Iranian Journal of Numerical Analysis and Optimization
Vol. 12, No. 3 (Special Issue), 2022, pp 533–541
DOI:10.22067/ijnao.2022.73913.1081
https://ijnao.um.ac.ir/

How to cite this article
Research Article

On stagnation of the DGMRES method

F. Kyanfar

Abstract

Let A be an n-by-n matrix with index $\alpha > 0$ and $b \in \mathbb{C}^n$. In this paper, the problem of stagnation of the DGMRES method for the singular linear system $Ax = b$ is considered. We show that DGMRES(A, b, α) has partial stagnation of order at least k if and only if $(0, \dots, 0)$ belongs to the the joint numerical range of matrices $\{B^{\alpha+1}, \dots, B^{\alpha+k}\}$, where B is a compression of A to the range of A^α. Also, we characterize the nonsingular part of a matrices A such that DGMRES(A, b, α) does not stagnate for all $b \in \mathbb{C}^n$. Moreover, a sufficient condition for non-existence of real stagnation vectors $b \in \mathcal{R}(A^\alpha)$ for the DGMRES method is presented, and the DGMRES stagnation of special matrices are studied.

AMS subject classifications (2020): 65F10; 15A06; 15A60.

Keywords: Stagnation; DGMRES method; Singular systems.

1 Introduction

Let A be an n-by-n matrix with index α. The index is the size of the largest Jordan block of A corresponding to the zero eigenvalue. The Drazin inverse A^D of A is the unique n-by-n matrix that satisfies

$$AA^D = A^D A, \quad A^{\alpha+1}A^D = A^\alpha, \quad A^D A A^D = A^D.$$

Since A^D can be written as a polynomial in A [2, p. 186], there is a possibility of using Krylov subspace methods to find the Drazin inverse solution $A^D b$ to a possibly inconsistent linear system $Ax = b$. Such an algorithm, called DGMRES, developed by Sidi [7]. DGMRES has been considered in several studies; see [1, 8]. This algorithm is similar to the GMRES algorithm developed by Saad and Schultz [6] for solving nonsingular linear systems.

Received 8 December 2021; revised 1 March 2022; accepted 15 March 2022

Faranges Kyanfar
Department of Applied Mathematics, Shahid Bahonar University of Kerman, Iran. e-mail: kyanfar@uk.ac.ir

The stagnation of GMRES was studied in [3, 5, 10] and the stagnation of DGMRES was studied in [11].

Note that while the linear system $Ax = b$ may have no solution, if we multiply each side by A^α, then the linear system $A^{\alpha+1}x = A^\alpha b$ is consistent and has $x = A^D b$ as a solution. The DGMRES algorithm works as follows. Given an initial guess x_0, compute the initial residual $r_0 = b - Ax_0$. We will choose approximate solutions x_k, $k = 1, 2, \dots, n-\alpha$, to be of the form x_0 plus a linear combination of vectors from the kth Krylov subspace

$$\mathcal{K}_k(A, A^\alpha r_0) = span\{A^\alpha r_0, \dots, A^{\alpha+k-1} r_0\}, \tag{1}$$

such that the residual vector $r_k = b - Ax_k$ satisfies

$$\begin{aligned} \|A^\alpha r_k\| &= \min_{x \in \mathcal{K}_k(A, A^\alpha r_0)} \|A^\alpha (b - A(x_0 + x)\| \\ &= \min_{c_1, \dots, c_k} \|A^\alpha (b - A(x_0 + c_1 A^\alpha r_0 + \cdots + c_k A^{\alpha+k-1} r_0))\| \\ &= \min_{c_1, \dots, c_k} \|A^\alpha r_0 - c_1 A^{2\alpha+1} r_0 - \cdots - c_k A^{2\alpha+k} r_0))\|. \end{aligned} \tag{2}$$

The DGMRES terminates with the exact Drazin-inverse solution in at most $n - \alpha$ iterations (i.e., $\|A^\alpha r_{n-\alpha}\| = 0$) [7]. Throughout this paper, $\|\cdot\|$ denotes the Euclidean norm for vectors and the spectral norm for matrices. Without loss of generality, we assume that $x_0 = 0$ and $\|A^\alpha r_0\| = \|A^\alpha b\| = 1$, because if $A^\alpha r_0 = 0$, then the DGMRES algorithm has the solution x_0 at the initial step, in other words, the DGMRES algorithm has no progress.

Definition 1. Let $\{A_1, A_2, \dots, A_k\}$ be $n \times n$ matrices. The joint numerical range for $(A_1, A_2, \dots, A_k)$ is defined and denoted by

$$W(A_1, A_2, \dots, A_k) := \{(x^* A_1 x, x^* A_2 x, \dots, x^* A_k x) : x \in \mathbb{C}^n, x^* x = 1\}.$$

Note that in Definition 1, if $k = 1$, then the joint numerical range coincide with the standard numerical range.

2 Partial stagnation of DGMRES

In this section, the problem of stagnation of the DGMRES algorithm for singular linear system $Ax = b$ is studied.

Definition 2. Let A be an n-by-n matrix with index α and a right-hand side vector $b \in \mathbb{C}^n$. We say that DGMRES (A, b, α) has partial stagnation of order k, if

$$\|A^\alpha r_0\| = \cdots = \|A^\alpha r_k\| > \|A^\alpha r_{k+1}\| \geq \cdots \geq \|A^\alpha r_{n-\alpha}\| = 0. \tag{3}$$

Also, if DGMRES (A, b, α) has partial stagnation of order $k = n - \alpha - 1$, then DGMRES (A, b, α) has complete stagnation. DGMRES (A, b, α) does not stagnate, if DGMRES (A, b, α) has not partial stagnation of any order.

In the following result, we state an equivalent definition for partial stagnation [11].

Lemma 1. Let A be an n-by-n matrix with index α and a right-hand side vector $b \in \mathbb{C}^n$. Then DGMRES (A, b, α) has partial stagnation of order at least k if and only if $A^\alpha b$ is perpendicular to $\text{span}\{A^{2\alpha+1}b, \dots, A^{2\alpha+k}b\}$.

Proof. By using (2), we obtain that for all $1 \le i \le k$,

$$\|A^\alpha b\| = \min_{c_1,\dots,c_i} \|A^\alpha b - c_1 A^{2\alpha+1} b - \cdots - c_i A^{2\alpha+i} b))\|.$$

Therefore, $A^\alpha b$ should be perpendicular to $\text{span}\{A^{2\alpha+1}b, \dots, A^{2\alpha+k}b\}$. □

By using the Core-Nilpotent decomposition and QR decomposition, we obtain the following decomposition [1].

Let $A \in \mathbb{C}^{n\times n}$ with $\alpha = ind(A) > 0$. Then there exists a unitary matrix $Q \in \mathbb{C}^{n\times n}$ such that

$$A = Q \begin{bmatrix} B & * \\ 0 & N \end{bmatrix} Q^*, \tag{4}$$

where $B \in \mathbb{C}^{m\times m}$ is the compression of A to $\mathcal{R}(A^\alpha)$ and N is nilpotent with index α.

Theorem 1. Let $A \in \mathbb{C}^{n\times n}$ with index α be as in (4). Then there exists a vector $b \in \mathbb{C}^n$ such that DGMRES(A, b, α) has partial stagnation of order at least k if and only if $(0, \dots, 0) \in W(B^{\alpha+1}, \dots, B^{\alpha+k})$.

Proof. By Lemma 1, we know that the DGMRES(A, b, α) has partial stagnation of order at least k, if and only if $(A^\alpha b)^* A^{2\alpha+i} b = 0,\ i = 1, \dots, k$. Then

$$(A^\alpha b)^*(A^{\alpha+i})(A^\alpha b) = 0, \qquad i = 1, \dots, k. \tag{5}$$

By using (4) and (5), for $i = 1, \dots, k$,

$$\begin{aligned}(A^\alpha b)^*(A^{\alpha+i})(A^\alpha b) &= (A^\alpha b)^* Q \begin{bmatrix} B^{\alpha+i} & * \\ 0 & N^{\alpha+i} \end{bmatrix} Q^*(A^\alpha b) \\ &= (Q^*(A^\alpha b))^* \begin{bmatrix} B^{\alpha+i} & * \\ 0 & 0 \end{bmatrix} Q^*(A^\alpha b) = 0. \end{aligned}\tag{6}$$

Define $z = \binom{z_1}{z_2} = Q^*(A^\alpha b)$, where $z_1 \in \mathbb{C}^m$. Since $0 \neq A^\alpha b \in \mathcal{R}(A^\alpha)$ and the last $n - m$ columns of Q form an orthonormal basis for the $\mathcal{R}(A^\alpha)^\perp$, we obtain that $z_2 = 0$ and hence $\|z_1\| = \|z\| = \|Q^*(A^\alpha b)\| = 1$. Therefore,

$$z^* \begin{bmatrix} B^{\alpha+i} & * \\ 0 & 0 \end{bmatrix} z = z_1^* B^{\alpha+i} z_1 = 0,\ i = 1, \dots, k. \tag{7}$$

This means that $(0, \dots, 0) \in W(B^{\alpha+1}, \dots, B^{\alpha+k})$.

Conversely, assume that $(0, \dots, 0) \in W(B^{\alpha+1}, \dots, B^{\alpha+k})$. Then there exists a unit vector $z_1 \in \mathbb{C}^m$ such that $z_1^* B^{\alpha+i} z_1 = 0,\ i = 1, \dots, k$. Define

$z = \binom{z_1}{0} \in \mathbb{C}^n$. Then (7) holds. We know that the first m columns of Q form an orthonormal basis for the range of A^α. Then $Qz = Q\binom{z_1}{0} \in \mathcal{R}(A^\alpha)$, and hence the equation $A^\alpha x = Qz$ has a solution $x = b$. Since $z = Q^*(A^\alpha b)$, by using (7)

$$(Q^*(A^\alpha b))^* \begin{bmatrix} B^{\alpha+i} & * \\ 0 & 0 \end{bmatrix} (Q^*(A^\alpha b)) = z_1^* B^{\alpha+i} z_1 = 0,\ i = 1, \ldots, k.$$

Therefore, $(A^\alpha b)^*(A^{\alpha+i})(A^\alpha b) = (A^\alpha b)^*(A^{2\alpha+i} b) = 0,\ i = 1, \ldots k$. This shows that $A^\alpha b$ is perpendicular to $A^{2\alpha+i}b,\ i = 1, \ldots, k$. Then by Lemma 1, DGMRES(A, b, α) has partial stagnation of order at least k. □

3 Complete stagnation of DGMRES

Let A be an n-by-n matrix with index α and let $b \in \mathbb{C}^n$. By Definition 2, we know that DGMRES(A, b, α) has complete stagnation if

$$\|A^\alpha r_0\| = \cdots = \|A^\alpha r_{n-\alpha-1}\| > \|A^\alpha r_{n-\alpha}\| = 0. \tag{8}$$

In the following result, we show that $\|A^\alpha r_m\| = 0$.

Theorem 2. Let $A \in M_n(\mathbb{C})$ with index α be as in (4) and let $b \in \mathbb{C}^n$. Then $A^\alpha r_m = 0$, where m is the dimension of $\mathcal{R}(A^\alpha)$, the range of A^α.

Proof. The matrix $B \in M_m(\mathbb{C})$ is nonsingular, so by using the Cayley–Hamilton theorem, there exists a polynomial of degree at most $m-1$ say $p(x) = a_{m-1}x^{m-1} + \cdots + a_1 x + a_0$ such that $(B^{-1})^{\alpha+1} = p(B)$. Then by [2, p. 186] the Drazin inverse $A^D = A^\alpha p(A)$. Then

$$\begin{aligned} \|A^\alpha r_m\| &= \min_{x \in \mathcal{K}_m(A, A^\alpha b)} \|A^\alpha (b - Ax)\| \\ &= \min_{t_0, \ldots, t_{m-1}} \|A^\alpha b - A^{2\alpha+1}(t_0 b + \cdots + t_{m-1} A^{m-1} b)\| \\ &\le \|A^\alpha b - A^{2\alpha+1}(a_0 b + \cdots + a_{m-1} A^{m-1} b)\| \\ &= \|A^\alpha b - A^{\alpha+1}[A^\alpha p(A)]b\| = \|(A^\alpha - A^{\alpha+1} A^D) b)\|. \end{aligned} \tag{9}$$

Since $A^{\alpha+1}A^D = A^\alpha$, we obtain that $\|A^\alpha r_m\| = 0$. □

Remark 1. Theorem 2 shows that the DGMRES method terminates at most after m iterations. Then the complete stagnation occurs if $m = n - \alpha$. This means that the nilpotent part N in (4) must be equal to the Jordan block of size α corresponding to zero eigenvalue, $N = J_\alpha(0)$.

4 Stagnation of real matrices

Let $A \in \mathbb{R}^{n\times n}$ with $\alpha = ind(A) > 0$. Then by the core-nilpotent and QR decompositions for real matrices, there exist an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$, an invertible matrix $B \in \mathbb{R}^{m\times m}$, and a nilpotent matrix $N \in \mathbb{R}^{n-m\times n-m}$ such that (4) holds. Let $A \in \mathbb{R}^{n\times n}$ and let $e \in \mathbb{R}^n$. Then easy computation shows that

$$e^T Ae = 0 \text{ if and only if } e^T(A + A^T)e = 0.$$

Let $A \in \mathbb{R}^{n\times n}$ be as in (4) with $\alpha = ind(A) > 0$. If we are looking for a real stagnation vector $e \in \mathcal{R}(A^\alpha)$, it is enough to consider the following polynomial system:

$$e^T(A^{\alpha+i} + (A^{\alpha+i})^T)e = 0, \qquad i = 1, 2, \ldots, k, \quad e^T e = 1. \tag{10}$$

Meurant [4, Theorem 2.2] presented a sufficient condition for non-existence of real stagnation vectors $b \in \mathbb{R}^n$ for the GMRES method. In the following result, we state a sufficient condition for non-existence of real stagnation vectors $b \in \mathcal{R}(A^\alpha)$ for DGMRES method.

Theorem 3. Let $A \in \mathbb{R}^{n\times n}$ with $\alpha = ind(A) > 0$ be as in (4) and let $B_i := B^i + (B^i)^T, \quad i = \alpha + 1, \alpha + 2, \ldots, \alpha + k$, where $k \leq m$ is a natural number. If there exist real scalars $\mu_i, \quad i = 1, 2, \ldots, k$ such that the matrix $\mu_1 B_{\alpha+1} + \cdots + \mu_k B_{\alpha+k}$ is a (positive or negative) definite matrix, then there is no real stagnation vector $e \in \mathcal{R}(A^\alpha)$.

Proof. Assume if possible there exist a real stagnation vector $e \in \mathcal{R}(A^\alpha)$. Then there exists $b \in \mathbb{R}^n$ such that $e = A^\alpha b$ and (5) holds. By using the notations $z = \binom{z_1}{z_2} = Q^T(A^\alpha b)$ with $\|z_1\| = 1$ in Theorem 1, we obtain that $z_1^T B^{\alpha+i} z_1 = 0, \ i = 1, \ldots, k$. By (10), $z_1^T(B^{\alpha+i} + (B^{\alpha+i})^T)z_1 = z_1^T B_{\alpha+i} z_1 = 0, \ i = 1, \ldots, k$, and hence $z_1^T(\mu_1 B_{\alpha+1} + \cdots + \mu_k B_{\alpha+k})z_1 = 0$. Since $\mu_1 B_{\alpha+1} + \cdots + \mu_k B_{\alpha+k}$ is (positive or negative) definite, we obtain that $z_1 = 0$, a contradiction with $\|z_1\| = 1$. $\square$

Example 1. Let A be as in (4), where $B = \begin{bmatrix} 1 & 2 & 1 \\ 1 & -1 & 2 \\ 1 & 0 & -1 \end{bmatrix}$ and $N = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$.
It is readily seen that $10B_2 + B_3 = \begin{bmatrix} 96 & 30 & 44 \\ 30 & 62 & -1 \\ 44 & -1 & 44 \end{bmatrix}$ is positive definite, where $B_2 = B^2 + (B^2)^T$ and $B_3 = B^3 + (B^3)^T$. Then by Theorem 3, there is no real stagnation vector.

5 Stagnation of special matrices

Let A be as in (4). If $m = 0$, then A is nilpotent with index α, which means that $A^\alpha = 0$, and hence $A^\alpha b = 0$ for all $b \in \mathbb{C}^n$. Then without loss of generality, we assume that $\|A^\alpha b\| = 1$ throughout this paper. Also, we assume that $m > 0$, which means that $B \in M_m(\mathbb{C})$ is invertible and A is not nilpotent. In this section, we are going to characterize all matrices $B \in M_m(\mathbb{C})$ such that DGMRES(A, b, α) does not stagnate, for all $b \in \mathbb{C}^n$ and unitary matrices $Q \in M_n(\mathbb{C})$.

The decomposition (4) is known as the core-nilpotent decomposition of A. Moreover, the matrix B is nonsingular. On the other hand, this decomposition is shown by $A = B \oplus N$.

Theorem 4. Let $B \in M_m(\mathbb{C})$ be an invertible matrix and let $N \in M_{n-m}(\mathbb{C})$ be a nilpotent matrix with index α. Then $B^{\alpha+1}$ is a scalar matrix if and only if DGMRES(A, b, α) does not stagnate for any $b \in \mathbb{C}^n$ and invertible $V \in M_n(\mathbb{C})$, where $A = V \begin{bmatrix} B & 0 \\ 0 & N \end{bmatrix} V^{-1}$.

Proof. Assume that$B^{\alpha+1} = \lambda I_m$ is a scalar matrix, where $\lambda \neq 0$. Let $b \in \mathbb{C}^n$ be an arbitrary vector and let $V \in M_n(\mathbb{C})$ be an arbitrary invertible matrix. Assume that $V = QR$ is the QR decomposition of V. Then

$$\begin{aligned} A = V \begin{bmatrix} B & 0 \\ 0 & N \end{bmatrix} V^{-1} =& Q \begin{bmatrix} R_1 & * \\ 0 & R_2 \end{bmatrix} \begin{bmatrix} B & 0 \\ 0 & N \end{bmatrix} \begin{bmatrix} R_1^{-1} & * \\ 0 & R_2^{-1} \end{bmatrix} Q^* \\ =& Q \begin{bmatrix} R_1 B R_1^{-1} & * \\ 0 & R_2 N R_2^{-1} \end{bmatrix} Q^*. \end{aligned}$$

Note that $R_2 N R_2^{-1}$ is again a nilpotent matrix with index $\alpha > 0$ and that $R_1 B R_1^{-1} = \lambda I_m$ is a scalar matrix. Since $0 \notin W((R_1 B R_1^{-1})^{\alpha+1}) = \{\lambda^{\alpha+1}\}$, by Theorem 1, DGMRES$(A, b, \alpha)$ does not stagnate, for any $b \in \mathbb{C}^n$ and $V \in M_n(\mathbb{C})$.

Conversely, let DGMRES(A, b, α) do not stagnate for any $b \in \mathbb{C}^n$ and let $V \in M_n(\mathbb{C})$. Assume if possible $B^{\alpha+1}$ is not a scalar matrix. Then by [9, Theorem 3], there exists an invertible matrix $V_1 \in M_m(\mathbb{C})$ such that $0 \in W(V_1 B^{\alpha+1} V_1^{-1})$. Let $V_1 = Q_1 R_1$ be the QR decomposition of V_1. Define the matrix $V := \begin{bmatrix} V_1 & 0 \\ 0 & I_{n-m} \end{bmatrix}$ and the unitary matrix $Q := \begin{bmatrix} Q_1 & 0 \\ 0 & I_{n-m} \end{bmatrix}$. Then

$$A = V \begin{bmatrix} B & 0 \\ 0 & N \end{bmatrix} V^{-1} = Q \begin{bmatrix} R_1 B R_1^{-1} & 0 \\ 0 & N \end{bmatrix} Q^*.$$

Since $0 \in W(V_1 B^{\alpha+1} V_1^{-1}) = W(R_1 B^{\alpha+1} R_1^{-1})$, by Theorem 1, DGMRES$(A, b, \alpha)$ has a partial stagnation of order at least one, a contradiction. Then $B^{\alpha+1}$ is a scalar matrix. □

Zhou and Wei [11, Section 3] showed that for 2×2 matrices, the stagnation system has no relation with condition number of V and that the stagnation system always has a real root, where V is the Jordan transformation matrix of A. Indeed, in the following result, we show that for any 2×2 matrix A, DGMRES(A, b, α) does not stagnate for any Jordan transformation matrix $V \in M_2(\mathbb{C})$ and $b \in \mathbb{C}^2$.

Proposition 1. Let A be a nonzero singular 2×2 matrix with index $\alpha = 1$ and let $b \in \mathbb{C}^2$ be an arbitrary vector. Then DGMRES(A, b, α) does not stagnate.

Proof. The Jordan decomposition of 2-by-2 matrix A has the following form:

$$A = V \begin{bmatrix} \lambda & 0 \\ 0 & 0 \end{bmatrix} V^{-1}.$$

Then $B^2 = [\lambda^2]$ is a scalar matrix, and hence by Theorem 4, DGMRES(A, b, α) does not stagnate for any $b \in \mathbb{C}^2$. □

In the following example, we show that by changing the right-hand side vector b, the stagnation of DGMRES(A, b, α) will be removed.

Example 2. Let $A = B \oplus N$, where

$$B = \begin{bmatrix} 2.5300 & -0.4147 & -0.6717 & -0.3570 \\ -0.4147 & 1.7306 & 0.8017 & -0.4718 \\ -0.6717 & 0.8017 & -0.5233 & 0.5021 \\ -0.3570 & -0.4718 & 0.5021 & 1.2627 \end{bmatrix}, \quad \text{and} \quad N = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

By choosing the vector $b = \begin{bmatrix} -0.5291 & -0.1187 & -1.2012 & -0.5129 & 0 & 0 \end{bmatrix}^T$ as the right-hand side vector, DGMRES$(A, b, 2)$ has partial stagnation of order one (see Figure 1 (a)).

By choosing $\hat{b} = \begin{bmatrix} 0.2277 & 0.4357 & 0.3111 & 0.9234 & 0.4302 & 0.1848 \end{bmatrix}^T$, as a random vector, DGMRES$(A, \hat{b}, 2)$ does not stagnate (see Figure 1 (b)).

6 Conclusion

Let A be an n-by-n matrix with index $\alpha > 0$ and let $b \in \mathbb{C}^n$. A necessary and sufficient condition for partial stagnation of DGMRES(A, b, α) is obtained, and also for $A \in M_n(\mathbb{R})$, a sufficient condition for the non-existence of real stagnation vector $b \in \mathcal{R}(A^\alpha)$ is studied. Moreover, a characterize for matrices $A \in M_n(\mathbb{C})$ such that DGMRES(A, b, α) does not stagnate for every $b \in \mathbb{C}^n$ are considered.

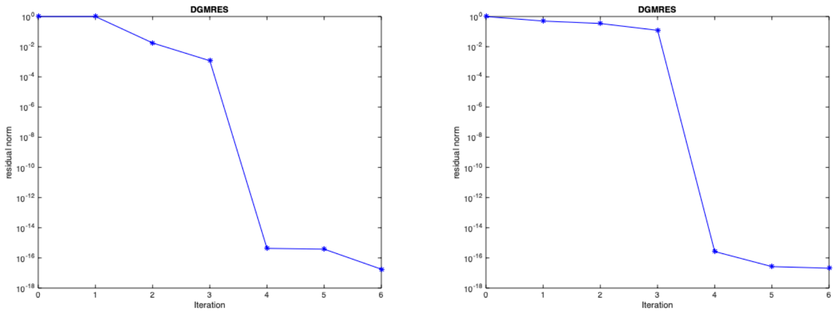

Figure 1: (a) DGMRES$(A, b, 2)$ (b) DGMRES$(A, \hat{b}, 2)$

Acknowledgement

The author would like to thank the anonymous referees for the careful reading and helpful comments to improve this paper.

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How to cite this article

F. Kyanfar On stagnation of the DGMRES method. *Iranian Journal of Numerical Analysis and Optimization*, 2022; 12(3 (Special Issue), 2022): 533-541. doi: 10.22067/ijnao.2022.73913.1081.