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EXPRESSIONS AND BOUNDS FOR THE GMRES RESIDUAL *

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Abstract.

Expressions and bounds are derived for the residual norm in GMRES. It is shown that the minimal residual norm is large as long as the Krylov basis is well-conditioned. For scaled Jordan blocks the minimal residual norm is expressed in terms of eigenvalues and departure from normality. For normal matrices the minimal residual norm is expressed in terms of products of relative eigenvalue differences.

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1 Introduction.

The generalised minimal residual method (GMRES) [34, 39] (and MINRES for Hermitian matrices [33]) is an iterative method for solving systems of linear equations $Ax = b$. The approximate solution in iteration i minimises the two-norm of the residual $b - Az$ over the Krylov space span$\{b, Ab, \ldots, A^{i-1}b\}$.

The goal of this paper is to express this minimal residual norm in terms of eigenvalues and departure of A from normality. Although it is known that the convergence of GMRES for a non-normal matrix is not determined by eigenvalues alone [1, 20, 30, 31, 12], our expressions for the residual norms of scaled Jordan blocks in §3 represent the first quantitative dependence of the minimal residual norm on the non-normality of the matrix.

Often the residual norm in Krylov space methods is bounded in terms of polynomials. With regard to GMRES, upper bounds on the residual norm in terms of polynomials are given in [4, 30, 34], and the tightness of these bounds is examined in [19, 21, 36]. Convergence analyses based on Ritz values are given in [5, 32, 38]. The case of nearly singular matrices is analysed in [3], and comparisons with other methods are made in [2, 25]. The approach here is different because we ignore the way GMRES is implemented (e.g. via Arnoldi's

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method) and we do not use polynomials to derive the bounds. Instead we exploit structure in the Krylov matrix.

1.1 Overview

In §2 the minimal residual norm is expressed in terms of the pseudo-inverse of the next Krylov matrix. In §3 the minimal residual norm of a scaled Jordan block is expressed in terms of eigenvalues and departure from normality. In §4 it is shown that the minimal residual norm for normal matrices is proportional to a product of relative eigenvalue diffferences. In §5 the current minimal residual norm is related to the previous one.

1.2 Notation

The norm $\|\cdot\|$ is the Euclidean two-norm, or spectral norm. The identity matrix of order k is $I_k \equiv \begin{pmatrix} e_1 & \dots & e_k \end{pmatrix}$ with columns e_i. The conjugate transpose of a matrix K is K^*; and the Moore-Penrose inverse of a full column rank matrix K is $K^\dagger \equiv (K^*K)^{-1}K^*$.

Let A be a complex square matrix and $b \neq 0$ a column vector. The Krylov space in iteration i is

$$\mathcal{K}_i \equiv \text{span}\{b, Ab, \dots, A^{i-1}b\}, \qquad i \geq 1,$$

and the corresponding Krylov matrix is

$$K_i \equiv \begin{pmatrix} b & Ab & \dots & A^{i-1}b \end{pmatrix}, \qquad i \geq 1.$$

2 Nothing Happens as Long as the Krylov Basis is Well-Conditioned.

It is shown that the minimal residual norm is related to the conditioning of the Krylov basis in the next larger space.

In iteration i a minimal residual method wants to find a vector $z \in \mathcal{K}_i$ that makes $\|b - Az\|$ small. But $z \in \mathcal{K}_i$ means that $z = K_i y$ for some y, hence

$$\|b - Az\| = \|b - AK_i y\|.$$

However since $K_{i+1} = \begin{pmatrix} b & AK_i \end{pmatrix}$, making the residual norm small means approximating the first column of K_{i+1} by the remaining columns. If the residual norm can be made small then the columns of K_{i+1} must be almost linearly dependent, which means $\|K_{i+1}^\dagger\|$ is large.

THEOREM 2.1. *If K_{i+1} has full column rank then*

$$\min_{z \in \mathcal{K}_i} \|b - Az\| = \frac{1}{\|e_1^* K_{i+1}^\dagger\|}.$$

PROOF. Let $B = \begin{pmatrix} b & B_1 \end{pmatrix}$ be a matrix with leading column b, and let y be the solution to the least squares problem $\min_z \|b - B_1 z\|$. With $r \equiv b - B_1 y$ one obtains [6, §8], [7, §5], [35, §§3,4]

$$e_1^* B^\dagger = \frac{1}{\|r\|^2}(b^* - y^* B_1^*) = \frac{r^*}{\|r\|^2}.$$

The proof follows by setting $B = K_{i+1}$ and $B_1 = AK_i$. □

Therefore if the columns of the next Krylov matrix are very linearly independent then the residual norm in the current iteration must be large. This can happen, for instance, with circulant matrices [2, Example 3.1], [30, Example C].

COROLLARY 2.2. *If K_{i+1} has full column rank then*

$$\min_{z\in\mathcal{K}_i} \frac{\|b - Az\|}{\|b\|} \geq \frac{1}{\|K_{i+1}\| \, \|K_{i+1}^{\dagger}\|}.$$

This means there is no convergence as long as the Krylov basis is well-conditioned. The following example illustrates that the bound in Corollary 2.2 can be tight for all iterations. In $Ax = b$ let

$$A = \begin{pmatrix} 1 & & & \\ & \omega & & \\ & & \ddots & \\ & & & \omega^{n-1} \end{pmatrix}, \qquad b = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix},$$

where $\omega \equiv e^{2\pi\sqrt{-1}/n}$ is the nth root of unity. In the last iteration the Krylov matrix is $K_n = \sqrt{n}F_n$, where F_n is the Fourier matrix. Hence $\|e_1^* K_n^{-1}\| = 1/\sqrt{n}$. Therefore the residual norms remain maximal until the last iteration

$$\min_{z\in\mathcal{K}_i} \frac{\|b - Az\|}{\|b\|} = 1 = \frac{1}{\|K_{i+1}\| \, \|K_{i+1}^{\dagger}\|}, \qquad 1 \leq i \leq n-1.$$

3 The Residual Norm Depends on the Departure From Normality.

It is shown that for a scaled Jordan block the minimal residual norm depends on how large the departure from normality is compared to the eigenvalue magnitude.

Let A be a scaled Jordan block of order n,

$$A \equiv \begin{pmatrix} \lambda & \eta & & \\ & \lambda & \ddots & \\ & & \ddots & \eta \\ & & & \lambda \end{pmatrix}.$$

The two-norm departure from normality [23, §1.2] of A is $|\eta|$. When $\eta \neq 0$ then A is diagonally similar to a Jordan block, i.e. $A = XJX^{-1}$, where

$$J \equiv \begin{pmatrix} \lambda & 1 & & \\ & \lambda & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{pmatrix}, \qquad X \equiv \begin{pmatrix} 1 & & & \\ & 1/\eta & & \\ & & \ddots & \\ & & & 1/\eta^{n-1} \end{pmatrix},$$

and the eigenvalue λ is maximally defective. When $\lambda = 0$ and $\eta \neq 0$ no solution to $Ax = b$ lies in a Krylov space [28, Theorem 2], so the interesting case is $\lambda \neq 0$.

Construct an upper triangular Toeplitz matrix T of order n from the right-hand side $b = (\, b_1 \quad \dots \quad b_n \,)^T$, and let T_{i+1} be the trailing $i+1$ columns of T,

$$T \equiv \begin{pmatrix} b_n & \dots & b_2 & b_1 \\ & \ddots & & b_2 \\ & & \ddots & \vdots \\ & & & b_n \end{pmatrix}, \qquad T_{i+1} \equiv T \begin{pmatrix} 0 \\ I_{i+1} \end{pmatrix}.$$

THEOREM 3.1. *Let A be a scaled Jordan block with $\lambda \neq 0$. If K_{i+1} has full column rank then*

$$\min_{z \in \mathcal{K}_i} \frac{\|b - Az\|}{\|b\|} = c_{i+1} \frac{|\tau|^i}{\sqrt{1 + |\tau|^2 + \dots + |\tau|^{2i}}}, \qquad \tau \equiv \frac{\eta}{\lambda},$$

where the constant c_{i+1} depends only on i and b, and

$$\frac{1}{\|b\| \, \|T_{i+1}^\dagger\|} \leq c_{i+1} \leq \frac{\|T_{i+1}\|}{\|b\|} \leq \sqrt{i+1}.$$

PROOF. The idea is to factor the Krylov matrix

$$K_{i+1} = T \begin{pmatrix} 0 \\ Z \end{pmatrix} D = T_{i+1} Z D,$$

where

$$D \equiv \begin{pmatrix} 1 & & & \\ & \lambda & & \\ & & \ddots & \\ & & & \lambda^i \end{pmatrix}$$

and

$$Z \equiv \begin{pmatrix} 0 & 0 & 0 & & \tau^i \\ 0 & 0 & 0 & \cdot^{\cdot^{\cdot}} & \alpha_{i,i-1}\tau^{i-1} \\ 0 & 0 & \tau^2 & \cdot^{\cdot^{\cdot}} & \vdots \\ 0 & \tau & \alpha_{21}\tau & \dots & \alpha_{i1}\tau \\ 1 & 1 & 1 & \dots & 1 \end{pmatrix},$$

with elements

$$\begin{aligned} &\alpha_{21} = 2 \\ &\alpha_{i1} = 1 + \alpha_{i-1,1}, \qquad 2 \leq i \\ &\alpha_{ij} = \alpha_{i-1,j-1} + \alpha_{i-1,j}, \qquad 2 \leq i, \quad 2 \leq j \leq i-2 \\ &\alpha_{i,i-1} = \alpha_{i-1,i-2} + 1, \qquad 2 \leq i. \end{aligned}$$

That is, $\alpha_{ij} = \binom{i}{j}$, $i \geq 1$. Hence

$$\|e_1^* K_{i+1}^\dagger\| = \|e_1^* D^{-1} Z^{-1} T_{i+1}^\dagger\| = \|e_1^* Z^{-1} T_{i+1}^\dagger\|.$$

This together with Theorem 2.1 implies

$$\min_{z\in\mathcal{K}_i} \frac{\|b-Az\|}{\|b\|} = c_{i+1}\frac{1}{\|e_1^* Z^{-1}\|},$$

where

$$\frac{1}{\|b\|\,\|T_{i+1}^{\dagger}\|} \le c_{i+1} \le \frac{\|T_{i+1}\|}{\|b\|}.$$

To express $\|e_1^*Z^{-1}\|$ in terms of τ, factor $Z = P\Delta R$, where

$$P \equiv \begin{pmatrix} & & 1 \\ & \cdot^{\cdot^{\cdot}} & \\ 1 & & \end{pmatrix}, \qquad \Delta \equiv \begin{pmatrix} 1 & & & \\ & \tau & & \\ & & \ddots & \\ & & & \tau^i \end{pmatrix},$$

and

$$R \equiv \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ & 1 & \alpha_{21} & \dots & \alpha_{i1} \\ & & \ddots & \ddots & \vdots \\ & & & \ddots & \alpha_{i,i-1} \\ & & & & 1 \end{pmatrix}.$$

Hence $e_1^*Z^{-1} = e_1^*R^{-1}\Delta^{-1}P^T$. An induction using the recurrences for α_{ij} shows

$$e_1^*R^{-1} = \begin{pmatrix} 1 & -1 & \dots & -(-1)^{i+1} \end{pmatrix},$$

which implies

$$e_1^*R^{-1}\Delta^{-1} = \begin{pmatrix} 1 & -\tau^{-1} & \dots & -(-1)^{i+1}\tau^{-i} \end{pmatrix}.$$

Hence

$$\|e_1^*Z^{-1}\|^2 = \sum_{l=0}^{i} |\tau|^{-2i} = |\tau|^{-2i}\,\left(1+|\tau|^2+\cdots+|\tau|^{2i}\right).$$

□

The following examples illustrate values for c_{i+1} in Theorem 3.1.

When b is a canonical vector, i.e. $b = e_k$, then $c_{i+1} = 1$.

When all elements of b have the same value, i.e. $b = \beta e$, then $c_{i+1} \ge 1/\sqrt{2(i+1)}$. This follows from the fact that $\|T_{i+1}^{\dagger}\| \le \|T_{i+1,i+1}^{-1}\|$, where $T_{i+1,i+1}$ contains the trailing $i+1$ rows of T_{i+1}, and $T_{i+1,i+1}^{-1}$ is an upper bidiagonal matrix with $1/\beta$ on the diagonal and $-1/\beta$ on the superdiagonal.

When b is of the form $b = \begin{pmatrix} b_1 & \dots & b_k & 0 \end{pmatrix}^T$, where b_k is an element of largest magnitude in b, then $c_{i+1} \ge 2^{-i}/\sqrt{k}$. This follows from the bound [24, Theorem 8.13] $\|T_{i+1,i+1}^{-1}\| \le 2^i/|\beta_k|$.

COROLLARY 3.2. *Let A be as in Theorem 3.1. If $|\eta| \ge |\lambda|$ then*

$$\min_{z\in\mathcal{K}_i} \frac{\|b-Az\|}{\|b\|} \ge c_{i+1}\,\frac{1}{\sqrt{i+1}}$$

and if $|\eta| \ll |\lambda|$ *then*

$$\min_{z\in\mathcal{K}_i} \frac{\|b-Az\|}{\|b\|} \approx c_{i+1} \left|\frac{\eta}{\lambda}\right|^i .$$

This means the residual norms decrease slowly when the scaled Jordan block is highly non-normal ($|\lambda| \leq |\eta|$), while they decrease faster when the Jordan block is only weakly non-normal ($|\lambda| \gg |\eta|$).

4 Normal Matrices.

For normal matrices it is shown that the minimal residual norm in iteration i is proportional to a product of i relative eigenvalue separations.

Let A be a normal matrix of order n with eigenvalue decomposition

$$A = Q \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} Q^*,$$

where Q is unitary, and let β_i be the norm of the orthogonal projection of b onto the eigenspace associated with λ_i. Denote by d the number of distinct eigenvalues of A minus the eigenvalues of A whose eigenspace is orthogonal to b.

THEOREM 4.1. *If A is normal and $1 \leq i \leq d-1$ then*

$$\min_{z\in\mathcal{K}_i} \frac{\|b-Az\|}{\|b\|} = c_{i+1} \min_{1\leq j\leq i+1} \left\{ \frac{\beta_j}{\|b\|} \prod_{l=1,l\neq j}^{i+1} \frac{|\lambda_l - \lambda_j|}{|\lambda_l|} \right\},$$

where $1/\sqrt{i+1} \leq c_{i+1} \leq \sqrt{(i+1)(d-i)}$, and $\lambda_1, \ldots, \lambda_{i+1}$ are $i+1$ distinct eigenvalues of A that maximise

$$\prod_{j=1}^{i+1} \beta_j \prod_{l=j+1}^{i+1} |\lambda_l - \lambda_j|.$$

In particular[1] $c_d \leq 1$.

PROOF. The idea is to factor the Krylov matrix as $K_{i+1} = QDV_{i+1}$, where

$$D \equiv \begin{pmatrix} b_1 & & \\ & \ddots & \\ & & b_n \end{pmatrix}, \qquad V_{i+1} \equiv \begin{pmatrix} 1 & \lambda_1 & \ldots & \lambda_1^i \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_n & \ldots & \lambda_n^i \end{pmatrix}.$$

Here V_{i+1} is a $n \times (i+1)$ Vandermonde matrix, and

$$\begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix} = Q^* b.$$

[1]We thank Anne Greenbaum for this observation.

Hence $\|e_1^* K_{i+1}^\dagger\| = \|e_1^*(DV_{i+1})^\dagger\|$. Before proceeding with the action in the proof we remove redundant quantities in DV_{i+1}.

First remove rows with multiple eigenvalues in V_{i+1} to create a Vandermonde matrix with distinct nodes. Suppose $\lambda_j = \lambda_k$ so that rows j and k of V_{i+1} are identical. Eliminate one of these rows in DV_{i+1}, say row k, by a plane rotation P_{jk},

$$P_{jk}\begin{pmatrix} b_j \\ b_k \end{pmatrix}\begin{pmatrix} \lambda_j & \lambda_j^2 & \dots & \lambda_j^i \end{pmatrix} = \begin{pmatrix} \gamma \\ 0 \end{pmatrix}\begin{pmatrix} \lambda_j & \lambda_j^2 & \dots & \lambda_j^i \end{pmatrix},$$

where $\gamma = \sqrt{|b_j|^2 + |b_k|^2}$. Aside from introducing a zero row, the plane rotation P_{jk} preserves the Vandermonde structure. At last, permute zero rows to the bottom of the matrices. The whole transformation can be expressed as a unitary matrix U,

$$\begin{pmatrix} \hat{D}\hat{V}_{i+1} \\ 0 \end{pmatrix} = U\, DV_{i+1},$$

where

$$\hat{D} = \begin{pmatrix} \beta_1 & & \\ & \ddots & \\ & & \beta_d \end{pmatrix}$$

is a non-singular diagonal matrix, and $\hat{V}_{i+1}$ is a $d \times (i+1)$ Vandermonde matrix with distinct nodes λ_j, $1 \le j \le d$. Fortunately the unitary transformation does not do any harm,

$$\|e_1^* K_{i+1}^\dagger\| = \|e_1^*(DV_{i+1})^\dagger\| = \|e_1^*(\hat{D}\hat{V}_{i+1})^\dagger\|.$$

Now we are back to the action. Let P be a permutation matrix such that

$$P\,\hat{D}\hat{V}_{i+1} = \begin{pmatrix} S \\ B \end{pmatrix} = \begin{pmatrix} I \\ Z \end{pmatrix} S, \qquad Z \equiv BS^{-1},$$

where S has order $i+1$ and $|\det(S)|$ is maximal. Hence

$$\|e_1^*(\hat{D}\hat{V}_{i+1})^\dagger\| = \|e_1^* S^{-1}\begin{pmatrix} I \\ Z \end{pmatrix}^\dagger\|$$

and

$$\|e_1^* S^{-1}\| / \|\begin{pmatrix} I \\ Z \end{pmatrix}\| \le \|e_1^*(\hat{D}\hat{V}_{i+1})^\dagger\| \le \|e_1^* S^{-1}\|\,\|\begin{pmatrix} I \\ Z \end{pmatrix}^\dagger\|.$$

With $\sigma_{min}(\cdot)$ denoting the smallest singular value of a matrix one obtains [16, §2]

$$\|\begin{pmatrix} I \\ Z \end{pmatrix}^\dagger\| = \frac{1}{\sqrt{1 + \sigma_{min}(Z)^2}} \le 1,$$

and

$$\|\begin{pmatrix} I \\ Z \end{pmatrix}\| = \sqrt{1 + \|Z\|^2}.$$

Since $|\det(S)|$ is maximal, one can show as in the proof of [22, Lemma 3.1] that $|Z_{lk}| \leq 1$. Hence [15, (2.3.8)] $1 + \|Z\|^2 \leq (i+1)(d-i)$. This, together with Theorem 2.1, yields

$$\min_{z \in \mathcal{K}_i} \|b - Az\| = \frac{d_{i+1}}{\|e_1^* S^{-1}\|},$$

where $1 \leq d_{i+1} \leq \sqrt{(i+1)(d-i)}$. In the case when $i = d-1$ then $Z = 0$ and $d_{i+1} = 1$.

Now bound $\|e_1^* S^{-1}\|$ by an element of largest magnitude,

$$\max_{1 \leq j \leq i+1} |(S^{-1})_{1j}| \leq \|e_1^* S^{-1}\| \leq \sqrt{i+1} \max_{1 \leq j \leq i+1} |(S^{-1})_{1j}|.$$

Hence

$$\min_{z \in \mathcal{K}_i} \|b - Az\| = c_{i+1} \min_{1 \leq j \leq i+1} \frac{1}{|(S^{-1})_{1j}|}.$$

Since S is a submatrix of $\hat{D}\hat{V}_{i+1}$, one can write $S = \tilde{D}\tilde{V}_{i+1}$, where

$$\tilde{D} \equiv \begin{pmatrix} \beta_1 & & \\ & \ddots & \\ & & \beta_{i+1} \end{pmatrix}, \qquad \tilde{V}_{i+1} \equiv \begin{pmatrix} 1 & \lambda_1 & \dots & \lambda_1^i \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_{i+1} & \dots & \lambda_{i+1}^i \end{pmatrix}$$

for eigenvalues λ_j and components β_j, $1 \leq j \leq i+1$, that maximise

$$|\det(S)| = \prod_{j=1}^{i+1} \beta_j \prod_{l=j+1}^{i+1} |\lambda_l - \lambda_j|.$$

Using the expressions for elements in the first row of the inverse of a Vandermonde matrix [17, Theorem 1] gives

$$|(S^{-1})_{1j}| = \frac{1}{\beta} \prod_{l=1, l \neq j}^{i+1} \frac{|\lambda_l|}{|\lambda_l - \lambda_j|}.$$

□

Theorem 4.1 suggests that GMRES converges fast for all normal matrices whose eigenvalues have small pairwise relative distances. In early iterations the minimal residual norm depends on eigenvalues that are far apart in an absolute sense. This suggests (in the absence of any information about b) that GMRES and MINRES tend to process outlying, far-apart eigenvalues first. In this sense Theorem 4.1 corroborates the convergence model for GMRES in [4]. After d iterations, GMRES has found the exact solution and $z \in \mathcal{K}_d$ solves $Ax = b$. This is well-known [34, Proposition 2], [28, §10] because d is the degree of the minimal polynomial of b with respect to A.

It is not obvious how the expression in Theorem 4.1 compares to existing polynomial bounds for GMRES. For instance, specializing the bound [34, Proposition 4], [30, §3] for diagonalizable matrices to normal matrices gives

$$\min_{z \in \mathcal{K}_i} \frac{\|b - Az\|}{\|b\|} \leq \min_{p_i} \max_{1 \leq j \leq n} |p_i(\lambda_j)|,$$

where the minimum ranges over all polynomials $p_i(\lambda)$ of degree i with $p_i(0) = 1$, and the maximum ranges over all n eigenvalues. This bound does not depend on b. In contrast, Theorem 4.1 can be written as

$$\min_{z \in \mathcal{K}_i} \frac{\|b - Az\|}{\|b\|} = c_{i+1} \min_{1 \le j \le i+1} \left\{ \frac{\beta_j}{\|b\|} |p_{ij}(\lambda_j)| \right\},$$

where

$$p_{ij}(\lambda) = \prod_{l=1, l \ne j}^{i+1} \frac{|\lambda_l - \lambda|}{|\lambda_l|}, \qquad 1 \le j \le i+1,$$

are polynomials of degree i with $p_{ij}(0) = 1$. This expression depends on b because the eigenvalues $\lambda_1, \ldots, \lambda_{i+1}$ are chosen to maximise

$$\prod_{j=1}^{i+1} \beta_j \prod_{l=j+1}^{i+1} |\lambda_l - \lambda_j|.$$

As a result, the maximum ranges only over a subset of $i+1$ eigenvalues. The form of the polynomials is the same as in [34, Theorem 5],

$$\min_{z \in \mathcal{K}_i} \frac{\|b - Az\|}{\|b\|} \le \left(\frac{R}{C} \right)^{i-k} \max_{k+1 \le j \le n} \prod_{l=1}^{k} \frac{|\lambda_l - \lambda_j|}{|\lambda_l|},$$

where $\lambda_1, \ldots, \lambda_k$ are eigenvalues of A with non-positive real parts and all other eigenvalues are situated in a circle with center $C > 0$ and radius $R < C$.

According to [8, §1] 'Vandermonde matrices have a reputation of being ill conditioned. This reputation is well-deserved for Vandermonde matrices whose nodes are real'. In particular, the condition number of a Vandermonde matrix grows exponentially when the nodes are positive [14, §2], or are located symmetrically around the origin on the real line [14, §3], or are either all less than one in magnitude or larger than one [37, §4]. This explains why GMRES and MINRES can converge fast (in exact arithmetic) when the matrix is positive-definite or even indefinite. The example at the end of §2 illustrates that allowing complex nodes makes it easier to construct well-conditioned Vandermonde matrices [8, §1], which in turn produce large residual norms for many iterations.

When b has the same contribution in all eigenvectors, i.e. $b = \beta Q^* e$, where e is the vector of all ones, Theorem 4.1 implies

$$\min_{z \in \mathcal{K}_i} \frac{\|b - Az\|}{\|b\|} = c_{i+1} \min_{1 \le j \le i+1} \prod_{l=1, l \ne j}^{i+1} \frac{|\lambda_l - \lambda_j|}{|\lambda_l|},$$

where $1/\sqrt{n(i+1)} \le c_{i+1} \le \sqrt{(i+1)(d-i)/n}$, and $\lambda_1, \ldots, \lambda_{i+1}$ are $i+1$ distinct eigenvalues of A that maximise

$$\prod_{j=1}^{i+1} \prod_{l=j+1}^{i+1} |\lambda_l - \lambda_j|.$$

For this particular case the following two examples illustrate how to interpret the bounds in Theorem 4.1 for different eigenvalue distributions.

In the first example A has one cluster of eigenvalues centered at a point c in the complex plane with radius $\epsilon > 0$, and a single outlier $c + \delta$. Then $|\delta|$ is the absolute distance between cluster and outlier. We make three assumptions: First the absolute separation between cluster and outlier is much larger than the absolute cluster radius, $|\delta| \gg \epsilon$; second, the relative cluster radius is small, $\epsilon/|c| < 1$; and third, the outlier is farther away from zero than the cluster, $|c + \delta| \geq |c|$. Then one can show [26, §5.2] that in iteration i,

$$\min_{z \in \mathcal{K}_i} \frac{\|b - Az\|}{\|b\|} \approx \left|\frac{\delta}{c+\delta}\right| \left(\frac{\epsilon}{|c|}\right)^{i-1},$$

which suggests that the minimal residual norm decreases as a power of the relative cluster radius. This agrees with the bounds [4, Corollary 4.2] and [34, Theorem 5].

In the second example A has one cluster of eigenvalues centered at c and a second cluster centered at $c + \delta$. The two clusters have the same number of eigenvalues and the same absolute cluster radius $\epsilon > 0$. The absolute cluster separation is $|\delta|$. We assume again that the absolute cluster separation is much larger than the absolute cluster radius, $|\delta| \gg \epsilon$, and that one of the clusters has a small relative cluster radius, $\epsilon/|c| < 1$. The minimal residual norm in iteration i is proportional to

$$\min_{z \in \mathcal{K}_i} \frac{\|b - Az\|}{\|b\|} \approx \min\left\{\left|\frac{\delta}{c}\right|, \left|\frac{\delta}{c+\delta}\right|\right\} \left|\frac{\delta}{c}\right|^{\frac{i-1}{2}} \left(\frac{\epsilon}{|c+\delta|}\right)^{\frac{i-1}{2}}.$$

The last factor represents a power of the relative cluster radius, and the preceding factors represent a power of the relative cluster separation. In contrast to the previous example, the relative cluster separation now has more influence on the residual norm. Again, this agrees with the more qualitative bound [4, Proposition 5.1].

These two examples suggest that, in general, indefinite matrices can produce larger residual norms than definite matrices because eigenvalues with opposite signs lead to larger relative cluster separations.

5 Relation Between Successive Residuals.

It is shown that successive minimal norm residuals are related by the sine of the angle between the current Krylov space and the new Krylov vector.

Let

$$\rho_i \equiv \min_{z \in \mathcal{K}_i} \frac{\|b - Az\|}{\|b\|}$$

be the relative residual in iteration i. An angle θ_i below is the largest principal angle between two subspaces [15, §12.4.3].

THEOREM 5.1. *If K_{i+1} has full column rank then*

$$\sin\theta_i \, \rho_{i-1} \leq \rho_i \leq \rho_{i-1},$$

where $0 < \theta_i \leq \pi/2$ *is the angle between* $\mathcal{K}_i$ *and* $A^i b$, *and*

$$\sin\theta_i = \|(I - K_i K_i^\dagger)A^i b\|/\|A^i b\|.$$

Proof. Applying Lemmas 5.2 and 5.3 below to $A \equiv K_{i+1}$, $B \equiv K_i$, $c \equiv A^i b$ and $\theta \equiv \theta_i$ gives

$$\|e_1^* K_{i+1}^\dagger\| \leq \|e_1^* K_i^\dagger\|/\sin\theta_i,$$

as well as the expression for $\sin\theta_i$. The proof follows with Theorem 2.1. □

The circulant system

$$A = \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ 1 & & & 0 \end{pmatrix}, \qquad b = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

presents an extreme case, where each new Krylov vector is orthogonal to the previous Krylov space, until the very last iteration. That is,

$$K_i = \begin{pmatrix} e_1 & e_n & \dots & e_{n-i+2} \end{pmatrix}, \qquad A^i b = e_{n-i+1},$$

and $K_{i+1}^\dagger A^i b = 0$. Hence $(I - K_i K_i^\dagger)A^i b = A^i b = e_{n-i+1}$ and $\sin\theta_i = 1$, $i \leq n-1$.

In many GMRES implementations a least squares problems is solved in each iteration by reducing a Hessenberg matrix to upper triangular form via plane rotations [34, §3.2], [18, §2.4]. At iteration i a plane rotation $\begin{pmatrix} c_i & s_i \\ -\bar{s}_i & c_i \end{pmatrix}$ is generated to eliminate the trailing element of the Hessenberg matrix. Successive residual norms satisfy $\rho_i = |s_i|\rho_{i-1}$ [34, §3.2], [2, §4] (see also [29, Lemma 6]). Thus

$$\sin\theta_i \leq |s_i|,$$

and the angle between the old space $\mathcal{K}_i$ and the new vector $A^i b$ is bounded by the angle of the plane rotation in iteration i. Bounds on ratios of successive residuals also follow from [5, Theorem 6] and [13, §1] but we did not see how to relate them to $\sin\theta_i$.

Lemma 5.2. *If* $A = \begin{pmatrix} B & c \end{pmatrix}$ *has full column rank then*

$$e_1^* A^\dagger = e_1^* B^\dagger\,(I - P),$$

where

$$P \equiv (1 - c^\dagger B B^\dagger c)^{-1}\, cc^\dagger (I - BB^\dagger)$$

is an oblique projector.

Proof. If A has full column rank then $e_1^* A^\dagger = e_1^*(A^*A)^{-1}A^*$. The partitioning of A gives

$$A^*A = \begin{pmatrix} B^*B & B^*c \\ c^*B & c^*c \end{pmatrix}.$$

Since A^*A is Hermitian, the first row of the inverse is [9, (4)]

$$e_1^*(A^*A)^{-1} = e_1^* S^{-1} \begin{pmatrix} I & -(c^*c)^{-1}B^*c \end{pmatrix},$$

where S is the Schur complement

$$S \equiv B^*B - B^*c\,(c^*c)^{-1}\,c^*B = B^*B - B^*cc^\dagger B.$$

Hence the first row of the pseudo-inverse can be expressed as

$$e_1 A^\dagger \quad = \quad e_1^* S^{-1}(B^* - B^*c(cc^*)^{-1}c^*) = e_1^* S^{-1} B^*(I - cc^\dagger).$$

Applying the Sherman-Morrison Woodbury formula [15, (2.1.4)] to S^{-1} gives

$$S^{-1} \quad = \quad (B^*B)^{-1} + \alpha^{-1}\, B^\dagger cc^\dagger B(B^*B)^{-1},$$

where

$$\alpha \equiv 1 - c^\dagger B(B^*B)^{-1}B^*c = 1 - c^\dagger BB^\dagger c.$$

Since A has full column rank, its columns are linearly independent and c does not lie in range(B). Hence $\alpha \neq 0$. Substitute the expression for S^{-1} into the expression for $e_1^*A^\dagger$,

$$\begin{aligned} e_1^*A^\dagger \quad &= \quad e_1^*\left[(B^*B)^{-1} + \alpha^{-1}\, B^\dagger cc^\dagger B(B^*B)^{-1}\right] B^*(I - cc^\dagger) \\ &= \quad e_1^* B^\dagger\,(I + \alpha^{-1}cc^\dagger BB^\dagger)(I - cc^\dagger), \end{aligned}$$

and multiply the last two factors to get

$$(I + \alpha^{-1}cc^\dagger BB^\dagger)(I - cc^\dagger) = I - P.$$

Since $P^2 = P$, P is a projector. $\square$

LEMMA 5.3. *If $A = \begin{pmatrix} B & c \end{pmatrix}$ has full column rank then*

$$\|e_1^*A^\dagger\| \leq \|e_1^*B^\dagger\| / \sin\theta,$$

where $0 < \theta \leq \pi/2$ is the angle between range(B) *and c, and*

$$\sin\theta = \|(I - BB^\dagger)c\| / \|c\|.$$

PROOF. The previous lemma implies $e_1^*A^\dagger = e_1^*B^\dagger(I - P)$, where

$$P = \alpha^{-1}\, cc^\dagger(I - BB^\dagger), \qquad \alpha = 1 - c^\dagger BB^\dagger c.$$

Thus $\|e_1^*A^\dagger\| \leq \|e_1^*B^\dagger\|\,\|I - P\|$. Since A has full column rank, $c \neq 0$ and $B \neq I$, and P has rank one. Hence [27, Corollary 5.3]

$$\|I - P\| = \|P\| = \|\alpha^{-1}c\|\,\|(I - BB^\dagger)c^\dagger\| = |\alpha|^{-1}\|(I - BB^\dagger)c\| / \|c\|.$$

But $I - BB^\dagger$ is the orthogonal projector onto the orthogonal complement of range(B). Hence [10, §6], [11, p 10] $\|(I - BB^\dagger)c\|/\|c\| = \sin\theta$, and $\|I - P\| = |\alpha|^{-1}\sin\theta$. At last

$$\alpha = 1 - \frac{c^* BB^\dagger c}{c^* c} = \frac{c^*(I - BB^\dagger)c}{c^* c}$$

implies

$$|\alpha| = \left(\frac{\|(I - BB^\dagger)c\|}{\|c\|}\right)^2 = (\sin\theta)^2.$$

Therefore $\|I - P\| = 1/\sin\theta$. □

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