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A block GMRES method augmented with eigenvectors ☆

Gui-Ding Gu, Zhi-Hao Cao *

Institute of Mathematics, Fudan University, Shanghai 200433, People's Republic of China

Abstract

The GMRES method augmented with some eigenvectors is extended to a block version for solving large nonsymmetric linear systems with multiple right-hand sides. Residual bound is established which has an improved convergence rate on the standard block GMRES method. This improvement displays a good efficiency when restarting is used. Also an improved residual norm estimate is derived by using matrix-valued polynomials. Numerical experiments show that the new algorithm is more efficient, compared with the block GMRES method. © 2001 Elsevier Science Inc. All rights reserved.

Keywords: Block GMRES; Iterative methods; Nonsymmetric linear systems; Multiple right-hand sides

1. Introduction

There are some techniques which are sometimes used to improve the convergence rate of Krylov subspace method; see, e.g., [2,4,7,12]. One of the simplest ideas employed is to add to the Krylov subspace some approximation to an invariant subspace associated with a few of the smallest eigenvalues. A projection process on this augmented subspace is then carried out.

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* Corresponding author.
E-mail address: zcao@fudan.edu.cn (Z.-H. Cao).

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We consider the following linear system with multiple right-hand sides:

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

where A is a large nonsymmetric real matrix of order n, and $X = [x_1, \ldots, x_p]$ and $B = [b_1, \ldots, b_p]$ are rectangular matrices of dimension $n \times p$ with modest block size p. The block system (1.1) arises in many areas such as chemistry, electromagnetics, structures and control; see Refs. in [13]. When A is a large spares matrix, block iterative methods, e.g., block CG method, block GMRES method (denoted by BGMRES) or block QMR method, are natural candidates for solving (1.1) (see, e.g., [3,8,9,13,14]).

An essential component of BGMRES is the block Arnoldi procedure; see [1]. Given an initial guess $X^{(0)}$, the initial block residual $R^{(0)} = B - AX^{(0)}$ can be assumed of full rank, otherwise, it can be deflated. BGMRES generates an approximate solution $X^{(m)} = X^{(0)} + Z_m$ over the block Krylov subspace $\mathscr{K}_m = \mathrm{span}\{R^{(0)}, AR^{(0)}, \ldots, A^{m-1}R^{(0)}\}$, generated by $R^{(0)}$, where Z_m solves the minimization problem

$$\min_{Z \in \mathscr{K}_m} \|R^{(0)} - AZ\|_F \tag{1.2}$$

with $\|\cdot\|_F$ the Frobenius norm. Simoncini and Gallopoulos [14] have shown that for $j = 1, \ldots, p$, the residual satisfies

$$\left(r_j^{(m)}, r_j^{(m)}\right) \leqslant S\left(\frac{a/e + \sqrt{(a/e)^2 - 1}}{|\, c/e\,| + \sqrt{|\, c/e\,|^2 - 1}}\right)^{2m}, \tag{1.3}$$

where the scalar S does not depend on m, and c is center, $c \pm e$ are foci, e^2 is real and a is major semiaxis of the ellipse $F(c, e, a)$ which contains eigenvalue $\lambda_p, \ldots, \lambda_n$ with assumption that

$$0 < \mathrm{Re}(\lambda_1) \leqslant \cdots \leqslant \mathrm{Re}(\lambda_n). \tag{1.4}$$

In this paper, we extend the GMRES method augmented with some approximate invariant subspace presented by Morgan [7] to a block version for solving the system (1.1). In this case, the subspace of projection is of the form

$$\mathscr{K} = \mathscr{K}_m + \mathscr{W},$$

where $\mathscr{K}_m = \mathrm{span}\{R^{(0)}, AR^{(0)}, \ldots, A^{m-1}R^{(0)}\}$ is the standard block Krylov subspace and $\mathscr{W}$ is some approximate invariant subspace. Thus, an approximate solution $X^{(m)} = X^{(0)} + Z_m$ belongs to $\mathscr{K}$ and Z_m should solve the problem (1.2) over the subspace $\mathscr{K}$, i.e.,

$$Z_m = \arg \min_{Z \in \mathscr{K}} \|R^{(0)} - AZ\|_F. \tag{1.5}$$

We analyzed the convergence behavior of the method and derive an improved convergence rate on the block GMRES method. This improvement is important when restarting is used in the block GMRES method. In addition, we use matrix-valued polynomials as a useful tool in studying the convergence of block iterative schemes to evaluate the residual norm. The implementation and the expenses of the method are discussed in Section 3. Numerical experiments in Section 4 show that the new block algorithm is efficient, compared with the block GMRES method when restarting is used.

Throughout the paper, we adopt the following notations: Uppercase letters denote matrices except for special illustration. $\lambda_1, \ldots, \lambda_n$ are eigenvalues of matrix A with assumption (1.4). A superscript on a matrix or vector denotes an iteration number. Columns of a matrix are indexed by subscript; elements of a matrix have row and column indices as subscripts. Thus, for example, $x_{ij}^{(k)}$ is the element of the matrix $X^{(k)}$ in the ith row and jth column, and $x_j^{(k)}$ is the jth column.

For simplicity, the span of the columns of a matrix X will be denoted by $\text{span}\{X\}$, and matrix $A \in \text{span}\{X\}$ means the columns of A, $a_j \in \text{span}\{X\}$.

2. Residual evaluation

In this section, we will give a residual evaluation, which improves the result (1.3) of BGMRES augmented with some invariant (or approximate invariant) subspace by assuming that A is diagonalizable. Also, we obtain an evaluation of residual norm for the method by using matrix-valued polynomials. The idea of our analysis is basicly originated from [14].

2.1. Basic results

Since A is real, its eigenvalues are symmetric with respect to the real axis. We can thus construct an ellipse $E(c, e, a)$ which contains $\lambda_{l+p}, \ldots, \lambda_n$ and has center c on the real axis, foci $c \pm e$, and major semiaxis a [5], and the ellipse is symmetric with respect to the real axis. Here, we should point out that e and a both can be purely imaginary.

For understanding and analysis, through this paper, we assume that the subspace $\mathscr{K}$ is full-rank, i.e., $\dim(\mathscr{K}) = mp + l$ with $\dim(\mathscr{K}_m) = mp$, though any implementation of the algorithm must take account of the possible rank loss, which can be handled by employing a deflation procedure [3,8]. Let T_m denote the Chebyshev polynomial of first kind and degree m.

Before giving the main results, we extend the conclusion of Lemma 2.4 in [14]. Define $\tilde{R}$ to be $R^{(0)}$ with the pth column omitted.

Lemma 2.1. *Suppose A has spectral decomposition $A = Z\Lambda Z^{-1}$ with $\Lambda =$ diag $(\lambda_1, \ldots, \lambda_n)$. Let $E(c, e, a)$ contain $\lambda_{l+p}, \ldots, \lambda_n$ and define an $n \times (p-1)$ matrix*

$$L = \begin{bmatrix} L_1 \\ L_2 \\ L_3 \end{bmatrix}$$

such that ZL is an orthogonal basis for span$\{A\tilde{R}\}$, *with an $l \times (p-1)$ matrix L_1 and a nonsingular matrix L_2 of order $p-1$. Let $\bar{L} = L_1 L_2^{-1} = (\bar{l}_{ij})$ and $\bar{\bar{L}} = L_3 L_2^{-1} = (\bar{\bar{l}}_{ij})$. Then, for each $j = 1, \ldots, p-1$ there is a vector $g_{l+j} \in$ span$\{A\tilde{R}, \ldots, A^m\tilde{R}\}$ such that*

$$g_{l+j} = \sum_{i=1}^{l} \delta_{ij} z_i + z_{l+j} + \sum_{i=l+p}^{n} \tau_{ij} z_i \tag{2.1}$$

with $\delta_{ij} = \bar{l}_{ij} T_{m-1}(\zeta_i)/T_{m-1}(\zeta_{l+j})$, $\tau_{ij} = \bar{\bar{l}}_{ij} T_{m-1}(\zeta_i)/T_{m-1}(\zeta_{l+j})$, and $\zeta_r = (c - \lambda_r)/e$.

Proof. First note that $ZLL_2^{-1} \in$ span$\{A\tilde{R}\}$. For $j = 1, \ldots, p-1$, define the vector $g_{l+j} = h_j(A)(ZLL_2^{-1})e_j$, where e_j is the jth $(p-1)$-dimensional coordinate vector and

$$h_j(\lambda) := T_{m-1}(\zeta)/T_{m-1}(\zeta_{l+j})$$

with $\zeta = (c - \lambda)/e$. Let $Z = [Z_1, Z_2, Z_3]$ with $Z_1 = [z_1, \ldots, z_l]$, $Z_2 = [z_{l+1}, \ldots, z_{l+p-1}]$ and $Z_3 = [z_{l+p}, \ldots, z_n]$. Since $h_j(\lambda_{l+j}) = 1$ and $(ZLL_2^{-1})e_j = (Z_1\bar{L} + Z_2 + Z_3\bar{\bar{L}})e_j = Z_1\bar{l}_j + z_{l+j} + Z_3\bar{\bar{l}}_j$, we have

$$\begin{aligned} g_{l+j} &= \sum_{i=1}^{l} h_j(\lambda_i) z_i \bar{l}_{ij} + z_{l+j} + \sum_{i=l+p}^{n} h_j(\lambda_i) z_i \bar{\bar{l}}_{ij} \\ &= \sum_{i=1}^{l} \delta_{ij} z_i + z_{l+j} + \sum_{i=l+p}^{n} \tau_{ij} z_i. \qquad \square \end{aligned}$$

The following theorem shows an evaluate of the residual after approximating the solution from $\mathscr{K}$:

Theorem 2.2. *Suppose A has spectral decomposition $A = Z\Lambda Z^{-1}$ with $\Lambda =$ diag$(\lambda_1, \ldots, \lambda_n)$. Let $E(c, e, a)$ contain $\lambda_{l+p}, \ldots, \lambda_n$ and be such that $c \in R^+$ is its center, e^2 is real, and the origin is exterior to the ellipse. Assume that*

the minimum residual solution $X^{(m)}$ *is extracted from the subspace* $\mathscr{K} \equiv \operatorname{span}\{R^{(0)}, AR^{(0)}, \ldots, A^{m-1}R^{(0)}, z_1, \ldots, z_l\}$. *Then*

$$\|R^{(m)}\|_F \leqslant S\left(\frac{a/e + \sqrt{(a/e)^2 - 1}}{|\,c/e\,| + \sqrt{|\,c/e\,|^2 - 1}}\right)^m, \tag{2.2}$$

where $R^{(m)} = B - AX^{(m)}$ *is the residual and the scalar* S *does not depend on* m.

Proof. It only needs to show the evaluate (2.2) for the jth residual vector $r_j^{(m)}$ $(j = 1, \ldots, p)$. From (1.5), the method computes $X^{(m)}$ in $\mathscr{K}$ so that the trace $\operatorname{tr}[(R^{(m)})^{\mathrm{T}} R^{(m)}]$ is minimized. This is achieved by minimizing $\|r_j^{(m)}\|_2$, for $j = 1, \ldots, p$.

To simplify notation, we derive the result for the pth residual vector $r^{(m)} \equiv r_p^{(m)}$ with omitting the subscript p in all related amount. The result also holds for other residuals. Any vector $x - x^{(0)}$ in the subspace $\mathscr{K}$ can be written in the form

$$x = x^{(0)} + \sum_{i=1}^{l} \alpha_i z_i + \sum_{j=1}^{p} t_j(A) r_j^{(0)},$$

where t_j is a polynomial of degree at most $m - 1$. Let

$$r_j^{(0)} = \sum_{i=1}^{n} \beta_{ij} z_i \tag{2.3}$$

and define the polynomial q as $q(\lambda) = 1 - \lambda t(\lambda)$. Then we can get that

$$\begin{aligned} r = b - Ax &= \sum_{i=1}^{n} \beta_i z_i - \sum_{i=1}^{l} \alpha_i \lambda_i z_i - \sum_{j=1}^{p} A t_j(A) r_j^{(0)} \\ &= \sum_{i=1}^{n} \beta_i q(\lambda_i) z_i - \sum_{i=1}^{l} \alpha_i \lambda_i z_i - \sum_{j=1}^{p-1} t_j(A) A r_j^{(0)}, \end{aligned}$$

where β_i is the expansion coefficient of $r_p^{(0)}$. The polynomial q is chosen such that

$$q(\lambda) = T_m\left(\frac{c - \lambda}{e}\right) / T_m(c/e) \tag{2.4}$$

and the remaining $p - 1$ polynomials are constructed as follows:

$$\sum_{j=1}^{p-1} t_j(A) A r_j^{(0)} = \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) g_{l+j}$$

with $g_{l+j} = \sum_{i=1}^{l} \delta_{ij} z_i + z_{l+j} + \sum_{i=l+p}^{n} \tau_{ij} z_i$ given by Lemma 2.1. Hence,

$$\begin{aligned} r &= \sum_{i=1}^{n} \beta_i q(\lambda_i) z_i - \sum_{i=1}^{l} \alpha_i \lambda_i z_i - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) g_{l+j} \\ &= \sum_{i=1}^{l} (\beta_i q(\lambda_i) - \lambda_i \alpha_i) z_i - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \sum_{i=1}^{l} \delta_{ij} z_i - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) z_{l+j} \\ &\quad - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \sum_{i=l+p}^{n} \tau_{ij} z_i + \sum_{i=l+1}^{n} \beta_i q(\lambda_i) z_i \\ &= \sum_{i=1}^{l} \left(\beta_i q(\lambda_i) - \lambda_i \alpha_i - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \delta_{ij} \right) z_i \\ &\quad + \sum_{i=l+p}^{n} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \tau_{ij} \right) z_i. \end{aligned} \tag{2.5}$$

By picking $\alpha_i = (1/\lambda_i)(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \delta_{ij})$ $(i = 1, \ldots, l)$, we obtain

$$r = \sum_{i=l+p}^{n} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \tau_{ij} \right) z_i. \tag{2.6}$$

Since the solution minimizes the residual norm, it will be at least as good as any choice we make, so $\|r_p^{(m)}\|_2 \leqslant \|r\|_2$. The desired result

$$\|r_p^{(m)}\|_2 \leqslant S_p \left(\frac{a/e + \sqrt{(a/e)^2 - 1}}{|\, c/e \,| + \sqrt{|\, c/e \,|^2 - 1}} \right)^m \tag{2.7}$$

follows from the standard bound in (1.3). □

Remark. Corresponding to (2.6), the residual expression in [14] is

$$r = \sum_{i=p}^{n} \left(q(\lambda_i) \beta_i - \sum_{j=1}^{p-1} \beta_j q(\lambda_j) \tau_{ij} \right) z_i,$$

i.e., the situation of (2.6) for $l = 0$. Then the evaluate (1.3) is obtained (cf. the proof of it in [14] for detail).

Clearly, the evaluation (2.2) improves the result of (1.3). When A has a cluster of smallest eigenvalues more than p, this improvement will be significant. Especially, when restarting is used, the improvement will be more beneficial, compared with the BGMRES method (see numerical experiments in Section 4). If A has both some very large eigenvalues and some very small eigenvalues, the augmented BGMRES method will give the following evaluation:

Corollary 2.3. *Suppose A has spectral decomposition $A = Z\Lambda Z^{-1}$ with $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Let $E(\bar{c}, \bar{e}, \bar{a})$ contain $\lambda_p, \ldots, \lambda_{n-l}$ and be such that $\bar{c} \in R^+$ is its center, $\bar{e}^2$ is real, and the origin is exterior to the ellipse. Assume that the minimum residual solution $X^{(m)}$ is extracted from the subspace $\mathscr{K} \equiv \mathrm{span}\{R^{(0)}, AR^{(0)}, \ldots, A^{m-1}R^{(0)}, z_{n-l+1}, \ldots, z_n\}$. Then*

$$\|R^{(m)}\|_F \leqslant S\left(\frac{\bar{a}/\bar{e} + \sqrt{(\bar{a}/\bar{e})^2 - 1}}{|\,\bar{c}/\bar{e}\,| + \sqrt{|\,\bar{c}/\bar{e}\,|^2 - 1}}\right)^m, \tag{2.8}$$

where the scalar S does not depend on m.

Proof. Set $t := n - l + 1$ and assume $t > p$. Similar to the Proof of Theorem 2.2, for $x - x^{(0)} \in \mathscr{K}$,

$$x = x^{(0)} + \sum_{i=t}^{n} \alpha_i z_i + \sum_{j=1}^{p} t_j(A) r_j^{(0)}.$$

We can derive

$$r = b - Ax = \sum_{i=1}^{n} \beta_i q(\lambda_i) z_i - \sum_{i=t}^{n} \alpha_i \lambda_i z_i - \sum_{j=1}^{p-1} t_j(A) A r_j^{(0)},$$

where

$$q(\lambda) = T_m\left(\frac{\bar{c} - \lambda}{\bar{e}}\right) / T_m(\bar{c}/\bar{e}).$$

We cite Lemma 2.1 for $l = 0$ and let

$$\sum_{j=1}^{p-1} t_j(A) A r_j^{(0)} = \sum_{j=1}^{p-1} \beta_j q(\lambda_j) g_j,$$

where $g_j = z_j + \sum_{i=p}^{n} \tau_{ij} z_i$. Thus, we can get

$$r = \sum_{i=t}^{n} \left(\beta_i q(\lambda_i) - \lambda_i \alpha_i - \sum_{j=1}^{p-1} \beta_j q(\lambda_j) \tau_{ij}\right) z_i + \sum_{i=p}^{t-1} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_j q(\lambda_j) \tau_{ij}\right) z_i.$$

We choose $\alpha_i = (1/\lambda_i)(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \tau_{ij})$, then

$$r = \sum_{i=p}^{t-1} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_j q(\lambda_j) \tau_{ij}\right) z_i.$$

The desired result follows from $\|r_p^{(m)}\|_2 \leqslant \|r\|_2$ and the standard bound in (1.3). □

The following theorem gives the residual evaluation when the standard Krylov subspace $\mathscr{K}_m$ is augmented with some approximate invariant subspace, i.e., $\mathscr{K} = \mathscr{K}_m + \mathscr{W} \equiv \mathrm{span}\{R^{(0)}, AR^{(0)}, \ldots, A^{m-1}R^{(0)}, y_1, \ldots, y_l\}$, where y_i is an approximate eigenvector to z_i:

Theorem 2.4. *Suppose A has spectral decomposition $A = Z\Lambda Z^{-1}$ with $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Let $E(c, e, a)$ be the same ellipse as in Theorem* 2.2, *and $\psi_i \equiv \angle(y_i, z_i)$, $\|z_i\|_2 = \|y_i\|_2 = 1$. Assume that the minimum residual solution $X^{(m)}$ is extracted from the subspace $\mathscr{K}$. Then*

$$\|r_p^{(m)}\|_2 \leqslant S\left(\frac{a/e + \sqrt{(a/e)^2 - 1}}{|\,c/e\,| + \sqrt{|\,c/e\,|^2 - 1}}\right)^m + \|A\|_2 \left\| \sum_{i=1}^{l} \frac{\tan\psi_i}{\lambda_i} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \delta_{ij} \right) \right\|_2, \tag{2.9}$$

where $q(\lambda)$ is given in (2.4).

Proof. For vector $x - x^{(0)}$ in $\mathscr{K}$,

$$x = x^{(0)} + \sum_{i=1}^{l} \alpha_i y_i + \sum_{j=1}^{p} t_j(A) r_j^{(0)}.$$

For $j = 1, \ldots, p$, decompose y_i as

$$y_i = \cos\psi_i \cdot z_i + \sin\psi_i \cdot u_i,$$

where u_i is unit vector and $u_i \perp z_i$. Then

$$\begin{aligned} r = b - Ax &= \sum_{i=1}^{n} \beta_i z_i - \sum_{i=1}^{l} \alpha_i (\lambda_i \cos\psi_i \cdot z_i + \sin\psi_i \cdot Au_i) - \sum_{j=1}^{p} A t_j(A) r_j^{(0)} \\ &= \sum_{i=1}^{n} \beta_i q(\lambda_i) z_i - \sum_{i=1}^{l} \alpha_i \lambda_i \cos\psi_i \cdot z_i - \sum_{i=1}^{l} \alpha_i \sin\psi_i \cdot Au_i - \sum_{j=1}^{p-1} t_j(A) A r_j^{(0)}, \end{aligned}$$

where $q(\lambda) = 1 - \lambda t(\lambda)$ is chosen as (2.4), and $\sum_{j=1}^{p-1} t_j(A) A r_j^{(0)} = \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) g_{l+j}$ is constructed with g_{l+j} given by Lemma 2.1. Similar to (2.5), we derive

$$\begin{aligned} r = &\sum_{i=1}^{l} \left(\beta_i q(\lambda_i) - \lambda_i \alpha_i \cos\psi_i - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \delta_{ij} \right) z_i \\ &+ \sum_{i=l+p}^{n} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \tau_{ij} \right) z_i - \sum_{i=1}^{l} \alpha_i \sin\psi_i \cdot Au_i. \end{aligned}$$

After picking $\alpha_i = (1/\lambda_i \cos\psi_i)(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j})\delta_{ij})$, we get

$$r = \sum_{i=l+p}^{n} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \tau_{ij} \right) z_i - \sum_{i=1}^{l} \frac{\tan\psi_i}{\lambda_i} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \delta_{ij} \right) A u_i.$$

Hence,

$$\|r\|_2 \leqslant \left\| \sum_{i=l+p}^{n} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \tau_{ij} \right) z_i \right\|_2 + \|A\|_2 \left\| \sum_{i=1}^{l} \frac{\tan\psi_i}{\lambda_i} \left(\beta_i q(\lambda_i) - \sum_{j=1}^{p-1} \beta_{l+j} q(\lambda_{l+j}) \delta_{ij} \right) \right\|_2.$$

The desired result is obtained by evaluating the first item of right-hand side above from (2.6) and (2.7). □

Remark. The evaluation (2.9) also holds for other residuals $r_j^{(m)}$ $(j < p)$ provided the subscript p is changed accordingly.

2.2. Matrix-valued polynomials

Let Φ_m be a matrix-valued polynomial of degree m and order p, defined by $\Phi_m(\lambda) = \sum_{i=0}^{m} \lambda^i \xi_i$ with $\xi_i \in R^{p\times p}$, and $\mathscr{P}_{m,p}$ be the space of matrix-valued polynomials Φ_m of degree not greater than m and order p, such that $\Phi_m(0) = I_p$. In particular, if $\Phi_m(\lambda) := I_p - \sum_{i=0}^{m-1} \lambda^{i+1}\alpha_i \in \mathscr{P}_{m,p}$ is the matrix-valued residual polynomial for BGMRES, i.e., $R^{(m)} = \Phi_m(A) \circ R^{(0)} \equiv R^{(0)} - \sum_{i=0}^{m-1} A^{i+1} R^{(0)} \alpha_i$ is the residual of BGMRES after m steps iteration, Φ_m solves the minimization problem

$$\min_{\Theta_m \in \mathscr{P}_{m,p}} \|\Theta_m(A) \circ R^{(0)}\|_F.$$

Then, the following evaluation is shown in [14]:

$$\|R^{(m)}\|_F \leqslant \kappa(Z)\sqrt{n}\|\Phi_m\|_\Lambda \cdot \|R^{(0)}\|_F,$$

where $\kappa(Z) = \|Z\|_F \|Z^{-1}\|_F$ and $\|\Phi_m\|_\Lambda := \sup_{\{\lambda_1,\ldots,\lambda_n\}} \|\Phi_m(\lambda)\|_F$. For the augmented BGMRES, we shall derive an analogous result. Let $\mathscr{K} \equiv \operatorname{span}\{R^{(0)}, AR^{(0)}, \ldots, A^{m-1}R^{(0)}, \bar{Z}\}$ be a block Krylov subspace augmented with some eigenvectors of A, $\bar{Z} = [z_1, \ldots, z_l]$. Then augmented BGMRES computes $X^{(m)}$ in $\mathscr{K}$ so that $\|R^{(m)}\|_F^2 = \operatorname{tr}[(R^{(m)})^{\mathrm{T}} R^{(m)}]$ is minimized.

Theorem 2.5. *Suppose A has spectral decomposition $A = Z\Lambda Z^{-1}$ with $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Let $R^{(0)} = \sum_{i=1}^{n} z_i\beta_i \equiv Z\beta$, where $\beta \in R^{n\times p}$ and β_i is the row vector of β. Assume that the minimum residual solution $X^{(m)}$ is extracted from the subspace $\mathscr{K}$. Then*

$$\|R^{(m)}\|_F \leqslant \kappa(Z)\sqrt{n-l}\,\|Q_m\|_{\bar{\Lambda}}^{=} \cdot \|R^{(0)}\|_F, \tag{2.10}$$

where $\|Q_m\|_{\bar{\Lambda}}^{=} = \sup_{\{\lambda_{l+1},\ldots,\lambda_n\}} \|Q_m(\lambda)\|_F$ and $Q_m(\lambda)$ satisfies

$$\left\|Q_m(A)\circ \overset{=}{R}^{(0)}\right\|_F = \min_{\Theta_m\in\mathscr{P}_{m,p}} \left\|\Theta_m(A)\circ \overset{=}{R}^{(0)}\right\|_F \tag{2.11}$$

with $\overset{=}{R}^{(0)} = \sum_{i=l+1}^{n} z_i\beta_i$.

Proof. For any $X - X^{(0)} \in \mathscr{K}$,

$$X = X^{(0)} + \bar{Z}\alpha + P(A)\circ R^{(0)},$$

where $P(\lambda)$ is a matrix-valued polynomial of degree $m-1$ and order p, and $\alpha \in R^{l\times p}$. Let $Q(\lambda) = I_p - \lambda P(\lambda) \equiv \sum_{i=0}^{m} \lambda^i\xi_i$ with $\xi_0 = I_p$ and $\bar{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_l)$. Then $Q \in \mathscr{P}_{m,p}$ and

$$\begin{aligned} R = B - AX &= R^{(0)} - A\bar{Z}\alpha - AP(A)\circ R^{(0)} = -\bar{Z}\bar{\Lambda}\alpha + Q(A)\circ R^{(0)} \\ &= -\bar{Z}\bar{\Lambda}\alpha + \sum_{i=0}^{m} A^i R^{(0)}\xi_i = -\bar{Z}\bar{\Lambda}\alpha + \sum_{i=0}^{m} Z\Lambda^i\beta\xi_i. \end{aligned}$$

Let $\beta = [\bar{\beta}^{\mathrm{T}}, \overset{=}{\beta}]^{\mathrm{T}}$ with $\bar{\beta} \in R^{l\times p}$ and $Z = [\bar{Z}, \overset{=}{Z}]$. Then

$$\begin{aligned} R &= -\bar{Z}\bar{\Lambda}\alpha + \sum_{i=0}^{m}(\bar{Z}\bar{\Lambda}^i\bar{\beta} + \overset{=}{Z}\overset{=}{\Lambda}^i\overset{=}{\beta})\xi_i \\ &= \sum_{j=1}^{l} z_j\left(\beta_j\sum_{i=0}^{m}\lambda_j^i\xi_i - \lambda_j\alpha_j\right) + \sum_{i=0}^{m} A^i\overset{=}{Z}\overset{=}{\beta}\xi_i \sum_{j=1}^{l} z_j(\beta_j Q(\lambda_j) - \lambda_j\alpha_j) + Q(A)\circ \overset{=}{R}^{(0)}, \end{aligned}$$

where α_j is the jth row vector of α. Now choose $Q(\lambda)$ to satisfy (2.11) and pick $\alpha_j = (1/\lambda_j)\beta_j Q(\lambda_j)$, $j = 1, \ldots, l$. Hence

$$R = Q(A)\circ \overset{=}{R}^{(0)} = \overset{=}{Z}Q(\overset{=}{\Lambda})\circ\overset{=}{\beta}.$$

Note that $\|Q(A)\circ B\|_F \leqslant \|Q(A)\|_F\|B\|_F$ (cf. Proof of Theorem 3.1 in [14]). We have that

$$\|R\|_F \leqslant \|\overset{=}{Z}\|_F\|Q(\overset{=}{\Lambda})\circ\overset{=}{\beta}\|_F \leqslant \|\overset{=}{Z}\|_F\|Q(\overset{=}{\Lambda})\|_F\|\overset{=}{\beta}\|_F \leqslant \|\overset{=}{Z}\|_F\sqrt{n-l}\,\|Q\|_{\bar{\Lambda}}^{=}\|\overset{=}{\beta}\|_F. \tag{2.12}$$

Since $\|\overset{=}{\beta}\|_F \leqslant \|\beta\|_F = \|Z^{-1}R^{(0)}\|_F \leqslant \|Z^{-1}\|_F\|R^{(0)}\|_F$, $\|\overset{=}{Z}\|_F \leqslant \|Z\|_F$ and $R^{(m)}$ is minimized in $\mathscr{K}$ in the sense of Frobenius norm, we derive (2.10). □

Remark. The bound in (2.12) probably is much smaller than in (2.10).

For approximate invariant subspace, we have

Theorem 2.6. *Suppose A has spectral decomposition $A = Z\Lambda Z^{-1}$ with $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Assume that the minimum residual solution $X^{(m)}$ is extracted from the subspace $\mathscr{K} \equiv \mathrm{span}\{R^{(0)}, AR^{(0)}, \ldots, A^{m-1}R^{(0)}, \bar{Y}\}$, where $\bar{Y} = [y_1, \ldots, y_l]$ satisfies $\bar{Y} = \bar{Z}\gamma + \bar{\bar{Z}}\eta, \gamma \in R^{l\times l}, \eta \in R^{(n-l)\times l}$. Then*

$$\|R^{(m)}\|_F \leqslant \kappa(Z)\sqrt{n-l}\|Q_m\|_{\bar{\bar{\Lambda}}} \cdot \|R^{(0)}\|_F + \sqrt{n-l}\max_{l+1\leqslant j\leqslant n}|\lambda_j|\|\alpha\|_F\|\eta\|_F, \quad (2.13)$$

where $Q_m(\lambda)$ satisfies (2.11) *and α is chosen in the following proof.*

Proof. For any $X - X^{(0)} \in \mathscr{K}$,

$$X = X^{(0)} + \bar{Y}\alpha + P(A)\circ R^{(0)},$$

where $\alpha \in R^{l\times p}$. Hence

$$R = B - AX = R^{(0)} - A\bar{Y}\alpha - AP(A)\circ R^{(0)} = Q(A)\circ R^{(0)} - A\bar{Z}\gamma\alpha - A\bar{\bar{Z}}\eta\alpha.$$

Let $\bar{\alpha} = \gamma\alpha \in R^{l\times p}$ and $\bar{\alpha}_j$ is the jth row vector of $\bar{\alpha}$. According to the proof procedure of Theorem 2.5, we have

$$R = \sum_{i=1}^{l} z_j(\beta_j Q(\lambda_j) - \lambda_j\bar{\alpha}_j) + Q(A)\circ\bar{\bar{R}}^{(0)} - A\bar{\bar{Z}}\eta\alpha.$$

Pick $\bar{\alpha}_j = (1/\lambda_j)\beta_j Q(\lambda_j)$. Then

$$R = Q(A)\circ\bar{\bar{R}}^{(0)} - A\bar{\bar{Z}}\eta\alpha.$$

So, we have

$$\begin{aligned}\|R\|_F &\leqslant \|Q(A)\circ\bar{\bar{\mathrm{R}}}^{(0)}\|_F + \|A\bar{\bar{Z}}\|_F\|\alpha\|_F\|\eta\|_F \\ &\leqslant \kappa(Z)\sqrt{n-l}\|Q\|_{\bar{\bar{\Lambda}}} \cdot \|R^{(0)}\|_F + \sqrt{n-l}\max_{l+1\leqslant j\leqslant n}|\lambda_j|\|\alpha\|_F\|\eta\|_F,\end{aligned}$$

where $\alpha = \gamma^{-1}\bar{\alpha}$. The result (2.13) is obtained since $R^{(m)}$ is minimized in $\mathscr{K}$. □

3. Implementation

The implementation of the algorithm presented here first generates the orthonormal basis of block Krylov subspace $\mathscr{K}_m$, then adds some approximate eigenvectors to it, and last solves a linear least-squares problem with a block upper-Hessenberg matrix and a generalized eigenvalue problem.

Suppose that block orthonormal sequences $V_1, \ldots, V_m, V_{m+1}$ with each matrix V_i being orthonormal have been produced by block Arnoldi process with initial matrix $R^{(0)}$, i.e., V_1 is obtained from the QR factorization: $R^{(0)} = V_1 R$, and l approximate eigenvectors $y_1, \ldots, y_l$ have been derived. Note: If there are complex eigenvectors in $\{y_i\}$, we add the real and imaginary part of them to $\mathscr{K}_m$, since A is a real matrix. Thus, the algorithm keeps real arithmetic. Let $W = [V_1, \ldots, V_m, y_1, \ldots, y_l]$ and $Q = [V_1, \ldots, V_m, V_{m+1}, q_1, \ldots, q_l]$, where q_i is formed by orthogonalizing the vectors Ay_i, $i = 1, \ldots, l$ against the previous columns of Q. Then, we have

$$AW = Q\bar{H}, \tag{3.1}$$

where $\bar{H}$ is an $(r+p) \times r$ block upper-Hessenberg matrix, and $r = mp + l$. Any $X - X^{(0)}$ in the subspace $\mathscr{K} = \operatorname{span}\{W\}$ can be written as

$$X = X^{(0)} + W\alpha.$$

where $\alpha \in R^{r \times p}$. Then, the relation (3.1) results in

$$B - AX = R^{(0)} - AW\alpha = V_1 R - Q\bar{H}\alpha = Q(E_1 R - \bar{H}\alpha), \tag{3.2}$$

where $E_1 = [I_p, 0]^{\mathrm{T}} \in R^{(r+p)\times p}$. The augmented block GMRES approximation solution $X^{(m)}$ will be derived by $X^{(m)} = X^{(0)} + W\alpha^{(m)}$, where $\alpha^{(m)}$ satisfies

$$\alpha^{(m)} = \arg \min_{\alpha \in R^{r\times p}} \|E_1 R - \bar{H}\alpha\|_F.$$

Set $(r+p)$-dimensional vector

$$\bar{g}_i = E_1 \operatorname{Re}_i. \tag{3.3}$$

It has the form $[r_{1i}, \ldots, r_{ii}, 0, \ldots, 0]^{\mathrm{T}}$, where r_{ij} is the entries of matrix R. Thus, the approximation $X^{(m)} = [x_1^{(m)}, \ldots, x_p^{(m)}]$ can be formed by $x_i^{(m)}$ which minimizes the 2-norm of the individual column of the block-residual (3.2), i.e.,

$$\|b_i - Ax_i^{(m)}\|_2 = \|\bar{g}_i - \bar{H}\alpha_i^{(m)}\|_2 = \min_{\alpha_i \in R^r} \|\bar{g}_i - \bar{H}\alpha_i\|_2.$$

Let

$$P\bar{H} = U = \begin{bmatrix} U_1 \\ 0 \end{bmatrix}, \tag{3.4}$$

where P is an orthogonal matrix of order $(r+p)$ and U_1 is an upper triangular matrix of order r. Then

$$\|b_i - Ax_i^{(m)}\|_2 = \min_{\alpha_i \in R^r} \|P\bar{g}_i - U\alpha_i\|_2. \tag{3.5}$$

As a byproduct, the residual norm of $x_i^{(m)}$ is the 2-norm of the vector consisting of the components $r+1$ through $r+p$ of $P\bar{g}_i$.

Next, to estimate the eigenvectors of A in the subspace span$\{W\}$, a projection technique is used onto span$\{W\}$. The approximate eigenvector y to be extracted from span$\{W\}$ can be expressed in the form $y = Wz$, where z is an r-dimensional vector. Let θ be an associated eigenvalue. We would require that the residual $(A - \theta I)y$ be orthogonal to span$\{W\}$ which gives us the problem

$$W^{\mathrm{T}}(A - \theta I)Wz = 0.$$

This requires solving a generalized eigenvalue problem

$$W^{\mathrm{T}}AWz = \theta W^{\mathrm{T}}Wz.$$

To find better approximations to the eigenvalues nearest to 0, Morgan [6,7] suggested to use the following version of Rayleigh–Ritz:

$$W^{\mathrm{T}}A^{\mathrm{T}}AWz = \theta W^{\mathrm{T}}A^{\mathrm{T}}Wz. \tag{3.6}$$

This means that using the basis AW for the orthogonality condition, the Galerkin condition gives the problem

$$(AW)^{\mathrm{T}}(A - \theta I)Wz = 0.$$

Let $F = W^{\mathrm{T}}A^{\mathrm{T}}W$ and $G = (AW)^{\mathrm{T}}(AW)$. Then (3.6) is an $r \times r$ generalized eigenvalue problem

$$Gz = \theta Fz. \tag{3.7}$$

This problem will give us l eigenvectors z_i associated with the l smallest eigenvalues $\theta_i, i = 1, \ldots, l$. Corresponding approximate eigenvectors of A is $y_i = Wz_i$. To calculate the matrices G and F, Morgan used (3.1) and (3.4):

$$G = (AW)^{\mathrm{T}}AW = \bar{H}^{\mathrm{T}}Q^{\mathrm{T}}Q\bar{H} = \bar{H}^{\mathrm{T}}\bar{H} = U_1^{\mathrm{T}}U_1.$$

For the matrix F, since

$$F = W^{\mathrm{T}}A^{\mathrm{T}}W = \begin{bmatrix} V^{\mathrm{T}}A^{\mathrm{T}}V & V^{\mathrm{T}}A^{\mathrm{T}}Y \\ Y^{\mathrm{T}}A^{\mathrm{T}}V & Y^{\mathrm{T}}A^{\mathrm{T}}Y \end{bmatrix},$$

where $V = [V_1, \ldots, V_m]$ and $Y = [y_1, \ldots, y_l]$, the first mp columns are the same as the first mp columns of $\bar{H}^{\mathrm{T}}$. For the entries of $V^{\mathrm{T}}A^{\mathrm{T}}Y$, p-dimensional vectors $f_{ij} = (AV_i)^{\mathrm{T}}y_j,\ i = 1, \ldots, m,\ j = 1, \ldots, l$. For the remaining entries of $Y^{\mathrm{T}}A^{\mathrm{T}}Y$, elements $f_{ij} = y_i^{\mathrm{T}}A^{\mathrm{T}}y_j = z_i^{\mathrm{T}}W_{\mathrm{old}}^{\mathrm{T}}A^{\mathrm{T}}W_{\mathrm{old}}z_j = z_i^{\mathrm{T}}F_{\mathrm{old}}z_j,\ i, j = 1, \ldots, l$, where F_{old} denotes the previous F.

For a brief description of the algorithm, we let l can be divided by p with no remainder, i.e., $l = t \cdot p$; otherwise, the Arnoldi process for the underlying subspace $\mathscr{K}$ should be kept a vectorwise computation, i.e., block Arnoldi–Ruhe's version (see [10,11]) should be used to generate the basis of $\mathscr{K}$. $(r + p) \times r$ block upper-Hessenberg matrix $\bar{H}$ and $r \times r$ matrix F have the following form ($m = 4, l = 2p$):

$$\bar{H} = \begin{bmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & H_{16} \\ H_{21} & H_{22} & H_{23} & H_{24} & H_{25} & H_{26} \\ 0 & H_{32} & H_{33} & H_{34} & H_{35} & H_{36} \\ 0 & 0 & H_{43} & H_{44} & H_{45} & H_{46} \\ 0 & 0 & 0 & H_{54} & H_{55} & H_{56} \\ 0 & 0 & 0 & 0 & H_{65} & H_{66} \\ 0 & 0 & 0 & 0 & 0 & H_{76} \end{bmatrix},$$

$$F = \begin{bmatrix} F_{11} & F_{12} & 0 & 0 & F_{15} & F_{16} \\ F_{21} & F_{22} & F_{23} & 0 & F_{25} & F_{26} \\ F_{31} & F_{32} & F_{33} & F_{34} & F_{35} & F_{36} \\ F_{41} & F_{42} & F_{43} & F_{44} & F_{45} & F_{46} \\ F_{51} & F_{52} & F_{53} & F_{54} & F_{55} & F_{56} \\ F_{61} & F_{62} & F_{63} & F_{64} & F_{65} & F_{66} \end{bmatrix}.$$

Now, we summarize the algorithm, the restarted Block GMRES method augmented with ($l = t \cdot p$) eigenvectors, denoted by ABGMRES($m, t \cdot p, p$), as the following:

ABGMRES($m, t \cdot p, p$)

Given initial value $X^{(0)} \in R^{n\times p}$, $Y = [Y_1, \ldots, Y_t] \in R^{n\times l}$ and integer m. Compute $R^{(0)} = B - AX^{(0)}$. For $k = 0, 1, \ldots,$

1. QR factorization: $R^{(k)} = V_1 R$; For $j = 1, \ldots, t$, $i = 1, \ldots, t$, Do if ($k = 0$) then $F_{m+i,m+j} = (AY_i)^{\mathrm{T}} Y_j$ else $F_{m+i,m+j} = Z_i^{\mathrm{T}} F Z_j$, EndDo.
2. For $j = 1, 2, \ldots, m$, Do$W_j = AV_j$; for $i = 1, \ldots, t$, do $F_{j,m+i} = W_j^{\mathrm{T}} Y_i$, enddo;

$$\text{for } i = 1, \ldots, j, \text{ do } \begin{cases} H_{ij} = V_i^{\mathrm{T}} W_j, \\ F_{ji} = H_{ij}^{\mathrm{T}}, \\ W_j := W_j - V_i H_{ij}. \end{cases}$$

   QR factorization: $W_j = V_{j+1} H_{j+1,j}$; if ($j < m$) then $F_{j,j+1} = H_{j+1,j}^{\mathrm{T}}$, EndDo.
3. For $r = 1, \ldots, t$, Do $j = m + r$, $W_j = AY_r$;

$$\text{for } i = 1, \ldots, j, \text{ do } \begin{cases} H_{ij} = V_i^{\mathrm{T}} W_j, \\ \textit{if } (i \leqslant m) \textit{ then } F_{ji} = H_{ij}^{\mathrm{T}}, \\ W_j := W_j - V_i H_{ij}. \end{cases}$$

   QR factorization: $W_j = V_{j+1} H_{j+1,j}$, EndDo.
4. According to (3.5), for $i = 1, \ldots, p$, find $\alpha_i^{(m)}$ that minimizes $\|P\bar{g}_i - U\alpha_i\|_2$ for all $\alpha_i \in R^r$, where $\bar{g}_i, P, U$ can be derived from (3.3) and (3.4). Then $x_i^{(m)} = x_i^{(0)} + W\alpha_i^{(m)}$.
5. Compute $R^{(k)} = B - AX^{(m)}$; if ($\|R^{(k)}\|_F < \epsilon$) then *stop* else $X^{(0)} := X^{(m)}$.
6. Compute $G = U_1^{\mathrm{T}} U_1$ and form F; seek l eigenvectors z_i associated with the l smallest eigenvalues θ_i from $Gz_i = \theta_i F z_i$ ($i = 1, \ldots, l$); form $Y = WZ$.

Remark 1. If l is divided by p with remainder, vectorwise computation should be used in part 3.

Remark 2. If some y_i is linearly expressed by $V_1, \ldots, V_m$, the standard Krylov subspace $\mathscr{K}_m$ has already included the component part of approximate eigenvector y_i, so y_i can be discarded.

Remark 3. If some individual residual satisfies $\|r_i^{(m)}\|_2 < \epsilon$, i.e., $x_i^{(m)}$ has become an acceptable solution, a deflation could be used so that the block size p would be reduced.

We now examine the expense requirements for the ABGMRES$(m, t \cdot p, p)$ method as compared to the restarted block GMRES method, denoted by BGMRES $(m + t, p)$. Note that the subspaces used in two methods keep the same size. The major computational costs for each iteration (on superscript k) of two methods to restart are shown in Table 1. We denote by $A \cdot x$ the cost for performing one matrix–vector multiplication with the (sparse) matrix A.

From Table 1, we see that since p, m and t are small, the additional expense in ABGMRES is little.

Remark 4. If A is not very sparse or n is very large, the computation of AY in ABGMRES can be derived through $AY = Q\bar{H}Z$, the expense of which is $l(r + p)$ n-vector DOT and r-vector DOT(products), respectively. Thus, the cost of l matrix–vector multiplication $A \cdot x$ of ABGMRES in Table 1 should be replaced by the cost of $Q\bar{H}Z$. At the same time, $nl + \frac{1}{2}r(r + 1)$ memories must be added to ABGMRES in Table 2.

Leading storage requirements for the ABGMRES method and the BGMRES method (excluding those for A, X, and B) are listed in Table 2. Since $r \ll n$, two methods have the same memory requirement essentially. However, if AY in ABGMRES is computed through $AY = Q\bar{H}Z$, $nl + \frac{1}{2}r(r + 1)$ memories must be added to ABGMRES in Table 2, which is not a small amount.

Table 1
Leading computational costs per iteration of methods to restart

	ABGMRES$(m, t \cdot p, p)$	BGMRES$(m + t, p)$
$A \cdot x$	$r + p$	$r + p$
n-vector DOT(products)	$\frac{3}{2}r(r + p) + (r + mp)tp$	$\frac{3}{2}r(r + p)$
r-vector DOT(products)	$(r + p)t^2p$	–
QR factorization on $n \times p$ matrix	$m + t + 1$	$m + t + 1$
Solve $(r + p) \times r$ Least-squared problem	p	p
Solve order r generalized Eigenvalue problem	1	

Table 2
The leading storage for each method

ABGMRES$(m, t \cdot p, p)$	$n(r+2p)+\frac{3}{2}r^2+\mathrm{O}(pr)$
BGMRES$(m+t, p)$	$n(r+2p)+\frac{1}{2}r^2+\mathrm{O}(pr)$

4. Numerical experiment

In this section, we present some numerical examples to illustrate the convergence behavior of ABGMRES compared with BGMRES when restarting is used. The algorithms are computed on the basis of the number of iteration for k (the superscript k denotes the number of restarting) necessary to achieve residual $\max_{1\leqslant j\leqslant p}\|r_j^{(k)}\|_2 < \epsilon = 10^{-6}$. We set the limited iteration number on k to be 200. The initial value $X^{(0)} = 0$ and $Y = [e_1, \ldots, e_l]$ are chosen, where e_i is the ith n-dimensional canonical coordinate vector. We use subspace method to solve the generalized eigenvalue problem (3.7). In all the examples, we let $l = p$, i.e., the number of augmented eigenvectors is equal to block size, and the right-hand vector b_j is produced by setting $b_j = Au_j$, where

$$u_j = (1, \ldots, 1, \underbrace{0, \ldots, 0}_{j-1})^{\mathrm{T}} \quad (j = 1, \ldots, p).$$

All the test codes were written by Fortran77 using double precision.

The first three examples were taken from [7] and the matrix A in these examples is all bidiagonal matrix with 0.1 in each superdiagonal position.

Example 1. Let matrix A have the entries $1, 2, 3, \ldots, 1000$ on the main diagonal, so A has eigenvalue $1, 2, 3, \ldots, 1000$. We choose different block size p (p now is also the number of augmented eigenvectors) and different m, the number of Krylov block basis in ABGMRES(m, p, p), compared with BGMRES$(m+1, p)$. Thus, the same size subspace is used. The computation results are listed in Table 3.

Table 3
Iteration number to convergence for Example 1 with different m and p

p	ABGMRES				BGMRES			
	$m=24$	$m=19$	$m=14$	$m=9$	$m=25$	$m=20$	$m=15$	$m=10$
1	11	16	26	56	16	23	37	76
2	7	9	13	25	12	15	22	29
3	5	7	10	18	14	17	20	28
4	4	6	10	19	11	15	22	28
8	3	3	3	7	10	14	18	26

From Table 3, we can see that for $p > 1$, $m \geqslant 14$, ABGMRES method converges essentially more than twice as fast as BGMRES method; especially for large p, the convergence is faster. Even with a smaller subspace, e.g., $p \geqslant 3$ and $m = 14$, ABGMRES(m, p, p) converges still faster than BGMRES$(25, p)$ with a larger subspace.

Example 2. In this example, the entries on the main diagonal are $0.01, 0.02, 0.03, 0.04, 10, 11, 12, \ldots, 1005$, so matrix A has four very small eigenvalues. The results can be seen in Table 4.

For all p and m, BGMRES does not converge essentially. For small p ($\leqslant 2$), the convergence behavior of ABGMRES is not very good; however, for $p \geqslant 4$, the convergence of ABGMRES keeps similar convergence behavior to Example 1.

Example 3. Let matrix A have diagonal elements $1, 1.01, 1.02, 1.03, 1.04, 2, 3, 4, \ldots, 996$. Though A has no very small eigenvalues, some eigenvalues are very close. They are difficult to compute by Morgan's single method, i.e., GMRES method augmented with eigenvector. So the standard GMRES method and Morgan's single method are roughly equivalent to compute this example when using the same size subspace; see [7]. However, in our computation of this example, ABGMRES is still much better than BGMRES; see Table 5.

Table 4
Iteration number to convergence for Example 2 with different m and p[a]

p	ABGMRES			BGMRES		
	$m = 24$	$m = 19$	$m = 14$	$m = 25$	$m = 20$	$m = 15$
1	×	×	×	×	×	×
2	15	37	×	×	×	×
3	18	27	118	×	×	185
4	4	6	9	69	×	×
8	3	3	4	×	×	132

[a] Note: the notation × means that the residual norms have not reached the accuracy ϵ after 200 iterations.

Table 5
Iteration number to convergence for Example 3 with different m and p

p	ABGMRES			BGMRES		
	$m = 24$	$m = 19$	$m = 14$	$m = 25$	$m = 20$	$m = 15$
1	12	16	26	16	23	37
2	7	10	15	14	16	19
3	7	8	13	14	17	21
4	7	7	13	14	16	20

Example 4. We consider the following Dirichlet problem:

$$-u_{xx} - u_{yy} + \sigma u_x = f, \quad \Omega = \{(x,y),\ 0 \leqslant x, y \leqslant 1\}$$
$$u = 0 \quad \text{on } \partial\Omega$$

with $\sigma \geqslant 0$. The five-point centered difference is used to discrete the equation on 31×31 grid with mush size $h = \frac{1}{32}$ and natural ordering. The resulting linear systems have a pentadiagonal coefficient matrix A of order $N = 961$. Tests are done with $\sigma = 0$ and $\sigma = 128$, which result in $A = (-1, -1, 4, -1, -1)$ and $A = (-1, -3, 4, 1, -1)$, respectively. See Tables 6 and 7 for the computational results. For $\sigma = 0$, the convergence rate of ABGMRES is about twice as fast as BGMRES; however, for $\sigma = 128$, the effect of using eigenvectors is not very great.

From the computation results of our test examples, we see that the ABGMRES method enjoys the good convergence behaviors as Morgan's single method. It has an improved convergence rate on BGMRES method. Furthermore, ABGMRES method still has a fast convergence rate than BGMRES method in some examples for which Morgan's single method is roughly equivalent with the standard GMRES method; see Example 3 in this section and Example 4 in [7].

Table 6
Iteration number to convergence for Example 4 with $\sigma = 0$

p	ABGMRES			BGMRES		
	$m = 24$	$m = 19$	$m = 14$	$m = 25$	$m = 20$	$m = 15$
1	4	5	7	6	7	15
2	4	5	7	6	7	15
3	3	4	6	6	7	14
4	3	4	6	6	7	14

Table 7
Iteration number to convergence for Example 4 with $\sigma = 128$

p	ABGMRES			BGMRES		
	$m = 24$	$m = 19$	$m = 14$	$m = 25$	$m = 20$	$m = 15$
1	10	10	13	9	13	13
2	6	9	11	8	14	15
3	7	9	12	8	12	12
4	7	9	11	7	10	14

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