Worst-case and ideal GMRES for a Jordan Block

Petr Tichý[*,†]

joint work with

Jörg Liesen[*]

[*] Technical University of Berlin,

[†] Institute of Computer Science AS CR.

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GMRES

Consider a system of linear algebraic equations

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

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

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

$$x_k \in x_0 + \mathcal{K}_k(\mathbf{A}, r_0)$$

such that

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

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

GMRES bounds

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

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

- Normal matrices: worst-case GMRES $=$ ideal GMRES.

  [Greenbaum & Gurvits '94, Joubert '94]

- Nonnormal matrices: worst-case GMRES can differ 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

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

Then, for $k = 3$,

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

[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

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

- Does it hold worst-case GMRES $=$ ideal GMRES?
- How to estimate the ideal GMRES approximation?

[Faber et al. '96]: Let $\mathbf{A}$ be n by n triangular Toeplitz matrix. Then

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

Outline

1. Structure behind the ideal GMRES convergence for $\mathbf{J}_\lambda$
2. Steps k such that k divides n
3. Estimating the ideal GMRES approximation
4. Observation for a general step k
5. Conclusions

1. Structure behind the ideal GMRES convergence

Ideal GMRES matrix

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

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

[Existence and uniqueness of φ_k $\longrightarrow$ Greenbaum & Trefethen '94]

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

Numerical experiment: Using MATLAB-software SDPT3 by Toh we can compute ideal GMRES matrices and display their structure!

Numerical experiment

Let $\mathbf{A} = \mathbf{J}_1 \in \mathbb{R}^{8\times 8}$, $\bullet$ . . . nonzero entries, $\circ$ . . . zero entries (or almost).

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

Numerical experiment

Let $\mathbf{A} = \mathbf{J}_1 \in \mathbb{R}^{8\times 8}$, $\bullet \ldots$ nonzero entries, $\circ \ldots$ zero entries (or almost).

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

Numerical experiment

Let $\mathbf{A} = \mathbf{J}_1 \in \mathbb{R}^{8\times 8}$, $\bullet \ldots$ nonzero entries, $\circ \ldots$ zero entries (or almost).

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

Numerical experiment

Let $\mathbf{A} = \mathbf{J}_1 \in \mathbb{R}^{8\times 8}$, $\bullet$ . . . nonzero entries, $\circ$ . . . zero entries (or almost).

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

Numerical experiment

Let $\mathbf{A} = \mathbf{J}_1 \in \mathbb{R}^{8\times 8}$, $\bullet \ldots$ nonzero entries, $\circ \ldots$ zero entries (or almost).

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

Numerical experiment

Let $\mathbf{A} = \mathbf{J}_1 \in \mathbb{R}^{8\times 8}$, $\bullet \ldots$ nonzero entries, $\circ \ldots$ zero entries (or almost).

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

Numerical experiment

Let $\mathbf{A} = \mathbf{J}_1 \in \mathbb{R}^{8\times 8}$, $\bullet$ ... nonzero entries, $\circ$ ... zero entries (or almost).

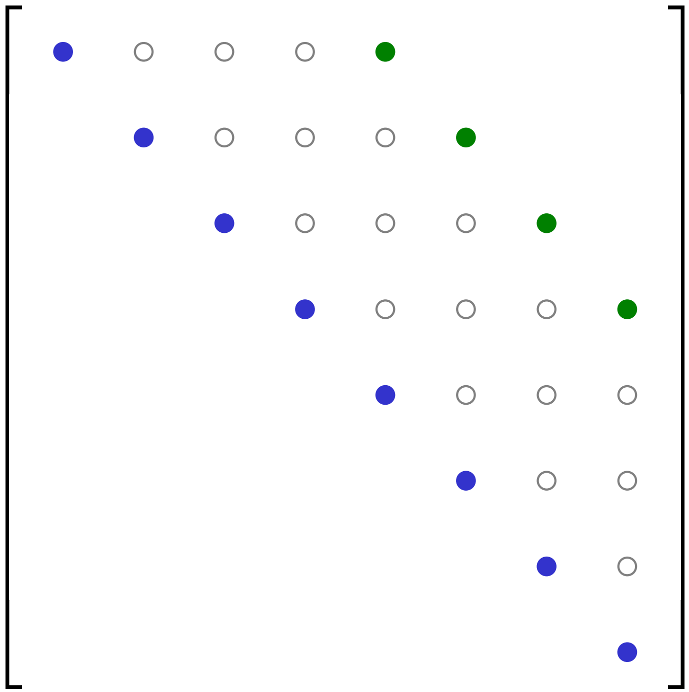
$$\varphi_7(\mathbf{J}_1) = \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \\ & & & & & & & \bullet \end{bmatrix},$$

The structure of $\varphi_k(\mathbf{J}_1)$ depends on relation between k and n.

2. Steps k such that k divides n

Steps k such that k divides n

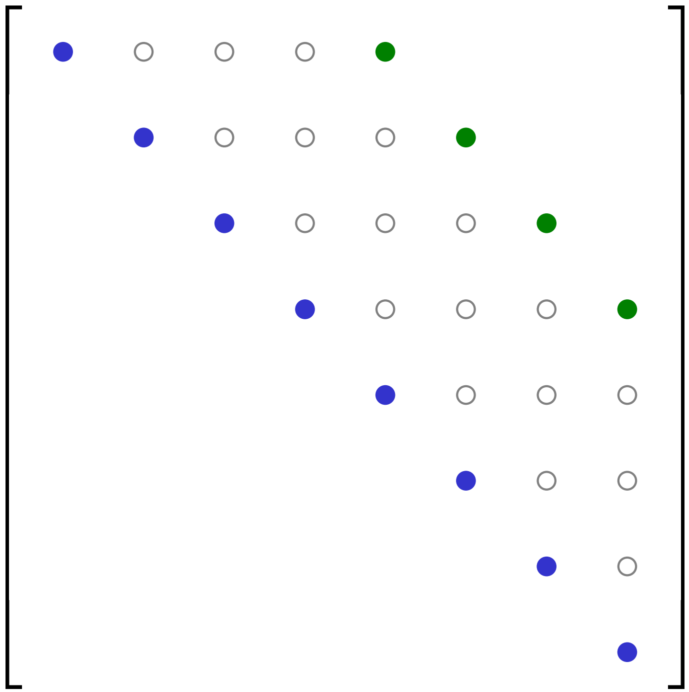
If k divides n then $\varphi_k(\mathbf{J}_1) =$



Steps k such that k divides n

If k divides n

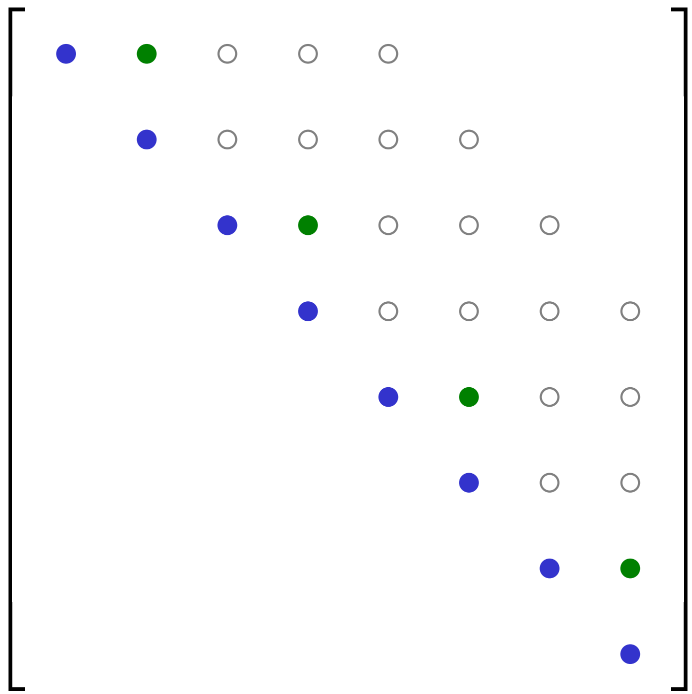
$$[I_{\frac{n}{k}} \otimes e_1, \ldots, I_{\frac{n}{k}} \otimes e_k]^T$$



$$[I_{\frac{n}{k}} \otimes e_1, \ldots, I_{\frac{n}{k}} \otimes e_k]$$

Steps k such that k divides n

If k divides n



Connection between the step k and 1

We proved: There is a strong connection between

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

Let e.g. $n = 8\,,\; k = 4\,.$

$$\varphi_k(\mathbf{J}_\lambda) = \begin{bmatrix} \bullet & & & & \pm\bullet & & & \\ & \bullet & & & & \pm\bullet & & \\ & & \bullet & & & & \pm\bullet & \\ & & & \bullet & & & & \pm\bullet \\ & & & & \bullet & & & \\ & & & & & \bullet & & \\ & & & & & & \bullet & \\ & & & & & & & \bullet \end{bmatrix} \longleftrightarrow \begin{bmatrix} \bullet & \bullet \\ & \bullet \end{bmatrix} = \varphi_1(\mathbf{J}_{\lambda^k})\,.$$

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

Using the transformation and results by [Greenbaum & Gurvits '94] we proved:

- If k divides n then

worst-case GMRES $=$ ideal GMRES.

- Ideal polynomial φ_k :

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

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

$$\|\varphi_k(\mathbf{J}_\lambda)\| \; = \; \frac{4\lambda^k}{4\lambda^{2k} + 1} \, .$$

[T. & Liesen '05]

3. Estimating the ideal GMRES approximation

Estimating using polynomial numerical hull

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

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

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

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

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

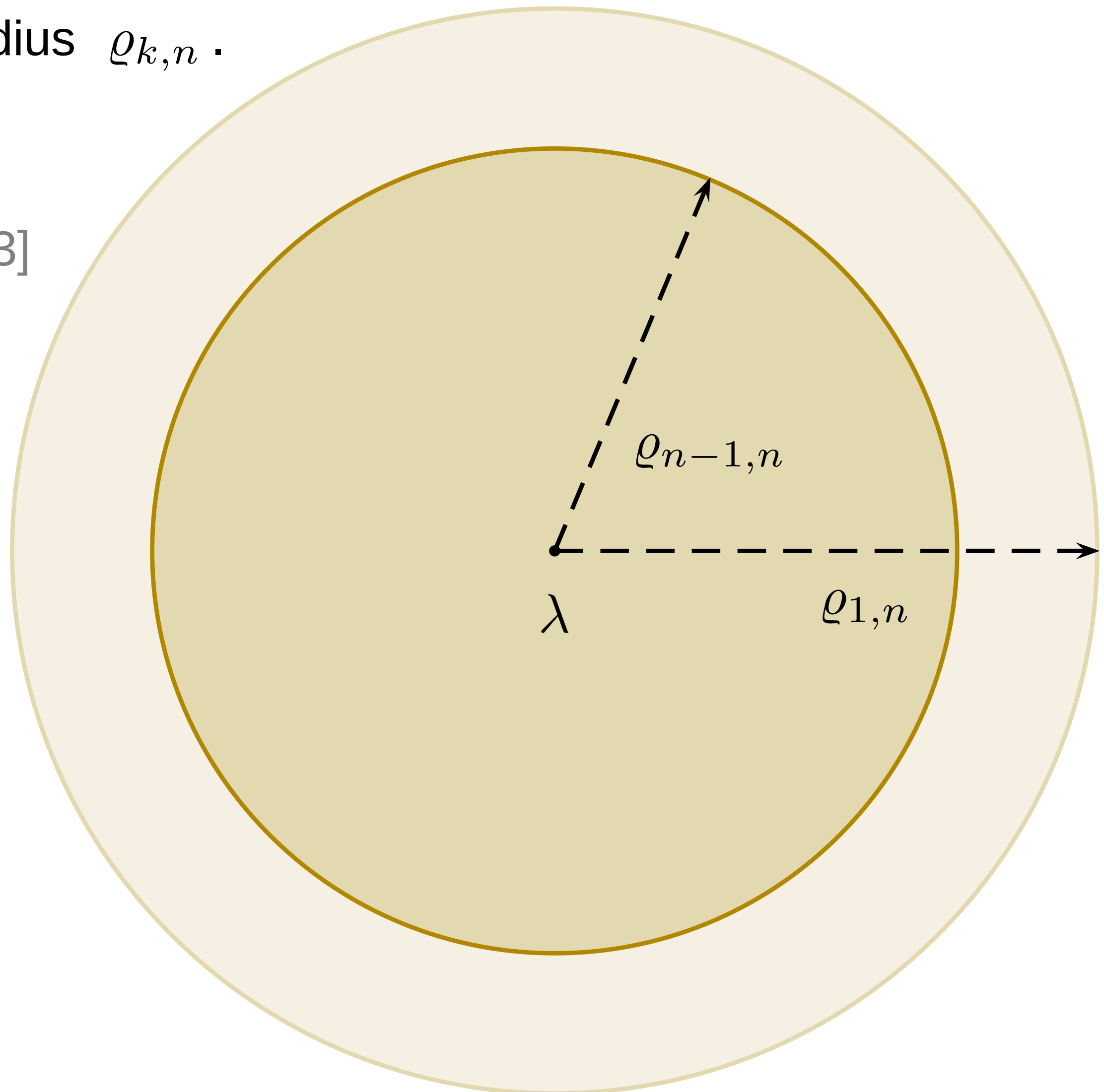
[Greenbaum '02]

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

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

$\varrho_{1,n}$ and $\varrho_{n-1,n}$ are known,
[Faber & Greenbaum & Marshall '03]

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



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

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

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

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

We proved the connection between

- the kth step of ideal GMRES for $\mathbf{J}_\lambda \in \mathbb{R}^{n\times n}$ and
- the 1st step of ideal GMRES for $\mathbf{J}_{\lambda^k} \in \mathbb{R}^{\frac{n}{k}\times\frac{n}{k}}$.

From this connection it follows

*We thank Anne Greenbaum for this observation.

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

and the bound

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

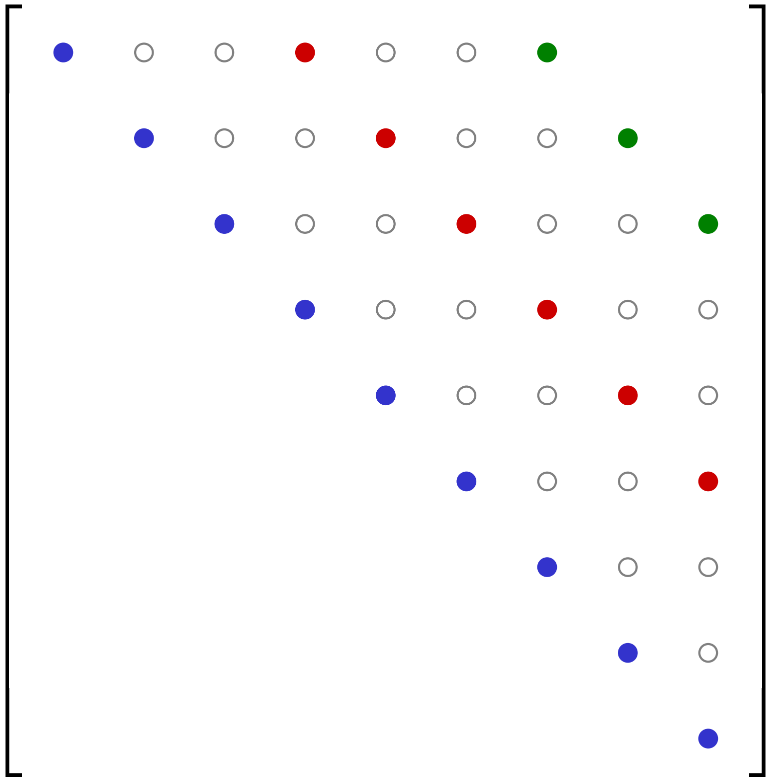
for $\lambda \ge \varrho_{k,n}$.

[T. & Liesen '05]

4. General step k

General step k (observation)

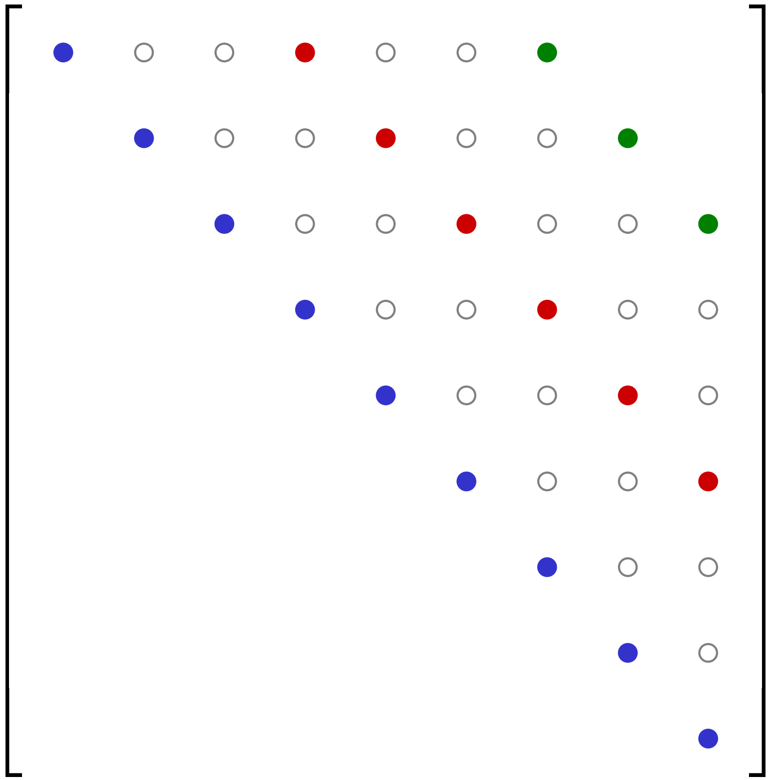
Let d be the greatest common divisor of n and k ($n = 9$, $k = 6$, $d = 3$).



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

General step k (observation)

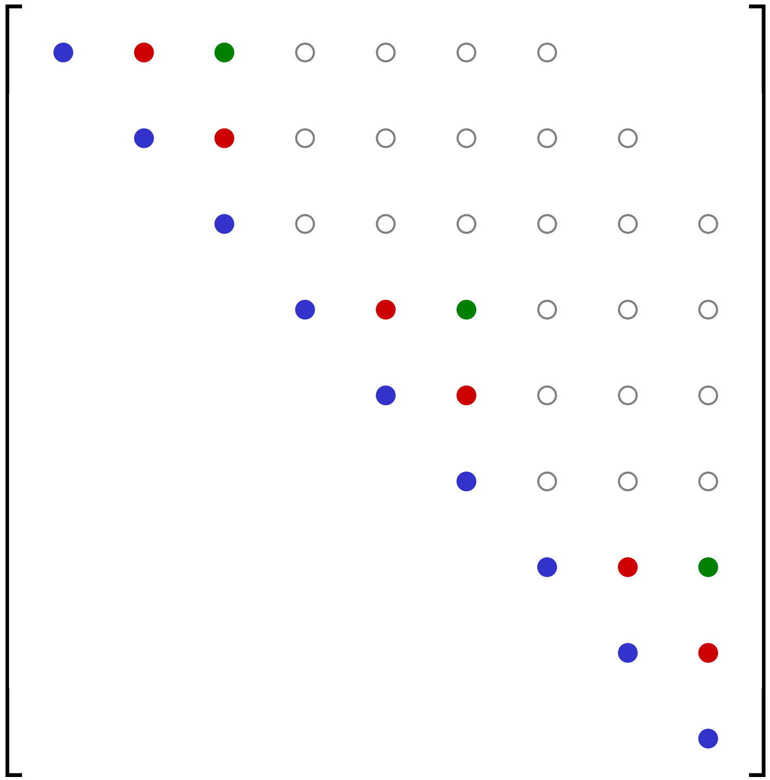
Let d be the greatest common divisor of n and k ($n = 9$, $k = 6$, $d = 3$).

$\mathbf{P}_{n,k}^T$  $\mathbf{P}_{n,k}$

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

General step k (observation)

Let d be the greatest common divisor of n and k ($n = 9$, $k = 6$, $d = 3$).



$$\mathbf{P}_{n,k}^T \, \varphi_k(\mathbf{J}_\lambda) \, \mathbf{P}_{n,k}$$

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

Let k divide n. At these steps k:

- we proved worst-case GMRES $=$ ideal GMRES,
- we determined the ideal GMRES **polynomial**,
- we know the **radius** of polynomial numerical hull,
- we derived tight **bounds** on $\|\varphi_k(\mathbf{J}_\lambda)\|$.

General k.

Our numerical experiments predict:

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

Thank you for your attention!

More details can be found in

Tichý, P. and Liesen, J., Worst-case and ideal GMRES for a Jordan block, submitted to Linear Algebra and its Applications, October 2004.

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