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Complementary cycles of restarted GMRES

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SUMMARY

Restarted GMRES is one of the most popular methods for solving large nonsymmetric linear systems. It is generally thought that the information of previous GMRES cycles is lost at the time of a restart; therefore, each cycle contributes to the global convergence individually. However, this is not the full story. In this paper, we shed light on the relationship between different GMRES cycles. It is shown that successive GMRES cycles can complement one another harmoniously. These groups of cycles, called complementary cycles, are defined and studied. Copyright © 2008 John Wiley & Sons, Ltd.

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KEY WORDS: nonsymmetric linear systems; iterative methods; GMRES; restarting; harmonic Ritz values

1. INTRODUCTION

Solution of the large system of linear equations

$$Ax = b, \quad A \in R^{n\times n}, \quad x, b \in R^n$$

with the iterative method GMRES [1, 2] is considered. GMRES extracts from a Krylov subspace the approximate solution with the minimum residual. However, as GMRES builds an orthogonal basis for the subspace, it may need to be restarted to reduce storage and expense. Restarted GMRES with restart frequency of m (cycles of length m) is called GMRES(m). The residual vector at the time of the restart can be expressed in terms of a polynomial in A. If the current problem at the beginning of a GMRES cycle is $A(x-x_0)=r_0$, where x_0 is the current approximate solution, then the residual vector at the end of the cycle is $r = p(A)r_0$, where p is a polynomial of degree m

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or less with value 1.0 at zero. The polynomial p is called the GMRES polynomial. Its roots are harmonic Ritz values [3–9]. The new approximate solution at the end of the GMRES(m) cycle is $x_m = x_0 + y$. Here, y is an element of the Krylov subspace $\mathrm{Span}\{r_0, Ar_0, A^2r_0, \ldots, A^{m-1}r_0\}$; therefore $y = q(A)r_0$ for q a polynomial of degree $m-1$ or less.

It is traditionally thought that the information of previous GMRES(m) cycles is discarded at the time of restarting so that the local minimization of GMRES(m) within each cycle can only contribute to its global convergence individually. However, this is not entirely true. It has been observed that successive GMRES cycles may differ from one another and complement each other in reducing the residual [10]. In this paper, we give a full description to this complementary behavior. In particular, *complementary cycles* of GMRES(m) are defined. This helps to present a new point of view on this algorithm.

In Section 2, complementary cycles of restarted GMRES are introduced with some examples. A definition of complementary cycle is given in Section 3 along with a theorem that helps explain complementary behavior. Then Section 4 has some further numerical examples including random matrices and a complex matrix from quantum chromodynamics (QCD) physics.

2. COMPLEMENTARY CYCLES

It has been noticed previously that GMRES(m) can behave in an alternating pattern [10, 11]. Baker *et al*. [11] note that there is a tendency for residuals from every other cycle to be nearly parallel. They developed an improved version of restarted GMRES, which attempts to prevent this pattern by augmenting it with differences between succeeding solutions. Here, we observe that this alternating can happen when two cycles complement each other. Therefore, the alternating is part of what makes restarted GMRES effective. We will also show that there can be more than two cycles working together. We call such a group of cycles a *complementary cycle* and say that the number of cycles is the *complementary frequency*. The first example is for complementary frequency of length two, which is the alternating behavior just mentioned.

Example 2.1

We consider the matrix Sherman4 from the Harwell–Boeing test collection [12]. It has size $n = 1104$. It is nonsymmetric, but is nearly symmetric. There is a random starting vector. Figure 1 gives the residual norm curves for restarted GMRES with restart frequencies of $m = 15$, 25, 30 and 40. We easily see complementary cycles with frequency two for the two larger values of m. For example, with $m = 40$ the residual norm has a steep drop about every 80 iterations or two cycles. When we look at the shorter restarting frequencies of $m = 15$ and 25, they do not show a pattern in the residual norms. Nevertheless, they actually do have cyclical patterns. Figure 2 has the GMRES polynomials that are generated during cycles 5–8 by GMRES(25). The polynomials for cycles 6 and 8 (shown with solid lines) are very similar. They almost overlie. The polynomials from 5 and 7 (shown with dotted lines) are also similar to each other. This shows the alternating pattern of GMRES, and indicates that successive cycles of GMRES(25) are complementing each other. To further support this, we show that the odd polynomials need the even ones and *vice versa*. Figure 3 has a test with the GMRES polynomials in a Richardson iteration (see, for example, [10, 13]). Each cycle of Richardson iteration involves multiplying the residual by a polynomial in A: $r = p(A)r_0$. If only the polynomial from cycle 5 is used, the method diverges fairly quickly. The cycle 6 polynomial causes even faster divergence. If we use all the odd cycle polynomials, starting with

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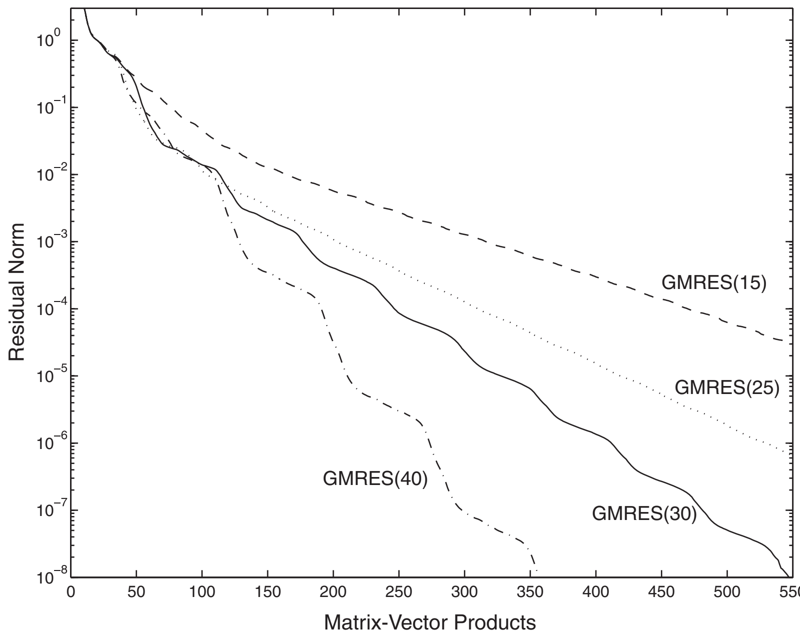

Figure 1. Example 2.1: restarted GMRES for matrix Sherman4.

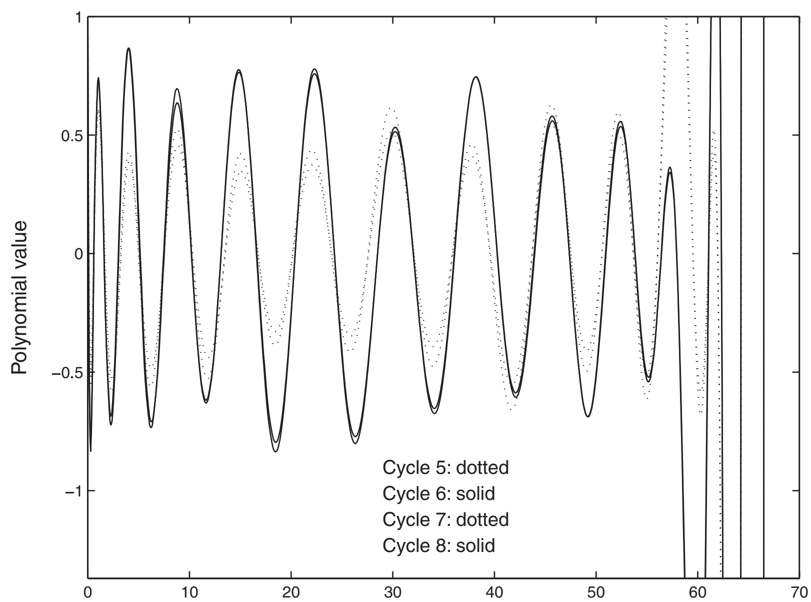

Figure 2. Example 2.1: GMRES(25) polynomials for cycles 5–8.

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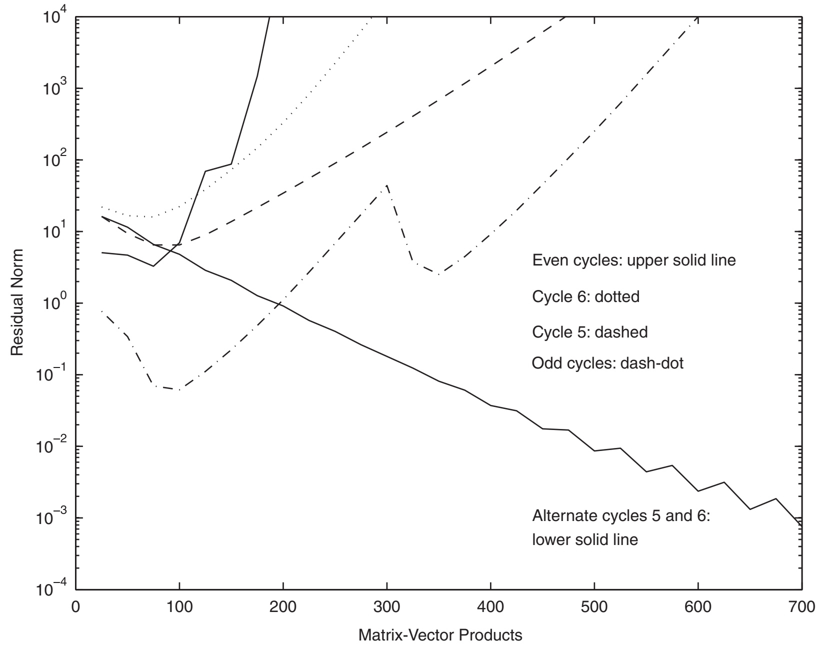

Figure 3. Example 2.1: GMRES polynomials used for the Richardson iteration.

cycle 1, the method is better, but still diverges. The even polynomials bring very quick divergence. Finally, if we alternate (as in [10]) between cycles 5 and 6, the method converges. This shows that the successive cycles of GMRES can work together in reducing the residual. As this example has complementary behavior for GMRES even when it is not obvious from the convergence curves, it suggests that such behavior may occur with other matrices even when it is not noticed.

As the GMRES polynomials in this last example are oscillating and of limited degree, they cannot be small everywhere. It makes sense that the next polynomial would try to be small where the previous one is not. Next, we consider cases where the matrix is not so close to being symmetric. We will see that it can require more than two polynomials to effectively complement each other.

Example 2.2
Consider the linear system $Ax=b$ where

$$A=\begin{pmatrix} 0.5 & \delta & & \\ & 1.0 & \delta & \\ & & 1.5 & \delta \\ & & & 2.0 \end{pmatrix}, \quad b=\begin{pmatrix} 0.5+\delta \\ 1.0+\delta \\ 1.5+\delta \\ 2.0 \end{pmatrix} \tag{1}$$

The exact solution is $x=(1,1,1,1)^{\mathrm{T}}$.

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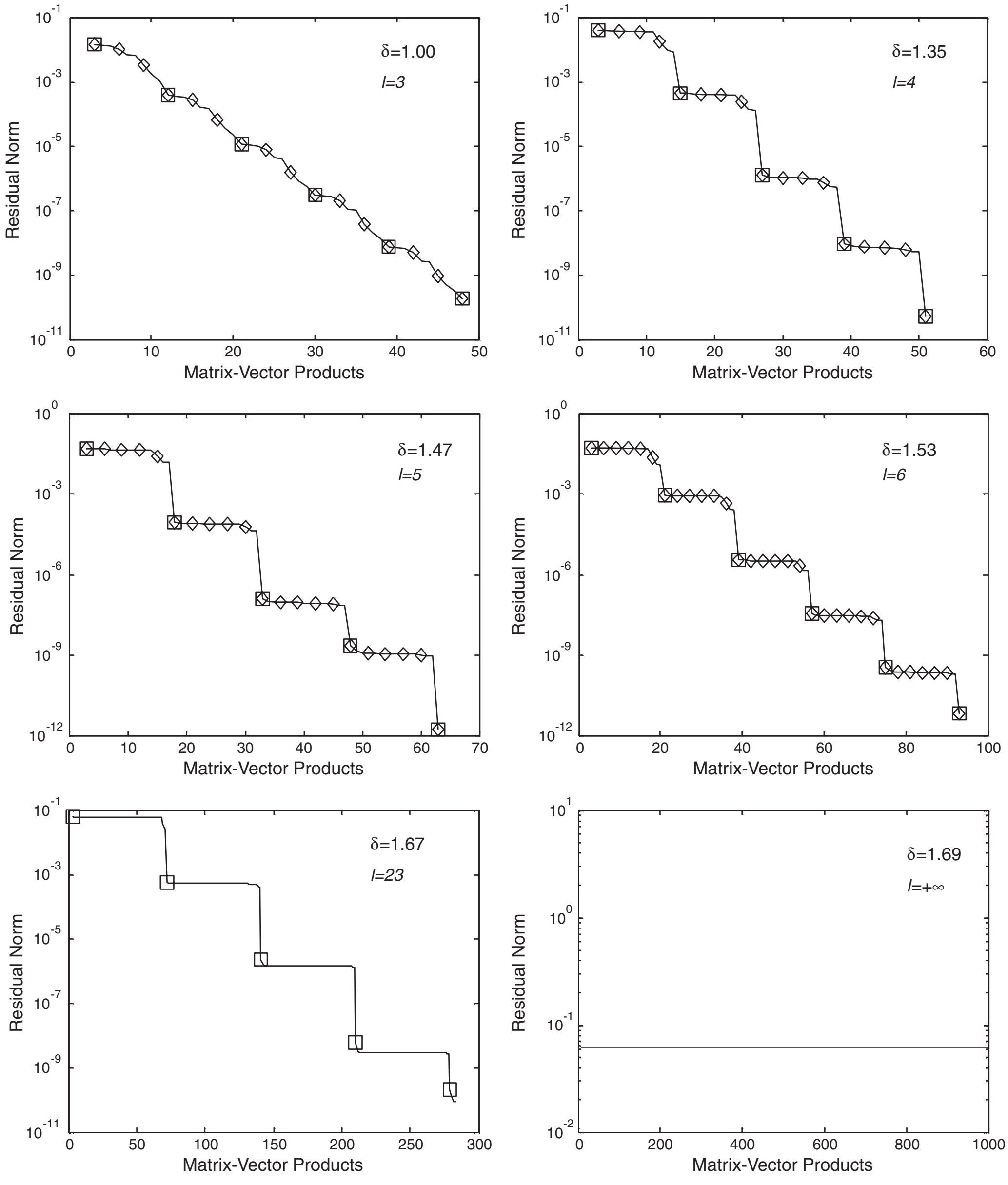

Figure 4. Example 2.2: convergence curves of GMRES(3). Restarting cycles: diamonds; complementary cycles: squares. (The restarting cycles are not marked out for $\delta = 1.67$ and 1.69.)

We will apply GMRES(3) with a convergence tolerance $\varepsilon = 10^{-10}$. Small values of δ again give complementary cycles of length two. We will use values large enough to give longer complementary frequencies, beginning with $\delta = 1.0$. The first plot in Figure 4 has the corresponding residual norm curve, and there is a pattern of complementary cycles with complementary frequency of 3. The

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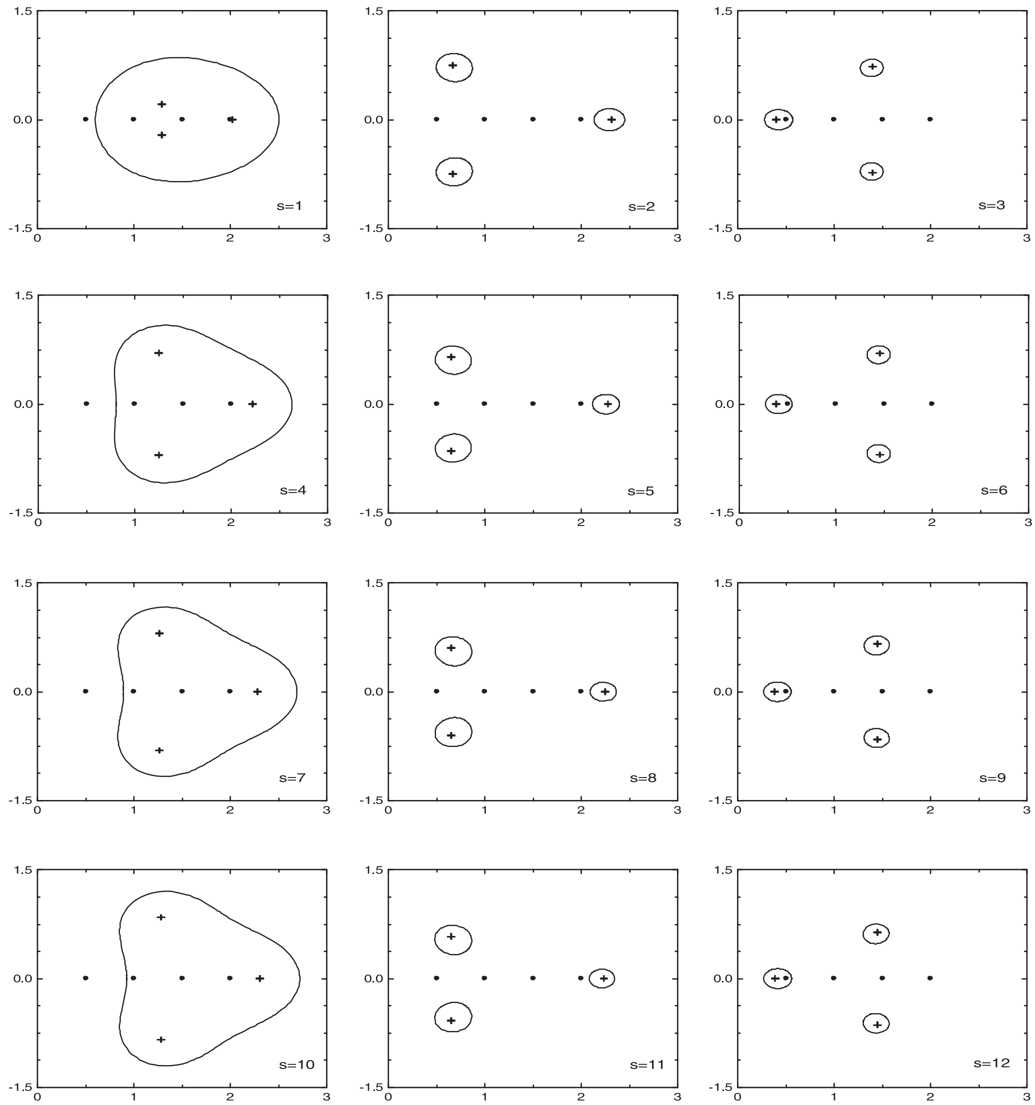

Figure 5. Example 2.2: GMRES lemniscates of the 1st–12th restarting cycles.
Eigenvalues: •; harmonic Ritz values: +.

GMRES lemniscates [13] can be examined to understand this. Let $p^{(s)}(z)$ be the GMRES residual polynomial of the sth cycle. Here, $\tau_k = \|r_{km}\|/\|r_{(k-1)m}\|$ is the convergence rate of the kth cycle for $k=1,2,\ldots,s$, and $\tau_{\text{average}} = (\tau_1\tau_2\cdots\tau_s)^{1/s}$ is computed by $(\|r_{sm}\|/\|r_0\|)^{1/s}$. Hence, τ_{average} is an average convergence rate of all the involved restarting cycles. The GMRES lemniscate is defined as

$$L_\tau = \{z\in C : |p^{(s)}(z)| = \tau_{\text{average}}\}$$

This average is used here instead of the choice in [13] of the convergence rate of a particular cycle, as we are interested in how each cycle contributes to the global convergence. Eigenvalues inside the lemniscate will have their corresponding eigenvector components of the residual significantly reduced. Figure 5 has the GMRES lemniscates of the 1st–12th cycles (those of the remaining cycles are very similar). Each group of three lemniscates is similar to the next three.

Figure 4 also has convergence for larger values of δ. The value l is the complementary frequency, and it increases as δ increases. The pseudospectrum [14, 15] can help to explain this. The ε-pseudospectrum is defined as $\Lambda_\varepsilon = \{\lambda \in C : \|(\lambda I - A)^{-1}\| \geqslant \varepsilon^{-1}\}$. Increasing nonnormality by increasing δ causes the pseudospectrum to spread out. In order to be effective, a product of polynomials needs to be small over the ε-pseudospectrum for small values of ε. For tougher pseudospectra, this takes more polynomials.

3. DEFINITION AND THEORY

3.1. A definition of complementary cycles

As mentioned previously, a complementary cycle can be thought of as a group of cycles that work together. The following definition is still somewhat vague, but it does attempt to make this more precise. We look at components of the residual vector when it is expanded in terms of an eigenvector basis and monitor how many cycles it takes before all components are reduced.

Definition 3.1

Starting from any cycle, a complementary cycle of GMRES(m) includes the cycles of restarted GMRES during which all the eigenvector components of the residual are significantly reduced, and at least one of them is significantly reduced just once. The number of cycles involved in the complementary cycle is referred to as the complementary frequency.

Here, a technique for dividing restarting cycles into complementary cycles is formulated. Denote the spectrum of A by Λ. Starting from the first (or any) cycle, a complementary cycle is a group of cycles that can be detected as follows:

1. At each cycle of the group, we obtain a subset of Λ:

$$\Lambda_s = \{\lambda \in \Lambda : |p^{(s)}(\lambda)| \leqslant \tau_{\text{average}}\} \quad (s = 1, 2, \ldots)$$

2. The complementary frequency l of the first complementary cycle satisfies

$$\bigcup_{s=1,2,\ldots,l} \Lambda_s = \Lambda \quad \text{while} \quad \bigcup_{s=1,2,\ldots,l-1} \Lambda_s \neq \Lambda$$

The input parameter τ_{average} is set to mark out the eigenvector components of the residual that are significantly reduced at a cycle (those associated with the eigenvalues in Λ_s). Sometimes restarted GMRES may be slowly convergent or nearly stagnant, causing τ_{average} to be very close to 1. In such cases, a smaller parameter should be used to detect the complementary cycles.

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Example 3.1
We use the technique to mark out the complementary cycles for the matrices from Example 2.2. For the first case of $\delta=1.0$, this gives

$$\Lambda_{3k-2}=\{\lambda_2,\lambda_3,\lambda_4\},\quad \Lambda_{3k-1}=\emptyset,\quad \Lambda_{3k}=\{\lambda_1\}\quad (k=1,2,\ldots,6)$$

Before convergence, six complementary cycles are detected, and each of them has a complementary frequency of three.

Next, the larger values of δ for system (1) are considered. In order for a more reasonable division, the first cycle is ignored, and we start from the second cycle for each choice of δ except the last one. Instead of τ_{average}, this input parameter is taken as $0.5\tau_{\text{average}}$ for $\delta=1.67$ and $\sqrt[3]{\tau_1\tau_2\tau_3}$ (the average convergence rate of the first three cycles) for $\delta=1.69$. The cycles are then divided into complementary cycles as marked off in Figure 4. The complementary frequency is fixed for each case: $l=4$, 5, 6, 23 and $+\infty$, respectively. When $\delta\to 1.69$, $l\to+\infty$ and GMRES(3) stagnates. In fact, when $\delta=1.69$, we have

$$\Lambda_1=\{\lambda_2,\lambda_3,\lambda_4\},\quad \Lambda_2=\Lambda_3=\cdots=\emptyset$$

As no complementary cycle is detected, it is defined that $l=+\infty$.

There is another fundamental consideration when the nonnormality of A increases. The eigenvalues of a nonnormal matrix may have little to do with its behavior [13, 14, 16]. The ε-pseudospectrum includes the spectrum but may be much larger than it. For such a case, the definition could be reworked with the requirement that the ε-pseudospectrum, for an ε small enough that the ε-pseudospectrum does not contain the origin, be covered by a collection of GMRES lemniscates.

3.2. *A supporting theorem*

We present a theorem that helps explain complementary cycles. It is similar to a theorem in [10]. First, an oblique projection process is introduced into the course of restarted GMRES. At the sth cycle, this process aims at approximating an eigenpair $\{\lambda,\varphi\}$ of A by a pair $\{\lambda^{(s)},\varphi^{(s)}\}$ satisfying

$$\varphi^{(s)}\in K_m(A,r_{(s-1)m}),\quad (A-\lambda^{(s)}I)\varphi^{(s)}\perp AK_m(A,r_{(s-1)m}) \tag{2}$$

where $K_m(A,v)=\operatorname{Span}\{A^i v\}_{i=0}^{m-1}$ denotes the Krylov subspace associated with a vector v and a matrix A. In order to interpret the above condition in terms of projection operators, we need the orthogonal projector $P^{(s)}$ onto $K_m(A,r_{(s-1)m})$ and the oblique projector $Q^{(s)}$ onto $K_m(A,r_{(s-1)m})$ and orthogonal to $AK_m(A,r_{(s-1)m})$. Then we can rewrite (2) as

$$(A^{(s)}-\lambda^{(s)}I)\varphi^{(s)}=0 \tag{3}$$

with $A^{(s)}=Q^{(s)}AP^{(s)}$.

The solutions $\{\lambda_i^{(s)}\}_{i=1}^m$ of the approximate problem (2) or (3) are the harmonic Ritz values. With each harmonic Ritz value $\lambda_i^{(s)}$ is associated a harmonic Ritz vector $\varphi_i^{(s)}$. Let $V^{(s)}=[v_1^{(s)},v_2^{(s)},\ldots,v_m^{(s)}]$ be a basis of $K_m(A,r_{(s-1)m})$ and $W^{(s)}=[w_1^{(s)},w_2^{(s)},\ldots,w_m^{(s)}]$ be a basis of $AK_m(A,r_{(s-1)m})$. We can solve the approximate problem by expressing the approximation $\varphi^{(s)}$

in the basis $V^{(s)}$ as $\varphi^{(s)} = V^{(s)} y^{(s)}$, in which case $\lambda^{(s)}$ and $y^{(s)}$ constitute an eigenpair of the m-dimensional eigenproblem derived from (2), see [17, 18]:

$$(G^{(s)} - \lambda^{(s)} I) y^{(s)} = 0$$

with $G^{(s)} = ((W^{(s)})^{\mathrm{T}} V^{(s)})^{-1} (W^{(s)})^{\mathrm{T}} A V^{(s)}$.

Assume, for simplicity, that the eigenvalues of A and $G^{(s)}$ are all simple. We express the residual as $r_{sm} = \sum_{i=1}^{n} \alpha_i^{(s)} \varphi_i$ $(s = 0, 1, 2, \ldots)$, in which $\{\varphi_i\}_{i=1}^{n}$ are the n normalized eigenvectors of A and $s = 0$ corresponds to the initial residual. We are interested in how each eigenvector component $\alpha_i^{(s)}$ $(i = 1, 2, \ldots, n)$ of the residual is reduced during the convergence of GMRES(m). The following theorem is established.

Theorem 3.2
Assuming that the eigenvalues of A and $G^{(s)}$ $(s = 1, 2, \ldots)$ are all simple, we have

$$|\alpha_i^{(s)}| \leqslant F_i^{(s)} \sum_{j=1, j \neq i}^{n} |\alpha_j^{(s-1)}| \quad (s = 1, 2, \ldots) \tag{4}$$

in which

$$F_i^{(s)} = \frac{\prod_{j=1}^{m} |\lambda_j^{(s)} - \lambda_i|}{\prod_{j=1}^{m} |\lambda_j^{(s)}| \cdot |\tilde{\lambda}_i^{(s)} - \lambda_i|} \gamma_i^{(s)} \kappa^{(s)} \frac{\varepsilon_i}{\| P^{(s)} \varphi_i \|}$$

with $\tilde{\lambda}_i^{(s)}$ being the harmonic Ritz value nearest to λ_i, $\gamma_i^{(s)} = \| Q^{(s)} (A - \lambda_i I)(I - P^{(s)}) \|$, $\kappa^{(s)}$ being the condition number of $G^{(s)}$, and

$$\varepsilon_i = \min_{\deg p \leqslant m-1;\, p(\lambda_i)=1} \; \max_{j=1,2,\ldots,n;\, j \neq i} |p(\lambda_j)|$$

The proof is similar to Theorem 5 of [10]. However, by a simple improvement of Lemma 3 of [10], the bound in the present theorem is improved by a factor of 2. We note that the bounds are still fairly rough, but nevertheless, the theorem adds something to the understanding of the convergence of restarted GMRES. It indicates that during the convergence of GMRES(m), each eigenvector component of the residual is in a way bounded by the others. If one of the components becomes much larger than the others, then a penalty of significant reduction will be imposed in the corresponding direction at the time of restarting. Simply put, if a cycle (or cycles) is not able to reduce certain components, then the next cycle will try. In such a manner, successive cycles of GMRES(m) complement one another in reducing the residual norm.

4. FURTHER EXAMPLES

Example 4.1
The purpose here is to demonstrate that the examples given in this paper have not been anomalous, rather that the complementary phenomenon is fairly common. We use several types of random matrices. First, diagonal matrices with diagonal elements distributed randomly on the interval from 0 to 1 are used. With several different sizes of matrices and several values of m, restarted GMRES does not show complementing in the residual curve. However, the polynomials do have alternating

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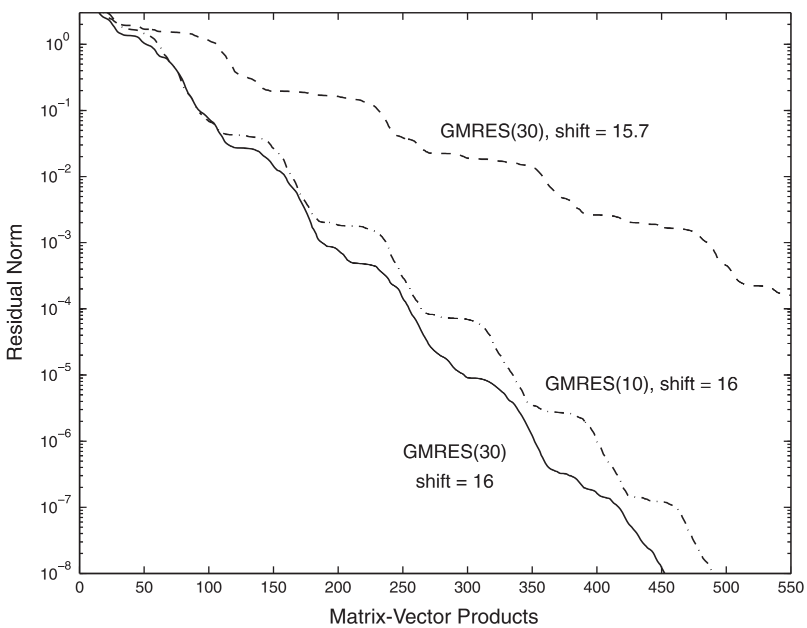

Figure 6. Example 4.1: shifted random matrix, $A+\text{shift}*I$.

behavior as in Example 2.1. We also try diagonal matrices with both positive and negative random eigenvalues (shifted slightly away from the origin so that restarted GMRES will converge). Again there are alternating polynomials that indicate complementary cycles with frequency of two.

Finally, we use full matrices with random elements distributed Normal(0,1). The matrices are then shifted so that restarted GMRES can converge. In tests with several different size matrices, the complementary cycles are visible in the residual norm curves. Figure 6 has a test with a 250×250 random matrix A that is shifted as $A+16*I$. We note that complementary frequencies for GMRES(10) and GMRES(30) are quite different. GMRES(30) has a frequency of 3 and GMRES(10) has a frequency decreasing from about 9 to about 7. However, the total number of iterations in each complementary cycle is similar. Next, for a tougher problem $A+15.7*I$, GMRES(10) does not converge and GMRES(30) has complementary frequency increasing to 4. Although not shown in the figure, the frequency for GMRES(30) goes to 5 with a shift of 15.65.

Example 4.2
The matrix ARC130 from Harwell–Boeing is used. Its dimension is 130. The right-hand side is taken such that the exact solution is $x=(1,1,\ldots,1)^{\mathrm{T}}$. All the eigenvalues of the matrix are located on the real axis, except for a few with a very small imaginary part. However, the ε-pseudospectrum, with $\varepsilon=10^{-5.9}$, expands widely on the complex plane; see the first plot in Figure 7 (plotted with Eigtool [19]). This is a characteristic phenomenon indicating high nonnormality.

Although the residual norm curve (not shown) does not have evidence of complementary cycles, they are there nevertheless. GMRES(6) has two complementary cycles of frequency two from the 4th to 7th restarting cycles; see the lower two plots in Figure 7. The GMRES lemniscates of two restarting cycles in each complementary cycle cover not only the exact spectrum but also the

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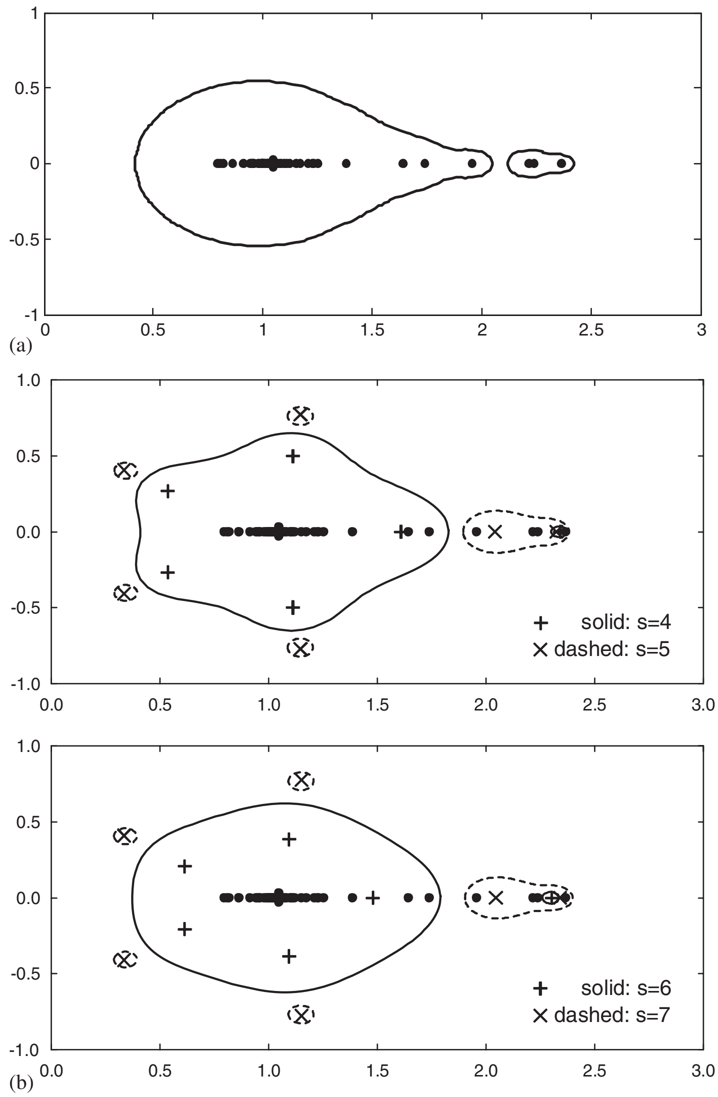

Figure 7. (a) ε-pseudospectrum of ARC130 and (b) Example 4.2: GMRES lemniscates of the 4th–7th restarting cycles. Eigenvalues: $\bullet$; harmonic Ritz values: $+$, $\times$.

pseudospectrum. The residual norm reaches 10^{-6} after the 7th cycle. Cycles beyond that are not as regular in their pattern, but still show some alternating behavior. This is another example (recall Example 2.1) showing that complementary behavior can occur with restarted GMRES even when it is not at first obvious.

Example 4.3

Finally, we test a typical Wilson–Dirac matrix from lattice QCD [20]. The matrix is complex non-Hermitian. Its size is $248\,832 \times 248\,832$. The right-hand side is a unit vector associated with

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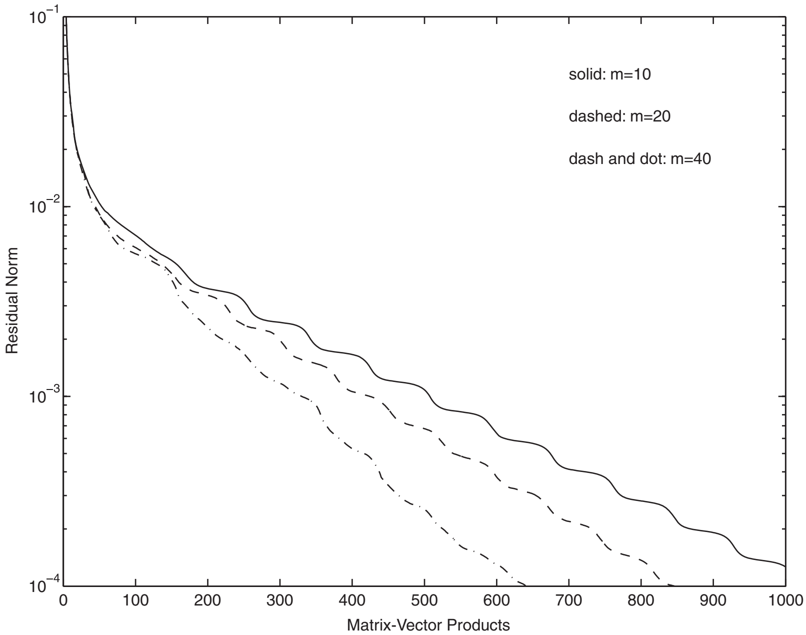

Figure 8. Example 4.3: QCD matrix. Convergence curves of GMRES with $m=10$, 20 and 40.

particular space-time, Dirac and color coordinates. Figure 8 shows convergence with different restarting frequencies. GMRES(10) has complementary frequencies of eight or nine. For GMRES(20), the frequencies are 3 or 4. The complementary behavior is not as clear from the residual norm curve for GMRES(40), but some complementary cycles can still be detected with frequency 2. This example shows complementary behavior in a large application matrix with complex entries.

5. CONCLUSIONS

We have observed that it can take several GMRES cycles working together to significantly reduce the residual norm. Awareness of this complementary behavior should improve understanding of restarted GMRES. Of course, GMRES does not always behave in such a regular manner as in the examples presented here. However, there are cases (Examples 2.1 and 4.2) that have complementing even when it is not obvious from observing the residual norm curve. It would be interesting to know how often in everyday use of GMRES there is complementary behavior.

Richardson iteration and polynomial preconditioning are examples of the application of this work. The product polynomial associated with a complementary cycle can be used to form an effective polynomial preconditioning scheme. This topic has been investigated by Zhong [10] for the Richardson iteration. However, in [10] s is generally taken as 2. Also, as Baker *et al.* [11] use alternating behavior of GMRES to develop their method, the longer complementary cycles of difficult nonnormal problems might lead to a new approach.

In future work, we plan to use complementary cycles to explain some instances of ‘tortoise and the hare’ behavior [21]. Also, superlinear convergence (see, for example, [22]) in nonrestarted

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GMRES has been studied; we plan to look at superlinear convergence of restarted GMRES. We are also interested in whether deflating eigenvalues [23, 24] in GMRES has an effect on complementary cycles.

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