On a New Proof of the Faber-Manteuffel Theorem

Petr Tichý

joint work with

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Outline

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Krylov subspace methods

Basis

Methods based on projection onto the Krylov subspaces

$$\mathcal{K}_j(\mathbf{A}, v) \equiv \text{span}(v, \mathbf{A}v, \ldots, \mathbf{A}^{j-1}v) \qquad j = 1, 2, \ldots .$$

$\mathbf{A} \in \mathbb{R}^{n \times n}$, $v \in \mathbb{R}^n$.

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Each method must generate a basis of $\mathcal{K}_j(\mathbf{A}, v)$.

- The trivial choice $v, \mathbf{A}v, \ldots, \mathbf{A}^{j-1}v$ is computationally infeasible (recall the Power Method).
- For numerical stability: Well conditioned basis.
- For computational efficiency: Short recurrence.

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- For numerical stability: Well conditioned basis.
- For computational efficiency: Short recurrence.
- Best of both worlds:
  Orthogonal basis computed by short recurrence.

Optimal Krylov subspace methods

with short recurrences

CG (1952), MINRES, SYMMLQ (1975)

- based on three-term recurrences

$$r_{j+1} = \gamma_j \mathbf{A} r_j - \alpha_j r_j - \beta_j r_{j-1} \,,$$

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  $\|x - x_j\|_{\mathbf{A}}$ in CG,
  $\|x - x_j\|_{\mathbf{A}^T\mathbf{A}} = \|r_j\|$ in MINRES,
  $\|x - x_j\|$ in SYMMLQ -here $x_j \in x_0 + \mathbf{A}\mathcal{K}_j(\mathbf{A}, r_0)$.

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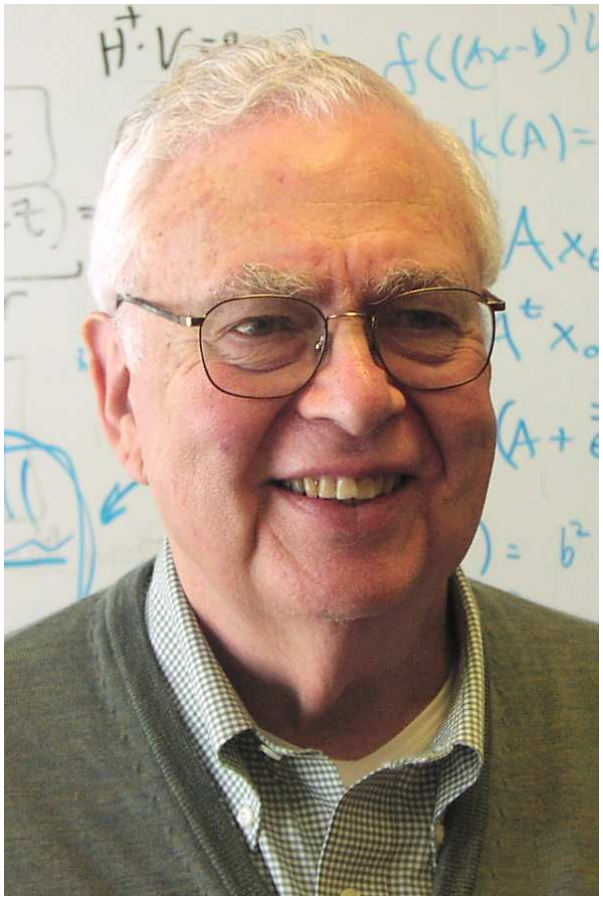
- An important assumption on $\mathbf{A}$:
  $\mathbf{A}$ is symmetric (MINRES, SYMMLQ) & pos. definite (CG).

Gene Golub



G. H. Golub, 1932–2007

- By the end of the 1970s it was unknown if such methods existed also for general unsymmetric $\mathbf{A}$.
- Gatlinburg VIII (now Householder VIII) held in Oxford from July 5 to 11, 1981.
- "A prize of $500 has been offered by Gene Golub for the construction of a 3-term conjugate gradient like descent method for non-symmetric real matrices or a proof that there can be no such method".

What kind of method Golub had in mind

- We want to solve $\mathbf{A}x = b$ using CG-like descent method: error is minimized in some given inner product norm, $\|\cdot\|_{\mathbf{B}} = \langle \cdot, \cdot \rangle_{\mathbf{B}}^{1/2}$.

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- Starting from x_0, compute

$$x_{j+1} = x_j + \alpha_j p_j\,, \qquad j = 0, 1, \ldots\,,$$

p_j is a direction vector, α_j is a scalar (to be determined),

$$\mathrm{span}\{p_0, \ldots, p_j\} = \mathcal{K}_{j+1}(\mathbf{A}, r_0), \qquad r_0 = b - \mathbf{A}x_0\,.$$

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- $p_0, \ldots, p_j$ has to be a $\mathbf{B}$-orthogonal basis of $\mathcal{K}_{j+1}(\mathbf{A}, r_0)$.

Faber and Manteuffel, 1984

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NECESSARY AND SUFFICIENT CONDITIONS FOR THE EXISTENCE OF A CONJUGATE GRADIENT METHOD*

VANCE FABER† AND THOMAS MANTEUFFEL†

Abstract. We characterize the class $CG(s)$ of matrices A for which the linear system $A\mathbf{x}=\mathbf{b}$ can be solved by an s-term conjugate gradient method. We show that, except for a few anomalies, the class $CG(s)$ consists of matrices A for which conjugate gradient methods are already known. These matrices are the Hermitian matrices, $A^*=A$, and the matrices of the form $A=e^{i\theta}(dI+B)$, with $B^*=-B$.

- Faber and Manteuffel gave the answer in 1984:
  For a general matrix $\mathbf{A}$ there exists *no* short recurrence for generating orthogonal Krylov subspace bases.
- **What are the details of this statement**?

Outline

Formulation of the problem

$\mathbf{B}$-inner product, Input and Notation

Without loss of generality, $\mathbf{B} = \mathbf{I}$. Otherwise change the basis:

$$\langle x, y \rangle_{\mathbf{B}} = \langle \mathbf{B}^{1/2} x, \mathbf{B}^{1/2} y \rangle, \quad \hat{\mathbf{A}} \equiv \mathbf{B}^{1/2} \mathbf{A} \mathbf{B}^{-1/2}, \quad \hat{v} \equiv \mathbf{B}^{1/2} v \,.$$

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- $\mathbf{A} \in \mathbb{C}^{n \times n}$, a nonsingular matrix.
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Notation:

- $d_{\min}(\mathbf{A})$ ... the degree of the minimal polynomial of $\mathbf{A}$.
- $d = d(\mathbf{A}, v)$ ... the grade of v with respect to $\mathbf{A}$,
  the smallest d s.t. $\mathcal{K}_d(\mathbf{A}, v)$ is invariant under mult. with $\mathbf{A}$.

Formulation of the problem

Our Goal

- Generate a basis $v_1, \ldots, v_d$ of $\mathcal{K}_d(\mathbf{A}, v)$ s.t.

  1. $\text{span}\{v_1, \ldots, v_j\} = \mathcal{K}_j(A, v), \quad \text{for} \quad j = 1, \ldots, d,$
  2. $\langle v_i, v_j \rangle = 0, \quad \text{for} \quad i \neq j, \quad i, j = 1, \ldots, d.$

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Arnoldi's method:
Standard way for generating the orthogonal basis
(no normalization for convenience): $v_1 \equiv v$,

$$v_{j+1} \quad = \quad \mathbf{A}v_j \; - \sum_{i=1}^{j} h_{i,j}\, v_i \,, \qquad\qquad h_{i,j} \quad = \quad \frac{\langle \mathbf{A}v_j, v_i \rangle}{\langle v_i, v_i \rangle} \,,$$

$j = 0, \ldots, d-1.$

Formulation of the problem

Arnoldi's method - matrix formulation

In matrix notation:

$$v_1 = v\,,$$

$$\mathbf{A}\underbrace{[v_1,\ldots,v_{d-1}]}_{\equiv \mathbf{V}_{d-1}} = \underbrace{[v_1,\ldots,v_d]}_{\equiv \mathbf{V}_d} \underbrace{\begin{bmatrix} h_{1,1} & \cdots & h_{1,d-1} \\ 1 & \ddots & \vdots \\ & \ddots & h_{d-1,d-1} \\ & & 1 \end{bmatrix}}_{\equiv \mathbf{H}_{d,d-1}},$$

$\mathbf{V}_d^*\mathbf{V}_d$ is diagonal, $\quad d = \dim \mathcal{K}_n(\mathbf{A}, v)\,.$

Formulation of the problem

Optimal short recurrences (Definition - Liesen and Strakoš, 2008)

$\mathbf{A}$ admits an optimal $(s+2)$-term recurrence, if

- for any v, $\mathbf{H}_{d,d-1}$ is at most $(s+2)$-band Hessenberg, and
- for at least one v, $\mathbf{H}_{d,d-1}$ is $(s+2)$-band Hessenberg.

$$\mathbf{A}\,\mathbf{V}_{d-1} \;=\; \mathbf{V}_d \overbrace{\begin{bmatrix} \bullet & \cdots & \bullet & & \\ \bullet & \ddots & & \ddots & \\ & \ddots & \ddots & & \bullet \\ & & \ddots & \ddots & \vdots \\ & & & \ddots & \bullet \\ & & & & \bullet \end{bmatrix}}^{d-1} \overbrace{\qquad\qquad}^{s+1}$$

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Basic question

What are sufficient and necessary conditions for $\mathbf{A}$ to admit an optimal $(s+2)$-term recurrence?

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Example of sufficiency: If $\mathbf{A}^* = \mathbf{A}$, then $s = 1$ and $\mathbf{A}$ admits an optimal 3-term recurrence.

Definition. If

$$\mathbf{A}^* = p_s(\mathbf{A}),$$

where p_s is a polynomial of the smallest possible degree s, $\mathbf{A}$ is called normal(s).

Outline

The Faber-Manteuffel theorem

Theorem. [Faber and Manteuffel, 1984], [Liesen and Strakoš, 2008]

Let $\mathbf{A}$ be a nonsingular matrix with minimal polynomial degree $d_{\min}(\mathbf{A})$. Let s be a nonnegative integer, $s+2 < d_{\min}(\mathbf{A})$:

$\mathbf{A}$ admits an optimal $(s+2)$-term recurrence

if and only if

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- Sufficiency is rather straightforward, necessity *is not*. Key words from the proof of necessity in (Faber and Manteuffel, 1984) include: "continuous function" (analysis), "closed set of smaller dimension" (topology), "wedge product" (multilinear algebra).

The Faber-Manteuffel theorem

Why is necessity so hard?

Optimal $(s+2)$-term recurrence:

$$\mathbf{A}\,\mathbf{V}_{d-1} \;=\; \mathbf{V}_d \underbrace{\overbrace{\begin{bmatrix} \bullet & \cdots & \bullet & & \\ \bullet & \ddots & & \ddots & \\ & \ddots & \ddots & & \bullet \\ & & \ddots & \ddots & \vdots \\ & & & \ddots & \bullet \\ & & & & \bullet \end{bmatrix}}^{s+1}}_{d-1}$$

Prove something about the linear operator $\mathbf{A}$, without complete knowledge of the structure of its matrix representation.

The Faber-Manteuffel theorem

Why is necessity so hard?

Since $\mathcal{K}_d(\mathbf{A}, v)$ is invariant, $\mathbf{A}v_d \in \mathcal{K}_d(\mathbf{A}, v)$ and

$$\mathbf{A}v_d = \sum_{i=1}^{d} h_{id}\, v_i.$$

$$\mathbf{A}\,\mathbf{V}_d \;=\; \mathbf{V}_d \overbrace{\begin{bmatrix} \bullet & \cdots & \bullet & & \bullet \\ \bullet & \ddots & & \ddots & \vdots \\ & \ddots & \ddots & & \bullet \\ & & \ddots & \ddots & \vdots \\ & & & \ddots & \bullet \\ & & & & \bullet \end{bmatrix}}^{s+1}_{d-1}$$

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V. Faber, J. Liesen and P. Tichý., 2008

The Faber-Manteuffel Theorem for Linear Operators

- Motivated by the paper [J. Liesen and Z. Strakoš, 2008] which contains a completely reworked theory of short recurrences for generating orthogonal Krylov subspace bases.

  "It is unknown if a simpler proof of the necessity part can be found. In view of the fundamental nature of the Faber-Manteuffel Theorem, such proof would be a welcome addition to the existing literature. It would lead to a better understanding of the theorem by enlightening some (possibly unexpected) relationships, and it would also be more suitable for classroom teaching."

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- We give two new proofs of the Faber-Manteuffel theorem that use more elementary tools,
- first proof - improved version of the Faber-Manteuffel proof,
- second proof - completely new proof based on orthogonal transformations of upper Hessenberg matrices.

Idea of the second proof (1)

V. Faber, J. Liesen and P. Tichý, 2008

(for simplicity, we omit indices by $\mathbf{V}_d$ and $\mathbf{H}_{d,d}$)

Let $\mathbf{A}$ admit an optimal $(s+2)$-term recurrence

$$\mathbf{A}\,\mathbf{V} \;=\; \mathbf{V}\,\mathbf{H}, \quad \mathbf{V}^*\mathbf{V} = \mathbf{I}\,.$$

Up to the last column, $\mathbf{H}$ is $(s+2)$-band Hessenberg.

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Let $\mathbf{G}$ be a $d \times d$ unitary matrix, $\mathbf{G}^*\mathbf{G} = \mathbf{I}$. Then

$$\mathbf{A}\,\underbrace{(\mathbf{V}\mathbf{G})}_{\mathbf{W}} \;=\; \underbrace{(\mathbf{V}\mathbf{G})}_{\mathbf{W}}\,\underbrace{(\mathbf{G}^*\mathbf{H}\mathbf{G})}_{\widetilde{\mathbf{H}}}\,.$$

$\mathbf{W}$ is unitary.

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$\mathbf{W}$ is unitary. If $\mathbf{G}$ is chosen such that $\widetilde{\mathbf{H}}$ is again unreduced upper Hessenberg matrix, then

$$\mathbf{A}\,\mathbf{W} \;=\; \mathbf{W}\,\tilde{\mathbf{H}}\,.$$

represents the result of Arnoldi's method applied to $\mathbf{A}$ and w_1.
Up to the last column, $\widetilde{\mathbf{H}}$ has to be $(s+2)$-band Hessenberg.

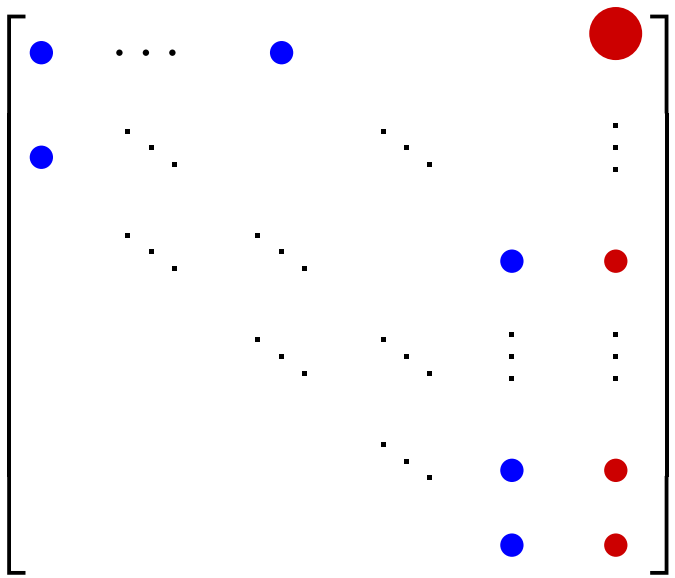
Idea of the second proof (2)

V. Faber, J. Liesen and P. Tichý, 2008

Proof by contradiction. Let $\mathbf{A}$ admit an optimal $(s+2)$-term recurrence and $\mathbf{A}$ not be normal(s).

Then there exists a starting vector v such that $h_{1,d} \neq 0$.

$$\mathbf{A}\ \mathbf{V} \quad = \quad \mathbf{V}$$



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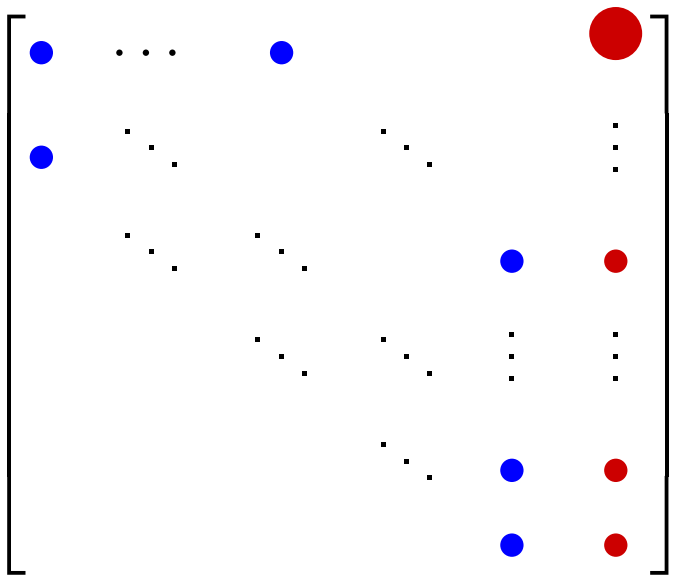


$$\mathbf{G}$$

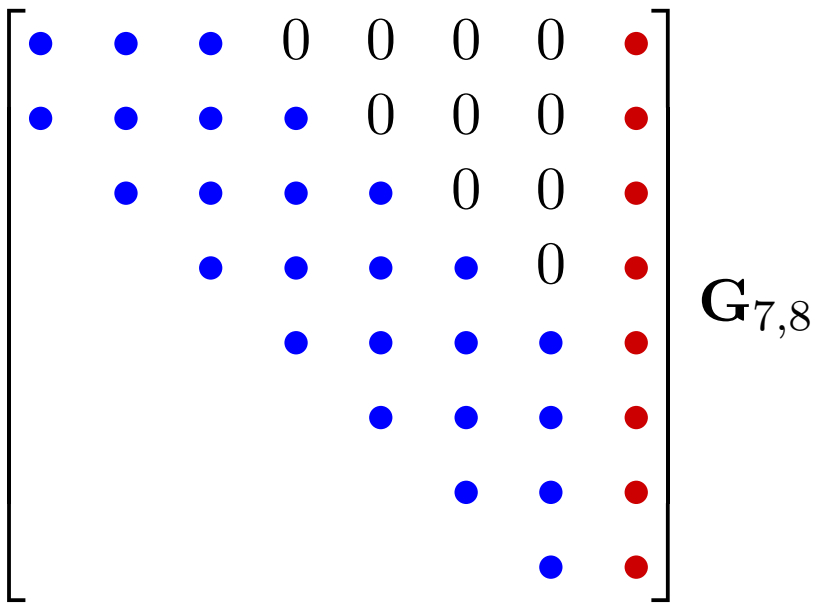
Find unitary $\mathbf{G}$ (a product of Givens rotations) such that $\widetilde{\mathbf{H}}$ is unreduced upper Hessenberg, but $\widetilde{\mathbf{H}}$ is not $(s+2)$-band (up to the last column) - **contradiction**.

Idea of the second proof (3)

V. Faber, J. Liesen and P. Tichý, 2008

Let v be a starting vector such that $h_{1,8} \neq 0$.

Choose Givens rotation $\mathbf{G}_{7,8}$.



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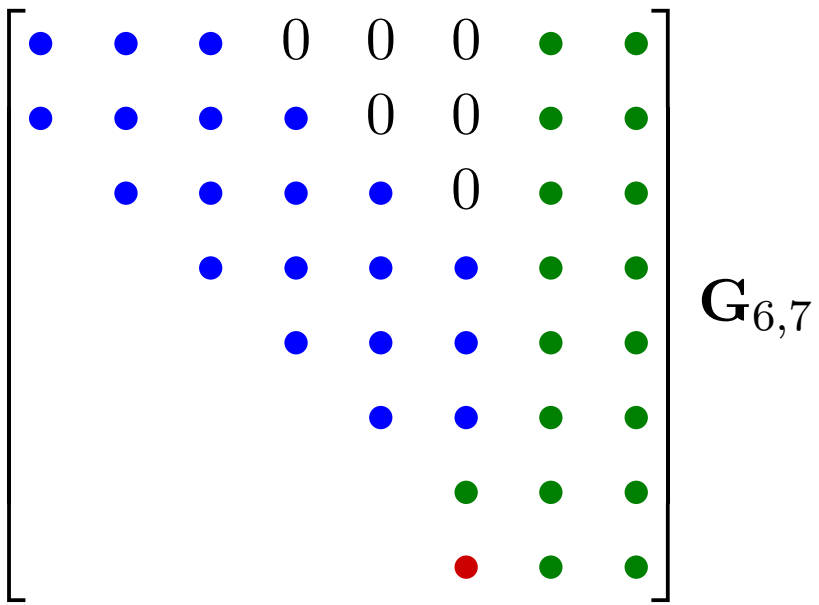

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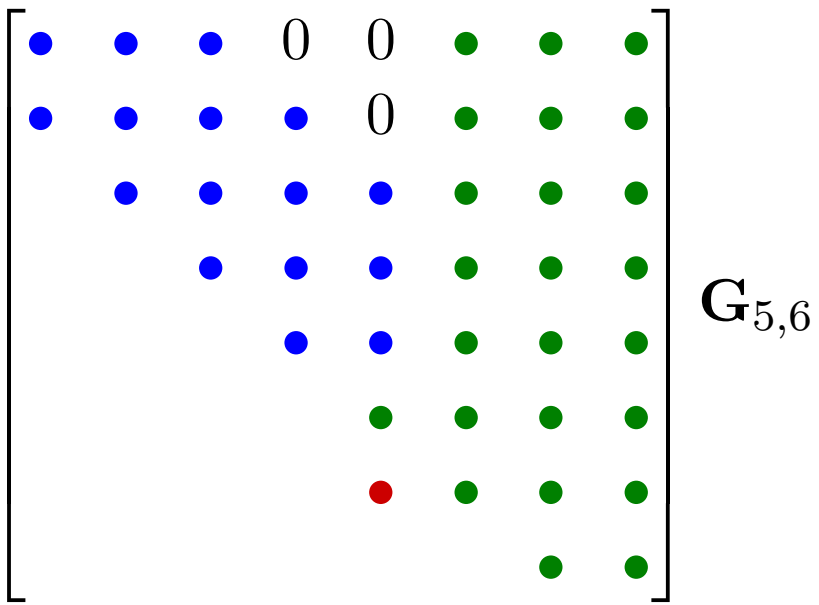

Idea of the second proof (3)

V. Faber, J. Liesen and P. Tichý, 2008

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$$\mathbf{G}_{5,6}^{*} \begin{bmatrix} \bullet & \bullet & \bullet & 0 & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \end{bmatrix}$$

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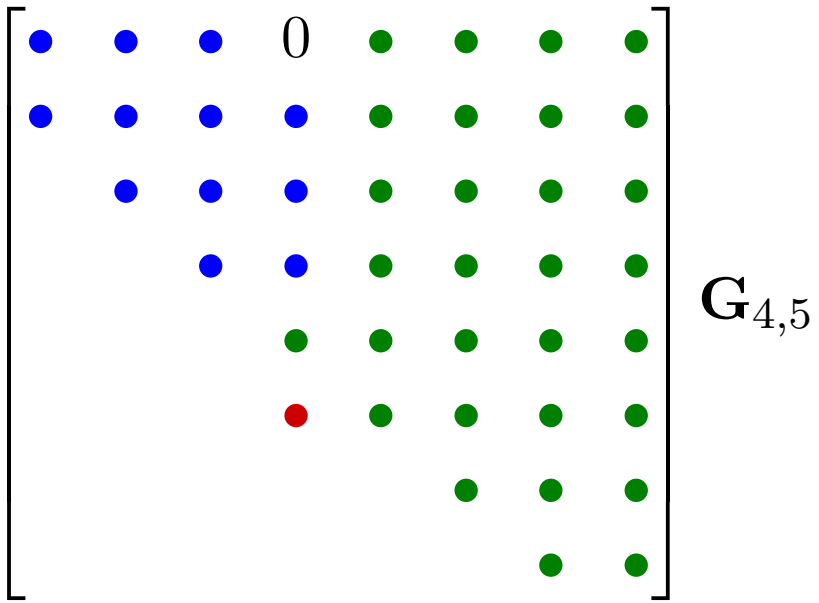

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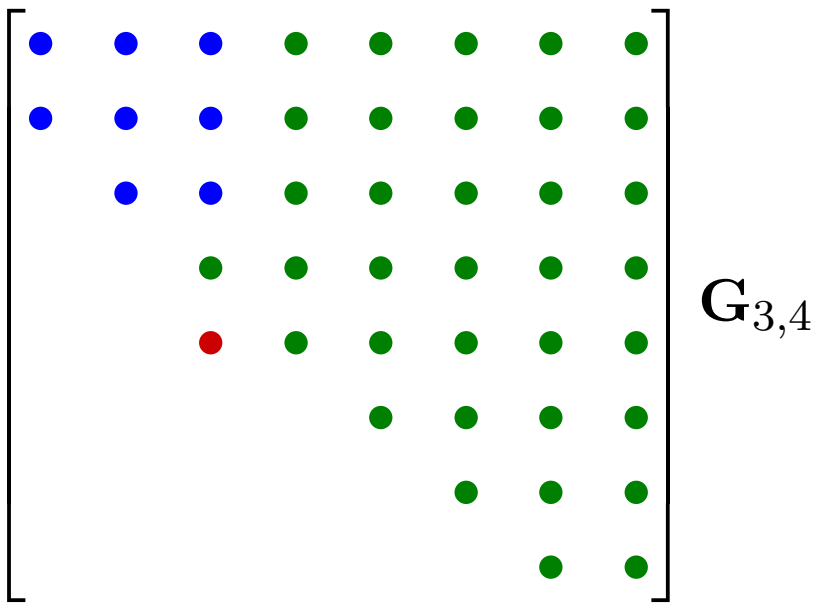

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$$\mathbf{G}_{3,4}^{*} \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \end{bmatrix}$$

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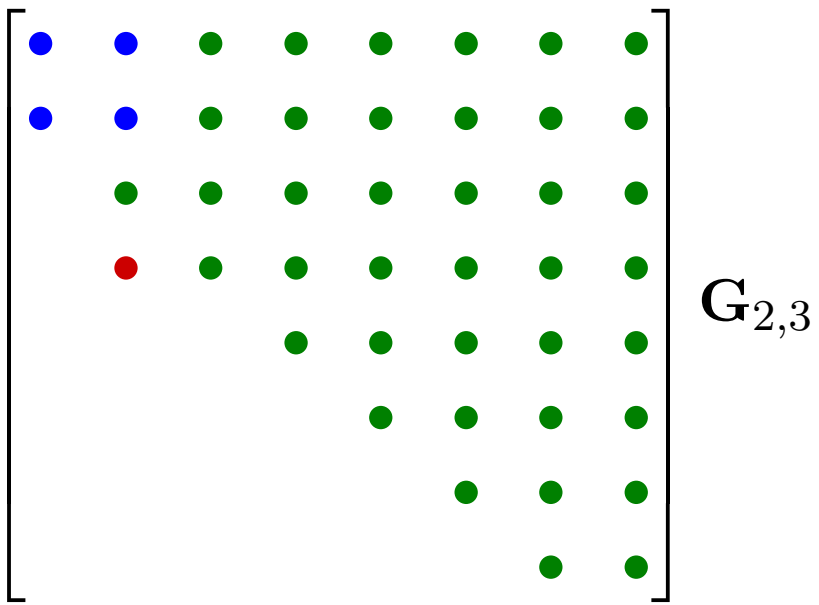

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$$\mathbf{G}_{2,3}^{*} \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \end{bmatrix}$$

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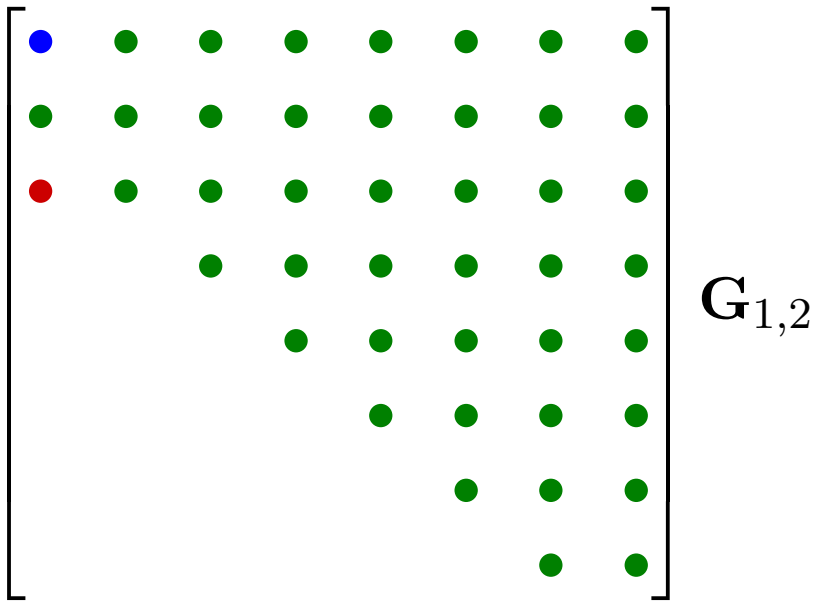

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$$\mathbf{G}_{1,2}^{*} \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \end{bmatrix}$$

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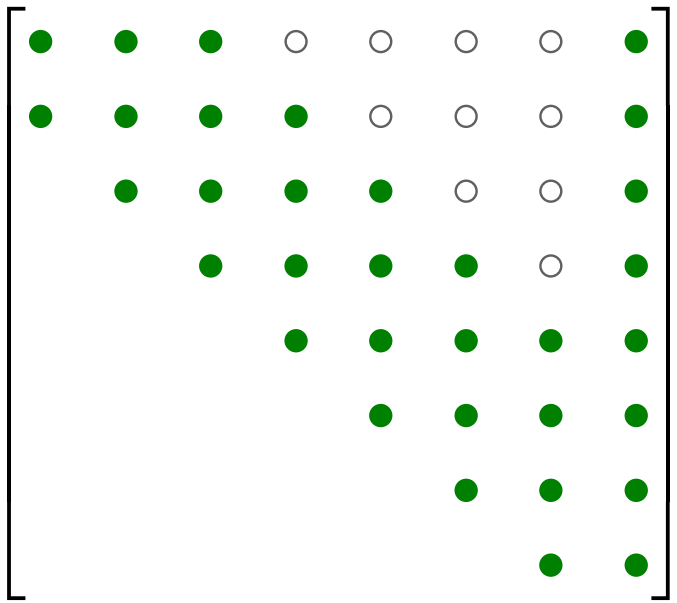

$$\mathbf{G} \equiv \mathbf{G}_{7,8}\mathbf{G}_{6,7}\ldots\mathbf{G}_{1,2}, \qquad \widetilde{\mathbf{H}} \equiv \mathbf{G}^* \mathbf{H}\, \mathbf{G}.$$

We proved: It is possible to choose $\mathbf{G}_{7,8}$ such that

$$h_{1,8} \neq 0 \quad \Longrightarrow \quad \tilde{h}_{1,7} \neq 0 \;\text{ or }\; \tilde{h}_{2,7} \neq 0\,.$$

Summary

Generating of orthogonal basis of $\mathcal{K}_d(\mathbf{A}, v)$ via short recurrences

Arnoldi-type recurrence
$(s+2)$-term

$\Updownarrow$

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- When is $\mathbf{A}$ normal(s)?

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- All classes of "interesting" matrices are known.

Related papers

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  Completely reworked theory of short recurrences for generating orthogonal Krylov subspace bases

- V. Faber, J. Liesen and P. Tichý, [The Faber-Manteuffel Theorem for Linear Operators, SIAM J. Numer. Anal., 2008, 46, 1323-1337].
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More details can be found at

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