On matrix approximation problems that bound GMRES convergence

Petr Tichý

Czech Academy of Sciences

joint work with

Vance Faber and Jörg Liesen

September 20, Mat Triad 2013,

Herzeg-Novi, Montenegro

Outline

Outline

Bounding GMRES residual norm

$\mathbf{A}x = b$, $\mathbf{A} \in \mathbb{R}^{n \times n}$ is nonsingular, $b \in \mathbb{R}^n$,

$x_0 = \mathbf{0}$ and $\|b\| = 1$ for simplicity, $\|\cdot\| =$ 2-norm.

GMRES computes $x_k \in \mathcal{K}_k(\mathbf{A}, b)$ such that $r_k \equiv b - \mathbf{A}x_k$ satisfies

$$\begin{aligned} \|r_k\| &= \min_{p \in \pi_k} \|p(\mathbf{A})b\| && \text{(GMRES)} \\ &\leq \max_{\|b\|=1} \min_{p \in \pi_k} \|p(\mathbf{A})b\| \equiv \mathcal{W}_k^{\mathbf{A}} && \text{(worst-case GMRES)} \\ &\leq \min_{p \in \pi_k} \|p(\mathbf{A})\| \equiv \mathcal{I}_k^{\mathbf{A}} && \text{(ideal GMRES)} \end{aligned}$$

where $\pi_k =$ degree $\leq k$ polynomials with $p(0) = 1$.

Questions

$$\|r_k\| \;\leq\; \underbrace{\max_{\|b\|=1}\min_{p\in\pi_k}\|p(\mathbf{A})b\|}_{\mathcal{W}_k^{\mathbf{A}}} \;\leq\; \underbrace{\min_{p\in\pi_k}\|p(\mathbf{A})\|}_{\mathcal{I}_k^{\mathbf{A}}}$$

- **Characterization** of solutions? Understanding?
- Existence and **uniqueness** of the solution?
- **Relationship** between ideal and worst case GMRES?

Normal matrices

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^*, \quad \mathbf{Q}^*\mathbf{Q} = \mathbf{I}\,.$$

- [Greenbaum, Gurvits '94; Joubert '94] showed:

$$\max_{\|b\|=1} \min_{p\in\pi_k} \|p(\mathbf{A})b\| \;=\; \min_{p\in\pi_k} \|p(\mathbf{A})\|$$

- Which (known) approximation problem is solved?

$$\min_{p\in\pi_k} \|p(\mathbf{A})\| \;=\; \min_{p\in\pi_k} \|\mathbf{Q}p(\mathbf{\Lambda})\mathbf{Q}^*\| \;=\; \min_{p\in\pi_k} \max_{\lambda_i} |p(\lambda_i)|\,.$$

- Is the solution unique? **Yes**

- Studied in [Greenbaum '79; Liesen, T. '04]

Nonnormal matrices – Toh's example

$$\|r_k\| \;\le\; \underbrace{\max_{\|b\|=1}\min_{p\in\pi_k} \|p(\mathbf{A})b\|}_{\mathcal{W}_k^{\mathbf{A}}} \;\le\; \underbrace{\min_{p\in\pi_k} \|p(\mathbf{A})\|}_{\mathcal{I}_k^{\mathbf{A}}}$$

Consider the 4 by 4 matrix

$$\mathbf{A} \;=\; \begin{bmatrix} 1 & \epsilon & & \\ & -1 & \epsilon^{-1} & \\ & & 1 & \epsilon \\ & & & -1 \end{bmatrix}, \qquad \epsilon > 0\,.$$

Then, for $k = 3$,

$$0 \;\overset{\epsilon\to 0}{\longleftarrow}\; \mathcal{W}_k^{\mathbf{A}} \;<\; \mathcal{I}_k^{\mathbf{A}} \;=\; \frac{4}{5}\,.$$

[Toh '97; another example in Faber, Joubert, Knill, Manteuffel '96]

Outline

Uniqueness

- Let $\mathbf{A}$ be a nonsingular matrix. Then the kth ideal GMRES polynomial that solves the problem

$$\min_{p \in \pi_k} \| p(\mathbf{A}) \|$$

is **unique**. [Greenbaum, Trefethen '94]

- Generalization of the uniqueness result to problems of the form

$$\min_{p \in \mathcal{P}_k} \| f(\mathbf{A}) - p(\mathbf{A}) \|$$

can be found in [Liesen, T. '09] .

Matrix approximation problems in spectral norm

and characterization of Ideal GMRES

- Ideal GMRES is a special case of the problem

$$\min_{\mathbf{M}\in\mathbb{A}} \| \mathbf{B} - \mathbf{M} \| = \| \mathbf{B} - \mathbf{A}_* \|$$

$\mathbf{A}_*$ is called a **spectral approximation** of $\mathbf{B}$ from $\mathbb{A}$.

- In our case,

$$\min_{p\in\pi_k} \|p(\mathbf{A})\| = \min_{\alpha_i\in\mathbb{C}} \left\| \mathbf{I} - \sum_{j=1}^{k} \alpha_j \mathbf{A}^j \right\| ,$$

i.e. $\mathbf{B} = \mathbf{I}$, $\mathbb{A} = \mathrm{span}\{\mathbf{A}, \ldots, \mathbf{A}^k\}$.

- General characterization by [Lau and Riha, 1981] and [Ziętak, 1993, 1996] $\to$ based on Singer's theorem [Singer, 1970] (a generalization of the classical results of approximation theory to Banach spaces).

Characterization of Ideal GMRES

by Faber, Joubert, Knill, Manteuffel '96

Given a polynomial $q \in \pi_k$ and $\mathbf{A}$, define the set

$$\Omega_k(q) \equiv \left\{ \begin{bmatrix} w^* \, q(\mathbf{A})^* \mathbf{A} \, w \\ \vdots \\ w^* \, q(\mathbf{A})^* \mathbf{A}^k \, w \end{bmatrix} : \; w \in \Sigma(q(\mathbf{A})), \; \|w\| = 1 \right\}$$

where $\Sigma(\mathbf{B})$ is the **span of maximal right singular vectors** of $\mathbf{B}$.

Theorem [Faber, Joubert, Knill, Manteuffel '96]

$p_* \in \pi_k$ is the kth ideal GMRES pol. of $\mathbf{A} \iff \mathbf{0} \in \mathrm{cvx}(\Omega_k(p_*))$.

Outline

Worst-case GMRES

For a given k, there exists a unit norm vector b such that

$$\|r_k\| = \min_{p\in\pi_k} \|p(\mathbf{A})b\| = \max_{\|v\|=1} \min_{p\in\pi_k} \|p(\mathbf{A})v\| = \mathcal{W}_k^{\mathbf{A}} .$$

b . . . a worst-case GMRES **initial vector**, the corresponding polynomial is a worst-case GMRES **polynomial** for $\mathbf{A}$ and k.

Theorem

[Zavorin '02; Faber, Liesen, T. '13]

$\mathcal{W}_k^{\mathbf{A}} = \mathcal{W}_k^{\mathbf{A}^T}$ holds for all $\mathbf{A}$ nad $k \geq 1$.

If b is a worst-case GMRES initial vector for $\mathbf{A}$ and k, then

$$b \xrightarrow{GMRES(\mathbf{A},b,k)} r_k \xrightarrow{GMRES(\mathbf{A}^T,r_k,k)} s_k = (\mathcal{W}_k^{\mathbf{A}})^2 b.$$

The cross equality

Definition

We say that b **satisfies the cross equality** for $\mathbf{A}$ and k if

$$b \xrightarrow{GMRES(\mathbf{A},b,k)} r_k \xrightarrow{GMRES(\mathbf{A}^T,r_k,k)} s_k \in \mathrm{span}\{b\}.$$

- A worst-case GMRES initial vector for $\mathbf{A}$ and k satisfies the cross equality for $\mathbf{A}$ and k.
- Satisfying the cross equality is **not sufficient** for b to be a worst-case initial vector.

Lemma

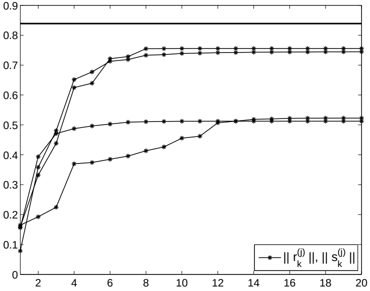
[Faber, Liesen, T. '13]

If A is nonderogatory ($d(\mathbf{A}) = n$), then each b with $d(\mathbf{A}, b) = n$ satisfies the cross equality for $\mathbf{A}$ and $n-1$.

Cross iteration algorithm [Faber, Liesen, T. '13]

- For each $\mathbf{A}$, k, and b, the following **seems to converge** to a vector satisfying the cross equality for $\mathbf{A}$ and k:

  Initialize $b^{(0)} = b$.
  For $j = 1, 2, \ldots$
  - $r_k^{(j)} = \text{GMRES}(\mathbf{A}, b^{(j-1)}, k)$
  - $c^{(j-1)} = r_k^{(j)} / \|r_k^{(j)}\|$
  - $s_k^{(j)} = \text{GMRES}(\mathbf{A}^T, c^{(j-1)}, k)$
  - $b^{(j)} = s_k^{(j)} / \|s_k^{(j)}\|$



Experiment with $\mathbf{A} = \mathbf{J}_1 \in \mathbb{R}^{11 \times 11}$, $k = 5$, and four random b.

Figure illustrates:

$\|r_k^{(j)}\| \leq \|s_k^{(j)}\| \leq \|r_k^{(j+1)}\| \leq \|s_k^{(j+1)}\|$

No convergence to a worst-case vector.

Worst-case polynomials for $\mathbf{A}$ and $\mathbf{A}^T$

Lemma [Faber, Liesen, T. '13]

Let b be a worst-case GMRES initial vector for $\mathbf{A}$ and k with corresponding $p_k \in \pi_k$, so that $r_k = p_k(\mathbf{A})b$.

- Then, by the cross equality, $r_k/\|r_k\|$ is a worst-case GMRES initial vector for $\mathbf{A}^T$ and k.
- Moreover, $p_k \in \pi_k$ **is the corresponding GMRES polynomial** for $\mathbf{A}^T$, k and $r_k/\|r_k\|$.

This implies:

$$p_k(\mathbf{A}^T)p_k(\mathbf{A})b = (\mathcal{W}_k^{\mathbf{A}})^2 b,$$

i.e., b is a **right singular vector** of the matrix $p_k(\mathbf{A})$.

Worst-case GMRES polynomials need not be unique

Theorem [Faber, Liesen, T. '13]

A worst-case GMRES polynomial for the Toh matrix

$$\mathbf{A} = \begin{bmatrix} 1 & \epsilon & & \\ & -1 & \epsilon^{-1} & \\ & & 1 & \epsilon \\ & & & -1 \end{bmatrix}, \qquad \epsilon > 0\,,$$

and $k = 3$ is **not unique**.

In particular, for this $\mathbf{A}$ and $k = 3$, we have shown that

- if $p(z) \in \pi_3$ is a worst-case polynomial $\Rightarrow p(-z)$ as well,
- if $p(z) \in \pi_3$ is a worst-case polynomial, then $p(z) \neq p(-z)$.

Outline

Ideal versus worst-case GMRES

- $\mathcal{W}_k^{\mathbf{A}} = \mathcal{I}_k^{\mathbf{A}}$ **iff** a worst-case initial vector b is a **maximal right singular vector** of $p_k(\mathbf{A})$.

  [Faber, Joubert, Knill, Manteuffel '96, T., Faber, Liesen, 2007]

- If $\Omega_k(p_*)$ is **convex** then $\mathcal{W}_k^{\mathbf{A}} = \mathcal{I}_k^{\mathbf{A}}$.

  [Faber, Joubert, Knill, Manteuffel '96]

- $\mathcal{W}_k^{\mathbf{A}} = \mathcal{I}_k^{\mathbf{A}}$ **iff**

$$\max_{v \in \mathbb{R}^n \setminus 0} \min_{c \in \mathbb{R}^k} F(c,v) = \min_{c \in \mathbb{R}^k} \max_{v \in \mathbb{R}^n \setminus 0} F(c,v) .$$

  where

$$F(c,v) \equiv \frac{\| v - K(v)c \|^2}{\| v \|^2} ,$$

$$K(v) \equiv [\mathbf{A}v, \mathbf{A}^2 v, \ldots, \mathbf{A}^k v].$$

  [Faber, Liesen, T. '13]

Summary

- Worst-case **initial vectors** satisfy the **cross equality**.
  This property is not sufficient for worst-case initial vectors.

- The **worst-case GMRES** problem is a nonlinear matrix approximation problem that can have **multiple solutions**.

- Worst-case **initial vector** b is a **right singular vector** of the corresponding GMRES matrix $p_k(\mathbf{A})$.

- $\mathcal{W}_k^{\mathbf{A}} = \mathcal{I}_k^{\mathbf{A}}$ **iff**
  b is a **maximal** right singular vector of $p_k(\mathbf{A})$.

- There are **many open questions** concerning the theory and the computation of $\mathcal{W}_k^{\mathbf{A}}$.

Related papers

- V. Faber, J. Liesen and P. Tichý, [Properties of worst-case GMRES, accepted to SIMAX (2013).]
- J. Liesen and P. Tichý, [On best approximations of polynomials in matrices in the matrix 2-norm, SIMAX, 31 (2009), pp. 853–863.]
- K. C. Toh, [GMRES vs. ideal GMRES, SIMAX, 18 (1997), pp. 30–36.]
- V. Faber, W. Joubert, E. Knill, and T. Manteuffel, [Minimal residual method stronger than polynomial preconditioning, SIMAX, 17 (1996), pp. 707–729.]
- A. Greenbaum and L. N. Trefethen, [GMRES/CR and Arnoldi/Lanczos as matrix approximation problems, SISC, 15 (1994), pp. 359–368.]

Thank you for your attention!