PRESCRIBING THE ERROR IN GMRES

GÉRARD MEURANT*

Abstract. In this paper we explain how, in the class of real matrices A having the same GMRES residual norm convergence curve, as defined by the parametrization of Arioli, Pták and Strakoš (BIT Numerical Mathematics, v 38 1998), we can choose the spectrum (or more exactly the coefficients of the characteristic polynomial) to obtain a given solution for the linear system $Ax = b$. This allows to be able, with a prescribed GMRES residual norm convergence curve, to compute the spectrum of A to prescribe the error vector at a given iteration. We also consider prescribing the norm of the error at every iteration. We exhibit a condition that has to be satisfied to be able to construct real matrices having the prescribed error norms as well as prescribed residual norms.

1. Introduction. We consider solving a linear system

$$Ax = b \tag{1.1}$$

where A is a real nonsingular matrix of order n with the Generalized Minimum RESidual method (GMRES) which is an iterative Krylov method based on the Arnoldi orthogonalization process; see Saad [6], [7] and Saad and Schultz [8].

During the last years, Strakoš and his co-workers studied the class of matrices giving the same GMRES residual norm convergence curve. Greenbaum and Strakoš [2] first proved that any GMRES residual norm convergence curve can be obtained with a non-derogatory matrix having prescribed eigenvalues. Then, it was proved in Greenbaum, Pták and Strakoš [3] that any nonincreasing sequence of residual norms can be produced by GMRES. A complete parametrization of all pairs $\{A, b\}$ generating a prescribed residual norm convergence curve was given by Arioli, Pták and Strakoš [1]. In [5] we gave more details on matrices and vectors that are linked to the Arioli, Pták and Strakoš parametrization. In particular, we provided expressions for the GMRES iterates and errors. The iterates do not depend on the eigenvalues of A, in the sense that in the parametrization we can change the companion matrix C corresponding to the eigenvalues of A (and thus the matrix A) without changing the iterates. Hence, there are non-derogatory matrices with different eigenvalue distributions and the same residual norm convergence curves and iterates. However, our results showed that the error vectors do depend on the matrix C, and therefore on the eigenvalues of A, through the exact solution of the linear system.

In this paper we are interested in computing the coefficients of the characteristic polynomial (and therefore the eigenvalues) of A, in the class of matrices with a prescribed residual norm convergence curve, to obtain a prescribed solution for the linear system (1.1). The coefficients are uniquely determined as functions of the matrices involved in the parametrization of [1]. This also allows to prescribe the error vector at a given iteration. Then we study the problem of prescribing the norm of the error at every iteration. This is not always possible since there is a relation between the errors and the residuals and the residual norms have to be monotonely decreasing. Hence we cannot choose the error norms arbitrarily. We exhibit a condition that has to be satisfied to be able to construct real matrices having the prescribed error norms as well as prescribed residual norms. Finally to show that there are cases for which this condition can be fulfilled we consider 2×2 and 3×3 matrices.

The contents of the paper are as follows. Section 2 recalls the results of Arioli, Pták and Strakoš [1] as well as some results from [5] giving expressions for the GMRES

*(gerard.meurant@gmail.com) started in Paris, version October 1, 2011

iterates and error vectors using the parametrization of [1]. In Section 3 we describe how to choose the coefficients of the characteristic polynomial to obtain a prescribed exact solution for the system (1.1). This result allows in Section 4 to choose the coefficients to obtain a prescribed error vector at a given iteration. In Section 5 we illustrate these results with some numerical experiments on small matrices. Section 6 considers the problem of prescribing the error norms for all iterations. To show that the condition for obtaining a real solution can sometimes be fulfilled we consider the case of 2×2 matrices in Section 7. Numerical experiments for matrices of order 3 are provided in Section 8. Finally we give some conclusions.

2. The Arioli, Pták and Strakoš parametrization. We recall the following results that were proved in [1] (Theorem 2.1 and Corollary 2.4).

THEOREM 2.1. *Assume we are given* $n+1$ *positive numbers*

$$f(0) \geq f(1) \geq \cdots \geq f(n-1) > 0, \quad f(n) = 0,$$

and n *complex numbers* $\lambda_1, \dots, \lambda_n$ *all different from* 0*. Let* A *be a matrix of order* n *and* b *an* n*-dimensional vector. The following assertions are equivalent:*

1- *The spectrum of* A *is* $\{\lambda_1, \dots, \lambda_n\}$ *and GMRES applied to* A *and* b *yields residuals* r^j, $j = 0, \dots, n-1$ *such that*

$$\|r^j\| = f(j), \quad j = 0, \dots, n-1.$$

2- *The matrix* A *is of the form* $A = WYCY^{-1}W^*$ *and* $b = Wh$*, where* W *is a unitary matrix,* Y *is given by*

$$Y = \begin{pmatrix} h & \begin{matrix} R \\ 0 \end{matrix} \end{pmatrix},$$

R being any nonsingular upper triangular matrix of order $n-1$, h a vector such that

$$h = (\eta_1, \dots, \eta_n)^T, \quad \eta_j = (f(j-1)^2 - f(j)^2)^{1/2}$$

and C *is the companion matrix corresponding to the polynomial* q*,*

$$q(z) = (z - \lambda_1) \cdots (z - \lambda_n) = z^n + \sum_{j=0}^{n-1} \alpha_j z^j,$$

$$C = \begin{pmatrix} 0 & \dots & & 0 & -\alpha_0 \\ 1 & 0 & \dots & 0 & -\alpha_1 \\ 0 & 1 & 0 & \dots & -\alpha_2 \\ & & \ddots & \ddots & \vdots \\ & & & 1 & -\alpha_{n-1} \end{pmatrix}. \tag{2.1}$$

We will call the parametrization, $A = WYCY^{-1}W^*$, the APS parametrization in reference to [1].

In the parametrization of Theorem 2.1, the prescribed residual norm convergence curve is implicitly contained in the vector h which is prescribed by the given residual norms defined by f. The degrees of freedom defining the class of matrices are the unitary matrix W, the upper triangular matrix R and the companion matrix C. Thus we can change R to obtain another matrix in the class for which we have the same residual convergence curve as long as the right-hand side is $b = Wh$. Changing W change the matrix A and also the right-hand side b but not the residual convergence curve. Keeping everything else (that is, W, R, h) the same, we can change the companion matrix C, and hence the eigenvalues of A, without changing the norms of the residuals. So we have a class of matrices all having different eigenvalue distributions and the same residual norms. This leads some researchers to write that "GMRES convergence does not depend on the eigenvalue distribution". However, we will see that we can compute the coefficients of the characteristic polynomial (and thus the eigenvalues of A) to obtain prescribed properties of the error. In particular we can construct matrices having a prescribed residual norm convergence curve and a small error vector at a given iteration. Hence, in this sense, one can say that GMRES convergence depends on the eigenvalues.

In this paper we are interested in real matrices and right-hand sides. In this case all the quantities defined in Theorem 2.1 are real, except the eigenvalues of A. Throughout the paper we will use the notation of [1] defined in Theorem 2.1. We will assume that the matrix A is non-derogatory and that the right-hand side is such that GMRES terminates at iteration n. Therefore all the Krylov subspaces are of maximal rank. For a square matrix B we denote as B_k the principal submatrix of order k and e^i denotes the ith column of the identity matrix of appropriate dimension. Without loss of generality, we will choose $x^0 = 0$ and $\|b\| = 1$; this yields the initial residual $r^0 = b$ and $\|h\| = 1$. Let us now recall results from [5].

Theorem 2.2. *The GMRES iterates x^k are*

$$x^k = WYC^{-1} \begin{pmatrix} 0 \\ R_k^{-1}h^k \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad k < n, \tag{2.2}$$

with only one zero element at the top of the vector on the right-hand side. The entries of the vector h^k are the first k components of h. Moreover, we have

$$YC^{-1} = \begin{pmatrix} z(\alpha) & h & \begin{pmatrix} R_{n-2} \\ 0 \\ 0 \end{pmatrix} \end{pmatrix},$$

where $z(\alpha)$ is a vector (depending on the coefficients α_j) given by

$$z(\alpha) = \begin{pmatrix} -\frac{\alpha_1}{\alpha_0}\hat{h} + Rt \\ -\frac{\alpha_1}{\alpha_0}\eta_n \end{pmatrix} = -\frac{\alpha_1}{\alpha_0}h + \begin{pmatrix} Rt \\ 0 \end{pmatrix} \tag{2.3}$$

with $\hat{h} = h^{n-1}$ the vector of the first $n-1$ components of h and

$$t = (\, -\tfrac{\alpha_2}{\alpha_0}, \quad \cdots \quad -\tfrac{\alpha_{n-1}}{\alpha_0}, \quad -\tfrac{1}{\alpha_0}\,)^T.$$

We see that only the first column of YC^{-1} depends on the coefficients α_j. In the expression (2.2) for the iterates x^k, this column is multiplied by zero. Therefore, the iterates do not depend on the eigenvalues of A. In the parametrization we can change the matrix C and hence the eigenvalues without changing the GMRES iterates.

3. Prescribing the solution of the linear system. In this section we show how to compute the coefficients α_j, $j = 0, \ldots, n$ of the characteristic polynomial for prescribing the solution of the linear system (1.1). Using the parametrization of Theorem 2.1, the exact solution is

$$x = (WYCY^{-1}W^T)^{-1}b = WYC^{-1}Y^{-1}W^Tb = WYC^{-1}e^1 = Wz(\alpha),$$

since $W^Tb = h$ and $Y^{-1}h = e^1$. The vector $z(\alpha)$, defined by (2.3), depends only on h, R and the coefficients α_j. One may ask if, given h, R and W, we can determine these n coefficients to obtain a prescribed solution $\tilde{x}$ to the linear system (1.1). We are looking for real parameters α_j (corresponding to real or complex conjugate eigenvalues). Their computation is described in the following theorem.

THEOREM 3.1. *Using the notation of Theorem 2.1, let h, R and W be given. Let $\tilde{x}$ be a prescribed vector and $p = W^T\tilde{x}$. Assume that $p_{n-1}\eta_n - p_n\eta_{n-1} \neq 0$. Then the vector $\tilde{x}$ is the solution of the linear system $Ax = WYCY^{-1}W^Tx = b = Wh$ if the coefficients α_j, $j = 0, \ldots, n-1$ in the companion matrix C defined in (2.1) are computed as the solutions of the following linear systems,*

$$\begin{pmatrix} p_{n-1} & \eta_{n-1} \\ p_n & \eta_n \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} -r_{n-1,n-1} \\ 0 \end{pmatrix}. \tag{3.1}$$

and

$$R_{n-2} \begin{pmatrix} \alpha_2 \\ \vdots \\ \alpha_{n-1} \end{pmatrix} = - \begin{pmatrix} r_{1,n-1} \\ \vdots \\ r_{n-2,n-1} \end{pmatrix} - \begin{pmatrix} p_1 & \eta_1 \\ \vdots & \vdots \\ p_{n-2} & \eta_{n-2} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix}. \tag{3.2}$$

Proof. We would like to find $\alpha_0, \ldots, \alpha_{n-1}$ such that $z(\alpha) = p$. From Theorem 2.2 this is equivalent to solving

$$-\frac{\alpha_1}{\alpha_0}h + \begin{pmatrix} Rt \\ 0 \end{pmatrix} = p, \tag{3.3}$$

where R, h and p are given. We have assumed that $\alpha_0 \neq 0$. Therefore we can rewrite (3.3) as

$$-\alpha_1 h - \begin{pmatrix} R \begin{pmatrix} \alpha_2 \\ \vdots \\ \alpha_{n-1} \\ 1 \end{pmatrix} \\ 0 \end{pmatrix} = \alpha_0 p.$$

This gives a linear system for the unknowns $\alpha_0, \ldots, \alpha_{n-1}$,

$$\begin{pmatrix} p_1 & \eta_1 & r_{1,1} & r_{1,2} & \cdots & r_{1,n-2} \\ p_2 & \eta_2 & 0 & r_{2,2} & \cdots & r_{2,n-2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ p_{n-2} & \eta_{n-2} & 0 & \cdots & 0 & r_{n-2,n-2} \\ p_{n-1} & \eta_{n-1} & 0 & \cdots & 0 & 0 \\ p_n & \eta_n & 0 & \cdots & 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{n-3} \\ \alpha_{n-2} \\ \alpha_{n-1} \end{pmatrix} = - \begin{pmatrix} r_{1,n-1} \\ r_{2,n-1} \\ \vdots \\ r_{n-2,n-1} \\ r_{n-1,n-1} \\ 0 \end{pmatrix}, \tag{3.4}$$

where $r_{i,j}$ denotes the entries of R which are known. The matrix in (3.4) has a very special structure. We see that, using the last two equations, we can first solve for α_0

and α_1 which are the solution of the linear system (3.1). With our hypothesis this system has a unique solution. We then compute $\alpha_2, \ldots, \alpha_{n-1}$ by solving the triangular system (3.2) of order $n-2$. This system has a unique solution since R is assumed to be nonsingular. This uniquely determines the coefficients α_j of the characteristic polynomial as functions of h, R and W. From the knowledge of the matrix C in (2.1), we can construct the matrix $A = WYCY^{-1}W^T$. The linear system with this matrix and $b = Wh$ has the prescribed solution $\tilde{x}$ and prescribed residual norms defined by f. The only condition to be satisfied is $p_{n-1}\eta_n - p_n\eta_{n-1} \neq 0$. □

Since we can prescribe the exact solution of the linear system (1.1), one may wonder if we can ask for an exact solution, say x, being equal to one of the iterates, say $x^m, m < n$. As we can guess, this is not possible since it will give $\|r^m\| = 0$ and this is contradictory with the fact that this norm has already been prescribed to be different from zero. This can be seen more formally since, if $x = x^m$, we have

$$p = W^T x = W^T x^m = YC^{-1} \begin{pmatrix} 0 \\ R_m^{-1} h^m \\ 0 \end{pmatrix}.$$

Let us denote by ρ the first element of the vector $R_m^{-1}h^m$. Using the structure of C^{-1}, we can see that ρ is the first element of the vector

$$C^{-1} \begin{pmatrix} 0 \\ R_m^{-1} h^m \\ 0 \end{pmatrix}.$$

hen the last two equations of $p = W^T x^m$ give

$$\begin{pmatrix} p_{n-1} \\ p_n \end{pmatrix} = \rho \begin{pmatrix} \eta_{n-1} \\ \eta_n \end{pmatrix}.$$

Therefore we have $p_{n-1}\eta_n - p_n\eta_{n-1} = 0$ and the linear system for α_0 and α_1 is singular.

4. Prescribing the error vector at a given iteration. In this section, using the previous results, we show how to obtain a prescribed error vector at a given iteration. Let ϵ be a given vector in $\mathbb{R}^n$ assumed to be different from zero. The problem we consider here is: Can we compute the coefficients α_j such that the error vector $\epsilon^k = x - x^k$ at iteration k is the given vector ϵ? From what we have seen in the previous section and Theorem 2.2, we have

$$W^T \epsilon^k = z(\alpha) - YC^{-1} \begin{pmatrix} 0 \\ R_k^{-1} h^k \\ 0 \end{pmatrix}. \tag{4.1}$$

Let

$$p = W^T \epsilon + YC^{-1} \begin{pmatrix} 0 \\ R_k^{-1} h^k \\ 0 \end{pmatrix}.$$

Then, the problem reduces to solving the equation $z(\alpha) = p$ where p is known since, according to the structure of YC^{-1} described in Theorem 2.2, the second term on the right-hand side does not depend on the coefficients α_j. Solving this problem has been done in the previous section. Therefore, in the class of matrices having the same residual norm convergence curve, we can construct a particular matrix having a prescribed (nonzero) error vector at a given iteration by computing appropriately the coefficients of the characteristic polynomial.

5. Numerical experiments. Let us consider a small (5×5) example. We choose a random R, a random orthogonal W and h as

$$R = \begin{pmatrix} -0.432565 & -1.14647 & 0.327292 & -0.588317 \\ 0 & 1.19092 & 0.174639 & 2.18319 \\ 0 & 0 & -0.186709 & -0.136396 \\ 0 & 0 & 0 & 0.113931 \end{pmatrix},$$

$$W = \begin{pmatrix} -0.767849 & 0.389048 & 0.079038 & -0.435081 & -0.252008 \\ -0.0426702 & -0.303441 & 0.907719 & -0.166331 & 0.233416 \\ 0.0688467 & -0.654749 & -0.108865 & -0.344183 & -0.660492 \\ 0.599116 & 0.411357 & 0.0385463 & -0.685803 & 0.00568851 \\ -0.211914 & -0.398314 & -0.395552 & -0.440738 & 0.667627 \end{pmatrix},$$

$$h^T = (\, 0.99995, \quad 0.00994987, \quad 0.000994987, \quad 9.94987\ 10^{-5}, \quad 10^{-5}\,).$$

This corresponds to GMRES residual norms equal to

$$1, \quad 0.01, \quad 0.001, \quad 0.0001, \quad 10^{-5},$$

for $k = 0, \ldots, 4$. Then, let us choose a random eigenvalue distribution with complex conjugate or real eigenvalues,

$$0.257304 - 1.05647i, \quad 0.257304 + 1.05647i, \quad 1.41514 - 0.80509i,$$

$$1.41514 + 0.80509i, \quad 0.528743.$$

From the eigenvalues we construct the corresponding companion matrix C and the matrix A. The linear system is

$$\begin{pmatrix} -87520.1 & 80969.9 & -229267 & 1873.1 & 231643 \\ 17942.1 & -16594.5 & 46997.5 & -381.358 & -47483 \\ 51341.7 & -47479.8 & 134472 & -1079.95 & -135847 \\ 18137.1 & -16798.5 & 47533.5 & -406.565 & -48044.5 \\ 11329.5 & -10463.9 & 29657.5 & -224.579 & -29946.7 \end{pmatrix} x = \begin{pmatrix} -0.763906 \\ -0.0447983 \\ 0.0621794 \\ 0.60315 \\ -0.216297 \end{pmatrix},$$

whose solution is

$$x = \begin{pmatrix} 2.83717 \\ -1.48457 \\ -4.046 \\ 2.05175 \\ -2.43021 \end{pmatrix}.$$

The matrix A has a condition number of $2.6\ 10^{11}$ having one small singular value. When running GMRES on this linear system, starting from $x^0 = 0$, we obtain the following residual norms

$$1, \quad 0.01, \quad 0.001, \quad 0.0001, \quad 10^{-5}, \quad 3.5478\ 10^{-11}$$

that are the prescribed ones. The error norms are

$$6.06129, \quad 6.27366, \quad 6.28074, \quad 6.28699, \quad 6.28649, \quad 7.65631\ 10^{-8}\,.$$

They are almost constant up to the last step. Now we would like to construct a matrix with the same residual norm convergence curve and an error vector at the third iteration which is $10^{-6}e$ where e is the vector of all ones. From the previous section we compute the coefficients of the characteristic polynomial and the companion matrix $\tilde{C}$. The new matrix is $\tilde{A} = WY\tilde{C}Y^{-1}W^T$ and the right-hand side is the same as before. We obtain

$$\tilde{A} = \begin{pmatrix} -89839.8 & 83755.7 & -236237 & 2704.11 & 239572 \\ 18451.3 & -17205.9 & 48527.5 & -563.751 & -49223.3 \\ 52831.2 & -49268.5 & 138948 & -1613.53 & -140938 \\ 18640.3 & -17402.8 & 49045.6 & -586.831 & -49764.5 \\ 11729.7 & -10944.5 & 30860.2 & -367.948 & -31314.6 \end{pmatrix}.$$

This matrix has a condition number of $1.7\ 10^8$. The spectrum of $\tilde{A}$ is

$$-10.1482 - 16.3584i, \quad -10.1482 + 16.3584i, \quad 10.5609 - 15.6928i,$$

$$10.5609 + 15.6928i, \quad -0.426482\,.$$

This matrix cannot be considered as a large modification of A since we have $\|A - \tilde{A}\|/\|A\| = 0.0333$. The largest singular values of A and $\tilde{A}$ are not much different ($4.1728\ 10^5$ and $4.3107\ 10^5$), however the smallest singular value of $\tilde{A}$ is larger than the smallest singular value of A. Note also that 0 is in the convex hull of the eigenvalues of $\tilde{A}$ when it was outside for A. When we run GMRES on the system $\tilde{A}x = b$, we obtain the following residual norms

$$1, \quad 0.01, \quad 0.001 \quad 0.0001, \quad 9.99995\ 10^{-6}, \quad 1.21344\ 10^{-11}\,.$$

They are (almost) the same as before. The error norms for $k = 0, 1, \ldots, 5$ are

$$2.33784, \quad 0.0269172, \quad 0.00641637, \quad 2.23604\ 10^{-6}, \quad 0.00403993, \quad 1.24166\ 10^{-9}\,.$$

We see that the norm $\|\epsilon^3\|$ is small. The error vectors for $k = 1, \ldots, 5$ are

0.0174532	−0.00223741	$9.99754\ 10^{-7}$	0.00330782	$1.00806\ 10^{-9}$
0.00310014	0.00195393	10^{-6}	0.000140114	$5.18857\ 10^{-11}$
0.00254853	0.00417422	$1.00007\ 10^{-6}$	−0.000673838	$-1.87872\ 10^{-10}$
−0.0183542	−0.00283306	$1.00013\ 10^{-6}$	−0.0021452	$-6.74045\ 10^{-10}$
0.00818142	0.00262596	$9.99977\ 10^{-7}$	0.000551208	$1.82237\ 10^{-10}$

Up to rounding errors, the error vector ϵ^3 is as prescribed. Note that the error norms are not monotonely decreasing in GMRES and the error norm increases at iteration 4. Nevertheless, the error norms are smaller than for the matrix A whence the residual norms are the same. In this sense, even though they belong to the same class of matrices with the prescribed residual norms, the matrix $\tilde{A}$ is "better" than the matrix A regarding the error norms.

6. Prescribing the error norm at every iteration. Since we have n parameters $\alpha_0, \ldots, \alpha_{n-1}$ at our disposal, one may ask the question: Can we prescribe the norm of the error $\|\epsilon^k\|$ for $k = 0, \ldots, n-1$? We will see that this is not always possible. The prescribed values for the norm of the errors have to satisfy some constraints. This makes sense since there is a close relation between the residuals and the errors ($A\epsilon^k = r^k$) and the residual norms have to be monotonely decreasing. Let us look for the real coefficients $\alpha_0, \ldots, \alpha_{n-1}$ of the characteristic polynomial that would give complex conjugate eigenvalues. Let $\omega_0, \ldots, \omega_{n-1}$ be n given real positive values. We would like to have $\|\epsilon^k\| = \omega_k$, $k = 0, \ldots, n-1$.

From Theorem 2.2 we know that

$$W^T \epsilon^k = Y C^{-1} \begin{pmatrix} 1 \\ -R_k^{-1} h^k \\ 0 \end{pmatrix}.$$

Let us denote

$$\gamma_j^{(k)} = (R_k^{-1} h^k)_j, \; j = 1, \ldots, k \tag{6.1}$$

with an upper index (k) since these elements change at each iteration k.

Let

$$t^k = \gamma_1^{(k)} h + \begin{pmatrix} R_{n-2} \begin{pmatrix} \gamma_2^{(k)} \\ \vdots \\ \gamma_k^{(k)} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} h & \begin{matrix} R_{k-1} \\ 0 \\ \vdots \\ 0 \end{matrix} \end{pmatrix} \begin{pmatrix} \gamma_1^{(k)} \\ \vdots \\ \gamma_k^{(k)} \end{pmatrix}, \tag{6.2}$$

for $k = 2, \ldots, n-1$ and $t^0 = 0$, $t^1 = \gamma_1^{(1)} h$ with $\gamma_1^{(1)} = \eta_1 / r_{1,1}$. Note that the vectors t^k are known. The GMRES iterates are $x^k = W t^k$. The exact solution is $x = W z(\alpha)$. Then the error ϵ^k satisfies

$$W^T \epsilon^k = z(\alpha) - t^k, \; k = 1, \ldots, n-1. \tag{6.3}$$

Since $x^0 = 0$, we have $\|\epsilon^0\|^2 = \|x\|^2 = \|z(\alpha)\|^2 = \omega_0^2$. The other norms are written as

$$\|\epsilon^k\|^2 = \|z(\alpha) - t^k\|^2 = \|z(\alpha)\|^2 - 2(z(\alpha), t^k) + \|t^k\|^2 = \omega_k^2, \; k = 1, \ldots, n-1.$$

We substitute the value of $\|z(\alpha)\|^2$ in this equation to obtain $n-1$ equations in n unknowns. Let $\delta_k = (\omega_0^2 + \|t^k\|^2 - \omega_k^2)/2$, then we have the linear equations

$$(z(\alpha), t^k) = \delta_k, \; k = 1, \ldots, n-1, \tag{6.4}$$

for the components of $z(\alpha)$. Let t_i^j be the components of the vector t^j. In matrix form, (6.4) is written as

$$\begin{pmatrix} t_1^1 & \cdots & t_n^1 \\ \vdots & \ldots & \vdots \\ t_1^{n-1} & \cdots & t_n^{n-1} \end{pmatrix} \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix} = \begin{pmatrix} \delta_1 \\ \vdots \\ \delta_{n-1} \end{pmatrix}, \tag{6.5}$$

where the values z_j are the components of $z(\alpha)$. Let T be the square matrix of order $n-1$ with elements $(T)_{i,j} = t_j^i$ (that is, the first $n-1$ columns of the matrix in (6.5)) and δ a vector with components δ_j, $j = 1, \ldots, n-1$. Then

$$T \begin{pmatrix} z_1 \\ \vdots \\ z_{n-1} \end{pmatrix} = -z_n \begin{pmatrix} t_n^1 \\ \vdots \\ t_n^{n-1} \end{pmatrix} + \delta. \tag{6.6}$$

Let us assume that T is nonsingular. This implies that the vectors t^k and therefore the iterates x^k are different. It excludes the case of GMRES stagnation. Let $p = T^{-1}\delta$ and

$$q = T^{-1} \begin{pmatrix} t_n^1 \\ \vdots \\ t_n^{n-1} \end{pmatrix}.$$

From (6.6) we have

$$\begin{pmatrix} z_1 \\ \vdots \\ z_{n-1} \end{pmatrix} = -z_n q + p.$$

Now we use this relation in the first equation $\|z(\alpha)\|^2 = \omega_0^2$. It yields a quadratic equation for z_n,

$$(1 + \|q\|^2) z_n^2 - 2(p,q) z_n + \|p\|^2 - \omega_0^2 = 0. \tag{6.7}$$

We need that (6.7) has real solutions. Hence, we obtain the constraint

$$(p,q)^2 - \|p\|^2 \, \|q\|^2 + \omega_0^2 (1 + \|q\|^2) - \|p\|^2 \geq 0. \tag{6.8}$$

If this condition is fulfilled then we have two real solutions for z_n and we can recover the other components of $z(\alpha)$ from (6.6). Note that the components of the vector q are functions of h and R and those of the vector p are functions of h, R and ω_j, $j = 0, \ldots, n-1$. If condition (6.8) is satisfied and T is nonsingular we obtain a real vector $z(\alpha)$ and we can compute the coefficients α_j using what was done in section 3.

The constraint (6.8) can be written as

$$(p,q)^2 + (\omega_0^2 - \|p\|^2)(1 + \|q\|^2) \geq 0.$$

Therefore, a sufficient condition for having real solutions is

$$\omega_0^2 \geq \|p\|^2. \tag{6.9}$$

On the other hand we have

$$\|p\|^2 - \omega_0^2 \leq \frac{(p,q)^2}{1 + \|q\|^2} \leq \frac{\|p\|^2 \, \|q\|^2}{1 + \|q\|^2},$$

by the Cauchy–Schwarz inequality. Therefore

$$\omega_0^2 \geq \frac{\|p\|^2}{1 + \|q\|^2} \tag{6.10}$$

is a necessary condition. Note that if $\|q\|$ is small, conditions (6.9) and (6.10) are close. This may happen if η_n is small since the vector q is proportional to η_n.

We will see in the next section that there are cases for which the condition (6.8) can be fulfilled. Finally, let us consider the question of the rank of the matrix T. Looking at the vectors t^k in (6.2), we see that T is the sum of two singular matrices of order $n-1$, T_1 and T_2,

$$T_1 = \begin{pmatrix} \gamma_1^{(1)} \\ \vdots \\ \gamma_1^{(n-1)} \end{pmatrix} \begin{pmatrix} \eta_1 & \cdots & \eta_{n-1} \end{pmatrix}, \quad T_2 = \begin{pmatrix} 0 & \cdots & 0 & 0 \\ & & & 0 \\ & L & & \vdots \\ & & & 0 \end{pmatrix},$$

where the matrix L is lower triangular. The matrix T_1 is of rank 1 and, generically, the matrix T_2 is of rank $n-2$ since L is nonsingular. If we assume that $\eta_j \neq 0$, $j = 1, \ldots, n$ we can apply the result about the rank of the sum of two matrices in [4]. With this hypothesis, generically, the intersections of the column spaces and row spaces of T_1 and T_2 is void and the rank of T is the sum of the ranks of T_1 and T_2 that is $n-1$.

7. Prescribing the error norms, the case $n = 2$. To see if there are cases for which the condition (6.8) can be satisfied we consider the class of 2×2 real matrices A with the APS parametrization $A = WYCY^{-1}W^T$. In the case $n = 2$ we have

$$Y = \begin{pmatrix} \eta_1 & r_{1,1} \\ \eta_2 & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & -\alpha_0 \\ 1 & -\alpha_1 \end{pmatrix}.$$

The matrix R is just a single real element $r_{1,1} \neq 0$. If η_1 and η_2 are given, all the matrices in this class have (when $b = Wh$) the same GMRES residual norms given by

$$\|r^0\| = \sqrt{\eta_1^2 + \eta_2^2}, \quad \|r^1\| = \eta_2, \quad \|r^2\| = 0.$$

As in the previous section, we would like to study if, in this class of matrices, we can find real matrices for which the error norms $\|\epsilon^0\|$ and $\|\epsilon^1\|$ have prescribed values, say ω_0 and ω_1 that are two positive numbers. If these two values are given, then there are some constraints on $r_{1,1}$. Conversely, for a given $r_{1,1}$, ω_0 and ω_1 cannot have any prescribed values.

We are looking for a real companion matrix $\tilde{C}$ (that is, real $\tilde{\alpha}_0, \tilde{\alpha}_1$) such that $\|\epsilon^0\| = \omega_0, \|\epsilon^1\| = \omega_1$. To do this it is enough to find a real vector $z(\alpha) = \begin{pmatrix} z_1 & z_2 \end{pmatrix}^T$ such that $Wz(\alpha)$ is the solution of

$$\tilde{A}x = (WY\tilde{C}Y^{-1}W^T)x = b = Wh,$$

and the norms of the errors have the prescribed values. From the vector $z(\alpha)$ we know how to compute $\tilde{\alpha}_0$ and $\tilde{\alpha}_1$. We use the same machinery as for the general case with some simplifications. Asking for the prescribed error norms yields two equations for z_1 and z_2,

$$z_1^2 + z_2^2 = \omega_0^2, \tag{7.1}$$

$$(z_1 - t_1^1)^2 + (z_2 - t_2^1)^2 = \omega_1^2. \tag{7.2}$$

Let us assume that $\eta_1 \neq 0$ since otherwise the two equations are the same (this corresponds to stagnation). Equation (7.2) can be written as

$$z_1^2 + z_2^2 - 2(z_1 t_1^1 + z_2 t_2^1) + (t_1^1)^2 + (t_2^1)^2 = \omega_1^2.$$

Using (7.1) we obtain

$$z_1 = \frac{r_{1,1}}{2\eta_1^2}\left[-2\frac{\eta_1\eta_2}{r_{1,1}} z_2 + \frac{\eta_1^2}{r_{1,1}^2}\|h\|^2 - \omega_1^2 + \omega_0^2\right].$$

As in the previous section, let us write this as

$$z_1 = -qz_2 + p, \quad q = \frac{\eta_2}{\eta_1}, \quad p = \frac{1}{2r_{1,1}}\|h\|^2 + \frac{r_{1,1}}{2\eta_1^2}(\omega_0^2 - \omega_1^2).$$

Putting this in (7.1) we obtain a quadratic equation for z_2,

$$(1+q^2)z_2^2 - 2pqz_2 + p^2 - \omega_0^2 = 0.$$

To obtain a real solution z_2 we have the constraint

$$p^2 \le (1+q^2)\omega_0^2.$$

Rewriting this using the values of p and q and simplifying, we obtain the constraint

$$\frac{\eta_1^2}{4r_{1,1}^2}\|h\|^4 - \frac{\|h\|^2}{2}(\omega_0^2+\omega_1^2) + \frac{r_{1,1}^2}{4\eta_1^2}(\omega_0^2-\omega_1^2)^2 \le 0. \tag{7.3}$$

7.1. $n = 2$**,** ω_0 **and** ω_1 **given.** In the constraint (7.3), assume that ω_0 and ω_1 are given and let us see for which values of $r_{1,1}$ it can be satisfied. We rewrite (7.3) as

$$\eta_1^2\|h\|^4 - 2r_{1,1}^2\,\|h\|^2(\omega_0^2+\omega_1^2) + r_{1,1}^4\frac{(\omega_0^2-\omega_1^2)^2}{\eta_1^2} \le 0.$$

Looking for the left-hand side to be zero, we have a quadratic equation in $r_{1,1}^2$. The two roots of this equation (if $\omega_1 \ne \omega_0$) are

$$\frac{\eta_1^2\|h\|^2}{(\omega_0-\omega_1)^2}, \quad \frac{\eta_1^2\|h\|^2}{(\omega_0+\omega_1)^2}.$$

Therefore we obtain four roots for $r_{1,1}$ which are plus or minus the square roots of these values. The constraint is satisfied if $r_{1,1}$ is in between the two positive roots or the two negative ones. If $\omega_1 = \omega_0$, there are only two possible values for $r_{1,1} = \pm\eta_1\|h\|/(2\omega_0)$. Hence only the real matrices in the class satisfying these restrictions on the value of $r_{1,1}$ can have the prescribed error norms.

Note that if ω_1 is small compared to ω_0 then, for each of these two intervals, the two ends are close meaning that the range of feasible values for $r_{1,1}$ is quite small.

7.2. $n = 2$**,** $r_{1,1}$ **given.** On the contrary, since this is our primary goal, we may assume that the value of $r_{1,1}$ is given and look for which values of ω_0 and ω_1 the constraint (7.3) can be satisfied. Let us write (7.3) with obvious notation as

$$\delta - \beta(x^2+y^2) + \gamma(x^2-y^2)^2 \le 0.$$

We are interested in the boundary of the region defined by this constraint in the positive quadrant. We remark that we have $\beta^2 = 4\delta\gamma$. Clearly the curve described by $\delta - \beta(x^2+y^2) + \gamma(x^2-y^2)^2 = 0$ is symmetric with respect to the line $y = x$. Let us look for the values on straight lines defined by $y = ax + c$. We obtain

$$\delta - \beta((1+a^2)x^2 + 2acx + c^2) + \gamma((1-a^2)x^2 - 2acx - c^2)^2 = 0.$$

Let us choose $a^2 = 1$. Then the third term simplifies and we get a quadratic equation in x. The constant coefficient is $\delta - \beta c + \gamma c^4$ and this gives $c = \pm\sqrt{\beta/(2\gamma)}$ since we have $\beta^2 = 4\delta\gamma$. The coefficient of x is $-2\beta c + 4\gamma c^3 = 0$ with the values of c we have obtained. Similarly the coefficient of x^2 is $-2\beta + 4\gamma c^2 = 0$. Therefore the intersections of the lines

$$y = \pm x \pm \sqrt{\frac{\beta}{2\gamma}}$$

with the quadrant $x \geq 0$, $y \geq 0$ are parts of the boundary. But, for a given value of $x > 0$ we obtain two values of y^2,

$$y^2 = \frac{\beta + 2\gamma x^2 \pm 2x\sqrt{2\beta\gamma}}{2\gamma} > 0.$$

Since we are interested only in $y > 0$ we obtain two values. Hence, we have found all the boundary. It is composed of the intersections of two lines of slope 1 and one of slope -1 with the positive quadrant $x \geq 0$, $y \geq 0$; see Figure 7.3 for an example. The intersections with the x and y-axis are $(\sqrt{\beta/(2\gamma)}, 0)$ and $(0, \sqrt{\beta/(2\gamma)})$. If the point (ω_0, ω_1) is within the semi-infinite rectangle defined by these three lines, the constraint (7.3) is satisfied.

7.3. Numerical examples for $n = 2$. Let us prescribe

$$h = (\,0.469946, \quad 0.882695\,)^T.$$

This gives $\|h\| = 1$ and corresponds to residual norms $1, \quad 0.882695$. Let $\omega_0 = 1$ and let us look at the positive interval that must contain $r_{1,1}$ as a function of ω_1. Figure 7.1 displays the region for the feasible values of $r_{1,1}$ as a function of ω_1. For a given value of ω_1 it must be contained in the interval given by the intersections of a vertical line with the dashed and solid curves. Hence, we see that when ω_1 is close to $\omega_0 = 1$ almost any value of $r_{1,1}$ can used. When ω_1 decreases to 0, the length of the feasible interval decreases very rapidly. For ω_1 small, the value of $r_{1,1}$ is very constrained. However there are still an infinite number of matrices having the prescribed error norms since we can pick W as we wish as long as it is orthogonal. As an example let us choose $\omega_1 = 0.95$. Then $r_{1,1}$ (if chosen to be positive) has to be in the interval $[\,0.240998, \quad 9.39891\,]$. We can pick, for instance, $r_{1,1} = 3$. Then the matrix Y is

$$Y = \begin{pmatrix} 0.469946 & 3 \\ 0.882695 & 0 \end{pmatrix}.$$

One of the two companion matrices that are obtained from Y and ω_0, ω_1 is

$$C = \begin{pmatrix} 0 & -2.87519 \\ 1 & 2.52981 \end{pmatrix}.$$

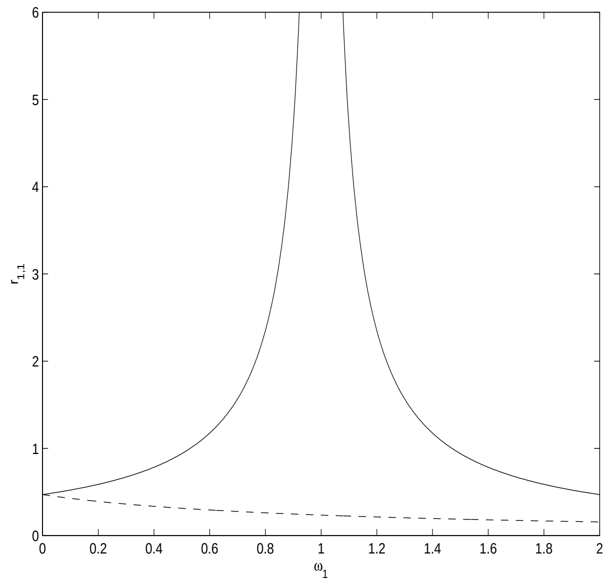

FIG. 7.1. *Feasible values of $r_{1,1}$ as a function of ω_1 when $\omega_0 = 1$*

Its eigenvalues are $1.2649 + 1.12925i, \quad 1.2649 - 1.12925i$. Let us now choose a random orthogonal matrix W

$$W = \begin{pmatrix} -0.399411 & -0.916772 \\ -0.916772 & 0.399411 \end{pmatrix}.$$

From this, one of the solutions is the matrix

$$\tilde{A} = \begin{pmatrix} 1.23962 & -0.480095 \\ 2.65748 & 1.29019 \end{pmatrix}$$

and the right-hand side is

$$\tilde{b} = Wh = \begin{pmatrix} -0.996932 \\ -0.0782748 \end{pmatrix}.$$

When running GMRES for the system $\tilde{A}x = \tilde{b}$, the residual norms are

$$1, \quad 0.882695, \quad 3.51083\ 10^{-16}$$

as prescribed and the error norms are

$$1, \quad 0.95, \quad 3.7238\ 10^{-16}$$

as given by the chosen values of ω_0 and ω_1.

The values of $r_{1,1}$ can be more severely constrained if, for instance, ω_0 is smaller. As an example Figure 7.2 shows the feasible region for $r_{1,1}$ as a function of ω_1 for $\omega_0 = 0.1$.

Now let us consider the matrix

$$A = \begin{pmatrix} 1 & -0.5 \\ -3 & 1 \end{pmatrix}.$$

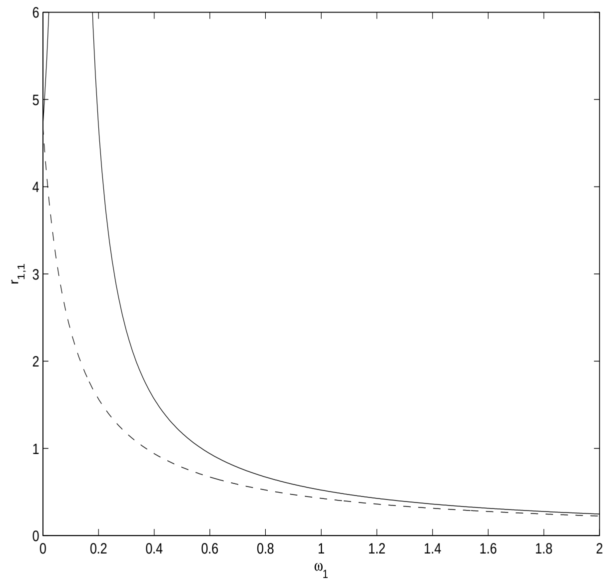

FIG. 7.2. *Feasible values of $r_{1,1}$ as a function of ω_1 when $\omega_0 = 0.1$*

This matrix has two real eigenvalues and a condition number of 22.455. The eigenvalues are $2.22474, \quad -0.224745$. We choose a random $b = (\,-0.25137, \quad -0.96789\,)^T$ of norm 1. The APS parametrization of A gives

$$W = \begin{pmatrix} 0.736229 & -0.676732 \\ -0.676732 & -0.736229 \end{pmatrix}, \quad Y = \begin{pmatrix} 0.469937 & 0.315901 \\ 0.8827 & 0 \end{pmatrix}.$$

Therefore $h = (\,0.469937, \quad 0.8827\,)^T$ as we had in the previous example and we have a fixed value of $R = r_{1,1} = 0.31590$. This matrix and the right-hand side give the same residual norm convergence curve as before. The norms of the residuals are $1, \quad 0.8827, \quad 5.55112\,10^{-17}$ and the error norms are $3.74485, \quad 5.22058, \quad 0$. The companion matrix C is

$$C = \begin{pmatrix} 0 & 0.5 \\ 1 & 2 \end{pmatrix}.$$

The boundary of the region ω_0, ω_1 for which the constraint (7.3) is satisfied is given by

$$0.55325 - 0.5(x^2 + y^2) + 0.11297(x^2 - y^2)^2 = 0.$$

This boundary is shown in Figure 7.3. We have positive solutions $\omega_0 = x$, $\omega_1 = y$ inside the semi-infinite rectangle. The star in the center of the figure corresponds to the error norms of the matrix A and right-hand side b. We also see that with these values of h and R we cannot ask for ω_0 and ω_1 to both be small. However we may look for matrices corresponding to the vertices of the rectangle (or to points close to that). The star on the x-axis is $(\sqrt{\beta/2\gamma},\, 0)$, the value of the square root being 1.4876.

Let us ask for $\|\epsilon^0\| = 1.4876$ and $\|\epsilon^1\| = 10^{-6}$. This point is within the feasible

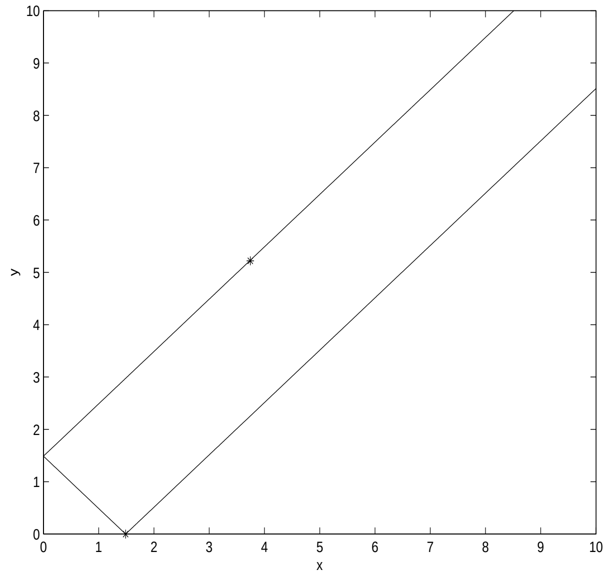

FIG. 7.3. *A part of the boundary of the region for which we have real solutions*

region so we find two solutions for $z(\alpha)$ that are

$$\begin{matrix} 0.699083 & 0.699084 \\ 1.31311 & 1.31311 \end{matrix}.$$

They are very close since the chosen point was close to a point on the x-axis where there is only one solution. However, this gives rise to two companion matrices

$$\tilde{C}_1 = \begin{pmatrix} 0 & -278579 \\ 1 & 414417 \end{pmatrix}, \quad \tilde{C}_2 = \begin{pmatrix} 0 & 278579 \\ 1 & -414417 \end{pmatrix}.$$

Up to rounding errors, they differ only by the signs of the coefficients α_0 and α_1. This gives two matrices

$$\tilde{A}_1 = \begin{pmatrix} 577619 & -150013 \\ 628401 & -163201 \end{pmatrix}, \quad \tilde{A}_2 = \begin{pmatrix} -577619 & 150013 \\ -628401 & 163202 \end{pmatrix},$$

with differences in signs of the entries. The eigenvalues of $\tilde{A}_1$ are $414416, \quad 0.67222$ and those of $\tilde{A}_2$ are $-414417, \quad 0.672218$. These two matrices are different from A. But, nevertheless, when we run GMRES with $\tilde{A}_1$ and b we obtain residual norms $1, \quad 0.8827, \quad 2.35162\ 10^{-11}$ as we should and

$$1.48761, \quad 1.00096\ 10^{-6} \quad 4.26339\ 10^{-11}$$

for the error norms as we have prescribed. It is the same for $\tilde{A}_2$. Therefore we have computed two matrices in the APS class defined by h that have the same prescribed residual norms as A and better error norms than those obtained with A even though the properties of these matrices do not look particularly good.

8. Numerical examples for $n = 3$. For a given matrix R, finding the boundary of the feasible region for ω_i, $i = 0, 1, 2$ seems difficult. So, let us consider a numerical example. Let

$$Y = \begin{pmatrix} 0.994987 & -1.14647 & 1.18916 \\ 0.099995 & 0 & -0.0376333 \\ 0.001 & 0 & 0 \end{pmatrix}.$$

This corresponds to residual norms $1, \; 0.1, \; 0.001$. We discretize the values of ω_i, $i = 0, 1, 2$ in intervals $[0, \omega]$ and we check the condition (7.3) for all the discretization points. This is shown in Figure 8.1 for $\omega = 1$ where we draw a '+' when the feasibility condition is satisfied. The volume of feasible values is semi-infinite as it can be seen by taking larger values of ω.

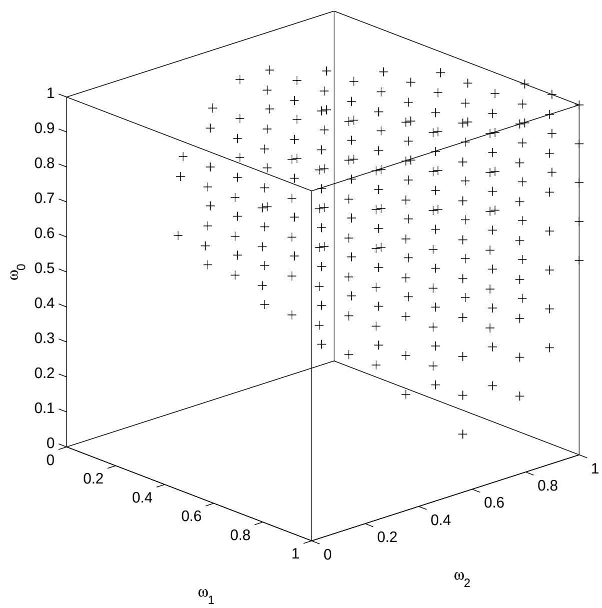

FIG. 8.1. *A part of the region for which we have real solutions*

Let us choose $W = I$ and therefore $b = h$. We pick values $\omega_0 = 0.7, \omega_1 = 0.5, \omega_2 = 0.2$ that are in the feasible region. One of the companion matrices we obtain is

$$C = \begin{pmatrix} 0 & 0 & 0.00195349 \\ 1 & 0 & -0.368311 \\ 0 & 1 & -1.35779 \end{pmatrix}.$$

It yields a matrix

$$A_1 = \begin{pmatrix} -1.03724 & -1.14283 & -0.15467 \\ 0.0328253 & -0.325746 & -0.087757 \\ 6.19296\ 10^{-22} & -5.19085\ 10^{-5} & 0.00519059 \end{pmatrix}.$$

Up to rounding errors this matrix is upper Hessenberg. Its eigenvalues are

$$-0.97989, \quad -0.383108, \quad 0.00520369 .$$

Running GMRES with A_1 and b we obtain residual norms

$$1, \quad 0.1, \quad 0.001, \quad 1.14439\ 10^{-16}$$

as prescribed. The error norms are

$$0.7, \quad 0.5, \quad 0.2, \quad 7.85046\ 10^{-17}$$

corresponding to the values ω_i we have chosen. Our algorithm also gives another solution

$$A_2 = \begin{pmatrix} -1.03724 & -1.1457 & 0.131783 \\ 0.0328253 & -0.327436 & 0.0812249 \\ -6.19296\ 10^{-22} & 5.19085\ 10^{-5} & -0.00519059 \end{pmatrix}$$

whose eigenvalues are $-0.979569, \quad -0.385118, \quad -0.00517823$. Note that zero is not in the convex hull of the eigenvalues of A_2 when it is in the convex hull for A_1. However the residual and error norm convergence curves are the same.

9. Conclusions. In this paper we have shown that in the class of matrices A having the same residual norm convergence curve, as defined in [1], we can choose the companion matrix C (and hence the eigenvalues of A) to obtain a prescribed error vector at a given iteration k. Moreover, when certain conditions are satisfied, we can compute the matrix C to have prescribed error norms at every iteration. It would be interesting to study if the eigenvalue distributions giving rise to “good” error norm convergence curves, for a given residual norm convergence curve, have any particular characteristics.

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