Characterization of worst-case GMRES

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joint work with

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GMRES

Consider a system of linear algebraic equations

$$\mathbf{A}x = b$$

$\mathbf{A} \in \mathbb{C}^{n \times n}$ is nonsingular, $b \in \mathbb{C}^n$.

For simplicity, $x_0 = \mathbf{0}$ and $\|b\| = 1$. GMRES computes x_k ,

$$x_k \in \mathcal{K}_k(\mathbf{A}, b)$$

such that

$$\|r_k\| = \|b - \mathbf{A}x_k\| = \min_{p \in \pi_k} \|p(\mathbf{A})\, b\| \,,$$

where $\pi_k = \{ \, p$ is a polynomial; $\deg(p) \le k; \; p(0) = 1\}$.

Bounding the GMRES residual norm

$$
\begin{aligned}
\|r_k\| &= \min_{p \in \pi_k} \|p(\mathbf{A})b\| && \text{(GMRES)} \\
&\le \max_{\|b\|=1} \min_{p \in \pi_k} \|p(\mathbf{A})b\| \equiv \psi_k(\mathbf{A}) && \text{(worst-case GMRES)} \\
&\le \min_{p \in \pi_k} \|p(\mathbf{A})\| \equiv \varphi_k(\mathbf{A}) && \text{(ideal GMRES)} \\
&\le 1\,.
\end{aligned}
$$

Questions

$$\|r_k\| \;\le\; \underbrace{\max_{\|b\|=1}\min_{p\in\pi_k} \|p(\mathbf{A})b\|}_{\psi_k(\mathbf{A})} \;\le\; \underbrace{\min_{p\in\pi_k} \|p(\mathbf{A})\|}_{\varphi_k(\mathbf{A})}$$

- Relationship between ideal and worst case GMRES?
- Existence and uniqueness of the solution?
- Characterization of solutions? Understanding?
- How to approximate ideal/worst-case quantities?

Normal matrices

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

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

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

- Is the solution unique? **Yes**
- Which (known) approximation problem is solved?

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

- How to approximate ideal/worst-case quantities?

[Greenbaum '79; Liesen, T. '04]

GMRES convergence for nonnormal matrices

Any Nonincreasing Convergence Curve Is Possible for GMRES

Theorem [Greenbaum, Pták, Strakoš '96]

Given a nonincreasing sequence

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

and a set of nonzero complex numbers $\{\lambda_1, \ldots, \lambda_n\}$, there exists a matrix $\mathbf{A}$ with eigenvalues $\lambda_1, \ldots, \lambda_n$ and a right-hand side b with $\|b\| = f(0)$ such that the residuals r_k of GMRES$(\mathbf{A}, b)$ satisfy

$$\|r_k\| = f(k), \qquad k = 1, 2, \ldots, n-1\,.$$

Nonnormal matrices – Toh's example

Worst-case GMRES can be very different from ideal GMRES!

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 $k = 3$,

$$0 \xleftarrow{\epsilon \to 0} \psi_k(\mathbf{A}) < \varphi_k(\mathbf{A}) = \frac{4}{5}\,.$$

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

Uniqueness

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

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

is unique. [Greenbaum, Trefethen '94]

Corrected proof and generalization to

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

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

Notation:

p_* . . . the kth ideal GMRES polynomial for $\mathbf{A}$,

$p_*(\mathbf{A})$ . . . the kth ideal GMRES matrix of $\mathbf{A}$.

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 the subspace $\mathbb{A}$.

In our case,

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

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]
$\rightarrow$ based on the Singer's theorem [Singer, 1970].

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]

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

Let p_* be the kth ideal GMRES polynomial of $\mathbf{A}$. If $\Omega_k(p_*)$ is convex then $\psi_k(\mathbf{A}) = \varphi_k(\mathbf{A})$.

[Faber, Joubert, Knill, Manteuffel '96]

Worst-case GMRES

For a given k, there exists a right hand side b such that

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

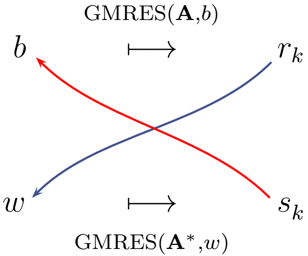
Theorem [Zavorin '02; Faber, T., Liesen '11]

Let $\mathbf{A} \in \mathbb{C}^{n\times n}$ be a nonsingular matrix. Then GMRES achieves the same worst-case behavior for $\mathbf{A}$ and $\mathbf{A}^*$ at every iteration.

- [Zavorin '02] $\rightarrow$ only for diagonalizable matrices.
- [Faber, T., Liesen '11] $\rightarrow$ for all nonsingular matrices.

Cross equality for worst-case GMRES vectors

Given: $\mathbf{A} \in \mathbb{C}^{n\times n}$, k, a worst-case starting vector b



$w \equiv \frac{r_k}{\|r_k\|}$

It holds that

$$\|s_k\| = \|r_k\| = \psi_k(\mathbf{A}), \qquad b = \frac{s_k}{\|s_k\|}.$$

[Zavorin '02; Faber, T., Liesen '11]

A new characterization of worst-case GMRES

Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be given. For $v \in \mathbb{R}^n$ and $c \in \mathbb{R}^k$ define

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

$K(v) \equiv [\mathbf{A}v, \mathbf{A}^2 v, \ldots, \mathbf{A}^k v]$. Denote $S \equiv \{u \in \mathbb{R}^n : \|u\| = 1\}$.

We want to characterize the solution of the problem

$$\max_{v \in S} \min_{c \in \mathbb{R}^k} f(c,v)\,. \tag{1}$$

Theorem [Faber, T., Liesen '11]

$\tilde{c} \in \mathbb{R}^k$ and $\tilde{v} \in S$ that solve the problem (1) satisfy

$$\frac{\partial F}{\partial c}(\tilde{c},\tilde{v}) = 0, \qquad \frac{\partial F}{\partial v}(\tilde{c},\tilde{v}) = 0,$$

i.e., $(\tilde{c},\tilde{v})$ is a stationary point of the function $F(c,v)$.

Consequences of the new characterization

Let $b \in S$ be a worst-case starting vector and

$$r_k = p_k(\mathbf{A})b, \qquad \|r_k\| = \psi_k(\mathbf{A})$$

the corresponding GMRES residual vector. Then

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

$$\psi_k(\mathbf{A})^2\, b \;=\; p_k(\mathbf{A}^T)p_k(\mathbf{A})\, b\,.$$

- p_k is also a worst-case GMRES polynomial for $\mathbf{A}^T$.
- $\psi_k(\mathbf{A}) = \varphi_k(\mathbf{A})$ **iff** a worst-case starting vector b is a maximal right singular vector of $p_k(\mathbf{A})$.
- $\psi_k(\mathbf{A}) = \varphi_k(\mathbf{A})$ **iff** the points $(\tilde{c}, \tilde{v}) \in \mathbb{R}^k \times S$ that solve

$$\max_{v \in S} \min_{c \in \mathbb{R}^k} f(c, v)\,.$$

  are also the saddle points of $f(c, v)$ in $\mathbb{R}^k \times S$.

[Faber, T., Liesen '11]

Worst-case GMRES polynomials need not be unique

Theorem [Faber, T., Liesen '11]

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 the step $k = 3$ is **not unique**.

Example: If $\varepsilon = 0.1$, then both

$$-39.9^{-1}(z - 1.181)(z + 0.939)(z + 35.96)$$

and

$$39.9^{-1}(z + 1.181)(z - 0.939)(z - 35.96)$$

are worst-case GMRES polynomials of $\mathbf{A}$.

Summary on worst-case GMRES

1. Worst-case starting vectors satisfy the cross equality.
2. Worst-case GMRES data $(\tilde{c}, \tilde{v})$ are stationary points of the function $F(c, v)$.
3. Worst-case starting vector b is a right singular vector of the corresponding GMRES matrix $p_k(\mathbf{A})$.
4. $\psi_k(\mathbf{A}) = \varphi_k(\mathbf{A})$ **iff** b is a maximal right singular vector of $p_k(\mathbf{A})$.
5. Worst-case GMRES polynomials need not be unique.

Thank you for your attention!

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