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Complete stagnation of GMRES ☆

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Abstract

We study problems for which the iterative method GMRES for solving linear systems of equations makes no progress in its initial iterations. Our tool for analysis is a nonlinear system of equations, the stagnation system, that characterizes this behavior. We focus on complete stagnation, for which there is no progress until the last iteration. We give necessary and sufficient conditions for complete stagnation of systems involving unitary matrices, and show that if a normal matrix completely stagnates then so does an entire family of nonnormal matrices with the same eigenvalues. Finally, we show that there are real matrices for which complete stagnation occurs for certain complex right-hand sides but not for real ones.

Keywords: Iterative methods; GMRES; Stagnation; Convergence

1. Introduction

GMRES [16] is one of the most widely used iterations for solving linear systems of equations $Ax = b$, where A is an $n \times n$ matrix and x and b are n-vectors. Although it is guaranteed to produce the exact solution in at most n iterations, it is useful for

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large systems of equations because a good approximate solution is often computed quite early, after very few iterations.

In this paper, we study an oddity: the class of problems for which the GMRES algorithm, when started with the initial guess $x^{(0)} = 0$ and using exact arithmetic, computes m iterates $x^{(1)} = \cdots = x^{(m)} = 0$ without making any progress at all. We call this *partial* or *m-step stagnation*. If $m = n - 1$, we call this *complete stagnation* of GMRES. In this case, GMRES will compute the exact solution at iteration n.

If GMRES frequently stagnated on practical problems, it would not be a popular algorithm. Clearly this set of problems is rather obscure. Why is it of interest? Saad and Schultz presented an example of 1-step stagnation in the original paper on GMRES [16]. Since then, a great deal of research has been invested in understanding the causes and cures for stagnation (see, for example, [1–5,7,17–19,21]). Despite the past 15 years of intense effort, the convergence of GMRES is not at all well-understood and a great number of open questions remain. Although we study the extreme case, we believe the new perspective lends insight into the factors that affect convergence rate and provides tools that may be of use in studying problems for which GMRES converges more favorably. In particular, this is demonstrated in [24, Chapter 5] and a forthcoming paper [23]. In addition, most common implementations of GMRES allow restarts after a small number of iterations to conserve storage space. The restarted GMRES algorithm often makes rapid progress in the beginning iterations but then nearly stagnates in the later ones. We hope that our study of stagnation will eventually shed light on restarted stagnation, too.

We begin with a new tool for studying GMRES convergence, the stagnation system. In Section 2, we derive this equation, which separates the effects of the eigenvalues of A, the eigenvectors of A, and the right-hand side. In the rest of the paper, we focus on complete stagnation. We present a geometric interpretation of complete stagnation that illustrates how this phenomenon can be studied through interaction between the eigenvalues and eigenvectors of A. In Section 3 we consider normal matrices. It is well known that GMRES can stagnate on a particular set of unitary matrices [14]; we show that this is the only set of stagnating problems for unitary matrices. We further show that if a normal matrix stagnates then so does an entire family of nonnormal matrices with the same eigenvalues. Results on real matrices and right-hand sides are given in Section 4.

2. The stagnation equation

We apply GMRES to the linear system

$$Ax = b, \quad x \in \mathscr{C}^n, \;\; b \in \mathscr{C}^n, \;\; A \in \mathscr{C}^{n\times n}$$

which we denote by GMRES(A, b). When the right-hand side vector is not specified, we use the notation GMRES(A). Throughout this paper, a barred quantity denotes a complex conjugate, and we make the following assumptions:

1. The matrix A is diagonalizable and has the spectral decomposition $A = V\Lambda V^{-1}$ where $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ and the columns of V are the right eigenvectors of A, which are linearly independent, and so the matrix $W = V^{\mathrm{H}}V = (\overline{V})^{\mathrm{T}}V$ is Hermitian positive definite.
2. The right-hand side b is normalized to Euclidean norm 1 and the initial guess for GMRES is $x_0 = 0$. We denote by r_m the GMRES residual after m steps, so that $r_m = b - Ax_m$ with $r_0 = b$.
3. The matrix V has a singular value decomposition of the form $P\Sigma Q^{\mathrm{H}}$, where Q contains right singular vectors of V and Σ is a diagonal matrix with singular values of V on the diagonal. Behavior of GMRES is essentially invariant to premultiplication of V by a unitary matrix. Therefore, when convenient, we may assume that P is the identity matrix. In other words, left singular vectors of V are irrelevant to the apparatus we develop in this paper. Also, without loss of generality, we may assume that columns of V have Euclidean norm 1.

The GMRES algorithm computes a sequence of approximate solutions to $Ax = b$ so that the mth approximation is the member of the Krylov subspace

$$\mathscr{K}_m(A, b) = \mathrm{span}\{b, Ab, \ldots, A^{m-1}b\}$$

with minimal residual norm

$$\|r_m\| = \min_{x \in \mathscr{K}_m(A,b)} \|b - Ax\|.$$

It is well known [16] and evident from this definition that the residual norms are monotonically nonincreasing with m, and that GMRES terminates with the exact solution in at most n iterations.

A standard approach for analysis of GMRES uses the inequality

$$\frac{\|r_m\|}{\|r_0\|} \leqslant \kappa(V) \min_{p_m(0)=1} \max_{\lambda_j} |p_m(\lambda_j)|, \tag{2.1}$$

where $\kappa(V)$ is the condition number of the matrix of eigenvectors of A and p_m is a polynomial of degree m. Typically, little is known about $\kappa(V)$, but insight into performance is obtained from studying the polynomial term.

In this section we develop a new approach for analysis of GMRES, establishing necessary and sufficient conditions for stagnation of GMRES. This is done using the *Krylov matrix*

$$K_m = \begin{bmatrix} b & Ab & \cdots & A^{m-1}b \end{bmatrix},$$

together with the eigenvalues and eigenvectors of the coefficient matrix A.

An important tool in our analysis is a factorization of K_m, separating the influence of the eigenvalues of A, the eigenvectors, and the right-hand side b. This factorization appears, for example, in [9, Proof of Theorem 4.1].

Lemma 2.1. *Let* $y = V^{-1}b$ *and let* $Y = \mathrm{diag}(y)$. *Then*

$$K_{m+1} = VYZ_{m+1}, \tag{2.2}$$

where Z_{m+1} is the Vandermonde matrix computed from eigenvalues of A,

$$Z_{m+1} = \begin{pmatrix} 1 & \lambda_1 & \dots & \lambda_1^m \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_n & \dots & \lambda_n^m \end{pmatrix} = \begin{pmatrix} e & \Lambda e & \dots & \Lambda^m e \end{pmatrix},$$

where e is the vector of ones.

Proof. The Krylov matrix satisfies

$$\begin{aligned} K_{m+1}(A,b) &= \begin{bmatrix} Vy & V\Lambda V^{-1}Vy & \cdots & V\Lambda^m V^{-1}Vy \end{bmatrix} \\ &= V\begin{bmatrix} Ye & \Lambda Ye & \cdots & \Lambda^m Ye \end{bmatrix} \\ &= VY\begin{bmatrix} e & \Lambda e & \cdots & \Lambda^m e \end{bmatrix} \\ &= VYZ_{m+1}. \qquad \square \end{aligned}$$

We are now ready to prove the main result of this section.

Theorem 2.2. *Let A be nonsingular with at least $m+1$ distinct eigenvalues. Let $y = V^{-1}b$. Then* GMRES(A, b) *m-stagnates if and only if y satisfies the* stagnation system

$$Z_{m+1}^{\mathrm{H}} \overline{Y} W y = e_1, \tag{2.3}$$

where $e_1 = [1, 0, \dots, 0]^{\mathrm{T}} \in \mathscr{C}^{m+1}$.

Proof. At the mth step, GMRES minimizes the residual over all vectors x in the span of the columns of K_m. This means that the resulting residual r_m is the projection of b onto the subspace orthogonal to the span of the columns of AK_m. Therefore, GMRES stagnates at step m if and only if b is orthogonal to the columns of AK_m, or, equivalently, orthogonal to the last m columns of K_{m+1}. Since the first column of K_{m+1} is b, this is equivalent to stagnation if and only if $K_{m+1}^{\mathrm{H}} b = e_1$. Substituting the factorization of K_{m+1} from Lemma 2.1 yields the desired result. $\square$

Note that without the assumption that $\|b\| = 1$, the right-hand side of the stagnation system would be multiplied by $\|b\|^2$.

If $m = n-1$, we have complete stagnation. Since complete stagnation is impossible if eigenvalues of A repeat, we assume a distinct spectrum, which yields a full-rank square Vandermonde matrix Z_n. In this case, Theorem 2.2 takes the following form:

Corollary 2.3. *Let A be nonsingular with distinct eigenvalues. Let $y = V^{-1}b$. Then* GMRES(A, b) *completely stagnates if and only if y satisfies*

$$\overline{Y} W y = Z_n^{-\mathrm{H}} e_1 = u, \tag{2.4}$$

where the elements of u are defined by

$$u_j = (-1)^{n+1} \operatorname{conj}\left(\prod_{\substack{k=1 \\ k\neq j}}^{n} \frac{\lambda_k}{\lambda_j - \lambda_k} \right), \tag{2.5}$$

where conj *denotes complex conjugate.*

Proof. Denote the elements of the first column of $Z_n^{-\mathrm{H}}$ by u_j, $j = 1, \dots, n$. The proof is a consequence of [8, Section 21.1], where an explicit construction of the entries of the inverse of a Vandermonde matrix is derived. □

We can make a similar statement for partial stagnation.

Corollary 2.4. *Let A be nonsingular with at least $m + 1$ distinct eigenvalues. Let $y = V^{-1}b$. Then* GMRES(A, b) *m-stagnates if and only if y satisfies*

$$\overline{Y}Wy = \left(Z_{m+1}^{\mathrm{H}}\right)^{\dagger} e_1 + t, \tag{2.6}$$

where $t \in \mathcal{N}(Z_{m+1}^{\mathrm{H}})$, the null space of Z_{m+1}^{H}, and $(Z_{m+1}^{\mathrm{H}})^{\dagger} = Z_{m+1}(Z_{m+1}^{\mathrm{H}} Z_{m+1})^{-1}$ is the pseudo-inverse of Z_{m+1}^{H} [10,20].

The usefulness of (2.3), as well as the related Eqs. (2.4) and (2.6), is that it separates the influence of the eigenvalues, which determine Z_n, and eigenvectors, which determine W. Stagnation is explored through the interaction of W and Z_n.

The systems (2.3) and (2.4) are not polynomial systems of equations since they involve complex conjugation of the entries of the variable y. They can, however, be rewritten as real polynomial systems with $2(m + 1)$ and $2n$ equations, respectively, by splitting all components into their respective real and imaginary parts. Partial or complete stagnation of GMRES corresponds to the existence of a *real* solution of such a polynomial system. If the total number of (real and complex) regular and infinite solutions is finite, then, according to a result of Bezout [12], the number does not exceed the total degree of the polynomial system, which in the case of (2.3) is $2^{2(m+1)}$. Therefore, in practical experiments, we need to use a solver such as POLSYS_PLP [22] that finds *all* solutions of the system. Stagnation takes place iff any of these solutions is regular and real.

Next we establish the equivalence of stagnation of GMRES for A with stagnation for A^{H}.

Theorem 2.5. *Let A be nonsingular with at least $m + 1$ distinct eigenvalues. Then* GMRES(A, b) *m-stagnates for some $b \in \mathscr{C}^n$ iff* GMRES(A^{H}, b) *stagnates for the same b.*

Proof. GMRES(A, b) m-stagnates if and only if b is orthogonal to the columns of AK_m; i.e., $b^{\mathrm{H}}[Ab \;\; A^2b \;\; \cdots \;\; A^m b] = 0$. Taking the conjugate transpose of each of the inner products yields $b^{\mathrm{H}}[A^{\mathrm{H}}b \;\; (A^{\mathrm{H}})^2 b \;\; \cdots \;\; (A^{\mathrm{H}})^m b] = 0$, so GMRES$(A^{\mathrm{H}}, b)$ also m-stagnates. □

The stagnation system can be used to completely analyze stagnation of GMRES in the case when $n = 2$, and this analysis is given in [24]. In that case, stagnation is determined by a simple relationship between the ratio of the eigenvalues and the condition number of the eigenvector matrix. More specifically, given *any* set of distinct nonzero eigenvalues $\lambda \in \mathscr{C}^2$ and a set of eigenvectors $V \in \mathscr{C}^{2\times 2}$, there exists a vector $b \in \mathscr{C}^2$ such that GMRES$(V\Lambda V^{-1}, b)$ stagnates iff the condition number of V is large enough with respect to the ratio of the largest eigenvalue to the smallest one. An explicit formula is provided for a stagnating right-hand side b. For more details, see [24,25].

2.1. The geometry of stagnation

The complete stagnation system (2.4) can be written as

$$F_V(y) = G(\lambda),$$

where $F_V(y) = \overline{Y}Wy$ and $G(\lambda) = u$. Let us look at the domains and ranges of F_V and G. Since

$$1 = \|b\|^2 = \|Vy\|^2 = y^{\mathrm{H}}Wy = \|y\|_W^2 = e^{\mathrm{T}}u,$$

it follows that the domain of $F_V(y)$ is the hyper-ellipsoid surface

$$E_V = \left\{ y \in \mathscr{C}^n \mid y^{\mathrm{H}}Wy = 1 \right\},$$

whose axes are determined by singular values and vectors of the matrix V. Moreover, u lies in the hyperplane

$$S_n = \left\{ u = [u_1 \quad \cdots \quad u_n]^{\mathrm{T}} \in \mathscr{C}^n \,\middle|\, \sum_{j=1}^{n} u_j = 1 \right\}.$$

The range of the operator $F_V(y)$ defined over E_V is

$$S_V = \left\{ u \in S_n \mid \text{there exists } y_u \in \mathscr{C}^n \text{ such that } F_V(y_u) = u \right\}$$

which is a subset of S_n. Due to scale-invariance of the function $G(\lambda)$, without loss of generality we can assume that all eigenvalue distributions lie in the box

$$B = \left\{ \lambda = [\lambda_1 \quad \cdots \quad \lambda_n]^{\mathrm{T}} \in \mathscr{C}^n \mid 0 \leqslant |\lambda_j| \leqslant 1 \right\}.$$

Therefore, the range of $G(\lambda)$ defined over B is

$$S_\lambda = \left\{ u \in S_n \mid \text{there exists } \lambda_u \in B \text{ such that } G(\lambda_u) = u \right\}$$

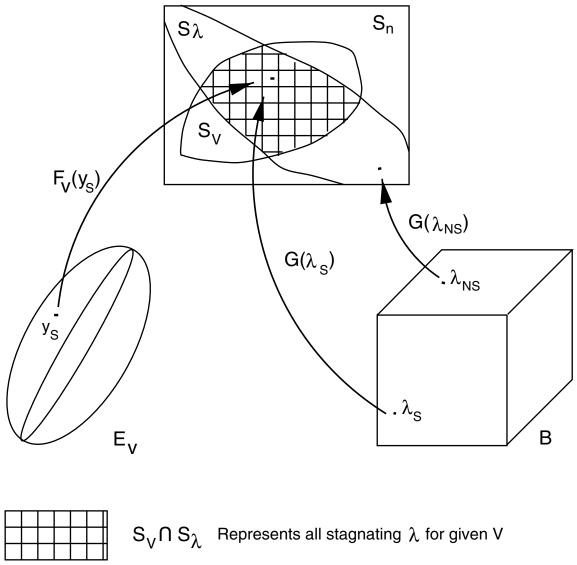

Fig. 1. A geometric interpretation of complete GMRES stagnation.

which is also a subset of S_n. To summarize,

$$F_V : E_V \to S_V \subset S_n, \quad G(\lambda) : B \to S_\lambda \subset S_n.$$

We can now give a geometric interpretation of complete stagnation of GMRES. It is illustrated in Fig. 1. Let us fix a set of eigenvectors V, which fixes the domain and range sets E_V and S_V, respectively. The intersection of S_V with S_λ, which is the meshed area in Fig. 1, can be thought of as a representation of all eigenvalue distributions λ which yield a stagnating matrix $A = V\Lambda V^{-1}$ for the given V. Why? Because, if we pick an eigenvalue distribution (labeled λ_S in the figure) such that it gets mapped by G inside $S_V \cap S_\lambda$, then there exists a vector $y_S \in E_V$ such that the stagnation equation is satisfied for the triple $\{V, \lambda_S, y_S\}$ and so GMRES$(V\Lambda_S V^{-1}, Vy_S)$ completely stagnates. Conversely, if $G(\lambda_{NS}) \notin S_V \cap S_\lambda$ for some λ_{NS} then no matter what $y \in E_V$ we pick, the stagnation equation (2.4) is never satisfied and so GMRES$(V\Lambda_{NS}V^{-1}, b)$ never stagnates.

We make two remarks. First, the above interpretation allows us to make a generic statement about what it means for a set of eigenvectors to be “good” or “bad” in terms of complete GMRES stagnation. We see that the larger $S_V \cap S_\lambda$ is for a given V, the more stagnating λ’s one can find, and so the smaller this intersection is the better. Second, this interpretation places primary emphasis on eigenvectors and then incorporates eigenvalues into the picture. This is different from the analysis based on (2.1), which uses only eigenvalues. So in order to get a better understanding of stagnation, we have to study properties of $F_V(y)$ and $G(\lambda)$ as operators defined over their respective domains. Compare with [6] for other results showing that eigenvalues do not provide a complete analysis.

Similar statements can be made for the domain and range for the partial stagnation equation, but perhaps the most intuitive interpretation is that we seek an element of E_V that is orthogonal to the columns 2 through $m+1$ of Z.

2.2. The nature of S_λ

It follows from (2.5) that $u \in S_n$ belongs to S_λ iff there exists a vector $\lambda \in B$ such that $G(\lambda) = u$. Since we may assume that all eigenvalues are distinct and nonzero, this is equivalent to the following system of equations:

$$\begin{aligned}
&\lambda_2\lambda_3\cdots\lambda_n = (-1)^{n+1}\bar{u}_1(\lambda_1-\lambda_2)\cdots(\lambda_1-\lambda_n)\\
&\vdots\\
&\lambda_1\cdots\lambda_{j-1}\lambda_{j+1}\cdots\lambda_n = (-1)^{n+1}\bar{u}_j(\lambda_j-\lambda_1)\cdots(\lambda_j-\lambda_n)\\
&\vdots\\
&\lambda_1\lambda_2\cdots\lambda_{n-1} = (-1)^{n+1}\bar{u}_n(\lambda_n-\lambda_1)\cdots(\lambda_n-\lambda_{n-1}).
\end{aligned} \tag{2.7}$$

It appears from extensive numerical experiments that, in the case of arbitrary complex eigenvalues, the system (2.7) has solutions for any $u \in S_n$, i.e. $S_\lambda = S_n$. Consequently, in our analysis of the stagnation region $S_V \cap S_\lambda$, we focus most of our attention on S_V.

The system (2.7) is a parametrized polynomial system in λ with elements of the given vector $u \in S_n$ being the parameters. For certain values of u, it is possible to compute solutions of (2.7) explicitly. For instance, any permutation of the vector

$$\lambda = \left[\mathrm{e}^{\mathrm{i}\theta_1}, \ldots, \mathrm{e}^{\mathrm{i}\theta_n}\right]^{\mathrm{T}}, \quad \theta_j = \frac{2\pi(j-1)}{n},$$

solves the system when $u_j = 1/n$, $j = 1, \ldots, n$. Thus, in order to establish equality of S_n and S_λ analytically, it may be possible to use the theory of coefficient-parameter polynomial continuation [13].

When only real or complex conjugate eigenvalues are allowed, S_n is significantly larger than S_λ. However, in this case experimental data suggest that for any two eigenvector distributions V_1 and V_2, the volume of $S_{V_1} \cap S_\lambda$ is larger than that of $S_{V_2} \cap S_\lambda$ iff the volume of S_{V_1} is larger than that of S_{V_2}.

2.3. The nature of S_V

Since E_V is compact and $F_V(y)$ is continuous, S_V is also compact, and we now derive an explicit bound for elements of S_V.

Lemma 2.6. *If V is nonsingular and $u \in S_V$, then $\|u\| \leqslant \kappa(V) \equiv \max_i \sigma_i / \min_i \sigma_i$.*

Proof. Since $\|y\|_W = 1$ we can bound the 2-norm of y in terms of the singular values of V:

$$\frac{1}{\max_i \sigma_i} \leqslant \|y\|_2 \leqslant \frac{1}{\min_i \sigma_i}.$$

Eq. (2.4) implies that

$$u = \overline{Y} W y = \overline{Y} V^{\mathrm{H}} b,$$

so

$$\|u\| \leqslant \|\overline{Y}\| \|V\| \|b\| \leqslant \frac{1}{\min_i \sigma_i} \max_i \sigma_i. \qquad \square$$

Lemma 2.6 implies that given eigenvectors V, any eigenvalue distribution λ such that $\|G(\lambda)\| > \kappa(V)$ necessarily yields a matrix $A = V \Lambda V^{-1}$ that does not completely stagnate.

3. Complete stagnation of normal matrices

A normal matrix A is one whose eigenvector matrix V is unitary. In this case, the stagnation system (2.4) simplifies to

$$\overline{Y} y = u = G(\lambda) \tag{3.1}$$

which is a system of n decoupled equations of the form,

$$|y_j|^2 = u_j, \quad j = 1, \ldots, n.$$

Theorem 3.1. *Let $A \in \mathscr{C}^{n \times n}$ be normal with distinct eigenvalues λ. If the vector $u = G(\lambda)$, defined by* (2.5), *satisfies $u \in \mathscr{R}^n$, and $0 \leqslant u_j \leqslant 1$, $j = 1, \ldots, n$, then* GMRES(A, b) *stagnates for $b = Vy$, where*

$$y_j = \sqrt{u_j}\, \mathrm{e}^{\mathrm{i}\theta_j}, \quad j = 1, \ldots, n, \tag{3.2}$$

and the phase angles θ_j are arbitrary. Conversely, if λ is such that the corresponding $G(\lambda)$ contains complex or real negative entries, then there is no right-hand side for which GMRES(A, b) *stagnates.*

Proof. If $u = G(\lambda)$ is real positive then y defined elementwise by (3.2) solves (3.1) and thus causes stagnation of GMRES. Conversely, if at least one element of u is either complex or real negative, the system (3.1) does not have a solution, so stagnation is impossible. $\square$

When A is normal, the corresponding S_V has a simple form.

Corollary 3.2. *Let $V \in \mathscr{C}^{n \times n}$ be unitary. Then the corresponding set E_V is the unit sphere and the range of $F_V(y)$ is a real simplex*

$$S_{\mathrm{I}} = \left\{ u \in \mathscr{R}^n \mid 0 \leqslant u_j \leqslant 1, \quad j = 1, \ldots, n \right\}.$$

When A is Hermitian or real symmetric, GMRES is equivalent to MINRES [15]. Proposition 3.3 below shows that in this case the two methods cannot stagnate, provided $n \geqslant 3$. This is a well known result, but we show how this fact is reflected in the framework of the stagnation equation.

Proposition 3.3. *Let $\lambda \in \mathscr{R}^n$ $(n \geqslant 3)$ have distinct elements and let $u = G(\lambda)$. Then at least one element of the vector u is negative. Therefore* GMRES *cannot stagnate when applied to a Hermitian or real symmetric matrix with distinct eigenvalues.*

Proof. Without loss of generality, assume that eigenvalues are ordered $\lambda_1 < \cdots < \lambda_n$. Choose an index j so that λ_j and λ_{j+1} have the same sign. Then the numerators in (2.5) have the same sign for j and $j+1$ while the denominators have opposite sign, so either u_j or u_{j+1} is negative. Theorem 3.1 leads to the second part of the result. □

Therefore, there are no normal matrices with real eigenvalues that stagnate, but there are stagnating normal matrices with complex eigenvalues. The eigenvalues constitute regular solutions with distinct nonzero elements of the polynomial system (2.7), and therefore they are quite rare. For instance, the eigenvalue distribution

$$\lambda = \begin{bmatrix} 1.00000000000000 \\ -0.30447006746090 - 0.06821372515028\,\mathrm{i} \\ 0.35306441656578 - 1.49970031360021\,\mathrm{i} \\ 0.10534543907217 + 1.04831885053493\,\mathrm{i} \end{bmatrix}$$

generates

$$u = G(\lambda) = \begin{bmatrix} 0.17225711241368 \\ 0.66327345135404 \\ 0.04991016520560 \\ 0.11455927102668 \end{bmatrix}.$$

3.1. Stagnation of unitary matrices

A normal matrix A is unitary iff its eigenvalues satisfy

$$\lambda_j = \mathrm{e}^{\mathrm{i}\phi_j}, \quad 0 \leqslant \phi_j \leqslant 2\pi, \quad j = 1, \ldots, n. \tag{3.3}$$

It has been shown that GMRES can stagnate when applied to a unitary matrix A with eigenvalues distributed uniformly over the unit circle in the complex plane [14]. Using Theorem 3.1 we now show that those are the only unitary matrices for which stagnation can occur.

Theorem 3.4. *Let $A \in \mathscr{C}^{n\times n}$ be unitary with distinct eigenvalues.* GMRES *stagnates iff the phase angles ϕ_j satisfy*

$$\phi_j = \phi + \frac{2\pi(j-1)}{n}, \quad j = 1, \ldots, n, \tag{3.4}$$

where ϕ is arbitrary, which represents n eigenvalues distributed uniformly over the unit circle in the complex plane.

We prove Theorem 3.4 in two steps. Given λ, a set of n distinct eigenvalues of the form (3.3), define its image under the transformation $G(\lambda)$ by

$$G(\lambda) = u = v + \mathrm{i}w, \quad v, w \in \mathscr{R}^n.$$

In Lemma 3.5, we derive explicit formulations for v and w. Then, in Lemma 3.6, we prove that the only set of phase angles $\{\phi_j\}$ that makes w zero is the one defined by (3.4). For this set of angles, it can be shown by direct computation that v contains only positive entries.

Lemma 3.5. *Let $\lambda \in \mathscr{C}^n$ be a set of n distinct eigenvalues of the form* (3.3). *Without loss of generality assume that*

$$0 = \phi_1 < \phi_2 < \cdots < \phi_n < 2\pi. \tag{3.5}$$

Then individual entries of the vector $u = (u_1, \ldots, u_n)^{\mathrm{T}}$ can be written in terms of the phase angles as follows:

$$u_j = \gamma^{(n)} C_j^{(n)} d_j^{(n)}, \tag{3.6}$$

where

$$\gamma^{(n)} = \begin{cases} (-1)^{(n-2)/2} & \text{if } n \text{ is even,} \\ (-1)^{(n-1)/2} & \text{if } n \text{ is odd,} \end{cases} \qquad C_j^{(n)} = \left(\frac{1}{2}\right)^{n-1} \prod_{\substack{k=1 \\ k \neq j}}^{n} \csc \frac{\phi_j - \phi_k}{2},$$

and

$$d_j^{(n)} = \begin{cases} \sin \frac{\alpha_j^{(n)}}{2} + \mathrm{i} \cos \frac{\alpha_j^{(n)}}{2} & \text{if } n \text{ is even,} \\ \cos \frac{\alpha_j^{(n)}}{2} - \mathrm{i} \sin \frac{\alpha_j^{(n)}}{2} & \text{if } n \text{ is odd,} \end{cases}$$

where

$$\alpha_j^{(n)} = (n-1)\phi_j - \sum_{\substack{k=1 \\ k \neq j}}^{n} \phi_k.$$

Proof. The jth element of u is u_j, defined by (2.5). Each term of (2.5) can be rewritten as follows using (3.3)

$$\begin{aligned} \frac{\lambda_k}{\lambda_j - \lambda_k} &= -\frac{\sin(\phi_j - \phi_k)/2 + \mathrm{i}\cos(\phi_j - \phi_k)/2}{2\sin(\phi_j - \phi_k)/2} \\ &= \left(-\frac{1}{2}\right) \csc \frac{\phi_j - \phi_k}{2}\, \mathrm{i} \exp\left\{\mathrm{i}\left(\frac{\phi_k - \phi_j}{2}\right)\right\}. \end{aligned}$$

This yields

$$u_j = (-1)^n \left(\frac{1}{2}\right)^{n-1} \prod_{\substack{k=1\\k\neq j}}^{n} \csc\frac{\phi_j - \phi_k}{2} \mathrm{i}^{n-1} \exp\left(\mathrm{i}\sum_{\substack{k=1\\k\neq j}}^{n} \frac{\phi_k - \phi_j}{2}\right). \tag{3.7}$$

Let us now assume that $n = 2k$ is even. The case for odd n is treated similarly. Since

$$(-1)^n\, \mathrm{i}^{n-1} = (-1)^{(n-2)/2}\, \mathrm{i},$$

we can rewrite (3.7) as

$$u_j = \gamma^{(n)} C_j^{(n)} \mathrm{i} \exp\left(-\mathrm{i}\frac{\alpha_j^{(n)}}{2}\right),$$

where

$$\mathrm{i} \exp\left(-\mathrm{i}\frac{\alpha_j^{(n)}}{2}\right) = \sin\frac{\alpha_j^{(n)}}{2} + \mathrm{i}\cos\frac{\alpha_j^{(n)}}{2}.$$

This completes the proof. □

Lemma 3.6. *The vector w, the imaginary part of u defined by* (3.6), *is zero iff the phase angles $\{\phi_j\}$ are given by* (3.4).

Proof. We present a proof for even values of n. The proof for odd n is similar. First we observe that since eigenvalues are distinct, the $C_j^{(n)}$ terms are all well-defined and nonzero. From (3.6) we see that u is real iff

$$\hat{w} = \left(\cos\frac{\alpha_1^{(n)}}{2}, \cos\frac{\alpha_2^{(n)}}{2}, \ldots, \cos\frac{\alpha_n^{(n)}}{2}\right)^{\mathrm{T}} = 0.$$

Thus

$$\alpha_k^{(n)} = \pi + 2\pi m_k, \quad k = 2, \ldots, n, \tag{3.8}$$

where m_k is an integer.

Our goal is to prove that the only combination of the indices m_k that yields phase angles ϕ_k that satisfy (3.5) is the one that gives (3.4). First we find phase angles $\phi_2, \ldots, \phi_n$ that set the bottom $n-1$ entries of $\hat{w}$ to zero; for this, we solve the $n-1 \times n-1$ system

$$M\hat{\phi} = \beta,$$

where

$$M = \begin{pmatrix} n-1 & -1 & -1 & \cdots & -1 \\ -1 & n-1 & -1 & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & n-1 \end{pmatrix}, \quad \hat{\phi} = \begin{pmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \phi_n \end{pmatrix},$$

$$\beta = \begin{pmatrix} \pi + 2\pi m_2 \\ \pi + 2\pi m_3 \\ \vdots \\ \pi + 2\pi m_n \end{pmatrix}.$$

Now

$$M^{-1} = \frac{1}{n}\begin{pmatrix} 2 & 1 & 1 & \cdots & 1 \\ 1 & 2 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 2 \end{pmatrix},$$

so

$$\hat{\phi} = M^{-1}\beta = \frac{\pi}{n}\begin{pmatrix} n + 2(m_2 + \cdots + m_n) + 2m_2 \\ n + 2(m_2 + \cdots + m_n) + 2m_3 \\ \vdots \\ n + 2(m_2 + \cdots + m_n) + 2m_n \end{pmatrix}.$$

From (3.5) it follows that $m_2 < m_3 < \cdots < m_n$, so we can write

$$m_j = m_{j-1} + \delta_j, \quad j = 3, \ldots, n,$$

where δ_j is a positive integer. We consider two cases.

Case I. $\delta_j = 1,\ j = 3, \ldots, n$. In this case $m_j = m_2 + (j-2)$ and so

$$\hat{\phi}_j = \frac{\pi}{n}\big(n^2 - 2n - 2 + 2nm_2 + 2j\big), \quad j = 2, \ldots, n.$$

In order to satisfy (3.5), $\hat{\phi}_2$ must be positive. Solving $\hat{\phi}_2 > 0$ for m_2, we obtain

$$m_2 > -\frac{n}{2} + 1 - \frac{1}{n} \;\Rightarrow\; m_2 \geqslant -\frac{n}{2} + 1,$$

because both m_2 and n are integers and $n > 1$. Similarly, solving $\hat{\phi}_n < 2\pi$, we get

$$m_2 < -\frac{n}{2} + 1 + \frac{1}{n} \;\Rightarrow\; m_2 \leqslant -\frac{n}{2} + 1.$$

We conclude that only when $m_2 = (2-n)/2$ do we get a valid set of phase angles $\hat{\phi}$, namely,

$$\hat{\phi} = \frac{2\pi}{n}(1, 2, \ldots, n-1)^{\mathrm{T}}. \tag{3.9}$$

Case II. First, suppose that $\delta_j = 1,\ j = 3, \ldots, n-1$ and $\delta_n = 2 + \epsilon$, where ϵ is a nonnegative integer. Then we obtain

$$\hat{\phi}_2 = \frac{\pi}{n}\big(n^2 - 2n + 2 + 2nm_2 + 2(1+\epsilon)\big),$$

$$\hat{\phi}_n = \frac{\pi}{n}\big(n^2 - 2 + 2nm_2 + 4(1+\epsilon)\big).$$

Solving $\hat{\phi}_2 > 0$ and $\hat{\phi}_n < 2\pi$ we obtain, respectively,

$$m_2 > \alpha \equiv -\frac{n}{2} + 1 - \frac{1}{n} - \frac{1+\epsilon}{n}, \quad m_2 < \beta \equiv -\frac{n}{2} + 1 - \frac{1}{n} - 2\frac{1+\epsilon}{n}.$$

It is easy to see that α is always bigger than β for any nonnegative integer ϵ. A similar result could be obtained if any other $\delta_j > 1$. We therefore conclude that (3.9) is the only valid combination of phase angles. Direct substitution also shows that this combination zeroes out the first entry of $\hat{w}$. □

3.2. Does normal stagnation imply nonnormal stagnation?

For $n = 2$, we found that, given $\lambda \in \mathscr{C}^2$, as long as $\kappa(V)$ is larger than a certain value that depends on λ, the corresponding $A = V\Lambda V^{-1}$ is stagnating [24]. In particular, this implies that if $A \in \mathscr{C}^{2\times 2}$ is normal and stagnating then so is $\tilde{A} = \widetilde{V}\Lambda\widetilde{V}^{-1}$ for any nonsingular $\widetilde{V}$. Does this extend to $n > 2$?

While running extensive testing to determine properties of S_V for low-dimensional real matrices V we have noticed that in all the tested cases, S_V included S_{I}, where S_{I} is the real simplex defined in Section 2.1 which constitutes the range of $F_V(y)$ for any orthonormal V.

Stagnation of a normal matrix does imply stagnation of an entire family of matrices with the same eigenvalues:

Theorem 3.7. *Suppose we have a vector $\lambda \in \mathscr{C}^n$ with distinct elements such that $u = G(\lambda)$ satisfies $u \in \mathscr{R}^n$ with $0 < u_i \leqslant 1$. Then for any nonsingular eigenvector matrix V with $W = V^{\mathrm{H}}V$ real,* GMRES(A, b) *stagnates for $A = V\Lambda V^{-1}$ and $b = Vy$, where $y \in \mathscr{R}^n$ satisfies $YWy = u$.*

Proof. If W is real, then it is symmetric positive definite. Solving the stagnation equation $YWy = u$ is equivalent to finding a diagonal scaling matrix Y so that YWY has row sums u. Since $0 < u_i \leqslant 1$, then [11, Corollary 2] tells us that such a scaling matrix exists. □

4. Complete stagnation of real matrices

In this section, we investigate the special form that the stagnation system (2.4) takes when A is real, and we determine whether it is sufficient to consider real right-hand side vectors when studying stagnation of GMRES for real matrices A.

When A is real, our stagnation equation (2.4) becomes a polynomial system in y, considerably simplifying analysis and numerical experimentation. To form this polynomial system, let $A \in \mathscr{R}^{n\times n}$ have eigenvalues $\lambda \in \mathscr{C}^{n\times n}$ and eigenvectors $V \in \mathscr{C}^{n\times n}$. Let $P \in \mathscr{R}^{n\times n}$ be the permutation matrix that interchanges the complex conjugate pairs in λ. Then

$$\bar{\lambda} = P\lambda, \quad \overline{V} = VP. \tag{4.1}$$

It follows that GMRES(A, b) stagnates for $b = Vy \in \mathscr{C}^n$ iff $\|b\| = 1$ and y solves

$$\overline{Y} P W_{\mathrm{T}} y = u, \tag{4.2}$$

where $W_{\mathrm{T}} = V^{\mathrm{T}} V$. Furthermore, GMRES$(A, b)$ stagnates for $b = Vy \in \mathscr{R}^n$ iff $\|b\| = 1$ and y solves the polynomial system

$$Y W_{\mathrm{T}} y = \bar{u}, \quad \bar{y} = Py. \tag{4.3}$$

4.1. Real eigenvalues

When the spectrum of A is real, the stagnation system simplifies even further. Both W and $G(\lambda)$ are real in this case, P is the identity matrix and $W_{\mathrm{T}} = W$. If we consider only real right-hand sides then we get the real polynomial stagnation system

$$YWy = u, \tag{4.4}$$

where $y \in \mathscr{R}^n$ satisfies $y^{\mathrm{T}} W y = 1$ and $u = G(\lambda)$.

Note that when (2.4) or (4.2) is solved, the corresponding domain for $F_V(y) = \overline{Y} W y$ is

$$E_V = \left\{ y \in \mathscr{C}^n \mid y^{\mathrm{H}} W y = 1 \right\}.$$

When we consider (4.3), the domain changes to

$$E_V = \left\{ y \in \mathscr{C}^n \mid \bar{y} = Py, \ \ y^{\mathrm{H}} W y = y^{\mathrm{T}} W_{\mathrm{T}} y = 1 \right\},$$

where $W_{\mathrm{T}} = V^{\mathrm{T}} V$ and P is defined by (4.1). Finally, for (4.4) the domain has the form

$$E_V = \left\{ y \in \mathscr{R}^n \mid y^{\mathrm{T}} W y = 1 \right\}.$$

4.2. When real vectors b are sufficient

Suppose A is real with real spectrum. Is it possible that GMRES(A, b) stagnates for some complex b but does not stagnate for any real b? If V is 3×3 or extreme, the answer is no: existence of a complex stagnating b implies existence of a real one.

Theorem 4.1. *Let $A \in \mathscr{R}^{n\times n}$ with real eigenvalues λ and eigenvectors V. If V is of size 3×3 then existence of a complex stagnating right-hand side vector implies existence of a real one.*

Proof. Let $u = G(\lambda) \in \mathscr{R}^n$. Suppose there exists stagnating $y \in \mathscr{C}^n$ of the form

$$y = \left(y_1 \mathrm{e}^{\mathrm{i}\phi_1}, \ldots, y_n \mathrm{e}^{\mathrm{i}\phi_n} \right)^{\mathrm{T}},$$

where, for every $j = 1, \ldots, n$, $y_j \in \mathscr{R}$ and $0 \leqslant \phi_j \leqslant 2\pi$. We may assume that $b = Vy$ has unit norm. This implies that y satisfies $\overline{Y} W y = u$.

We show that if V is 3×3, the phase angles ϕ_1, ϕ_2, and ϕ_3 are all equal. This implies that the real vector $y_R = e^{-i\phi_1} y$ satisfies and therefore corresponds to a stagnating right-hand side.

We expand $\overline{Y} W y$ and conclude that y must satisfy

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} x_1^2 + x_1 x_2 e^{i(\phi_2-\phi_1)} + x_1 x_3 e^{i(\phi_3-\phi_1)} \\ x_2^2 + x_2 x_1 e^{i(\phi_1-\phi_2)} + x_2 x_3 e^{i(\phi_3-\phi_2)} \\ x_3^2 + x_3 x_1 e^{i(\phi_1-\phi_3)} + x_3 x_2 e^{i(\phi_2-\phi_3)} \end{bmatrix}. \tag{4.5}$$

Each entry on the left of Eq. (4.5) is real, so, clearly, each entry on the right must also be real. The first term, x_j^2, $j = 1, 2, 3$ is real. In order for two complex numbers to have a real sum, they must have identical magnitudes and opposite phases. Therefore

$$\phi_2 - \phi_1 = \phi_1 - \phi_3, \quad \phi_1 - \phi_2 = \phi_2 - \phi_3.$$

Solving the above pair of equations we conclude that $\phi_1 = \phi_2 = \phi_3$. □

We say that a matrix is an *extreme matrix* if its singular values can be ordered to satisfy $\sigma_1 = \sigma_2 = \cdots = \sigma_{n-1} \neq \sigma_n$, The theorem above also holds for extreme matrices [24, Section 4.3.2, Lemma 7]. If V is not extreme or three-dimensional, however, it is possible for a corresponding matrix A to have a complex, but no real, stagnating right-hand side.

Example. Let the matrix A be defined by its eigenvector matrix

$$V = \begin{pmatrix} -0.3998204 & 0.2414875 & -0.0877858 & -0.4306034 \\ -0.5786559 & -0.8362391 & 0.4920379 & 0.3213318 \\ 0.6984230 & 0.0537175 & -0.7499413 & 0.5155494 \\ -0.1323115 & 0.4893898 & -0.4333364 & -0.6674844 \end{pmatrix}$$

and its eigenvalues

$$\lambda = (1.0000000, -0.7658066, -0.2656295, 0.8705277).$$

The mapping $G(\lambda)$ is

$$G(\lambda) = (-0.6120, -0.1600, 0.9269, 0.8451).$$

The vector

$$y = \begin{bmatrix} 1.5564116 + 1.5564116\,i \\ -1.2084570 - 0.3414864\,i \\ 0.7066397 + 1.5089330\,i \\ -1.8679775 - 1.2644748\,i \end{bmatrix}$$

solves (2.4) and it can be verified directly that GMRES(A, b) stagnates when $b = Vy$. In order to determine whether any real stagnating b exists, we solve the polynomial system (4.4) with W and u as above. Note that if a complex y solves (4.4) then so do $-y$, $\bar{y}$, and $-\bar{y}$. Applying the POLSYS_PLP solver we obtain exactly $2^4 = 16$ complex solutions. The four "fundamental" ones are listed below:

$$y_{\mathrm{I}} = \begin{bmatrix} 0.7391037 + 0.2570027\,\mathrm{i} \\ -0.1534853 + 0.5091449\,\mathrm{i} \\ 1.2414730 + 0.3333155\,\mathrm{i} \\ -1.2276988 + 0.1269897\,\mathrm{i} \end{bmatrix},$$

$$y_{\mathrm{II}} = \begin{bmatrix} 0.1578663 + 0.9757913\,\mathrm{i} \\ 0.1463589 + 0.0364812\,\mathrm{i} \\ 0.9548215 + 0.3991290\,\mathrm{i} \\ 0.8611411 - 0.2115472\,\mathrm{i} \end{bmatrix},$$

$$y_{\mathrm{III}} = \begin{bmatrix} -0.9785711 - 2.1552377\,\mathrm{i} \\ 3.4382447 + 2.1527698\,\mathrm{i} \\ 1.8727147 - 0.2306006\,\mathrm{i} \\ 2.7341793 + 2.2536406\,\mathrm{i} \end{bmatrix},$$

$$y_{\mathrm{IV}} = \begin{bmatrix} 2.4426010 + 0.4870174\,\mathrm{i} \\ -1.1947469 - 0.5787159\,\mathrm{i} \\ 1.7072389 + 0.0030895\,\mathrm{i} \\ -2.3718795 - 0.5254314\,\mathrm{i} \end{bmatrix}.$$

The degree of the system is 16, and all 16 solutions are verified to be isolated. We conclude that the given system (4.4) has no other real or complex solutions. On the other hand, a complex solution of (4.4) does not produce a stagnating b.

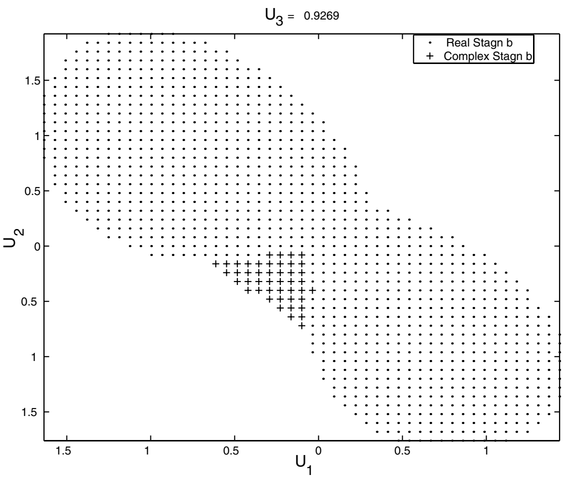

Fig. 2. Real vectors b are not sufficient (Section 4.2).

It appears, however, that at least for small n, A can be expected to have a real stagnating right-hand side if it has a complex one. For instance, let us examine Fig. 2, which shows a slice of S_V for the matrix V defined above. The slice is the intersection of S_V with the plane $u_3 = 0.9269$. The dotted points correspond to vectors $u \in S_n$ for which there are both real and complex stagnating vectors b. For the points marked with '+', only complex ones exist. We see that the dotted region is significantly larger.

5. Conclusions

We have presented several results on the stagnation behavior of GMRES. We gave necessary and sufficient conditions for stagnation of systems involving unitary matrices, and showed that if a normal matrix stagnates then so does an entire family of nonnormal matrices with the same eigenvalues. Finally, we showed that there are real matrices for which stagnation occurs for certain complex right-hand sides but not for real ones.

The stagnation system was a crucial tool in developing these results and we believe its analysis will contribute to the solution of other open problems as well.

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