos-based BiCG/BiCGStab and the Arnoldi-based FOM are the extreme cases of ML\((n)\)BiCG /ML\((n)\)BiCGStab.

In this paper, we did not assume that \( A \) is a nonsingular matrix. When a singular system (1.1) is solved, selecting an appropriate initial guess \( x_0 \) is a crucial step. If \( x_0 \) is selected such that the affine subspace \( x_0 + K(A, \bar{r}_0) \) contains a solution of (1.1), ML\((n)\)BiCG will almost surely converge (see Theorem 3.9). Otherwise, we shall have \( p_{\min}(0, A, \bar{r}_0) = 0 \) (see Remark 3.8(ii)) which yields \( \det(\bar{S}_n) = 0 \) (see Lemma 3.6(c)). In this case, in the last iteration \( k = \nu \), the \( LU \)-factorization in the construction of ML\((n)\)BiCG does not exist (see Remark 3.3(iii)). As a result, it is likely that \( \| \bar{r}_\nu \|_2 \) blows up to \( \infty \).\(^{11}\) A similar remark also applies to ML\((n)\)BiCGStab.

In the solution of a sequence of linear systems where BiCGStab is convergent throughout the sequence, the parameter \( n \) in ML\((n)\)BiCGStab can be chosen dynamically.

\(^{11}\)Lemma 3.6, together with Remark 3.3(ii), indicates that ML\((n)\)BiCG will run almost surely without encountering zero division from iteration \( k = 1 \) to iteration \( k = \nu - 1 \) in any situation.
9. Appendix. In this section, we present the preconditioned ML(n)BiCGStab algorithms together with their Matlab codes.

9.1. ML(n)BiCGStab with Definition (4.3). Algorithm 9.1 is a preconditioned version of Algorithm 4.1.

Algorithm 9.1. ML(n)BiCGStab with preconditioning associated with Definition (4.3).

1. Choose an initial guess $x_0$ and $n$ vectors $q_1, q_2, \ldots, q_n$.
2. Compute $r_0 = b - Ax_0$ and set $g_0 = r_0$.
3. Compute $g_0 = M^{-1}g_0$, $w_0 = A^Hg_0$, $c_0 = q_1^Hw_0$ and $e_0 = q_1^Hr_0$.
4. For $j = 0, 1, 2, \ldots$
5. \( \alpha_{jn+1} = e_{(j-1)n+n}/e_{(j-1)n+n} \); \( u_{jn+1} = r_{(j-1)n+n} - \alpha_{jn+1}w_{(j-1)n+n} \);
6. \( x_{jn+1} = x_{(j-1)n+n} + \alpha_{jn+1}g_{(j-1)n+n} \);
7. \( \bar{u}_{jn+1} = M^{-1}u_{jn+1} \);
8. \( \omega_{j+1} = (A\bar{u}_{jn+1})^Hw_{jn+1}/\|A\bar{u}_{jn+1}\|_2^2 \);
9. \( x_{jn+1} = x_{jn+1} + \omega_{j+1}u_{jn+1} \);
10. \( r_{jn+1} = -\omega_{j+1}A\bar{u}_{jn+1} + u_{jn+1} \);
11. For $i = 1, 2, \ldots, n-1$
12. \( f_{jn+i} = q_i^Hw_{jn+i} \);
13. If $j \geq 1$
14. \( \beta_{(j-1)n+i} = -f_{jn+i}/e_{(j-1)n+i} \);
15. If $i \leq n-2$
16. \( z_d = u_{jn+i} + \beta_{(j-1)n+i}d_{(j-1)n+i} \);
17. \( g_{jn+i} = \beta_{(j-1)n+i}g_{(j-1)n+i} \);
18. \( z_w = \beta_{(j-1)n+i}w_{(j-1)n+i} \);
19. \( \beta_{(j-1)n+i+1} = -q_{i+2}^Hz_d/e_{(j-1)n+i+1} \);
20. For $s = i+1, \ldots, n-2$
21. \( z_d = z_d + \beta_{(j-1)n+i}d_{(j-1)n+s} \);
22. \( g_{jn+i} = g_{jn+i} + \beta_{(j-1)n+i}g_{(j-1)n+s} \);
23. \( z_w = z_w + \beta_{(j-1)n+i}w_{(j-1)n+s} \);
24. \( \beta_{(j-1)n+i+1} = -q_{i+2}^Hz_d/e_{(j-1)n+i+1} \);
25. End
26. \( g_{jn+i} = g_{jn+i} + \beta_{(j-1)n+i}g_{(j-1)n+n} - g_{(j-1)n+n-1} \);
27. \( z_w = z_w + \beta_{(j-1)n+i}w_{(j-1)n+n-1} \);
28. \( z_w = r_{jn+i} - \omega_{j+1}z_w \);
29. Else
30. \( g_{jn+i} = \beta_{(j-1)n+i}g_{(j-1)n+n} - g_{(j-1)n+n-1} \);
31. \( z_w = r_{jn+i} - \omega_{j+1}g_{(j-1)n+i} \);
32. End
33. \( \beta_{(j-1)n+n} = q_1^Hz_w/\|\omega_{j+1}c_{(j-1)n+n}\|_2 \);
34. \( z_w = z_w - \omega_{j+1}\beta_{(j-1)n+n}w_{(j-1)n+n} \);
35. \( g_{jn+i} = g_{jn+i} + z_w + \beta_{(j-1)n+n}g_{(j-1)n+n} \);
36. Else
37. \( \beta_{(j-1)n+n} = q_1^HR_{jn+i}/\|\omega_{j+1}c_{(j-1)n+n}\|_2 \);
MATLAB code of Algorithm 9.1

```matlab
M = (A,x,b,Q,M,max_it,tol,kappa)
```

1. function [x, err, iter, flag] = mlbigeststb(A, x, b, Q, M, max_it, tol, kappa)
2. 
4. % Q: N-by-n auxiliary matrix [q_1, \ldots, q_n]. x: initial guess.
5. % b: right hand side vector. max_it: maximum number of iterations.
6. % tol: error tolerance.
7. % kappa: (real number in [0, 1]) minimization step controller:
8. % kappa = 0, standard minimization
9. % kappa > 0, Sleijpen-van der Vorst minimization
% output: \( x \): solution computed. \( err \): error norm. \( iter \): number of iterations performed.

10. \( flag \) = 0, solution found to tolerance
11. \( flag \) = 1, no convergence given \( max \_it \) iterations
12. \( flag \) = -1, breakdown.
13. \( G, Q, W \): \( N \times n \) matrices. \( A, M \): \( N \times N \) matrices.
14. \( x, r, g, u, z, b \): \( N \times 1 \) matrices. \( c \): \( 1 \times n \) matrix.

15. \( N = size(A, 2); n = size(Q, 2); \)
16. \( G = zeros(N, n); W = zeros(N, n); \) initialize work spaces
17. if \( n > 2, D = zeros(N, n - 2); \) end
18. \( c = zeros(1, n); \) end initialization
19. iter = 0; \( flag = 1; bnrm2 = norm(b); \)
20. if \( bnrm2 == 0.0, bnrm2 = 1.0; \) end
21. if \( err < tol, flag = 0; \) return, end
22. \( G(:, n) = r; g \_J = M \_r; W(:, n) = A \_g \_J; c(n) = Q(:, 1) \_W(:, n); \)
23. if \( c(n) == 0, flag = -1; \) return, end
24. \( e = Q(:, 1) \_r; \)
25. for \( j = 0 : max \_it \)
26. \( alpha = e/c(n); x = x + alpha \_g \_J; \)
27. \( u = r - alpha \_W(:, n); err = norm(u)/bnrm2; \)
28. if \( err < tol, flag = 0; iter = iter + 1; \) return, end
29. \( g \_J = M \_u; z = A \_g \_J; omega = z' \_z; \)
30. if \( omega == 0, flag = -1; \) return, end
31. \( rho = z' \_u; omega = rho/omega; \)
32. if \( kappa > 0 \)
33. \( rho = rho/norm(z) \_norm(u)); abs \_rho = abs(rho); \)
34. if \( (abs \_rho < kappa) \) & \( (abs \_rho \sim = 0), omega = omega \_kappa/abs \_rho; \) end
35. end
36. \( x = x + omega \_g \_J; r = -omega \_z + u; \)
37. \( err = norm(r)/bnrm2; iter = iter + 1; \)
38. if \( err < tol, flag = 0; \) return, end
39. if \( iter >= max \_it, \) return, end
40. \( rc = omega \_c(n); \)
41. if \( rc == 0, flag = -1; \) return, end
42. for \( i = 1 : n - 1 \)
43. \( f = Q(:, i + 1) \_u; \)
44. if \( j >= 1 \)
45. \( beta = -f/c(i); \)
46. if \( i <= n - 2 \)
47. \( D(:, i) = u + beta \_D(:, i); G(:, i) = beta \_G(:, i); \)
48. \( W(:, i) = beta \_W(:, i); beta = -Q(:, i + 2) \_D(:, i)/c(i + 1); \)
49. end
50. end
51. end
52. end
53. end
54. end
55. end
56. end
57. end
58. end
for $s = i + 1 : n - 2$

$D(:, i) = D(:, i) + \text{beta} \ast D(:, s)$;

$G(:, i) = G(:, i) + \text{beta} \ast G(:, s)$;

$W(:, i) = W(:, i) + \text{beta} \ast W(:, s)$;

$\beta = -Q(:, s + 2)' \ast D(:, i)/c(s + 1)$;

end

$G(:, i) = G(:, i) + \text{beta} \ast G(:, n - 1)$;

$W(:, i) = W(:, i) + \text{beta} \ast W(:, n)$;

$W(:, i) = r - \omega \ast W(:, i)$;

else

$G(:, n - 1) = \beta \ast G(:, n - 1)$;

$W(:, n - 1) = r - (\omega \ast \beta) \ast W(:, n - 1)$;

end

$\text{beta} = Q(:, 1)' \ast W(:, i)/rc$;

$W(:, i) = W(:, i) - (\omega \ast \beta) \ast W(:, n)$;

$G(:, i) = G(:, i) + W(:, i) + \beta \ast G(:, n)$;

else

$\beta = Q(:, 1)' \ast r/rc$;

$W(:, i) = r - (\omega \ast \beta) \ast W(:, n)$;

$G(:, i) = W(:, i) + \beta \ast G(:, n)$;

end

for $s = 1 : i - 1$

$\beta = -Q(:, s + 1)' \ast W(:, i)/c(s)$;

$G(:, i) = G(:, i) + \beta \ast G(:, s)$;

$W(:, i) = W(:, i) + \beta \ast D(:, s)$;

end

if $i < n - 1$

$D(:, i) = W(:, i) - u$; $c(i) = Q(:, i + 1)' \ast D(:, i)$;

if $c(i) == 0$, $\text{flag} = -1$; return, end

$\alpha = -f/c(i)$; $u = u + \alpha \ast D(:, i)$;

else

$c(i) = Q(:, i + 1)' \ast (W(:, i) - u)$;

if $c(i) == 0$, $\text{flag} = -1$; return, end

$\alpha = -f/c(i)$;

end

$g_J = M \ast G(:, i)$; $W(:, i) = A \ast g_J$;

$\alpha = \omega \ast \alpha$; $x = x + \alpha \ast g_J$; $r = r - \alpha \ast W(:, i)$;

$\text{err} = \text{norm} (r)/\text{bnrm2}$; $\text{iter} = \text{iter} + 1$;

if $\text{err} < \text{tol}$, $\text{flag} = 0$; return, end

if $\text{iter} > = \text{maxit}$, return, end

end

$e = Q(:, 1)' \ast r$; $\beta = e/rc$; $W(:, n) = r - (\omega \ast \beta) \ast W(:, n)$;

$G(:, n) = W(:, n) + \beta \ast G(:, n)$;

if $n > = 2$

$\beta = -Q(:, 2)' \ast W(:, n)/c(1)$;

for $s = 1 : n - 2$

$G(:, n) = G(:, n) + \beta \ast G(:, s)$;

$W(:, n) = W(:, n) + \beta \ast D(:, s)$;

$\beta = -Q(:, s + 2)' \ast W(:, n)/c(s + 1)$;

end

$G(:, n) = G(:, n) + \beta \ast G(:, n - 1)$;
Algorithm 9.2 is a preconditioned version of Algorithm 5.1.

Algorithm 9.2. ML\((n)\)BiCGStab with preconditioning associated with definition (5.2).

1. Choose an initial guess \(x_0\) and \(n\) vectors \(q_1, q_2, \ldots, q_n\).
2. Compute \(r_0 = b - Ax_0\), \(\bar{g}_0 = M^{-1}r_0\), \(w_0 = A\bar{g}_0\), \(c_0 = q_1^Hw_0\) and \(e_0 = q_1^Hr_0\).
3. For \(j = 0, 1, 2, \ldots\)
   4. For \(i = 1, 2, \ldots, n - 1\)
      5. \(\alpha_{jn+i} = c_{jn+i-1}/c_{jn+i-1};\)
      6. \(x_{jn+i} = x_{jn+i-1} + \alpha_{jn+i}\bar{g}_{jn+i-1};\)
      7. \(r_{jn+i} = r_{jn+i-1} - \alpha_{jn+i}w_{jn+i-1};\)
      8. \(c_{jn+i} = q_{i+1}^Hr_{jn+i};\)
      9. If \(j \geq 1\)
         10. \(\beta_{(j-1)n+i} = -c_{jn+i}/c_{(j-1)n+i};\)
         11. \(z_w = r_{jn+i} + \beta_{(j-1)n+i}w_{(j-1)n+i};\)
         12. \(\bar{g}_{jn+i} = \bar{g}_{jn+i-1}\); \(\beta_{(j-1)n+i} = \bar{g}_{jn+i};\)
         13. For \(s = i + 1, \ldots, n - 1\)
            14. \(\beta_{(j-1)n+s} = -q_{i+1}^Hz_w/c_{(j-1)n+s};\)
            15. \(z_w = z_w + \beta_{(j-1)n+s}w_{(j-1)n+s};\)
            16. \(\bar{g}_{jn+i} = \bar{g}_{jn+i} + \beta_{(j-1)n+s}\bar{g}_{(j-1)n+s};\)
            17. \(\bar{g}_{jn+i} = M^{-1}z_w - \frac{1}{\omega_j}\bar{g}_{jn+i};\)
         18. \(\bar{g}_{jn+i} = M^{-1}r_{jn+i};\)
      19. Else
         20. \(\bar{g}_{jn+i} = M^{-1}r_{jn+i};\)
      21. End
      22. \(w_{jn+i} = A\bar{g}_{jn+i};\)
      23. For \(s = 0, \ldots, i - 1\)
         24. \(\beta_{jn+s} = -q_{i+1}^Hw_{jn+i}/c_{jn+s};\)
         25. \(w_{jn+i} = w_{jn+i} + \beta_{jn+s}w_{jn+s};\)
         26. \(\bar{g}_{jn+i} = \bar{g}_{jn+i} + \beta_{jn+s}\bar{g}_{jn+s};\)
      27. End
      28. \(c_{jn+i} = q_{i+1}^Hw_{jn+i};\)
   4. End
   5. \(\alpha_{jn+n} = c_{jn+n-1}/c_{jn+n-1};\)
   6. \(x_{jn+n} = x_{jn+n-1} + \alpha_{jn+n}\bar{g}_{jn+n-1};\)
   7. \(u_{jn+n} = r_{jn+n-1} - \alpha_{jn+n}w_{jn+n-1};\)
   8. \(\tilde{u}_{jn+n} = M^{-1}u_{jn+n};\)
   9. \(\omega_j = (A\tilde{u}_{jn+n})^Hu_{jn+n}/\|A\tilde{u}_{jn+n}\|_2;\)
   10. \(x_{jn+n} = x_{jn+n} + \omega_ju_{jn+n};\)
   11. \(r_{jn+n} = -\omega_j\bar{u}_{jn+n} + u_{jn+n};\)
   12. \(c_{jn+n} = q_{i+1}^Hr_{jn+n};\)
   13. end


\[ \tilde{\beta}^{(j+n)} = -c_{j+n}/c_{(j-1)n+n}; \quad \tilde{\beta}^{(j+n)} = -\omega_{j+1}\tilde{\beta}^{(j+n)} \]

\[ z_w = r_{j+n} + \beta^{(j+n)} w_{(j-1)n+n}; \]

\[ \tilde{g}_{j+n} = \tilde{\beta}^{(j+n)} g_{(j-1)n+n}; \]

\[ g_{j+n} = \tilde{g}_{j+n} + \tilde{\beta}^{(j+n)} g_{j+n}; \]

\[ g_{j+n} = M^{-1} z_w - \frac{1}{\omega_{j+1}} \tilde{g}_{j+n}; \quad w_{j+n} = A\tilde{g}_{j+n}; \]

**Code #2: Matlab code of Algorithm 9.2**

```
function [x, err, iter, flag] = mlbicgstab(A, x, b, Q, M, max_it, tol, kappa)
    % The input/output arguments are described as in Code #1.
    % storage: c: 1 x n matrix. x, r, b, u, f, z: N-by-1 matrices.

    N = size(A, 2); n = size(Q, 2);
    G = zeros(N, n); W = zeros(N, n); % initialize work spaces
    c = zeros(1, n); % end initialization

    iter = 0; flag = 1; bnrm2 = norm(b);
    if bnrm2 == 0.0, bnrm2 = 1.0; end
    r = b - A * x; err = norm(r)/bnrm2;
    if err < tol, flag = 0; return, end

    G(:, 1) = M \ r; W(:, 1) = A * G(:, 1); c(1) = Q(:, 1)' * W(:, 1);
    if c(1) == 0, flag = -1; return, end
    e = Q(:, 1)' * r;

    for j = 0 : max_it
        for i = 1 : n - 1
            alpha = c(i)/c(i); x = x + alpha * G(:, i); r = r - alpha * W(:, i);
            err = norm(r)/bnrm2; iter = iter + 1;
            if err < tol, flag = 0; return, end
            if iter >= max_it, return, end
            e = Q(:, i + 1)' * r;
        if j > 0
            beta = -e/c(i + 1); W(:, i + 1) = r + beta * W(:, i + 1);
            G(:, i + 1) = beta * G(:, i + 1);
            for s = i + 1 : n - 1
                beta = -Q(:, s + 1)' * W(:, i + 1)/c(s + 1);
                W(:, i + 1) = W(:, i + 1) + beta * W(:, s + 1);
                G(:, i + 1) = G(:, i + 1) + beta * G(:, s + 1);
            end
            \[ g_{j+n} = \tilde{g}_{j+n} + \tilde{\beta}^{(j+n)} g_{j+n}; \]
    ```
\[ G(:, i + 1) = (M \setminus W(:, i + 1)) - (1/\omega) \ast G(:, i + 1); \]
else
\[ G(:, i + 1) = M \setminus r; \]
end
\[ W(:, i + 1) = A \ast G(:, i + 1); \]
for \( s = 0 : i - 1 \)
\[ \beta = -Q(:, s + 1)' \ast W(:, i + 1)/c(s + 1); \]
\[ W(:, i + 1) = W(:, i + 1) + \beta \ast W(:, s + 1); \]
\[ G(:, i + 1) = G(:, i + 1) + \beta \ast G(:, s + 1); \]
end
\[ c(i + 1) = Q(:, i + 1)' \ast W(:, i + 1); \]
if \( c(i + 1) == 0, \text{flag} = -1; \) return, end
end
\[ \alpha = e/c(n); \quad x = x + \alpha \ast G(:, n); \]
\[ r = r - \alpha \ast W(:, n); \quad \text{err} = \text{norm}(r)/\text{bnrm2}; \]
if \( \text{err} < \text{tol}, \text{flag} = 0; \) iter = iter + 1; return, end
\[ u_f = M \setminus r; \quad z = A \ast u_f; \quad \omega = z' \ast z; \]
if \( \omega == 0, \text{flag} = -1; \) return, end
\[ \rho = z' \ast r; \quad \omega = \rho/\omega; \]
if \( \kappa > 0 \)
\[ \rho = \rho/(\text{norm}(z) \ast \text{norm}(r)); \quad \text{abs}_r = \text{abs}(\rho); \]
if \( (\text{abs}_r < \kappa) \) & \( (\text{abs}_r \sim 0) \)
\[ \omega = \omega \ast \kappa/\text{abs}_r; \]
end
end
if \( \omega == 0, \text{flag} = -1; \) return, end
\[ x = x + \omega \ast u_f; \quad r = r - \omega \ast z; \]
\[ \text{err} = \text{norm}(r)/\text{bnrm2}; \quad \text{iter} = \text{iter} + 1; \]
if \( \text{err} < \text{tol}, \text{flag} = 0; \) return, end
if \( \text{iter} >= \text{max}_it, \) return, end
\[ e = Q(:, 1)' \ast r; \quad \beta = -e/c(1); \]
\[ W(:, 1) = r + \beta \ast W(:, 1); \quad G(:, 1) = \beta \ast G(:, 1); \]
for \( s = 1 : n - 1 \)
\[ \beta = -Q(:, s + 1)' \ast W(:, 1)/c(s + 1); \]
\[ W(:, 1) = W(:, 1) + \beta \ast W(:, s + 1); \]
\[ G(:, 1) = G(:, 1) + \beta \ast G(:, s + 1); \]
end
\[ G(:, 1) = (M \setminus W(:, 1)) - (1/\omega) \ast G(:, 1); \]
\[ W(:, 1) = A \ast G(:, 1); \]
\[ c(1) = Q(:, 1)' \ast W(:, 1); \]
if \( c(1) == 0, \text{flag} = -1; \) return, end
end

9.3. Sample Executions of ML(n)BiCGStab. We provide two sample executions: Code #3 for a single system and Code #4 for a sequence of systems.

Code #3: A sample run of ML(n)BiCGStab
1. \( N = 100; A = \text{randn}(N); M = \text{randn}(N); b = \text{randn}(N, 1); \)
2. \( n = 10; \text{tol} = 10^{-7}; \max_{it} = 3 \ast N; \kappa = 0; \quad \% \text{or, say,} \kappa = 0.7 \)
3. \( Q = \text{sign}(\text{randn}(N, n)); x = \text{zeros}(N, 1); Q(:, 1) = b - A \ast x; \)
4. \([x, \text{err}, \text{iter}, \text{flag}] = \text{mlbicgstab}(A, x, b, Q, M, \max_{it}, \text{tol}, \kappa); \)
Code #4: Solution of a sequence of linear systems

1. % Suppose mlbicgstab is used to solve a sequence of m systems \( A_i x = b_i \) with
2. % preconditioners \( M_i \). This code dynamically searches for \( n \) in an user-provided
3. % interval \([n_{\text{min}}, n_{\text{max}}]\) so that the time per iteration is as small as possible.
4. %
5. \( n_{\text{min}} = 2; n_{\text{max}} = 20; \text{step} = 3; \) % step size, an integer \( \geq 1 \).
6. \( \text{max_it} = 3 * N; \text{tol} = 10^{-7}; \kappa = 0; \) % or, say, \( \kappa = 0.7 \)
7. \( Q = \text{sign(randn}(N, n_{\text{max}})); \) % a random sign shadow matrix.
8. \( n = 10; \) % initial value for \( n \), an integer picked from \([n_{\text{min}}, n_{\text{max}}]\).
9. \( \text{walk} = 1; \) % \( \text{walk} = 1 \), search forward; \( = -1 \), search backward.
10. \( t_1 = \inf; \) % solution time of the previous system.
11. %
12. for \( i = 1 : m \)
13. \( x = \text{zeros}(N,1); \) % choose an initial guess for the \( i \)th system.
14. \( Q(:,1) = b_i - A_i x; \)
15. tic
16. \([x, \text{err}, \text{iter}, \text{flag}] = \text{mlbicgstab}(A_i, x, b_i, Q(:, 1 : n), M_i, \text{max_it}, \text{tol}, \kappa); \)
17. \( t_2 = \text{toc} / \text{iter}; \) % time per iteration of the current system.
18. if \( \text{walk} == 1 \)
19. if \( t_2 < t_1 \)
20. \( n = \text{min}(n + \text{step}, n_{\text{max}}); t_1 = t_2; \)
21. else
22. \( n = \text{max}(n - \text{step}, n_{\text{min}}); t_1 = t_2; \text{walk} = -1; \)
23. end
24. else
25. if \( t_2 < t_1 \)
26. \( n = \text{max}(n - \text{step}, n_{\text{min}}); t_1 = t_2; \)
27. else
28. \( n = \text{min}(n + \text{step}, n_{\text{max}}); t_1 = t_2; \text{walk} = 1; \)
29. end
30. end
31. end

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