On Ideal and Worst-case GMRES

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GMRES, Worst-case GMRES and Ideal GMRES

$\mathbf{A}x = b$, $\mathbf{A} \in \mathbb{C}^{n\times n}$ is nonsingular, $b \in \mathbb{C}^n$,
$x_0 = \mathbf{0}$ and $\|b\| = 1$ for simplicity.
GMRES computes $x_k \in \mathcal{K}_k(\mathbf{A}, b)$ such that $r_k \equiv b - \mathbf{A}x_k$ satisfies

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

How well does ideal GMRES characterize the GMRES worst-case behavior?

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 $k = 3$,

$$0 \overset{\epsilon \longrightarrow 0}{\longleftarrow} \psi_k(\mathbf{A}) < \varphi_k(\mathbf{A}) = \frac{4}{5}\,.$$

[Toh '97, another example in Faber et al. '96]

Outline

1. Basic results concerning $\psi_k(A)$ and $\varphi_k(A)$
2. Theoretical tools
3. Cross equality for worst-case GMRES vectors
4. Results for a Jordan block

Basic results concerning $\psi_k(\mathbf{A})$ and $\varphi_k(\mathbf{A})$

Theorem [Joubert '94, Faber et al. '96]

Let $\mathbf{A} \in \mathbb{C}^{n\times n}$ be a matrix with minimal polynomial degree $d(\mathbf{A})$. Then the following statements hold:

1. $\psi_0(\mathbf{A}) = \varphi_0(\mathbf{A}) = 1$.
2. $\psi_k(\mathbf{A})$ and $\varphi_k(\mathbf{A})$ are both nonincreasing in k .
3. $0 < \psi_k(\mathbf{A}) \le \varphi_k(\mathbf{A})$ for $0 < k < d(\mathbf{A})$.
4. If $\mathbf{A}$ is nonsingular, then $\psi_k(\mathbf{A}) = \varphi_k(\mathbf{A}) = 0$ for all $k \ge d(\mathbf{A})$.
5. If $\mathbf{A}$ is singular, then $\psi_k(\mathbf{A}) = \varphi_k(\mathbf{A}) = 1$ for all $k \ge 0$.

Basic results concerning $\psi_k(\mathbf{A})$ and $\varphi_k(\mathbf{A})$

When does it hold that

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

[Greenbaum & Gurvits '94, Joubert '94]:

- if $\mathbf{A}$ is **normal**,
- for $k = 1$.

Theoretical tools

Ideal GMRES polynomial and ideal GMRES matrix

Definition

The polynomial $p_* \in \pi_k$ is called the kth ideal GMRES polynomial of $\mathbf{A} \in \mathbb{C}^{n \times n}$, if it satisfies

$$\|p_*(\mathbf{A})\| = \min_{p \in \pi_k} \|p(\mathbf{A})\| .$$

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

Existence and uniqueness of p_* proved by

[Greenbaum & Trefethen '94]

Simple maximal singular value of $p_*(\mathbf{A})$

Lemma [Greenbaum & Gurvits '94]

If $p_*(\mathbf{A})$ has a simple max. singular value then $\psi_k(\mathbf{A}) = \varphi_k(\mathbf{A})$.

Is this situation frequent or rare for nonnormal matrices?

Normal case: $\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^*$, $\mathbf{Q}^*\mathbf{Q} = \mathbf{I}$

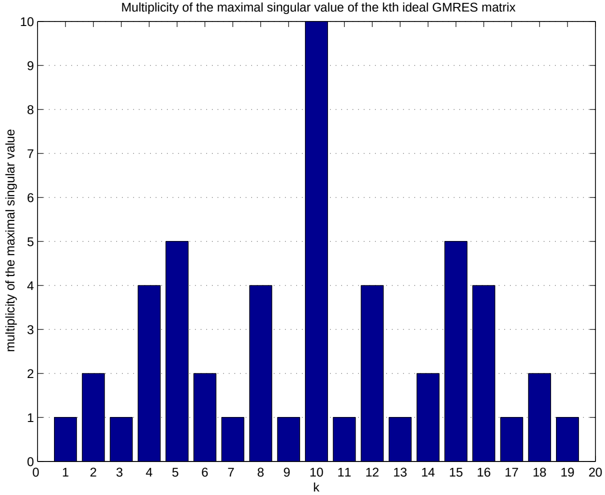
$$\min_{p\in\pi_k} \|p(\mathbf{A})\| = \min_{p\in\pi_k} \|\mathbf{Q}p(\mathbf{\Lambda})\mathbf{Q}^*\| = \min_{p\in\pi_k} \max_{\lambda_i} |p(\lambda_i)| .$$

$p_*(\xi)$ attains its maximum value on at least $k+1$ eigenvalues, i.e. **the multiplicity** of max. sing. value of $p_*(\mathbf{A})$ **is at least** $k+1$.

Multiplicity of the maximal singular value of $p_*(\mathbf{J}_\lambda)$

computed using the software SDPT3 by Toh

Jordan block $\mathbf{J}_\lambda$, $\lambda = 1$, $n = 20$.



Characterization of the situation $\psi_k(\mathbf{A}) = \varphi_k(\mathbf{A})$

Let $\Sigma(\mathbf{B})$ be the span of maximal right singular vectors of $\mathbf{B}$.

Lemma [T & Liesen & Faber '07, Faber et al. '96]

Suppose that a nonsingular matrix $\mathbf{A}$ and a positive integer $k < d(\mathbf{A})$ are given.

Then $\psi_k(\mathbf{A}) = \varphi_k(\mathbf{A})$ **if and only if** there exist a polynomial $q \in \pi_k$ and a unit norm vector $b \in \Sigma(q(\mathbf{A}))$, such that

$$q(\mathbf{A})b \perp \mathbf{A}\mathcal{K}_k(\mathbf{A}, b)\,.$$

If such q and b exist, then $q = p_*$.

k-dimensional generalized field of values of $\mathbf{A}$

$$F_k(\mathbf{A}) \equiv \left\{ \begin{pmatrix} v^*\mathbf{A}v \\ \vdots \\ v^*\mathbf{A}^k v \end{pmatrix} \in \mathbb{C}^k \ : v^*v = 1 \right\}$$

Theorem [Faber et al. '96]

For a nonsingular matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$ the following statements hold:

- $\psi_k(\mathbf{A}) = 1 \iff \mathbf{0} \in F_k(\mathbf{A})$,
- $\varphi_k(\mathbf{A}) = 1 \iff \mathbf{0} \in \mathrm{cvx}[\,F_k(\mathbf{A})\,]$.

If $F_k(\mathbf{A})$ is convex then

$$\psi_k(\mathbf{A}) = 1 \quad \iff \quad \varphi_k(\mathbf{A}) = 1\,.$$

A possible connection

Using $F_k(\mathbf{A})$, it is possible to define two sets

$$
\begin{aligned}
\mathscr{G}_k(\mathbf{A}) &= \{\xi \in \mathbb{C} \;:\; \mathbf{0} \in F_k(\mathbf{A} - \xi\mathbf{I})\} \\
\mathscr{H}_k(\mathbf{A}) &= \{\xi \in \mathbb{C} \;:\; \mathbf{0} \in \mathrm{cvx}[\, F_k(\mathbf{A} - \xi\mathbf{I})\,]\}.
\end{aligned}
$$

[Nevanlinna '93, Greenbaum '02]

Equivalent definitions:

$$
\begin{aligned}
\mathscr{G}_k(\mathbf{A}) &= \{\xi \in \mathbb{C} \;:\; \exists b \; \forall p \in \mathcal{P}_k \; |p(\xi)| \;\leq\; \|p(\mathbf{A})b\| \,\}, \\
\mathscr{H}_k(\mathbf{A}) &= \{\xi \in \mathbb{C} \;:\; \qquad \forall p \in \mathcal{P}_k \; |p(\xi)| \;\leq\; \|p(\mathbf{A})\| \,\},
\end{aligned}
$$

[Greenbaum '02, T. & Faber & Liesen '08]

where $\mathcal{P}_k$ denotes the set of polynomials of degree k or less.

There might be a connection between convexity of $F_k(\mathbf{A})$ and the relation between ideal and worst-case GMRES.

Worst-case GMRES and the cross equality

Worst-case GMRES

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

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

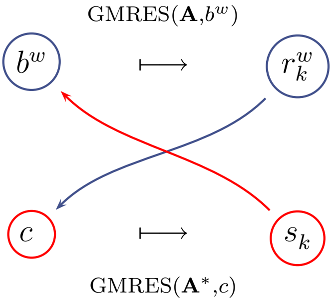
Theorem [Zavorin '02, T. & Faber & Liesen '08]

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
- T '07 $\rightarrow$ for all nonsingular matrices

Cross equality for worst-case GMRES vectors

Given: $\mathbf{A} \in \mathbb{C}^{n\times n}$, k



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

It holds that

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

[Zavorin '02, T. & Faber & Liesen '08]

Results for a Jordan block

Results for a Jordan block $\mathbf{J}_\lambda$

Consider an $n \times n$ Jordan block $\mathbf{J}_\lambda$, $\lambda \in \mathbb{C}$,

$\varrho_{k,n}$ ... the radius of the polynomial numerical hull $\mathscr{H}_k(\mathbf{J}_\lambda)$

$$\frac{1}{2} \leq \varrho_{k,n} < 1 .$$

$\psi_k(\mathbf{J}_\lambda) = \varphi_k(\mathbf{J}_\lambda)$ if

- $|\lambda| \leq \varrho_{k,n}$,
- $|\lambda| \geq \varrho_{k,n-k}^{-1}$ and $k < n/2$,
- k divides n ,
- $k \geq n/2$, $n-k$ divides n and $|\lambda| \geq 1$.

[T. & Liesen & Faber '07, Greenbaum '04]

Conclusions

1. The relation between ideal and worst-case GMRES for nonnormal matrices is not well understood.

2. There might be a connection between the convexity of the generalized field of values and the relation between ideal and worst-case GMRES.

3. Worst-case GMRES achieves the same convergence behavior for $\mathbf{A}$ and $\mathbf{A}^*$. Worst-case GMRES vectors satisfy a cross equality.

4. Based on numerical observation and theoretical results we conjecture that **ideal GMRES = worst-case GMRES** for a Jordan block.

Thank you for your attention!

More details can be found in

TICHÝ, P., LIESEN, J. AND FABER, V., *On worst-case GMRES, ideal GMRES, and the polynomial numerical hull of a Jordan block*, submitted to Electronic Transactions on Numerical Analysis (ETNA), March 2007.

http://www.cs.cas.cz/~tichy