On ideal GMRES for a Jordan Block

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joint work with

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A system of linear algebraic equations

Consider a system of linear algebraic equations

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

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

- How to construct an approximation to the solution?

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- How to construct an approximation to the solution?

Projection methods $\longmapsto$ Given x_0. Find an approximation x_i,

$$x_i \in x_0 + \mathcal{S}_i \qquad \texttt{such that} \qquad r_i \perp \mathcal{C}_i,$$

where $r_i = b - \mathbf{A}x_i$.

GMRES - a Krylov subspace method

Krylov subspace methods $\mapsto$ $\mathcal{S}_i \equiv \mathcal{K}_i(\mathbf{A}, r_0) \equiv \text{span}\,\{r_0, \cdots, \mathbf{A}^{i-1} r_0\}$.

Given $x_0 \in \mathbb{R}^n$, $r_0 = b - \mathbf{A} x_0$. GMRES computes iterates x_i such that

$$x_i \in x_0 + \underbrace{\mathcal{K}_i(\mathbf{A}, r_0)}_{\mathcal{S}_i} \quad \texttt{and} \quad r_i \perp \underbrace{\mathbf{A}\mathcal{K}_i(\mathbf{A}, r_0)}_{\mathcal{C}_i}.$$

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$$\updownarrow \quad r_i = b - \mathbf{A}x_i$$

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$$r_i = b - \mathbf{A}x_i$$

$$r_i \in r_0 + \mathbf{A}\mathcal{K}_i(\mathbf{A}, r_0) \qquad \|r_i\| = \min_{p \in \pi_i} \|p(\mathbf{A})\, r_0\|\,,$$

where $\pi_i \equiv \{\, p$ is a polynomial; $\deg(p) \leq i;\ p(0) = 1\}\,.$

The GMRES problem

GMRES constructs approximations $x_i \in x_0 + \mathcal{K}_i(\mathbf{A}, r_0)$ to the solution x of the system $\mathbf{A}x = b$ such that

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- **Our aim:**

Description and understanding of this minimization process.

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- **Our aim:**

Description and understanding of this minimization process.

- **Considered classes of matrices in this talk:**

Normal matrices and Jordan blocks.

- **For simplicity:**

Let $x_0 = 0$, i.e. $r_0 = b - Ax_0 = b$ and let $\|b\| = 1$.

Outline

1. Introduction
2. Bounds and Questions
3. GMRES for normal matrices
4. GMRES for nonnormal matrices
5. GMRES for a Jordan block
6. Polynomial numerical hull for a Jordan block
7. Conclusions

Bounds and Questions

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

$$\|r_i\| \quad = \quad \min_{p \in \pi_i} \|p(\mathbf{A})b\| \qquad \text{(GMRES)}$$

Bounds and Questions

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

$$\begin{aligned} \|r_i\| &= \min_{p \in \pi_i} \|p(\mathbf{A})b\| && \text{(GMRES)} \\ &\leq \max_{\|b\|=1} \min_{p \in \pi_i} \|p(\mathbf{A})b\| && \text{(worst-case GMRES)} \end{aligned}$$

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&\leq \min_{p \in \pi_i} \|p(\mathbf{A})\| && \text{(ideal GMRES).}
\end{aligned}
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Our questions:

- When ideal GMRES = worst-case GMRES?
- How to evaluate or estimate the ideal GMRES bound?
- Which b yields the worst-case residual norm?
- Relevance of the bound?

GMRES for normal matrices

Let $\mathbf{A}$ be nonsingular and normal,

$$\mathbf{A} \ = \ \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^H, \quad \mathbf{Q}^H\mathbf{Q} = \mathbf{I}, \quad \mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_n).$$

Then

worst-case GMRES $=$ ideal GMRES .

[Greenbaum & Gurvits '94, Joubert '94]

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Moreover

$$\min_{p \in \pi_i} \|p(\mathbf{A})\| = \min_{p \in \pi_i} \max_{\lambda_j \in L} |p(\lambda_j)|$$

where $L \equiv \{\lambda_1, \ldots, \lambda_n\}$.

Evaluation of the bound ($\mathbf{A}$ normal)

Conjecture: There exists a subset of $i+1$ (distinct) eigenvalues $\{\mu_1, \ldots, \mu_{i+1}\} \subseteq \{\lambda_1, \ldots, \lambda_n\}$ such that

$$\min_{p \in \pi_n} \max_{\lambda_j \in L} |p(\lambda_j)| \approx \left(\sum_{j=1}^{i+1} \prod_{\substack{k=1 \\ k \neq j}}^{i+1} \frac{|\mu_k|}{|\mu_k - \mu_j|} \right)^{-1} . \tag{1}$$

- **real eigenvalues** : [Liesen & T. '04, Greenbaum '79]

  (1) is equality (proved),

- **complex eigenvalues** : [Liesen & T. '04]

  (1) is equality up to a factor between 1 and $\frac{4}{\pi}$ (conjecture).

Nonnormal matrices $\mathbf{A}$

What is the GMRES behavior for nonnormal matrices?

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

- Eigenvalues may have nothing to do with the convergence behavior.

  [Arioli, Greenbaum, Pták, Strakoš 1992–2000]

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

  [Faber & Joubert & Knill & Manteuffel ’96, Toh ’97]

Toh's example

Worst-case GMRES can be very different from ideal GMRES for nonnormal $\mathbf{A}$!

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 $i = 3$,

$$\frac{\max_{\|b\|=1} \min_{p \in \pi_i} \|p(\mathbf{A})b\|}{\min_{p \in \pi_i} \|p(\mathbf{A})\|} \rightarrow 0 \qquad \text{as} \qquad \epsilon \rightarrow 0.$$

[Toh '97]

Toh's matrix

$$\mathbf{A} = \mathbf{V}\mathbf{J}\mathbf{V}^{-1},$$

where

$$\mathbf{J} = \begin{bmatrix} 1 & 1 & & \\ & 1 & & \\ & & -1 & 1 \\ & & & -1 \end{bmatrix}, \qquad \mathbf{V} = \frac{1}{4}\begin{bmatrix} \epsilon & \epsilon & \epsilon & -\epsilon \\ -2 & -1 & 0 & 1 \\ 0 & -2\epsilon & 0 & 2\epsilon \\ 0 & 4 & 0 & 0 \end{bmatrix},$$

and

$$\kappa(\mathbf{V}) \sim \frac{4}{\epsilon}\,.$$

GMRES for a Jordan block

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

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

What is the situation for a Jordan block? Does it hold

worst-case GMRES = ideal GMRES?

How to describe ideal GMRES convergence?

Known result

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

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

[Faber & Joubert & Knill & Manteuffel '96]

What is the situation if $\min_{p\in\pi_i} \|p(\mathbf{A})\| < 1$?

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What is the situation if $\min_{p \in \pi_i} \|p(\mathbf{A})\| < 1$?

Definition: The polynomial $\varphi_i \in \pi_i$ is called the ith ideal GMRES polynomial of $\mathbf{A} \in \mathbb{R}^{n \times n}$, if it satisfies

$$\|\varphi_i(\mathbf{A})\| = \min_{p \in \pi_i} \|p(\mathbf{A})\| \,.$$

[Existence and uniqueness of $\varphi_i \rightarrow$ Greenbaum & Trefethen '94]

We call the matrix $\varphi_i(\mathbf{A})$ the ith ideal GMRES matrix.

Numerical Experiment

The MATLAB-software SDPT3 by Toh $\rightarrow$ we can compute ideal GMRES matrices!

Let $\mathbf{A} = \mathbf{J}_1 \in \mathbb{R}^{8\times 8}$. We display the structure of $\varphi_i(\mathbf{J}_1)$.

$\bullet$ ... nonzero entries, $\circ$ ... zero entries (or almost)

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$$\varphi_1(\mathbf{J}_1) = \begin{bmatrix} \bullet & \bullet & & & & & & \\ & \bullet & \bullet & & & & & \\ & & \bullet & \bullet & & & & \\ & & & \bullet & \bullet & & & \\ & & & & \bullet & \bullet & & \\ & & & & & \bullet & \bullet & \\ & & & & & & \bullet & \bullet \\ & & & & & & & \bullet \end{bmatrix},$$

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$$\varphi_2(\mathbf{J}_1) = \begin{bmatrix} \bullet & \circ & \bullet & & & & & \\ & \bullet & \circ & \bullet & & & & \\ & & \bullet & \circ & \bullet & & & \\ & & & \bullet & \circ & \bullet & & \\ & & & & \bullet & \circ & \bullet & \\ & & & & & \bullet & \circ & \bullet \\ & & & & & & \bullet & \circ \\ & & & & & & & \bullet \end{bmatrix},$$

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$$\varphi_3(\mathbf{J}_1) = \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & & & & \\ & \bullet & \bullet & \bullet & \bullet & & & \\ & & \bullet & \bullet & \bullet & \bullet & & \\ & & & \bullet & \bullet & \bullet & \bullet & \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \\ & & & & & & & \bullet \end{bmatrix},$$

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$$\varphi_4(\mathbf{J}_1) = \begin{bmatrix} \bullet & \circ & \circ & \circ & \bullet & & & \\ & \bullet & \circ & \circ & \circ & \bullet & & \\ & & \bullet & \circ & \circ & \circ & \bullet & \\ & & & \bullet & \circ & \circ & \circ & \bullet \\ & & & & \bullet & \circ & \circ & \circ \\ & & & & & \bullet & \circ & \circ \\ & & & & & & \bullet & \circ \\ & & & & & & & \bullet \end{bmatrix},$$

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$$\varphi_5(\mathbf{J}_1) = \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & & \\ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \\ & & & & & & & \bullet \end{bmatrix},$$

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$$\varphi_6(\mathbf{J}_1) = \begin{bmatrix} \bullet & \circ & \bullet & \circ & \bullet & \circ & \bullet & \\ & \bullet & \circ & \bullet & \circ & \bullet & \circ & \bullet \\ & & \bullet & \circ & \bullet & \circ & \bullet & \circ \\ & & & \bullet & \circ & \bullet & \circ & \bullet \\ & & & & \bullet & \circ & \bullet & \circ \\ & & & & & \bullet & \circ & \bullet \\ & & & & & & \bullet & \circ \\ & & & & & & & \bullet \end{bmatrix},$$

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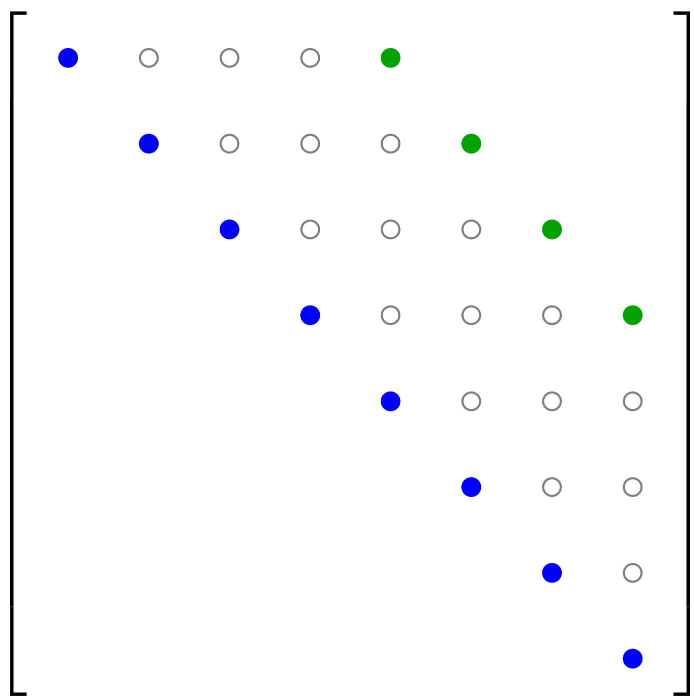
Structure behind ideal GMRES convergence

There is a structure behind the ideal GMRES convergence.

The structure of $\varphi_i(J_1)$ depends on relation between i and n.

E.g. if i divides n, $m \equiv n/i$, then $\varphi_i(\mathbf{J}_1) =$



(in general, the greatest common divisor of i and n plays an important role)

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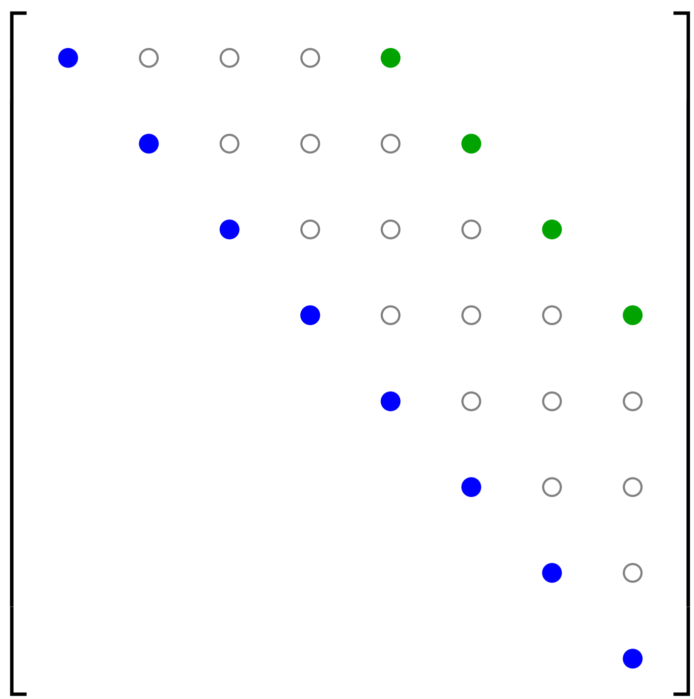

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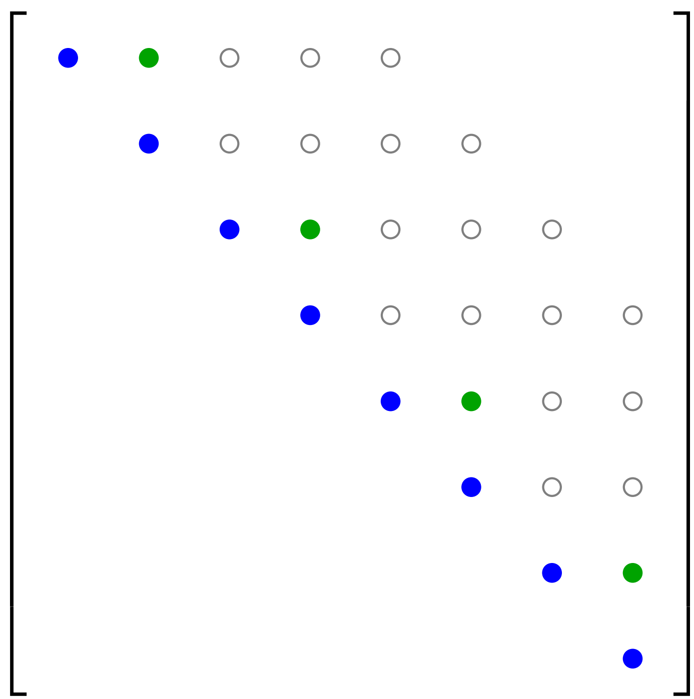

(in general, the greatest common divisor of i and n plays an important role)

Lemma

From [Greenbaum & Gurvits ’94] it follows:

Lemma: Let $A \in \mathbb{R}^{n \times n}$. The following statements are equivalent:

1. The ith worst-case GMRES approximation $=$ the ith ideal GMRES approx.
2. There exists a unit norm vector b and a polynomial $\psi \in \pi_i$, such that

$$\psi(\mathbf{A})b \perp \mathbf{A}\mathcal{K}_i(\mathbf{A}, b),$$

   and b lies in the span of right singular vectors of $\psi(A)$ corresponding to its maximal singular value.

In addition, if 2. holds, then $\psi = \varphi_i$.

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In addition, if 2. holds, then $\psi = \varphi_i$.

Using the orthogonal transformation and this lemma **we proved:** If i divides n then

ideal GMRES $=$ worst-case GMRES

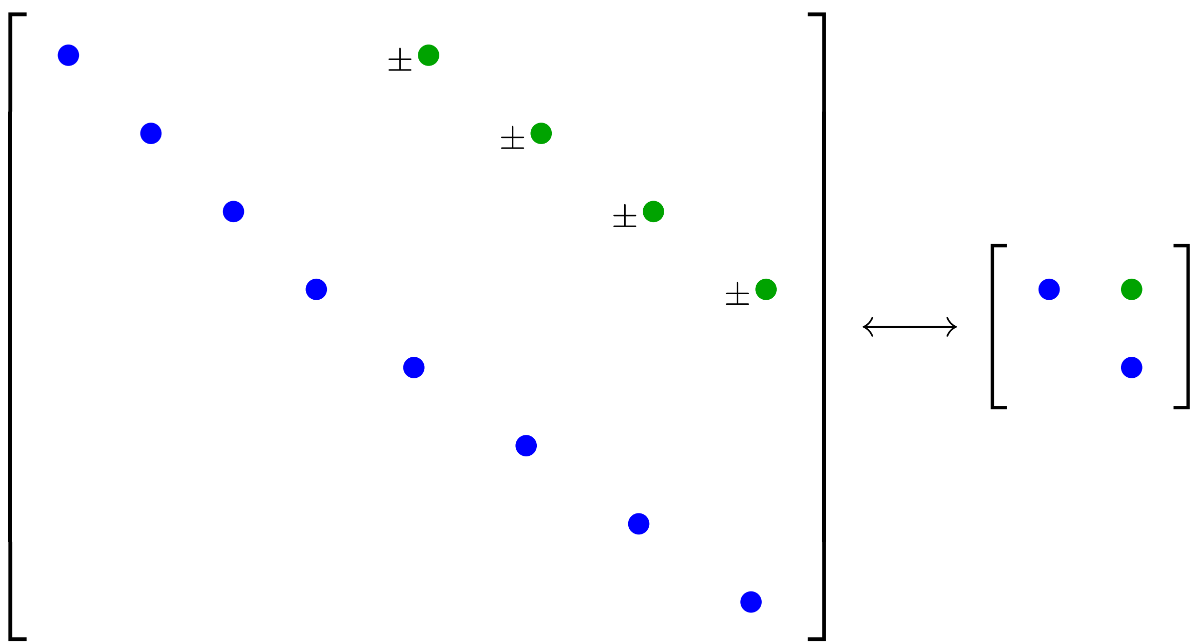
for a Jordan block $\mathbf{J}_\lambda$. [T.& Liesen '05]

In more details

We proved: There is a strong connection between

the i**th step** of ideal GMRES for $\mathbf{J}_\lambda \in \mathbb{R}^{n\times n}$ $\longleftrightarrow$ the 1**st step** of ideal GMRES for $\mathbf{J}_{\lambda^i} \in \mathbb{R}^{m\times m}$

where $m = n/i$. Let e.g. n is even, $i = n/2$, $m = 2$.

$\varphi_i(\mathbf{J}_\lambda) =$  $= \varphi_1(\mathbf{J}_{\lambda^i})$.

Interesting details (i divides n)

Ideal polynomial φ_i: [T.& Liesen ’05]

$$\varphi_i(z) = \bullet \; + \; \bullet \; (\lambda - z)^i.$$

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Let $\lambda = 1$. Based on numerical experiments we know that

$$\varphi_i(z) = \frac{m}{2m+1} + \frac{m+1}{2m+1}(1 - z)^i ,$$

where $m = n/i$, but we were unable to determine $\|\varphi_i(\mathbf{J}_1)\|$.

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Ideal polynomial φ_i: [T.& Liesen '05]

$$\varphi_i(z) = \color{blue}{\bullet} \;+\; \color{green}{\bullet}\; (\lambda - z)^i .$$

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where $m = n/i$, but we were unable to determine $\|\varphi_i(\mathbf{J}_1)\|$.

Let e.g. n be even, $i = n/2$, and let $\lambda^i \geq \frac{1}{2}$. Then

$$\|\varphi_i(\mathbf{J}_\lambda)\| = \frac{4\lambda^i}{4\lambda^{2i}+1} .$$

Estimating the ideal GMRES approximation

How to estimate the ideal GMRES approximation $\min_{p\in\pi_i} \|p(\mathbf{A})\|$?

We try to determine sets $\Omega \subset \mathbb{C}$ that are somehow associated with $\mathbf{A}$, and satisfy

$$\min_{p\in\pi_i} \|p(\mathbf{A})\| \sim \min_{p\in\pi_i} \max_{z\in\Omega} |p(z)|.$$

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- If $\mathbf{A}$ is normal then $\Omega = L$.
- If $\mathbf{A}$ is nonnormal then there are several possibilities how to choose Ω, e.g.
  - ε-pseudospectrum of $\mathbf{A}$, [Trefethen]
  - polynomial numerical hull of $\mathbf{A}$. [Nevanlinna, Greenbaum]

Polynomial numerical hull

Definition: Let $\mathbf{A}$ be n by n matrix. Polynomial numerical hull of degree i is a sets $\mathcal{H}_i$ in the complex plane defined as

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

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

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

The set $\mathcal{H}_i$ provides a lower bound on the ideal GMRES approximation

$$\min_{p \in \pi_i} \|p(\mathbf{A})\| \geq \min_{p \in \pi_i} \max_{z \in \mathcal{H}_i} |p(z)|.$$

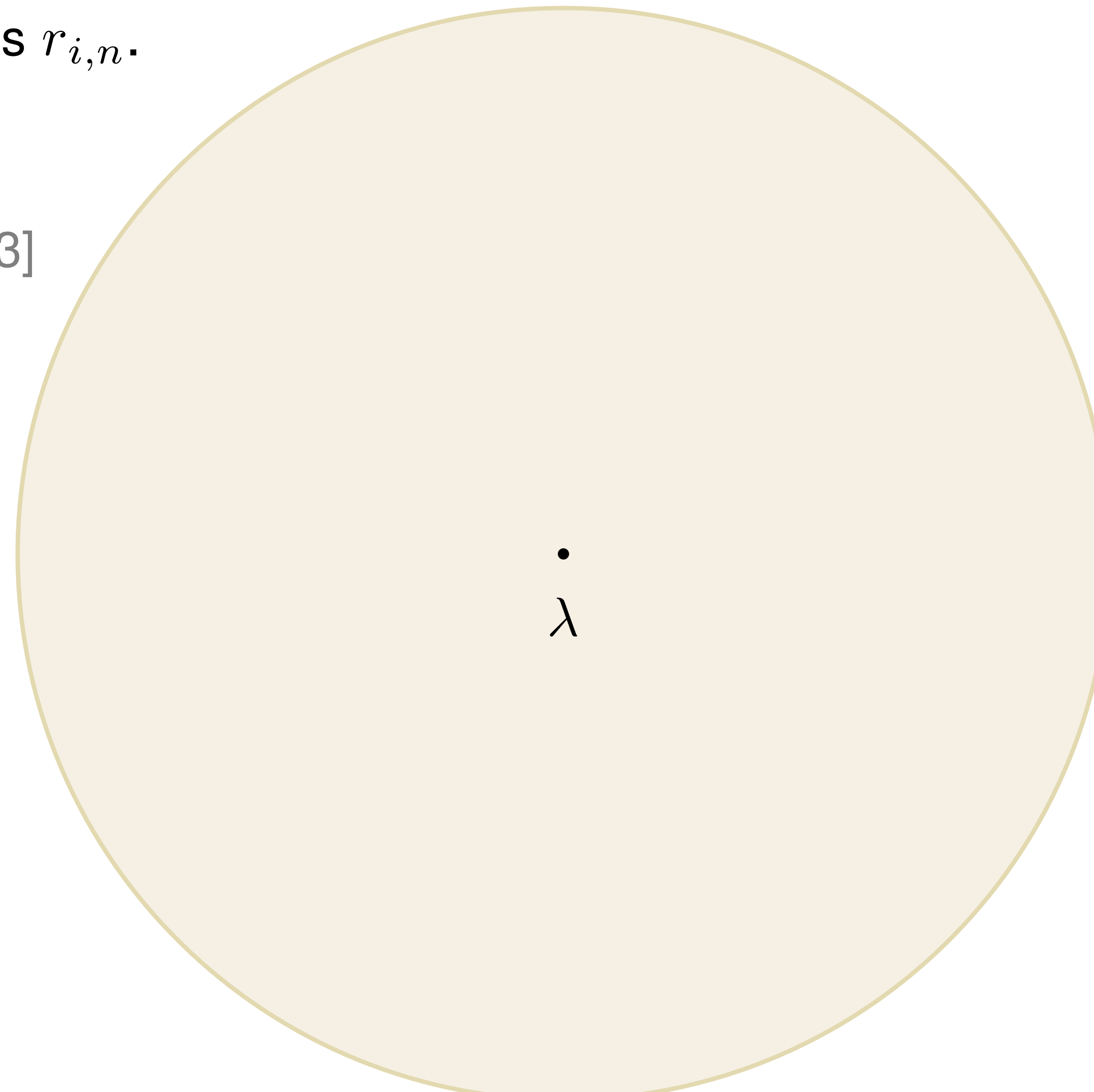
How do these sets look like for a given class of nonnormal matrices?

[papers by Greenbaum et al. 2000-2004]

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

$\mathcal{H}_i$ is a circle around λ with a radius $r_{i,n}$.

$r_{1,n}$ and $r_{n-1,n}$ are known,
[Faber & Greenbaum & Marshall ’03]



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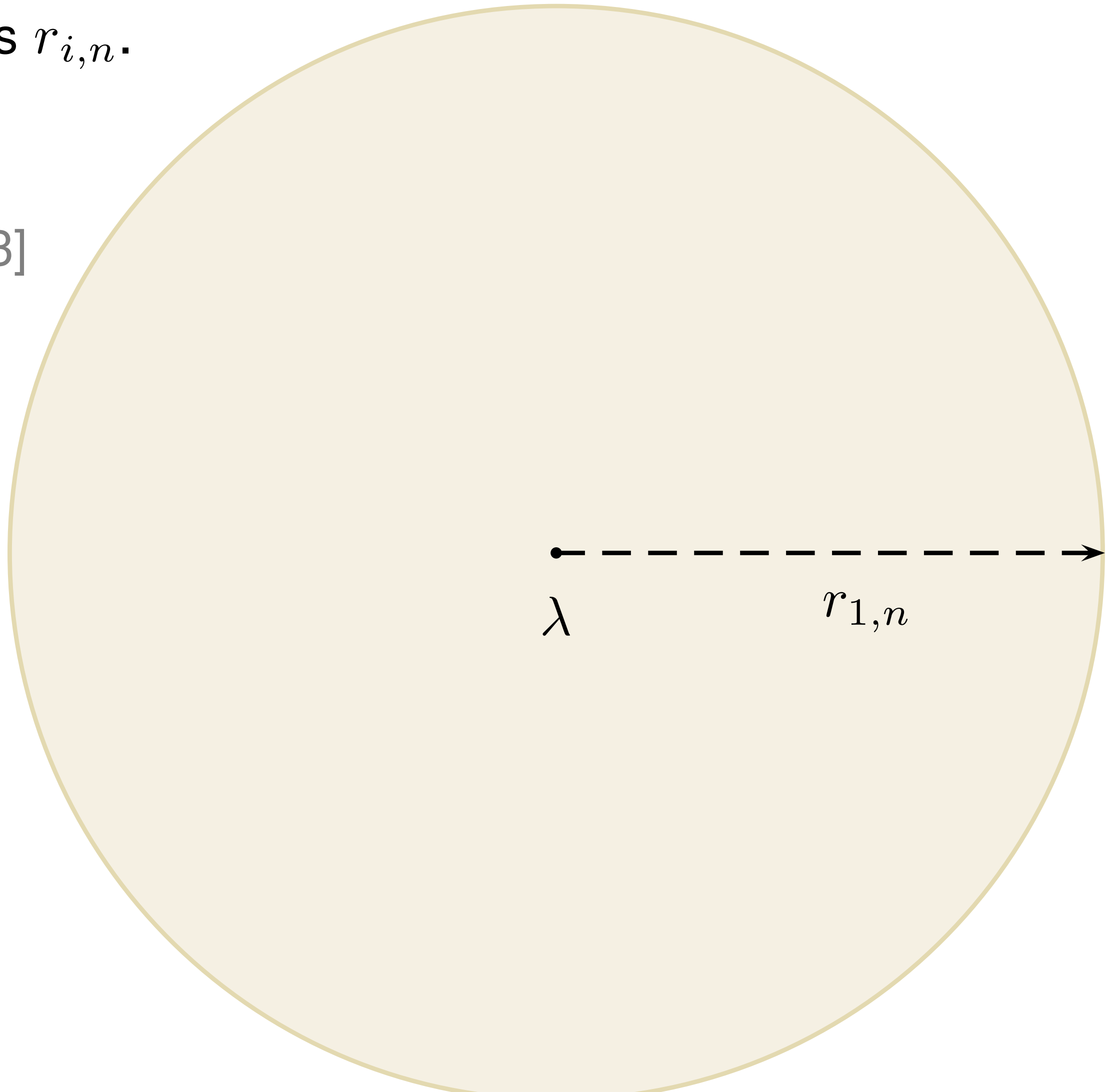
$$r_{1,n} = \cos\left(\frac{\pi}{n+1}\right).$$



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

$\mathcal{H}_i$ is a circle around λ with a radius $r_{i,n}$.

$r_{1,n}$ and $r_{n-1,n}$ are known,

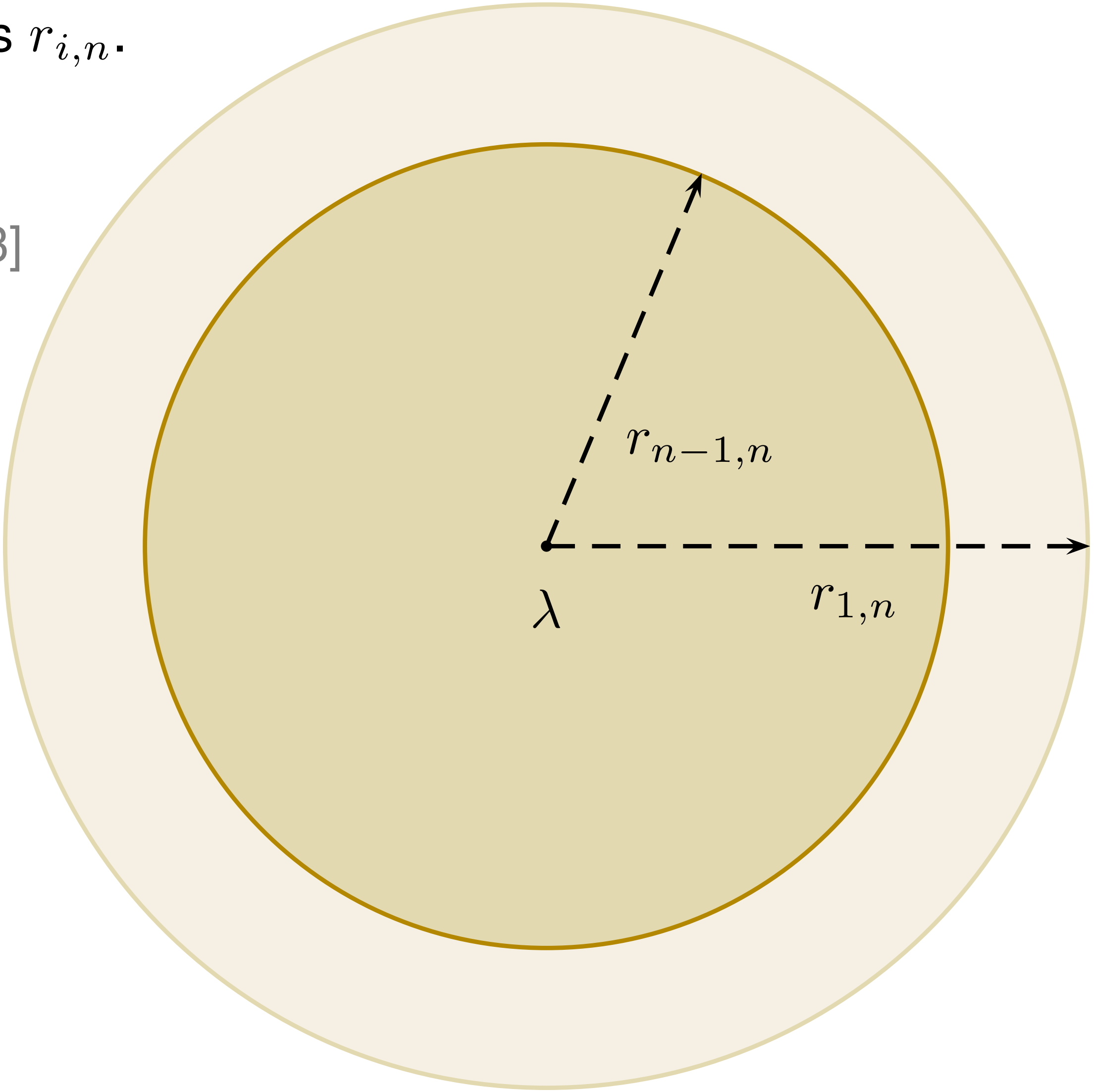
[Faber & Greenbaum & Marshall '03]

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

if n even, $r_{n-1,n}$ is the positive root of

$$2r^n + r - 1 = 0\,.$$

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



$\mathcal{H}_i$ for a Jordan block $\mathbf{J}_\lambda$ (i divides n)

We proved a connection between

- the ith step of ideal GMRES for $\mathbf{J}_\lambda \in \mathbb{R}^{n\times n}$ and
- the 1th step of ideal GMRES for $\mathbf{J}_{\lambda^i} \in \mathbb{R}^{m\times m}$, $m = n/i$.

From this connection it follows

$$r_{i,n} = \left[\cos\left(\frac{\pi}{m+1}\right)\right]^{1/i}$$

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and the bound

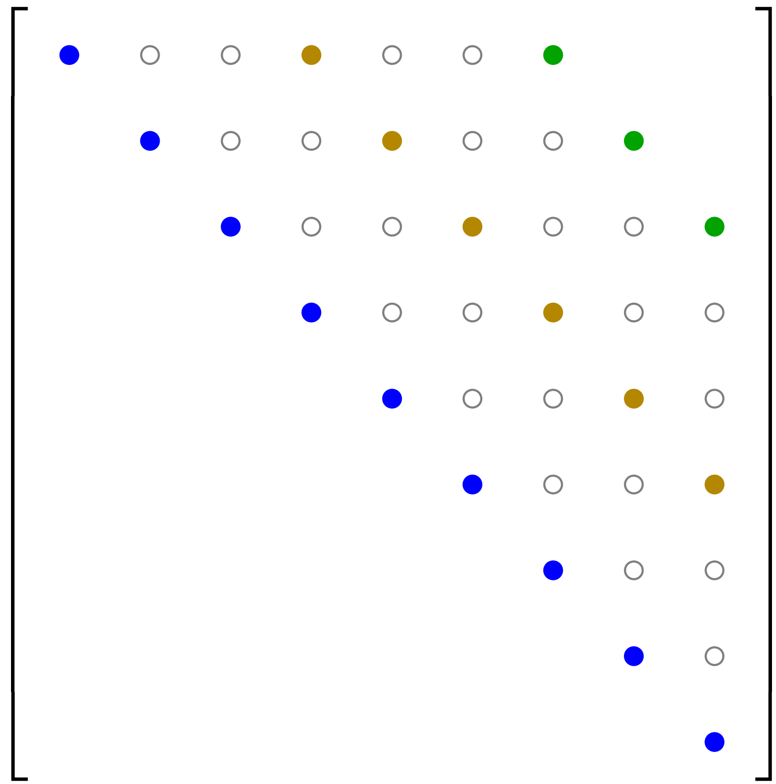
$$\lambda^{-i}\cos\left(\tfrac{\pi}{m+1}\right) \;\leq\; \min_{p\in\pi_i}\|p(\mathbf{J}_\lambda)\| \;\leq\; \lambda^{-i},$$

for $\lambda \geq r_{i,n}$.

[T. & Liesen '05]

General step i (observation), $n = 9$, $i = 6$

Let d be the greatest common divisor of n and i, $n_d = n/d$, $i_d = i/d$.



$$\varphi_i(\mathbf{J}_\lambda)$$

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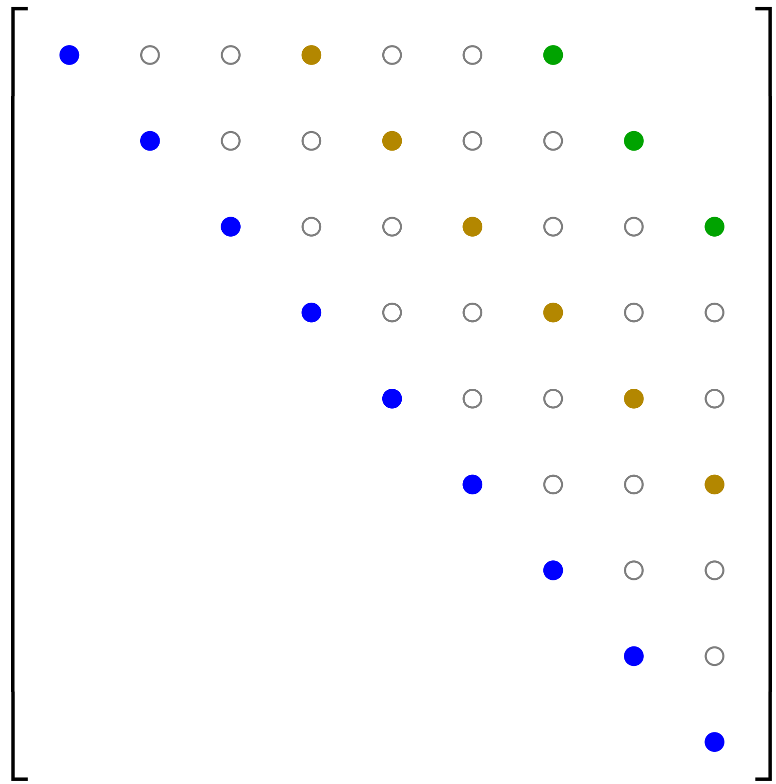

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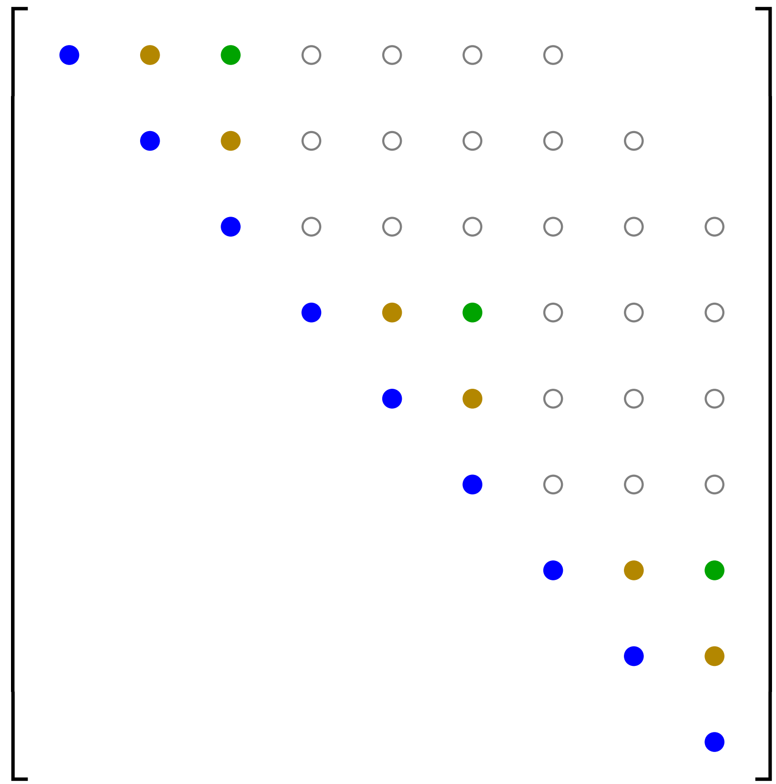

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Two observations (based on numerical experiments):

A. There is a strong connection between:

the i**th step** of ideal GMRES for $\mathbf{J}_\lambda \in \mathbb{R}^{n \times n}$ $\longleftrightarrow$ the i_d**st step** of ideal GMRES for $\mathbf{J}_{\lambda^d} \in \mathbb{R}^{n_d \times n_d}$

B. If i and n are relative primes then $\varphi_i(\mathbf{J}_\lambda)$ has a simple maximal singular value.

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if **A.** and **B.** hold then

worst-case GMRES $=$ ideal GMRES for $\mathbf{J}_\lambda$ in each step i.

Conclusions for a Jordan block

Let i divide n. In these steps i:

- we proved worst-case GMRES $=$ ideal GMRES,
- we determined the ideal GMRES **polynomial**,
- we know the **radius** of polynomial numerical hull,
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General step i :

Our numerical experiments predict:

worst-case GMRES $=$ ideal GMRES for $\mathbf{J}_\lambda$ in each step i.

Which approximation problem solves ideal GMRES for $\mathbf{J}_\lambda$?

Thank you for your attention!