# Ideal GMRES and polynomial numerical hull for a Jordan block

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joint work with

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# GMRES and Ideal GMRES

Consider a system $\mathbf{A}x = b$, $\mathbf{A} \in \mathbb{R}^{n \times n}$ is nonsingular, $b \in \mathbb{R}^n$.
GMRES computes iterates $x_k \in x_0 + \mathcal{K}_k(\mathbf{A}, r_0)$ such that

$$\|r_k\| = \|b - \mathbf{A}x_k\| = \min_{p \in \pi_k} \|p(\mathbf{A})\, r_0\| .$$

For simplicity assume $x_0 = 0$ and $\|b\| = 1$. Then

$$\|r_k\| = \min_{p \in \pi_k} \|p(\mathbf{A})b\| \le \min_{p \in \pi_k} \|p(\mathbf{A})\| \qquad \text{(ideal GMRES)}$$

It can happen that for all $b$

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

[Faber et al. '96, Toh '97]

# Toh's example

Ideal GMRES can be very different from worst-case 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 $k = 3$, and for all $b$, $\|b\| = 1$,

$$0 \overset{\epsilon \longrightarrow 0}{\longleftarrow} \|r_k\| < \min_{p \in \pi_k} \|p(\mathbf{A})\| = \frac{4}{5}\,.$$

[Toh '97]

# Outline

1. Known results about ideal GMRES
2. Ideal GMRES for a Jordan block
3. Polynomial numerical hull
4. Quality of the bound based on polynomial numerical hull

# Ideal GMRES polynomial and ideal GMRES matrix

**Definition**

The polynomial $\varphi_k \in \pi_k$ is called the $k$th ideal GMRES polynomial of $\mathbf{A} \in \mathbb{R}^{n \times n}$, if it satisfies

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

We call the matrix $\varphi_k(\mathbf{A})$ the $k$th ideal GMRES matrix of $\mathbf{A}$.

Existence and uniqueness of $\varphi_k$ proved by

[Greenbaum & Trefethen '94]

# Known results about ideal GMRES

When does it hold that

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

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

- if $\mathbf{A}$ is normal,
- for $k = 1$,
- if $\varphi_k(\mathbf{A})$ has a simple maximal singular value.

[Faber et al. '96]:

Let $\mathbf{A}$ be $n$ by $n$ triangular Toeplitz matrix. Then

$$\max_{\|b\|=1} \min_{p\in\pi_k} \|p(\mathbf{A})b\| = 1 \quad \Longleftrightarrow \quad \min_{p\in\pi_k} \|p(\mathbf{A})\| = 1\,.$$

# A model problem - Jordan block

Let $\lambda > 0$. Consider an $n$ by $n$ Jordan block

$$\mathbf{J}_\lambda = \begin{bmatrix} \lambda & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

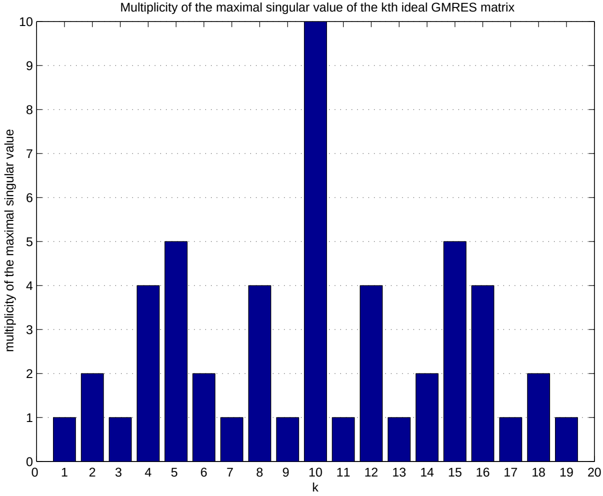
## Open question

- Does ideal GMRES coincide with worst-case GMRES?

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

computed using the software SDPT3 by Toh

$\lambda = 1$, $n = 20$.



# Observation

- If $k$ and $n$ are relatively prime, $\varphi_k(\mathbf{J}_\lambda)$ has a simple maximal singular value (i.e. ideal GMRES $=$ worst-case GMRES).

- Let $d$ be the greatest common divisor of $k$ and $n$. Then the maximal singular value of $\varphi_k(\mathbf{J}_\lambda)$ has multiplicity $d$.

## Theorem

[Tichý & Liesen '06]

Let $d$ be the greatest common divisor of $n$ and $k$. Let $\lambda > 0$ be given and define

$$\ell = \frac{k}{d}, \quad m = \frac{n}{d}, \quad \mu = \lambda^d.$$

If

$$\max_{\|b\|=1} \min_{p \in \pi_\ell} \|p(\mathbf{J}_\mu)b\| = \min_{p \in \pi_\ell} \|p(\mathbf{J}_\mu)\|$$

where $\mathbf{J}_\mu \in \mathbb{R}^{m \times m}$, then

$$\max_{\|b\|=1} \min_{p \in \pi_k} \|p(\mathbf{J}_\lambda)b\| = \min_{p \in \pi_k} \|p(\mathbf{J}_\lambda)\|$$

where $\mathbf{J}_\lambda \in \mathbb{R}^{n \times n}$.

# Two special cases

1. Consider the step $k$ such that $k$ divides $n$, i.e. $d = k$,

$$\ell = 1, \quad m = \frac{n}{k}, \quad \mu = \lambda^k.$$

2. Consider the step $n - k$ such that $k$ divides $n$, i.e. $d = k$,

$$\ell = m - 1, \quad m = \frac{n}{k}, \quad \mu = \lambda^k.$$

In both cases, the assumption of the previous Theorem

$$\max_{\|b\|=1} \min_{p \in \pi_\ell} \|p(\mathbf{J}_\mu) b\| = \min_{p \in \pi_\ell} \|p(\mathbf{J}_\mu)\|$$

is satisfied ($\lambda \geq 1$).

[Tichý & Liesen '06]

# Some results for the Jordan block $\mathbf{J}_\lambda$

Let $k$ divide $n$.

- At steps $k$ and $n-k$ $(\lambda \geq 1)$

$$\text{worst-case GMRES} = \text{ideal GMRES}\,.$$

- Ideal GMRES polynomial $\varphi_k$ :

$$\varphi_k(z) = \bullet \;+\; \bullet\; (\lambda - z)^k\,.$$

- Let $\lambda \geq 1$ . Then

$$\min_{p \in \pi_{n-k}} \|p(\mathbf{J}_\lambda)\| = \frac{1}{\lambda^{n-k}} \left[ \sum_{i=0}^{n/k-1} \lambda^{-2ki} 4^{-2i} \binom{2i}{i}^2 \right]^{-1}.$$

[T. & Liesen '06]

# Polynomial numerical hulls for a Jordan block

# Polynomial numerical hull

**Definition**

Let $\mathbf{A}$ be $n$ by $n$ matrix. Polynomial numerical hull of degree $k$ is a set in the complex plane defined by

$$\mathcal{H}_k \equiv \{z \in \mathbb{C} : \; |p(z)| \leq \|p(\mathbf{A})\| \;\; \forall \, p \in \mathcal{P}_k\},$$

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

The set $\mathcal{H}_k$ provides a lower bound

$$\min_{p \in \pi_k} \max_{z \in \mathcal{H}_k} |p(z)| \; \leq \; \min_{p \in \pi_k} \|p(\mathbf{A})\| \, .$$

[Greenbaum '02]

# $\mathcal{H}_k$ for a Jordan block $\mathbf{J}_\lambda$

$\mathcal{H}_k$ is a circle around $\lambda$ with a radius $\varrho_{k,n}$,

$1 > \varrho_{1,n} > \cdots > \varrho_{n-1,n} > 0$,

$\varrho_{1,n}$ and $\varrho_{n-1,n}$ are known,

[Faber & Greenbaum & Marshall '03]

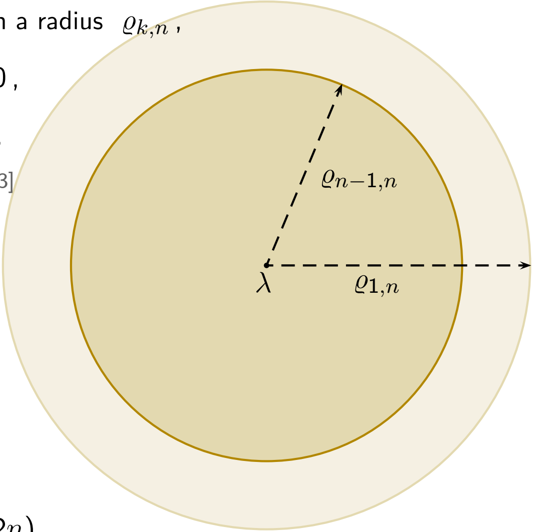
$$\varrho_{1,n} = \cos\left(\frac{\pi}{n+1}\right).$$

if $n$ is even,

$\varrho_{n-1,n}$ is the positive root of

$$2\varrho^n + \varrho - 1 = 0.$$

$$\varrho_{n-1,n} \geq 1 - \frac{\log(2n)}{n}$$



# Radius of polynomial numerical hull for $\mathbf{J}_\lambda$

**Theorem**

Let $d$ be the greatest common divisor of $n$ and $k$ and define

$$\ell = \frac{k}{d}, \quad m = \frac{n}{d}.$$

Then

$$\varrho_{k,n} = \varrho_{\ell,m}^{1/d}.$$

Consider $k$ such that $k$ divides $n$. Then

$$\varrho_{k,n} = \left[\cos\left(\frac{\pi}{m+1}\right)\right]^{\frac{1}{k}}, \qquad \varrho_{n-k,n} = \varrho_{m-1,m}^{\frac{1}{k}}.$$

[T. & Liesen '06]

# Bound based on polynomial numerical hull

$$\min_{p\in\pi_k} \max_{z\in\mathcal{H}_k} |p(z)| \;\le\; \min_{p\in\pi_k} \|p(\mathbf{J}_\lambda)\| \,.$$

For a Jordan block $\mathbf{J}_\lambda$

$$\lambda^{-k}\,\varrho_{k,n}^{k} \le \min_{p\in\pi_k} \|p(\mathbf{J}_\lambda)\| \le \lambda^{-k}\,.$$

[Greenbaum '04]

If $k$ divides $n$, then

$$\lambda^{-k}\cos\left(\frac{\pi}{\frac{n}{k}+1}\right) \;\le\; \min_{p\in\pi_k} \|p(\mathbf{J}_\lambda)\| \;\le\; \lambda^{-k}\,.$$

In particular, if $n$ is even, then it holds that for all $k \le n/2$

$$\lambda^{-k}\,\frac{1}{2} \;\le\; \min_{p\in\pi_k} \|p(\mathbf{J}_\lambda)\| \;\le\; \lambda^{-k}\,.$$

[T. & Liesen '06]

# Quality of the bound in later iterations

$$\lambda^{-k}\,\varrho_{k,n}^{k} \;\le\; \min_{p\in\pi_k} \|p(\mathbf{J}_\lambda)\|\,.$$

For simplicity, we concentrate on step $n-1$ and $\lambda = 1$.

From our results it follows that

$$\min_{p\in\pi_{n-1}} \|p(\mathbf{J}_\lambda)\| \;\sim\; \frac{1}{1+\log(n)}\,.$$

Using the bounds on $\varrho_{n-1,n}$ one can show that, for $n > 2$

$$\frac{1}{2n} \;\le\; \varrho_{n-1,n}^{n-1} \;\le\; \frac{\log(n)}{2n}.$$

Ideal GMRES converges slower that the lower bound predicts.

# Conclusions for the Jordan block $\mathbf{J}_\lambda$

1. Based on numerical observation for $k$ and $n$ being relatively prime, and based on our theorem we can conclude that **ideal GMRES = worst-case GMRES** for a Jordan block.

2. Theoretically, we were able to prove this only at steps $k$ and $n-k$ such that $k$ divides $n$.

3. There is a relation among radii of polynomial numerical hulls.

4. The bound based on polynomial numerical hull is tight up to the step $n/2$. In later iterations, this bound underestimates the ideal GMRES convergence (for $\lambda \geq 1$).

# Thank you for your attention!

**More details can be found in**

Tichý, P. and Liesen, J., *GMRES convergence and the polynomial numerical hull for a Jordan block*, submitted to Linear Algebra and its Applications.

http://www.math.tu-berlin.de/~tichy