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. For problems of dimension 2 we can solve this system explicitly, determining that every choice of eigenvalues leads to a stagnating problem for eigenvector matrices that are sufficiently poorly conditioned. We partially extend this result to higher dimensions for a class of eigenvector matrices called extreme. We give necessary and sufficient conditions for stagnation of systems involving unitary matrices, and show that if a normal matrix stagnates then so does an entire family of nonnormal matrices with the same eigenvalues. Finally, we show that there are real matrices for which stagnation occurs for certain complex right-hand sides but not for real ones.

Key words. Iterative methods, GMRES, stagnation, convergence.

Running Title: Stagnation of GMRES

1. Introduction. GMRES [8] 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 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 $x^{(1)} = \ldots = x^{(m)} = 0$ 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? Despite fifteen 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 [15, Chap. 5] and a forthcoming paper [14]. 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 Section 3 we present results of application of this formalism to analysis of complete GMRES stagnation for $n = 2$.

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In Section 4 we study the special case of *extreme matrices*, those whose eigenvector matrix has only two distinct singular values. In Section 5 we consider normal matrices. It is well known that GMRES can stagnate on a particular set of unitary matrices [5]; 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 6.

2. The Stagnation Equation. We apply GMRES to the linear system

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

Throughout this paper, 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.
2. These eigenvectors are linearly independent, so the matrix $W = V^H V$ is Hermitian positive definite.
3. 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 $r_0 = b$.
4. The matrix V has a singular value decomposition of the form $P \Sigma Q^H$, 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 pre-multiplication 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

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

with minimal residual norm

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

It is well known [8] 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.

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*

$$K_m = [b \; Ab \; \ldots \; A^{m-1}b].$$

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 Ipsen [2, Proof of Theorem 4.1]); a version of this result can also be found in [9].

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

$$K_{m+1} = VYZ_{m+1}, \tag{2.1}$$

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

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

Proof. The Krylov matrix satisfies

$$\begin{aligned} K_{m+1}(A,b) &= [Vy \;\; V\Lambda V^{-1}Vy \;\; \dots \;\; V\Lambda^m V^{-1}Vy] \\ &= V\,[Ye \;\; \Lambda Ye \;\; \dots \;\; \Lambda^m Ye] \\ &= VY\,[e \;\; \Lambda e \;\; \dots \;\; \Lambda^m e] \\ &= VYZ_{m+1}. \end{aligned}$$

□

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

$$Z_{m+1}^H \bar{Y} W y = e_1\,, \tag{2.2}$$

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

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 $K_{m+1}^H b = e_1$. Substituting the factorization of K_{m+1} from Lemma 2.1 yields the desired result. □

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. 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*

$$\bar{Y} W y = Z^{-H} e_1 = u \tag{2.3}$$

where the elements of u are defined by

$$u_j = (-1)^{n+1} \mathrm{conj}\left(\prod_{\substack{k=1 \\ k \neq j}}^{n} \frac{\lambda_k}{\lambda_j - \lambda_k} \right). \tag{2.4}$$

Proof. Denote the elements of the first column of Z^{-H} by u_j, $j = 1, \dots, n$. The proof is a consequence of [1, 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 distinct eigenvalues. Let $y = V^{-1}b$. Then* GMRES(A,b) *m-stagnates if and only if y satisfies*

$$\bar{Y}Wy = (Z_{m+1}^H)^\dagger e_1 + t \tag{2.5}$$

where t is in the null space of Z_{m+1}^H.

The usefulness of (2.2), as well as the related equations (2.3) and (2.5), is that it separates the influence of the eigenvalues, which determine Z, and eigenvectors, which determine W. Stagnation is explored through the interaction of W and Z.

The systems (2.2) and (2.3) 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 [3], the number does not exceed the total degree of the polynomial system, which in the case of (2.2) is $2^{2(m+1)}$. Therefore, in practical experiments, we need to use a solver such as `POLSYS_PLP` [12] that finds *all* solutions of the system. Stagnation takes place iff any of these solutions is regular and real.

We conclude this section by establishing the equivalence of stagnation of GMRES for A with stagnation for A^H.

THEOREM 2.5. GMRES *stagnates for the problem $Ax = b$ if and only if it stagnates for $A^H x = \hat{b}$ where $b = Vy$, $\hat{y} = \bar{Y}^{-1}u$, and $\hat{b} = V^{-H}\hat{y}$.*

Proof. From (2.3), we obtain $\bar{Y}V^H V y = u$, so

$$Y^{-1}V^{-1}V^{-H}\bar{Y}^{-1}u = e\,.$$

Let $U = diag(u)$ which yields $\bar{u} = \bar{U}e$. Multiplying the above equation by $\bar{U}$, we obtain the stagnation equation for $A^H x = \hat{b}$:

$$\overline{\hat{Y}}V^{-1}V^{-H}\hat{y} = \bar{u}.$$

□

2.1. The Geometry of Stagnation. The complete stagnation system (2.3) can be written as

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

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

$$1 = ||b||^2 = ||Vy||^2 = y^H W y = ||y||_W^2 = e^T u,$$

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

$$E_V = \{y \in \mathcal{C}^n \mid y^H W y = 1\},$$

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

$$S_n = \{u = [u_1 \ \dots \ u_n]^T \in \mathcal{C}^n \mid \sum_{j=1}^{n} u_j = 1\}.$$

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

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

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

$$B = \{\lambda = [\lambda_1 \ \dots \ \lambda_n]^T \in \mathcal{C}^n \mid 0 \leq |\lambda_j| \leq 1\}.$$

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

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

which is also a subset of S_n. To summarize,

$$\begin{aligned} F_V &: E_V \to S_V \subset S_n \\ G(\lambda) &: B \to S_\lambda \subset S_n. \end{aligned}$$

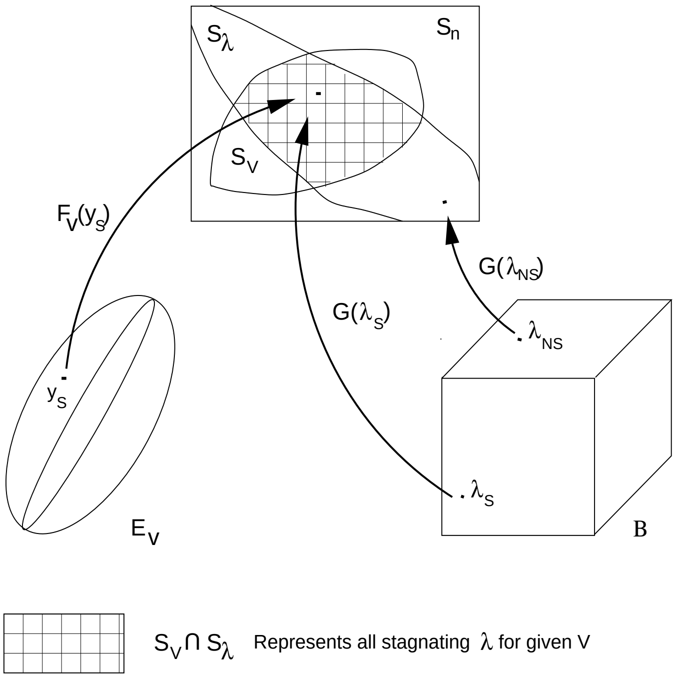

FIG. 2.1. *A Geometric Interpretation of Complete* GMRES *Stagnation*

We can now give a geometric interpretation of complete stagnation of GMRES. It is illustrated in Figure 2.1. 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 Figure 2.1, 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 $S_V \bigcap S_\lambda$, 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 $G(\lambda_{NS}) \notin S_V \bigcap S_\lambda$ for some λ_{NS} then no matter what $y \in E_V$ we pick, the stagnation equation (2.3) 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 $S_V \bigcap S_\lambda$ 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 existing literature on convergence of Krylov methods, where eigenvalues are considered more important. 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.

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 whose elements sum to one and that is orthogonal to the columns 2 through $m+1$ of Z.

2.2. The Nature of S_λ. It follows from (2.4) 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

$$
\begin{aligned}
\lambda_2\ \lambda_3\ \ldots\ \lambda_n &= (-1)^{n+1}\ u_1\ (\lambda_1 - \lambda_2)\ \ldots\ (\lambda_1 - \lambda_n) \\
&\ \ \vdots \\
\lambda_1\ \ldots\ \lambda_{j-1}\ \lambda_{j+1}\ \ldots\ \lambda_n &= (-1)^{n+1}\ u_j\ (\lambda_j - \lambda_1)\ \ldots\ (\lambda_j - \lambda_n) \\
&\ \ \vdots \\
\lambda_1\ \lambda_2\ \ldots\ \lambda_{n-1} &= (-1)^{n+1}\ u_n\ (\lambda_n - \lambda_1)\ \ldots\ (\lambda_n - \lambda_{n-1}).
\end{aligned}
\tag{2.6}
$$

It appears from extensive numerical experiments that, in the case of arbitrary complex eigenvalues, the system (2.6) has solutions for any $u \in S_n$, i.e. $S_\lambda = S_n$. Consequently, in our analysis of the stagnation region $S_V \bigcap S_\lambda$, we focus most of our attention on S_V.

The system (2.6) 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 (2.6) explicitly. For instance, any permutation of the vector

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

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 [4].

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 $S_{V_1} \bigcap S_\lambda$ is larger than that of $S_{V_2} \bigcap S_\lambda$ 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 $F_V(x)$ 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 $\|u\| \le \kappa(V) \equiv \max_i \sigma_i / \min_i \sigma_i$* . $\blacksquare$

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

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

If $u \in S_V$ with the corresponding $y_u \in E_V$, then

$$\|u\| = \|\overline{Y_u} W y_u\| \le \|Y_u\| \|W y_u\| \le \|y_u\| \|W y_u\|.$$

If we define r_u by $y_u = Q r_u$, then

$$1 = y_u^H W y_u = r_u^T \Sigma^2 r_u = \|\Sigma r_u\|,$$

so

$$\|W y_u\| = \|Q \Sigma^2 Q^H Q r_u\| = \|\Sigma^2 r_u\| \le \|\Sigma\| \|\Sigma r_u\| = \max_i \sigma_i.$$

Combining these expressions, we obtain

$$\|u\| \le \|y_u\| \|W y_u\| \le \frac{\max_i \sigma_i}{\min_i \sigma_i} = \kappa(V).$$

$\square$

Lemma 2.6 implies that given eigenvectors V, any eigenvalue distribution λ such that $\|G(\lambda)\| > \kappa(V)$ necessarily yields a non-stagnating matrix $A = V \Lambda V^{-1}$.

3. Results for Problems of Size 2×2. In this section we use the stagnation system to analyze stagnation of GMRES in the simplest possible case, when $n = 2$. We show that stagnation is determined by a simple relationship between the ratio of the eigenvalues and the condition number of the eigenvector matrix. More specifically, we show that given *any* set of distinct nonzero eigenvalues $\lambda \in \mathcal{C}^2$ and a set of eigenvectors $V \in \mathcal{C}^{2\times 2}$, there exists a vector $b \in \mathcal{C}^2$ 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. We also provide an explicit formula for a stagnating right-hand side b.

Let V have the form ΣQ^H and let $r = Q^H y$. We can rewrite the stagnation system (2.3) as follows,

$$G(\lambda) = \overline{Y} V^H V y = \overline{Y}(Q\Sigma)(\Sigma Q^H)(Qr) = \overline{Y} Q \Sigma^2 r. \tag{3.1}$$

Without loss of generality, we make the following assumptions. *First*, the unitary matrix Q has the form

$$Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ e^{i\alpha} & e^{i\alpha} \end{pmatrix}, \quad \alpha \in [0, 2\pi]. \tag{3.2}$$

Second, let $\kappa(V) \equiv \kappa \ge 1$. Due to the column scaling of V and the fact that the order of singular values is not important, we let

$$\Sigma = \sqrt{\frac{2}{\kappa^2 + 1}} \begin{pmatrix} \kappa & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.3}$$

Third, it is easy to see that y solves (2.3) iff $e^{i\gamma}y$ also does, where γ is any phase angle. Therefore we assume

$$r = \begin{bmatrix} r_1 \\ r_2 e^{i\phi} \end{bmatrix}, \quad r_1, r_2 \in \mathcal{R} \setminus \{0\}, \ \phi \in [0, 2\pi]. \tag{3.4}$$

Note that if vector r contains a zero entry, the corresponding right-hand side vector b can never cause stagnation. Therefore we assume that r_1 and r_2 are nonzero. Also note that we allow the two variables to be negative. This gives us more flexibility when solving the resulting polynomial system. On the other hand, if either variable takes a negative value, the corresponding polar representation of the entry of r can be obtained by adjusting the phase angle ϕ.

Finally, for our *fourth* assumption, since $G(\lambda)$ is scale invariant, we let

$$\lambda = \begin{bmatrix} 1 \\ \lambda_0 e^{i\theta} \end{bmatrix}, \quad \lambda_0 > 1, \ \theta \in [0, 2\pi]. \tag{3.5}$$

We plug (3.2) – (3.5) into (3.1), simplify, separate both sides of the stagnation system into real and imaginary parts and obtain the following system of four equations:

$$\begin{aligned}
\frac{\kappa^2 r_1^2 + r_2^2}{\kappa^2+1} - r_1 r_2 \cos\phi &= \frac{1 - \lambda_0 \cos\theta}{1 - 2\lambda_0\cos\theta + \lambda_0^2} \\
\frac{\kappa^2 r_1^2 + r_2^2}{\kappa^2+1} + r_1 r_2 \cos\phi &= \frac{\lambda_0(\lambda_0 - \cos\theta)}{1 - 2\lambda_0\cos\theta + \lambda_0^2} \\
\frac{(\kappa^2-1) r_1 r_2 \sin\phi}{\kappa^2+1} &= \frac{\lambda_0 \sin\theta}{1 - 2\lambda_0\cos\theta + \lambda_0^2} \\
-\frac{(\kappa^2-1) r_1 r_2 \sin\phi}{\kappa^2+1} &= -\frac{\lambda_0 \sin\theta}{1 - 2\lambda_0\cos\theta + \lambda_0^2}.
\end{aligned}$$

The fourth equation is redundant and can be dropped. The remaining three nonlinear equations have three unknowns $\{r_1, r_2, \phi\}$. We need to determine the conditions on the parameters of the system, λ_0, κ and θ, under which system has appropriate solutions.

There are four pairs of solutions $\{r_1, r_2\}$: [1],

$$\begin{aligned}
&\{\{-\frac{1}{2}\sqrt{1+\frac{1-\frac{c_4}{c_3}}{\kappa^2}}, -\frac{c_2 c_5\sqrt{1+\frac{1-\frac{c_4}{c_3}}{\kappa^2}}}{c_1}\}, \\
&\{\frac{1}{2}\sqrt{1+\frac{1+\frac{c_4}{c_3}}{\kappa^2}}, -\frac{c_2 c_6\sqrt{1+\frac{1+\frac{c_4}{c_3}}{\kappa^2}}}{c_1}\}, \\
&\{-\frac{1}{2}\sqrt{1+\frac{1+\frac{c_4}{c_3}}{\kappa^2}}, -\frac{c_2 c_6\sqrt{1+\frac{1+\frac{c_4}{c_3}}{\kappa^2}}}{c_1}\}, \\
&\{\frac{1}{2}\sqrt{1+\frac{1-\frac{c_4}{c_3}}{\kappa^2}}, -\frac{c_2 c_5\sqrt{1+\frac{1-\frac{c_4}{c_3}}{\kappa^2}}}{c_1}\}\},
\end{aligned} \tag{3.6}$$

[1]Computations were performed using `Mathematica` version 4 [13].

where

$$c = \begin{bmatrix} 4((\kappa^2-1)^2+8\kappa^2\lambda_0^2+(\kappa^2-1)^2\lambda_0^4-2(1+\kappa^2)^2\lambda_0^2\cos\theta), \\ \sqrt{(\kappa^2-1)^2(\lambda_0^2-1)^2+4(\kappa^2+1)^2\lambda_0^2\sin^2\theta}, \\ (\kappa^2-1)(1-2\lambda_0\cos\theta+\lambda_0^2), \\ \sqrt{c_7+c_8}, \\ c_4+(\kappa^4-1)(1-2\lambda_0\cos\theta+\lambda_0^2), \\ c_4-(\kappa^4-1)(1-2\lambda_0\cos\theta+\lambda_0^2), \\ (\kappa^2-1)^4+4(1-10\kappa^4+\kappa^8)\lambda_0^2, \\ (\kappa^2-1)^4\lambda_0^4-4(\kappa^4-1)^2\lambda_0(\lambda_0^2+1)\cos\theta+2(\kappa^2+1)^4\lambda_0^2\cos 2\theta \end{bmatrix}.$$

Although the above expressions are quite complicated, we observe that there exists a real pair of solutions $\{r_1, r_2\}$ iff c_4 is real. The expression $c_4^2 = c_7 + c_8$ is a fourth-degree polynomial in κ^2 with the positive leading coefficient $(1-2\lambda_0\cos\theta+\lambda_0^2)^2$. In order to determine regions corresponding to stagnating matrices A, we need to determine values of κ^2 for which the expression c_4^2 is positive. To this end, we solve $c_4^2 = 0$ for κ^2 and obtain the following four zeros,

$$\kappa_1^2(\lambda_0,\theta) = \frac{1+\lambda_0(\lambda_0-4)-2\sqrt{2(\lambda_0-1)^2\lambda_0(\cos\theta-1)}+2\lambda_0\cos\theta}{1-2\lambda_0\cos\theta+\lambda_0^2},$$

$$\kappa_2^2(\lambda_0,\theta) = \frac{1+\lambda_0(\lambda_0-4)+2\sqrt{2(\lambda_0-1)^2\lambda_0(\cos\theta-1)}+2\lambda_0\cos\theta}{1-2\lambda_0\cos\theta+\lambda_0^2},$$

(3.7)

$$\kappa_3^2(\lambda_0,\theta) = \frac{(1+\lambda_0-2\sqrt{\lambda_0}\cos\frac{\theta}{2})^2}{1-2\lambda_0\cos\theta+\lambda_0^2},$$

$$\kappa_4^2(\lambda_0,\theta) = \frac{(1+\lambda_0+2\sqrt{\lambda_0}\cos\frac{\theta}{2})^2}{1-2\lambda_0\cos\theta+\lambda_0^2}.$$

We now examine the sign of c_4^2 depending on where κ^2 is relative to $\kappa_j^2(\lambda_0,\theta)$, $j = 1,2,3,4$. We consider three separate cases.

(i) *Real Eigenvalues of the Same Sign.* Eigenvalues of A are real and of the same sign iff $\theta = 0$. In this case, (3.7) simplifies to

$$\kappa_1^2(\lambda_0,0) = \kappa_2^2(\lambda_0,0) = 1,$$
$$\kappa_3^2(\lambda_0,0) = \frac{1}{\kappa_{same}(\lambda_0)^2}, \quad \kappa_4^2(\lambda_0,0) = \kappa_{same}(\lambda_0)^2,$$

where

$$\kappa_{same}(\lambda_0) = \frac{\sqrt{\lambda_0}+1}{\sqrt{\lambda_0}-1},$$

and so

$$\kappa_3^2(\lambda_0,0) \le \kappa_1^2(\lambda_0,0) = 1 = \kappa_2^2(\lambda_0,0) \le \kappa_4^2(\lambda_0,0).$$

For any V, $\kappa(V) \ge 1$, so we need only consider only two cases, when $1 \le \kappa^2 < \kappa_4^2(\lambda_0,0)$ and $\kappa_4^2(\lambda_0,0) \le \kappa^2$. As noted above, the leading coefficient of c_4^2 as a function of κ^2 is positive, so that

$$\lim_{\kappa\to+\infty} c_4^2 = +\infty.$$

We conclude that if

$$\kappa(V) \geq \kappa_{same}(\lambda_0),$$

then $c_4^2 \geq 0$ and so there exists a real pair of $\{r_1, r_2\}$ that yields a stagnating right-hand side b. Conversely, if $1 \leq \kappa(V) < \kappa_{same}(\lambda_0)$, then there is no stagnating b. Note that $\lambda_0 > 1$ is just the ratio of the larger and smaller eigenvalues of A.

(ii) *Real Eigenvalues of Opposite Signs.* Eigenvalues of A are real and of opposite signs iff $\theta = \pi$. We first observe that unless $\theta = 0$, $\kappa_1^2(\lambda_0, \theta)$ and $\kappa_2^2(\lambda_0, \theta)$ are complex, so in order to determine the sign of c_4^2, we consider $\kappa_3^2(\lambda_0, \theta)$ and $\kappa_4^2(\lambda_0, \theta)$ only. After simplification we obtain

$$\kappa_3^2(\lambda_0, \pi) = \kappa_4^2(\lambda_0, \pi) = 1.$$

Again, since the leading coefficient is positive, we conclude that if

$$\kappa(V) \geq 1$$

then there exists a stagnating vector b. This implies that any $A \in \mathcal{C}^{2\times 2}$ with real eigenvalues of opposite signs is stagnating.

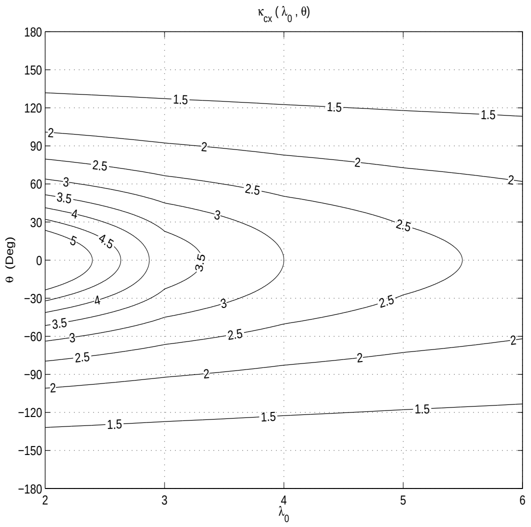

FIG. 3.1. *Contours of $\kappa_{cx}(\lambda_0, \theta)$*

(iii) *Complex Eigenvalues.* Finally, we consider $\theta \in (0, \pi) \bigcup (\pi, 2\pi)$, which corresponds to A with complex eigenvalues. Again, since $\kappa_{1,2}^2(\lambda_0, \theta)$ are complex, we only consider $\kappa_{3,4}^2(\lambda_0, \theta)$. First, we determine that

$$\kappa_3^2(\lambda_0, \theta)\ \kappa_4^2(\lambda_0, \theta) = 1.$$

Moreover, if $0 < \theta < \pi$ then $\kappa_3^2(\lambda_0, \theta) < 1$ and $\kappa_4^2(\lambda_0, \theta) > 1$. If $\pi < \theta < 2\pi$ then the opposite holds.

Once more referring to the positive leading coefficient, we conclude that a matrix $A \in \mathcal{C}^{2\times 2}$ with complex eigenvalues is stagnating iff the condition number of its eigenvector matrix V is larger than the biggest of the two zeros, i.e. it satisfies

$$\kappa(V) \geq \kappa_{cx}(\lambda_0, \theta),$$

where

$$\kappa_{cx}(\lambda_0,\theta) = \begin{cases} \kappa_4(\lambda_0,\theta) = \frac{1+\lambda_0+2\sqrt{\lambda_0}\cos\frac{\theta}{2}}{\sqrt{1-2\lambda_0\cos\theta+\lambda_0^2}}, & 0 < \theta < \pi \\ \\ \kappa_3(\lambda_0,\theta) = \frac{1+\lambda_0-2\sqrt{\lambda_0}\cos\frac{\theta}{2}}{\sqrt{1-2\lambda_0\cos\theta+\lambda_0^2}}, & \pi < \theta < 2\pi \end{cases}$$

where λ_0 and θ are determined by the ratio of moduli of the larger and smaller eigenvalues. As $\theta \to 0$ and π, $\kappa_{cx}(\lambda_0,\theta) \to \kappa_{same}(\lambda_0)$ and 1, respectively.

We can summarize the findings on 2×2 stagnation as follows.

1. Given an eigenvalue distribution $\lambda \in \mathcal{C}^2$, there exists $b \in \mathcal{C}^2$ for which GMRES($V\Lambda V^{-1}$,b) stagnates whenever $\kappa(V)$ is large enough with respect to $|\lambda_2|/|\lambda_1|$. Conversely, given a nonsingular $V \in \mathcal{C}^{2\times 2}$ one can find $\lambda \in \mathcal{C}^2$ that will yield a stagnating A.
2. For some $\lambda \in \mathcal{C}^2$ (specifically, real with eigenvalues of opposite signs), *every* V gives a stagnating matrix.
3. Whether a given matrix A yields stagnation of GMRES(A,b) for some b is completely determined by the relationship between the eigenvalue ratio $\lambda_0 e^{i\theta}$ and the condition number of V.
4. When $\kappa(V)$ is large enough to cause stagnation, it is possible to compute a stagnating right-hand side vector b explicitly from (3.6).

Item 1 is illustrated graphically in Figure 3.1, which shows contour lines of $\kappa_{cx}(\lambda_0,\theta)$ for $2 \le \lambda_0 \le 6$ and $-180° \le \theta \le 180°$. Each contour line $\kappa_{cx}(\lambda_0,\theta) = \kappa$ corresponds to eigenvalue distributions λ such that $A = V\Lambda V^{-1}$ is stagnating for every V with $\kappa(V) \ge \kappa$. The inside of the region enclosed by a contour line corresponds to non-stagnating distributions λ. As expected, this region becomes smaller as $\kappa_{cx}(\lambda_0,\theta)$ grows. Next we investigate to what extent these findings generalize to problems of larger dimensions.

4. Complete Stagnation of Matrices with Extreme Eigenvalue Distributions. We call V *extreme* if its singular values can be ordered to satisfy

$$\sigma_1 = \sigma_2 = \cdots = \sigma_{n-1} \neq \sigma_n,$$

In this section, we explore the structure of S_V derived from such extreme matrices and show in particular that two different, but equally conditioned, extreme eigenvector distributions have essentially the same range sets S_V. Since columns of V are assumed to have Euclidean norm 1, the condition number of V is within a factor of $\sqrt{n}$ of optimal [10], and the singular values satisfy

$$\sigma_1^2 + \ \cdots + \ \sigma_n^2 = n. \tag{4.1}$$

For extreme matrices V, the stagnation system $\bar{Y}Wy = u$ has a particularly simple form. Let the singular values of W be $\sigma_j^2 = \alpha$, $j = 1,\ldots,n-1$, and $\sigma_n^2 = \alpha+\beta$, where α is nonnegative and β is real. By (4.1), $n\alpha + \beta = n$, and, since the singular values are nonnegative, we must have $0 \le \alpha \le n/(n-1)$ and $\sigma_n^2 = \alpha + n(1-\alpha)$. The matrix Σ^2 then has the form

$$\Sigma^2 = \alpha I + n(1-\alpha)e_n e_n^T$$

where e_n is the nth unit vector. We can then conclude that

$$W = Q\Sigma^2 Q^H = Q(\alpha I + n(1-\alpha)e_n e_n^T)Q^H = \alpha I + n(1-\alpha)qq^H,$$

where q is the last column of Q, the right singular vector corresponding to the singular value σ_n. Therefore, the stagnation system (2.3) becomes

$$u = \bar{Y}Wy = \alpha\bar{Y}y + n(1-\alpha)\bar{Y}qq^Hy. \tag{4.2}$$

The singular vector q has the property that every entry has the same magnitude:

LEMMA 4.1. *Suppose $V \in \mathcal{C}^{n\times n}$ is extreme and the corresponding W has singular values parameterized by α and β as defined above. Then*

$$q = \frac{1}{\sqrt{n}}\left(e^{i\theta_1}, \ldots, e^{i\theta_n}\right)^T,$$

where $\theta_j \in [0, 2\pi]$ are certain phase angles.

Proof. Let elements of the vector q have the form $q_j = r_j e^{i\theta_j}$, where $r_j \in \mathcal{R}$ and $\theta_j \in [0, 2\pi]$. Since V is properly scaled, the main diagonal elements of W are

$$1 = w_{jj} = \alpha + n(1-\alpha)q_j\bar{q}_j = \alpha + n(1-\alpha)r_j^2, \quad j = 1, \ldots, n\,.$$

Consequently

$$r_j = \sqrt{\frac{1-\alpha}{n(1-\alpha)}} = \frac{1}{\sqrt{n}}.$$

□

4.1. Structure of S_V for an Extreme V. We now use this lemma to prove that the range set S_V of an extreme V is symmetric with respect to the "center" point $u_c = (1/n)\, e$, i.e., if $u \in S_V$ then $u_P = Pu \in S_V$, where P is any permutation matrix.

THEOREM 4.2. *Suppose a properly scaled matrix V is extreme, with singular values Σ and right singular vectors defined by Q. Then*

$$u \in S_V \quad \Rightarrow \quad u_P = Pu \in S_V,$$

where P is a permutation matrix.

Proof. Suppose we have a solution to the stagnation equation

$$u = \alpha\bar{Y}y + n(1-\alpha)\bar{Y}qq^Hy.$$

Since the basis in Q for the space orthogonal to q is arbitrary, we can establish our result just by proving it for a permutation P that interchanges the first and last components of a vector. Let $\hat{y} = \hat{Y}e$ where

$$\hat{Y} = PYPD,$$

and

$$D = \mathrm{diag}(e^{i(\theta_1-\theta_n)}, 1, \ldots, 1, e^{i(\theta_n-\theta_1)})\,.$$

Then $\bar{D} = PDP$, so that

$$\overline{\hat{Y}} = P\bar{Y}P\bar{D} = P\bar{Y}DP.$$

Therefore

$$\overline{\hat{Y}}\hat{y} = (P\bar{Y}DP)(PYPDe) = P\bar{Y}DYPDe = P\bar{Y}Y(DPD)e = P\bar{Y}y,$$

since $DPD = P$. Similarly, since $DPq = q$,

$$\begin{aligned}\overline{\hat{Y}}qq^H\hat{y} &= P\overline{Y}DPqq^HPYPDe \\ &= P\overline{Y}qq^HPYPDPPe \\ &= P\bar{Y}qq^HPY\bar{D}Pe \\ &= P\bar{Y}qq^HP\bar{D}Ye \\ &= P\bar{Y}qq^Hy.\end{aligned}$$

Therefore,

$$\alpha\overline{\hat{Y}}\hat{y} + n(1-\alpha)\overline{\hat{Y}}qq^H\hat{y} = Pu,$$

so $Pu \in S_V$. □

We have run extensive numerical experiments that suggest that the set S_V of an extreme V is convex. The range set S_V also appears to be convex for any 3×3 real matrix V. However, in general S_V is not convex.

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

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

If we consider only real right-hand sides b, then the dotted region in Figure 4.1 corresponds to the slice of S_V that is its intersection with the plane $u_3 = 0.9269$. Clearly, the range set is not convex. This figure was constructed by solving the stagnation system using globally convergent probability-one homotopy algorithms [11], as implemented in the POLSYS_PLP package [12]. Further details are given in [15].

We conclude this section with a result that relates the range sets S_V of two different extreme matrices.

THEOREM 4.3. *Let Q be a unitary matrix with last column q. Let κ be a real constant greater than 1. Define two extreme matrices $V_1 = \Sigma_1 Q^H$ and $V_2 = \Sigma_2 Q^H$ so that*

$$\frac{\alpha_1}{\alpha_1 + \beta_1} = \frac{\alpha_2 + \beta_2}{\alpha_2} = \kappa,$$

and thus $\kappa(W_1) = \kappa(W_2) = \kappa$. Then $u \in S_{V_1}$ iff $\bar{u} \in S_{V_2}$.

Proof. The proof is constructive. Suppose we are given a vector $y_1 \in E_{V_1}$ such that $F_{V_1}(y_1) = u$. Then we may express y_1 as

$$y_1 = r_1 e^{i\alpha_1}\hat{q} + r_n e^{i\alpha_n} q$$

for some $\hat{q}$ orthogonal to q, where $r_1, r_n \in \mathcal{R}$ and $0 \le \alpha_1, \alpha_n \le 2\pi$. Now let

$$y_2 = c_1 r_1 e^{-i\alpha_n}\hat{q} + c_n r_n e^{-i\alpha_1} q$$

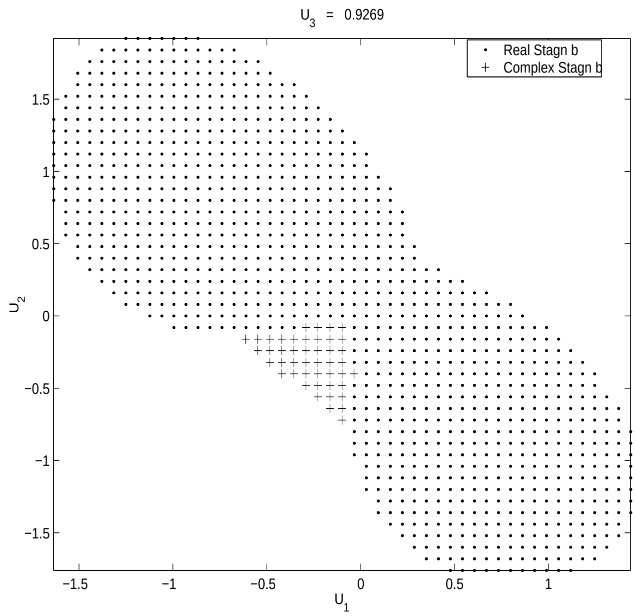

FIG. 4.1. *The range of $F_V(y)$ can fail to be convex (Section 4.1), and real vectors b are not sufficient (Section 6.2).*

where

$$c_1 = \sqrt{\frac{\kappa(\kappa+n-1)}{\kappa(n-1)+1}}, \quad c_n = \sqrt{\frac{\kappa+n-1}{\kappa(\kappa(n-1)+1)}}.$$

It is easy, but tedious, to verify that $F_{V_2}(y_2) = \bar{u}$. The details can be found in [15, Section 4.6]. □

Theorem 4.3 shows that the two equally conditioned extreme matrices are essentially identical in terms of stagnation, i.e. the matrix $A_1 = V_1 \Lambda V_1^{-1}$ is stagnating iff $A_2 = V_2 \bar{\Lambda} V_2^{-1}$ is, too.

5. Complete Stagnation of Normal Matrices. A normal matrix A is one whose eigenvector matrix V is unitary. In this case, the stagnation system (2.3) simplifies to

$$\overline{Y} y = u = G(\lambda), \tag{5.1}$$

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

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

THEOREM 5.1. *Let $A \in \mathcal{C}^{n\times n}$ be normal with distinct eigenvalues λ. If the vector $u = G(\lambda)$, defined by (2.4), satisfies $u \in \mathcal{R}^n$, and $0 \le u_j \le 1, \quad j = 1, \ldots, n$, then* GMRES($A$,$b$) *stagnates for $b = Vy$, where*

$$y_j = \sqrt{u_j} e^{i\theta_j}, \quad j = 1, \ldots, n, \tag{5.2}$$

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 (5.2) solves (5.1) and thus causes stagnation of GMRES. Conversely, if at least one element of u is either complex or real negative, the system (5.1) does not have a solution, so stagnation is impossible. □

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

COROLLARY 5.2. *Let $V \in \mathcal{C}^{n\times n}$ be unitary. Then the corresponding set E_V is the unit sphere and the range of $F_V(y)$ is a real simplex*

$$S_I = \{\ u \in \mathcal{R}^n \mid 0 \le u_j \le 1,\ j = 1,\dots,n\ \}.$$

When A is Hermitian or real symmetric, GMRES is equivalent to MINRES [7]. Proposition 5.3 below shows that in this case the two methods cannot stagnate, provided $n \ge 3$. This is a well known result, but we show how this fact is reflected in the framework of the stagnation equation.

PROPOSITION 5.3. *Let $\lambda \in \mathcal{R}^n$ and let $u = G(\lambda)$. Then all elements of $u = [u_1,\dots,u_n]^T$ are nonzero. Furthermore,*

- *If $n = 2\hat{n} - 1$ is odd then $\hat{n}$ elements of u are negative.*
- *If $n = 2\hat{n}$ is even then either $\hat{n}$ or $\hat{n} - 1$ elements of u are negative.*

Therefore GMRES *cannot stagnate when applied to a Hermitian or real symmetric matrix with distinct eigenvalues.*

Proof. See [15, Proposition 4]. □

5.1. Stagnation of Unitary Matrices. A normal matrix A is unitary iff its eigenvalues satisfy

$$\lambda_j = e^{i\phi_j},\quad 0 \le \phi_j \le 2\pi,\quad j = 1,\dots,n. \tag{5.3}$$

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 [5]. Using Theorem 5.1 we now show that those are the only unitary matrices for which stagnation can occur.

THEOREM 5.4. *Let $A \in \mathcal{C}^{n\times n}$ be unitary with distinct eigenvalues.* GMRES *stagnates iff the phase angles ϕ_j satisfy*

$$\phi_j = \phi + \frac{2\pi(j-1)}{n},\quad j = 1,\dots,n, \tag{5.4}$$

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

We prove Theorem 5.4 in two steps. Given λ, a set of n distinct eigenvalues of the form (5.3), define its image under the transformation $G(\lambda)$ by

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

In Lemma 5.5, we derive explicit formulations for v and w. Then, in Lemma 5.6, we prove that the only set of phase angles $\{\phi_j\}$ that makes w zero is the one defined by (5.4). For this set of angles, it can be shown by direct computation that v contains only positive entries.

LEMMA 5.5. *Let $\lambda \in \mathcal{C}^n$ be a set of n distinct eigenvalues of the form (5.3). Without loss of generality assume that*

$$0 = \phi_1 < \phi_2 < \ \dots < \phi_n < 2\pi. \tag{5.5}$$

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

$$u_j = \gamma^{(n)}\ C_j^{(n)}\ d_j^{(n)}, \tag{5.6}$$

where

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

and

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

where

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

Proof. The jth element of u satisfies $u_j = u_{1j}$, where u_{1j} is defined by (2.4). Each term of (2.4) can be rewritten as follows using (5.3)

$$\frac{\lambda_k}{\lambda_j - \lambda_k} = -\frac{\sin\frac{\phi_j-\phi_k}{2} + i\cos\frac{\phi_j-\phi_k}{2}}{2\sin\frac{\phi_j-\phi_k}{2}} = \left(-\frac{1}{2}\right)\csc\frac{\phi_j-\phi_k}{2}\ i\ e^{i\left(\frac{\phi_k-\phi_j}{2}\right)}$$

This yields

$$u_j = (-1)^n \left(\frac{1}{2}\right)^{n-1} \prod_{\substack{k=1\\k\neq j}}^{n} \csc\frac{\phi_j-\phi_k}{2}\ i^{n-1}\ exp\left(i\ \sum_{\substack{k=1\\k\neq j}}^{n} \frac{\phi_k-\phi_j}{2}\right). \tag{5.7}$$

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

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

we can rewrite (5.7) as

$$u_j = \gamma^{(n)}\ C_j^{(n)}\ i\ e^{-i\frac{\alpha_j^{(n)}}{2}},$$

where

$$i\ e^{-i\frac{\alpha_j^{(n)}}{2}} = \sin\frac{\alpha_j^{(n)}}{2} + \ \cos\frac{\alpha_j^{(n)}}{2}.$$

This completes the proof. ☐

LEMMA 5.6. *The vector w, the imaginary part of u defined by (5.6), is zero iff the phase angles $\{\phi_j\}$ are given by (5.4).*

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 (5.6) we see that u is real iff

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

Thus

$$\alpha_k^{(n)} = \pi + 2\pi m_k, \;\; k = 2, \ldots, n, \tag{5.8}$$

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 (5.5) is the one that gives (5.4). To find phase angles $\phi_2, \ldots, \phi_n$ that set the bottom $n-1$ entries of $\hat{w}$ to zero, we have to solve the $n-1 \times n-1$ system

$$M\phi = \beta,$$

where

$$M = \begin{pmatrix} n-1 & -1 & -1 & \ldots & -1 \\ -1 & n-1 & -1 & \ldots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \ldots & n-1 \end{pmatrix}, \quad \phi = \begin{pmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \phi_n \end{pmatrix}, \quad \beta = \begin{pmatrix} \pi + 2\pi m_2 \\ \pi + 2\pi m_3 \\ \vdots \\ \pi + 2\pi m_n \end{pmatrix}.$$

Now

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

so

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

From (5.5) it follows that $m_2 < m_3 < \ldots < m_n$, so we can write

$$m_j = m_2 + \delta_j, \;\; j = 3, \; \ldots, \; n,$$

where δ_j is a positive integer, increasing with j. We consider two cases.

Case I: $\delta_j = 1$, $j = 3, \ldots, n$. In this case

$$\hat{\phi}_k = \frac{\pi}{n}(n^2 - 2n - 2 + 2nm_2 + 2k), \;\; k = 2, \ldots, n.$$

We know that $m_2 \in [2-n, 0]$, so let $m_2 = (2-n)/2 - \mu$, where $m \in [1, (n-2)/2]$. Then

$$\hat{\phi}_2 = \frac{2\pi}{n}(1 - \mu n) < 0,$$

which violates (5.5). Now let $m_2 = (2-n)/2 + \mu$ with μ in the same range. Then

$$\hat{\phi}_n = \frac{2\pi}{n}(n - 1 + n\mu) > 2\pi,$$

which also violates (5.5). Only when $m_2 = (2-n)/2$ do we get a valid set of phase angles $\hat{\phi}_k$, namely,

$$\hat{\phi} = \frac{2\pi}{n}\,(1,\ 2,\ \ldots,\ n-1)^T. \tag{5.9}$$

Case II: $\delta_j > 1,\ j \geq j_0 \geq 3$. Clearly, in this case, regardless of j_0, $\hat{\phi}_2$ is negative and $\hat{\phi}_n$ exceeds 2π when m_2 equals $(2-n)/2 - \mu$ and $(2-n)/2 + \mu$, respectively. On the other hand, when $m_2 = (2-n)/2$,

$$\hat{\phi}_n \geq \frac{2\pi(n-1)}{n} + \frac{4\pi}{n} > 2\pi.$$

We conclude that the only combination of phase angles which satisfies (5.5) and sets the bottom $n-1$ entries of $\hat{w}$ to zero is the one defined by (5.9). It is easy to show by direct computation that it also zeroes out the first entry of $\hat{w}$. □

5.2. Does Normal Stagnation Imply Non-Normal Stagnation?. In Section 3 we found that, given $\lambda \in \mathcal{C}^2$, as long as $\kappa(V)$ is larger than a certain value that depends on λ, the corresponding $A = V\Lambda V^{-1}$ is stagnating. In particular, this implies that if $A \in \mathcal{C}^{2\times 2}$ is normal and stagnating then so is $\tilde{A} = \tilde{V}\Lambda\tilde{V}^{-1}$ for any $\tilde{V} \in \mathcal{V}^2$. 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 normal V. If this is true in general then that would imply that normal stagnation does indeed imply non-normal stagnation.

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

THEOREM 5.7. *Suppose A has distinct eigenvalues λ and a real eigenvector matrix V, and that $u = G(\lambda)$ satisfies $u \in \mathcal{R}^n$ with $0 < u_i \leq 1$. Then* GMRES(A,b) *stagnates for $b = Vy$ where $y \in \mathcal{R}^n$ satisfies $YWy = u$.*

Proof. If V is real, then W 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 $0 < u_i \leq 1$, the main theorem in [6] tells us that such a scaling matrix exists.
□

6. Complete Stagnation of Real Matrices. In this section, we investigate the special form that the stagnation system (2.3) 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, its spectrum consists of real eigenvalues and complex conjugate pairs of eigenvalues. Let $A \in \mathcal{R}^{n\times n}$ have eigenvalues λ and eigenvectors V. Then there exists a symmetric permutation matrix $P \in \mathcal{R}^{n\times n}$ such that

$$\overline{V} = VP, \quad \bar{\lambda} = P\lambda. \tag{6.1}$$

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

$$\overline{Y}PW_T y = u \tag{6.2}$$

where $W_T = V^T V$. Furthermore, GMRES(A,b) stagnates for $b = Vy \in \mathcal{R}^n$ iff $\|b\| = 1$ and y solves

$$YW_T y = \bar{u}, \quad \bar{y} = Py. \tag{6.3}$$

Unlike (2.3), equation (6.3) constitutes a polynomial system of size n in y. This makes numerical experiments easier.

6.1. 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 $W_T = W$. If we consider only real right-hand sides then we get the real polynomial stagnation system

$$YWy = u, \tag{6.4}$$

where $y \in \mathcal{R}^n$ satisfes $y^T Wy = 1$ and $u = G(\lambda)$.

Note that when (2.3) or (6.2) is solved, the corresponding domain for $F_V(y) = \overline{Y}Wy$ is

$$E_V = \{\ y \in \mathcal{C}^n \mid y^H Wy = 1\}.$$

When we consider (6.3), the domain changes to

$$E_V = \{\ y \in \mathcal{C}^n \mid \bar{y} = Py, \ \ y^H Wy = y^T W_T y = 1\},$$

where $W_T = V^T V$ and P is defined by (6.1). Finally, for (6.4) the domain has the form

$$E_V = \{\ y \in \mathcal{R}^n \mid y^T Wy = 1\}.$$

6.2. 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 6.1. *Let $A \in \mathcal{R}^{n\times n}$ with real eigenvalues λ and eigenvectors V. If V is of size 3×3 or is an extreme matrix, then existence of a complex stagnating right-hand side vector implies existence of a real one.*

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

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

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

We show that if V is 3×3 and/or extreme, the phase angles $\phi_1, \ldots, \phi_n$ are all equal. Then we can conclude that the real vector $y_R = e^{-i\phi_1} y$ satisfies $Y_R W y_R = u$ and, therefore, also corresponds to a stagnating right-hand side.

We first consider the 3×3 case. We expand $\overline{Y} W y$ and conclude that y must satisfy

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} x_1^2 + x_1 x_2 e^{i(\phi_2 - \phi_1)} + x_1 x_3 e^{i(\phi_3 - \phi_1)} \\ x_2^2 + x_2 x_1 e^{i(\phi_1 - \phi_2)} + x_2 x_3 e^{i(\phi_3 - \phi_2)} \\ x_3^2 + x_3 x_1 e^{i(\phi_1 - \phi_3)} + x_3 x_2 e^{i(\phi_2 - \phi_3)} \end{bmatrix}. \tag{6.5}$$

Each entry on the left of equation (6.5) 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

$$\begin{aligned} \phi_2 - \phi_1 &= \phi_1 - \phi_3 \\ \phi_1 - \phi_2 &= \phi_2 - \phi_3. \end{aligned}$$

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

Now assume V is extreme with singular vectors Q. Then, as in the proof of Theorem 4.3, y can be expressed as

$$y = r_1 e^{i\alpha_1} \hat{q} + r_n e^{i\alpha_n} q$$

for some $\hat{q}$ orthogonal to q, where $r_1, r_n \in \mathcal{R}$ and $0 \leq \alpha_1, \alpha_n \leq 2\pi$. Using the extreme matrix stagnation equation (4.2), we obtain

$$u_j = (\hat{q}_j r_1 \sigma_1)^2 + (q_j r_n \sigma_n)^2 + \hat{q}_j q_j r_1 r_n (\sigma_1^2 e^{i(\alpha_1 - \alpha_n)} + \sigma_n^2 e^{i(\alpha_n - \alpha_1)}), \quad j = 1, \ldots, n.$$

Unless V is unitary, $\sigma_1 \neq \sigma_n$. Therefore in order for u_j to be real, α_1 must be equal to α_n. This yields y with $\phi_1 = \ldots = \phi_n$. $\square$

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: Consider the matrix from Example 4.1. 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 (2.3) 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 (6.4) with W and u as above. Note that if a complex y solves (6.4) 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,

$$y_I = \begin{bmatrix} 0.7391037 + 0.2570027\, i \\ -0.1534853 + 0.5091449\, i \\ 1.2414730 + 0.3333155\, i \\ -1.2276988 + 0.1269897\, i \end{bmatrix}, \quad y_{II} = \begin{bmatrix} 0.1578663 + 0.9757913\, i \\ 0.1463589 + 0.0364812\, i \\ 0.9548215 + 0.3991290\, i \\ 0.8611411 - 0.2115472\, i \end{bmatrix},$$

$$y_{III} = \begin{bmatrix} -0.9785711 - 2.1552377\, i \\ 3.4382447 + 2.1527698\, i \\ 1.8727147 - 0.2306006\, i \\ 2.7341793 + 2.2536406\, i \end{bmatrix}, \quad y_{IV} = \begin{bmatrix} 2.4426010 + 0.4870174\, i \\ -1.1947469 - 0.5787159\, i \\ 1.7072389 + 0.0030895\, i \\ -2.3718795 - 0.5254314\, i \end{bmatrix}.$$

The degree of the system is 16, and all sixteen solutions are verified to be isolated. We conclude that the given system (6.4) has no other real or complex solutions. On the other hand, a complex solution of (6.4) does not produce a stagnating b.

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 again examine Figure 4.1, which shows a slice of S_V for the matrix V defined above. 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.

7. Conclusions. We have presented several results on the stagnation behavior of GMRES . For problems of dimension 2 we determined that every choice of eigenvalues leads to a stagnating problem for eigenvector matrices that are sufficiently poorly conditioned. We partially extended this result to higher dimensions for a class of eigenvector matrices called extreme. 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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