

Numerical Matrix Analysis

Notes #26
GMRES

Peter Blomgren
(blomgren@sdsu.edu)

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

<http://terminus.sdsu.edu/>

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Outline

- 1 GMRES
 - Setup and Notation
 - Moving Forward
 - Polynomial Approximation, and Convergence

- 2 GMRES: Matrix Polynomials
 - $\|p_n(A)\|$
 - Example: T&B-35.1
 - Example: T&B-35.2

Arnoldi Iteration $\rightsquigarrow A\vec{x} = \vec{b}$

Last time we looked at the Arnoldi Iteration as a procedure for finding eigenvalues. Next, we leverage it to solve $A\vec{x} = \vec{b}$; introducing GMRES, the “Generalized Minimal RESiduals” strategy.

Algorithm (Arnoldi Iteration)

```
1:  $\vec{b} \leftarrow \text{random}(\mathbb{R}^{m \times 1})$ ,  
2:  $\vec{q}_1 \leftarrow \vec{b} / \|\vec{b}\|$   
3: for  $n \in \{1, 2, \dots\}$  do  
4:    $\vec{v} \leftarrow A\vec{q}_n$   
5:   for  $j \in \{1, \dots, n\}$  do  
6:      $h_{j,n} \leftarrow \vec{q}_j^* \vec{v}$   
7:      $\vec{v} \leftarrow \vec{v} - h_{j,n} \vec{q}_j$   
8:   end for  
9:    $h_{n+1,n} \leftarrow \|\vec{v}\|$   
10:   $\vec{q}_{n+1} \leftarrow \vec{v} / h_{n+1,n}$   
11: end for
```

TB-33.2: $h_{n+1,n} = 0$ (Breakdown due to Convergence)

Structure, Notation, Idea

Problem Structure and Notation

We consider $A \in \mathbb{C}^{m \times m}$, with $\dim(\text{null}(A)) = 0$; $\vec{b} \in \mathbb{C}^m$;
 $K(A, \vec{b}, n) = \text{span}(\vec{b}, A\vec{b}, \dots, A^{n-1}\vec{b})$; and $\vec{x}_* = A^{-1}\vec{b}$ (exact solution).

GMRES Idea

At the n^{th} step, $\vec{x}_n \approx \vec{x}_*$ is the vector $\vec{x}_n \in K(A, \vec{b}, n)$ which minimizes $\|\vec{r}_n\|$, where $\vec{r}_n = (\vec{b} - A\vec{x}_n)$; *i.e.* each \vec{x}_n is the solution to a least squares problem over an n -dimensional (Krylov) subspace.

Many iterative optimization methods do something similar (at least in “spirit”) — seeking approximately optimal approximations in carefully nested sequences of subspaces. (See [MATH 693A])

GMRES: “Obvious” Strategy

With the Krylov matrix

$$K_n = \left[\begin{array}{c|c|c|c} \vec{b} & A\vec{b} & \dots & A^{n-1}\vec{b} \end{array} \right],$$

on hand, the “obvious” (ill-conditioned) way is to form

$$AK_n = \left[\begin{array}{c|c|c|c} A\vec{b} & A^2\vec{b} & \dots & A^n\vec{b} \end{array} \right],$$

which has the column space $\text{range}(AK_n)$. We seek \vec{c}_n

$$\vec{c}_n = \arg \min_{\vec{c} \in \mathbb{C}^n} \|(AK_n)\vec{c} - \vec{b}\|, \quad \text{and } \vec{x}_n = K_n\vec{c}_n.$$

Note: $\arg \min$ “returns” the argument-that-minimizes the given function (objective).

The “Obvious” Strategy Fails (in Finite Precision)

A $Q_n R_n$ -factorization of AK_n would provide the necessary components of the pseudo-inverse necessary for identification of the solution to the least squares problem.

But, alas, this approach is numerically unstable, and wasteful (the R_n factor is not needed.)

Instead, we use the Arnoldi Iteration to construct Krylov Matrices Q_n , whose columns satisfy

$$\text{span}(\vec{q}_1, \vec{q}_2, \dots, \vec{q}_n) = K(A, \vec{b}, n),$$

thus we can represent $\vec{x}_n = Q_n \vec{y}_n$ rather than $\vec{x}_n = K_n \vec{c}_n$; the associated Least Squares Problem is

$$\vec{y}_n = \arg \min_{\vec{y} \in \mathbb{C}^n} \|AQ_n \vec{y} - \vec{b}\|.$$

"Shrinking" the Problem

1 of 2

As stated $\vec{y}_n = \arg \min_{\vec{y} \in \mathbb{C}^n} \|AQ_n \vec{y} - \vec{b}\|$ is an $(m \times n)$ -dimensional Least Squares Problem, but using the structure of Krylov subspaces, its essential dimension is reduced to $((n+1) \times n)$:

We use the "Arnoldi relation" $AQ_n = Q_{n+1} \tilde{H}_n$ to transform the problem into

$$\vec{y}_n = \arg \min_{\vec{y} \in \mathbb{C}^n} \|Q_{n+1} \tilde{H}_n \vec{y} - \vec{b}\|,$$

multiplication by Q_{n+1}^* preserves the norm, since both $(Q_{n+1} \tilde{H}_n \vec{y})$ and \vec{b} are — by construction — in the column space of Q_n ; we get

$$\vec{y}_n = \arg \min_{\vec{y} \in \mathbb{C}^n} \|\tilde{H}_n \vec{y} - Q_{n+1}^* \vec{b}\|.$$

“Shrinking” the Problem

2 of 2

Finally, by construction of Q_n^\dagger , we get $Q_{n+1}^* \vec{b} = \|\vec{b}\| \vec{e}_1$, so our problem is

$$\vec{y}_n = \arg \min_{\vec{y} \in \mathbb{C}^n} \|\tilde{H}_n \vec{y} - \beta \vec{e}_1\|, \quad \text{where } \beta = \|\vec{b}\|;$$

and $\vec{x}_n = Q_n \vec{y}_n$.

\vec{e}_1 is as usual the first standard basis vector in the appropriate space; it has a single “1” in the first component, and the remaining components are “0”.

[‡] $\text{span}(Q_1) = \text{span}(\vec{b})$

GMRES Algorithm

Algorithm (GMRES)

- 1: $\vec{b} \leftarrow \text{random}(\mathbb{R}^{m \times 1})$,
- 2: $\beta \leftarrow \|\vec{b}\|$
- 3: $\vec{q}_1 \leftarrow \vec{b}/\beta$
- 4: **for** $n \in \{1, 2, \dots\}$ **do**
- 5: $\vec{v} \leftarrow A\vec{q}_n$
- 6: **for** $j \in \{1, \dots, n\}$ **do**
- 7: $h_{j,n} \leftarrow \vec{q}_j^* \vec{v}$
- 8: $\vec{v} \leftarrow \vec{v} - h_{j,n}\vec{q}_j$
- 9: **end for**
- 10: $h_{n+1,n} \leftarrow \|\vec{v}\|$
- 11: $\vec{q}_{n+1} \leftarrow \vec{v}/h_{n+1,n}$
- 12: $\vec{y}_n \leftarrow \arg \min_{\vec{y} \in \mathbb{C}^n} \|\tilde{H}_n \vec{y} - \beta \vec{e}_1\|$
- 13: $\vec{x}_n \leftarrow Q_n \vec{y}_n$
- 14: **end for**

Comments

- In each step we solve an $((n + 1) \times n)$ Least Squares Problem with Hessenberg structure; the cost via QR -factorization is $\mathcal{O}(n^2)$ (exploiting the Hessenberg structure).
 - It is possible to save work by identifying an updating strategy for the $Q_n R_n$ factorization of \tilde{H}_n from $Q_{n-1} R_{n-1} = \tilde{H}_{n-1}$. The cost is then one *Givens rotation** [T&B PROBLEMS 10.4 & 35.4] and $\mathcal{O}(n)$ work.
- * The Givens rotations are the building blocks for a slightly (50%) more expensive alternative to the Householder reflection method for computing the QR -factorization.

Polynomial Approximation

1 of 2

Polynomial Class P_n

$$P_n = \{ \text{POLYNOMIALS OF DEGREE } \leq n, \text{ WITH } p(0) = 1 \},$$

i.e. the constant coefficient $c_0 = 1$.

Just as in the Arnoldi Iteration case, we can discuss the GMRES iteration in terms of polynomial approximations:

$$\vec{x}_n = q_n(A)\vec{b}$$

where $q_n(\cdot)$ is a polynomial of degree $(n - 1)$ with coefficients from the vector $\vec{c}_n = \arg \min_{\vec{c} \in \mathbb{C}^n} \|AK_n\vec{c} - \vec{b}\|$.

Polynomial Approximation

2 of 2

With $p_n(z) = 1 - zq_n(z)$, we have

$$\vec{r}_n = \vec{b} - A\vec{x}_n = (I - Aq_n(A))\vec{b} = p_n(A)\vec{b},$$

for some $p_n \in P_n$.

GMRES solves the following problem

GMRES Approximation Problem

Find $p_n \in P_n$ such that

$$p_n = \arg \min_{p \in P_n} \|p(A)\vec{b}\|.$$

Invariance Properties

Theorem

Let the GMRES iteration be applied to a matrix $A \in \mathbb{C}^{m \times m}$, then the following holds:

- [SCALE-INVARIANCE] If A is changed to σA for some $\sigma \in \mathbb{C}$, and \vec{b} is changed to $\sigma \vec{b}$, the residuals \vec{r}_n change to $\sigma \vec{r}_n$.
- [INVARIANCE UNDER UNITARY TRANSFORMATIONS] If A is changed to UAU^* for some unitary matrix U , and \vec{b} is changed to $U\vec{b}$, the residuals \vec{r}_n change to $U^* \vec{r}_n$.

Convergence

Theorem (GMRES Convergence Property#1: Monotonic Convergence)

GMRES converges monotonically,

$$\|\vec{r}_{n+1}\| \leq \|\vec{r}_n\|.$$

This must be the case since we are minimizing over expanding subspaces, *i.e.* $K(A, \vec{b}, n) \subset K(A, \vec{b}, n+1)$.

Theorem (GMRES Convergence Property#2: m -step Convergence)

In infinite precision, GMRES converges in at most m steps

$$\|\vec{r}_m\| = 0.$$

This must be the case since $K(A, \vec{b}, m) = \mathbb{C}^m$.

Convergence

The factor that gives us more useful convergence estimates is related to the polynomial p_n :

$$\frac{\|\vec{r}_n\|}{\|\vec{b}\|} \leq \inf_{p_n \in P_n} \|p_n(A)\|,$$

which brings us back to studying matrix polynomials related to Krylov subspaces.

How small can $\|p_n(A)\|$ be?

The standard way to get bounds on the behavior of $\|p_n(A)\|$ is to study polynomials on the spectrum $\lambda(A)$.

Definition

If p is a polynomial and $S \subset \mathbb{C}$, then

$$\|p\|_S := \sup_{z \in S} |p(z)|.$$

In the case where S is a finite set of points in the complex plane, the supremum (sup) is just the maximum (max).

When A is diagonalizable $A = V\Lambda V^{-1}$, then

$$\|p(A)\| \leq \|V\| \|p(\Lambda)\| \|V^{-1}\| = \kappa(V) \|p\|_{\lambda(A)}.$$

$\kappa(V)$ is the conditioning of the Eigenbasis.

How small can $\|p_n(A)\|$ be?

Theorem

At step n of the GMRES iteration, the residual \vec{r}_n satisfies

$$\frac{\|\vec{r}_n\|}{\|\vec{b}\|} \leq \inf_{p_n \in P_n} \|p_n(A)\| \leq \kappa(V) \inf_{p_n \in P_n} \|p_n\|_{\lambda(A)},$$

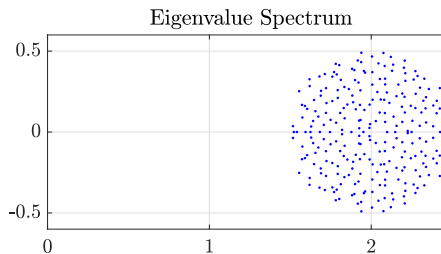
where $\lambda(A)$ is the set of eigenvalues of A , V is a non-singular matrix of eigenvectors (assuming A is diagonalizable), and $\|p_n\|_{\lambda(A)} = \sup_{z \in \lambda(A)} |p_n(z)|$.

As long as $\kappa(V)$ is not too large — *i.e.* the closer A is to being normal (unitarily diagonalizable) — and if polynomials p_n which decrease quickly on $\lambda(A)$ exist, then GMRES converges quickly.

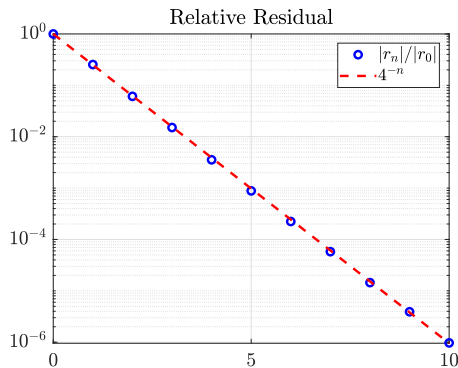
T&B-35.1

1 of 2

```
m = 256; b = ones(m,1);  
A = 2*eye(m) + 0.5 * randn(m)/sqrt(m);
```



$$\kappa(A) = 2.065$$



$$\kappa(V) = 216.490$$

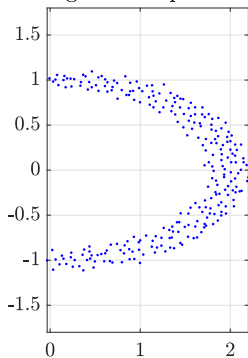
- The eigenvalue spectrum of A is roughly contained in the disk of radius $\frac{1}{2}$, centered at $z = 2$.
- $\|p(A)\|$ is approximately minimized by $p(z) = (1 - z/2)^n$;
- $\lambda(I - A/2)$ is roughly contained in the disc of radius $\frac{1}{4}$, centered at $z = 0$, so the convergence rate is $\|p_n(A)\| = \|(I - A/2)^n\| \sim \frac{1}{4^n}$.
- A is quite well-conditioned: $\kappa(A) = 2.065$.
- A is “not too far” from normal: $\kappa(V) = 216.490$.

T&B-35.2

1 of 2

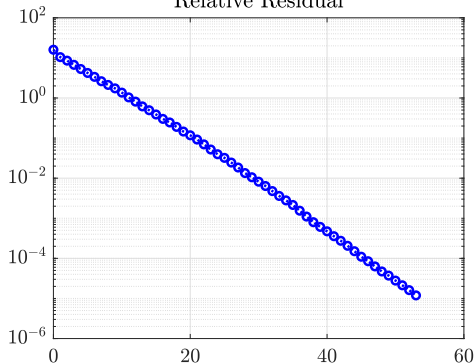
```
m = 256; b = ones(m,1); th = (0:(m-1))*pi / (m-1);  
A = 2*eye(m) + 0.5 * randn(m)/sqrt(m) + diag(-2+2*sin(th)+i*cos(th));
```

Eigenvalue Spectrum



$$\kappa(A) = 3.802$$

Relative Residual

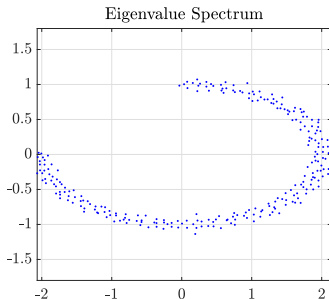


$$\kappa(V) = 150.711$$

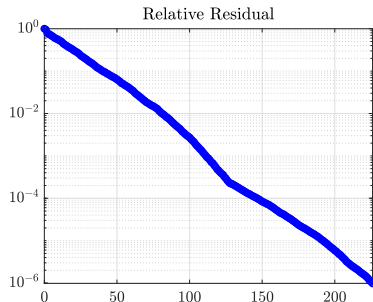
- The eigenvalue spectrum of A now “surrounds” the origin.
- A is quite well-conditioned: $\kappa(A) = 3.802$.
- A is not too far from normal: $\kappa(V) = 150.711$.
- The convergence is quite slow in this case (observed $\sim 1.23^{-n}$).
- Note that the slowdown in convergence does not depend on conditioning, but on the location of the eigenvalues.
- Clearly, understanding the impact of the “structure” of the eigenvalue spectrum is a non-trivial topic...

T&B-35.2⁺

```
m = 256; b = ones(m,1); th = 1.5*(0:(m-1))*pi / (m-1);  
A = 2*eye(m) + 0.5 * randn(m)/sqrt(m) + diag(-2+2*sin(th)+i*cos(th));
```



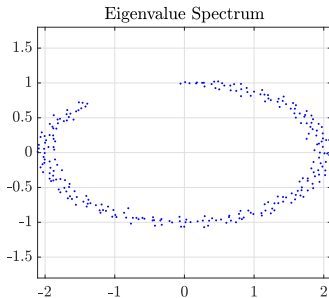
$$\kappa(A) = 3.9371$$



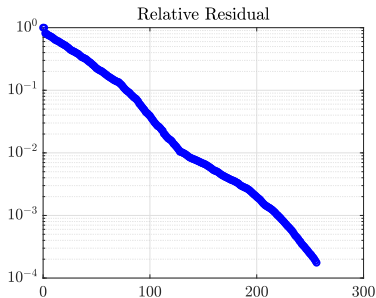
$$\kappa(V) = 73.7831$$

T&B-35.2⁺⁺

```
m = 256; b = ones(m,1); th = 1.75*(0:(m-1))*pi / (m-1);  
A = 2*eye(m) + 0.5 * randn(m)/sqrt(m) + diag(-2+2*sin(th)+i*cos(th));
```



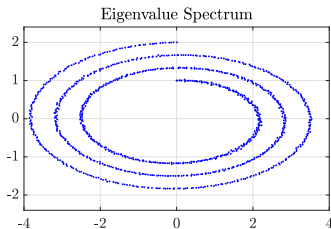
$$\kappa(A) = 3.7551$$



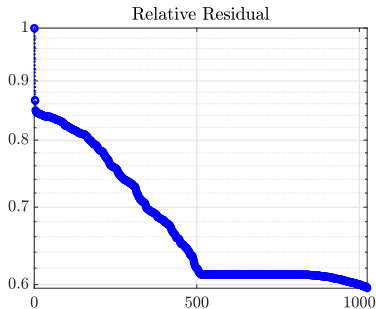
$$\kappa(V) = 58.6277$$

T&B-35.2+++

```
m = 1024; b = ones(m,1); th = 6.00*(0:(m-1))*pi / (m-1);  
A = 2*eye(m) + 0.5 * randn(m)/sqrt(m) + diag(-2+(1+th/(6*pi)).*(2*sin(th)+i*cos(th)));
```



$$\kappa(A) = 4.7704$$



$$\kappa(V) = 40.2912$$