

# On a New Proof of the Faber-Manteuffel Theorem

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joint work with

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# Outline

- 1 Introduction
- 2 Formulation of the problem
- 3 The Faber-Manteuffel theorem
- 4 The ideas of a new proof

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# Krylov subspace methods

Given  $\mathbf{A} \in \mathbb{R}^{n \times n}$ ,  $v \in \mathbb{R}^n$ . Define the  $j$ th Krylov subspace

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

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Krylov subspace methods:

- Iterative methods for solving large and sparse linear systems or eigenvalue problems,
- they are based on projection onto the Krylov subspaces,
- examples: Lanczos, CG, Arnoldi, GMRES, BiCG.

# Krylov subspace methods

## Basis

Each method **must generate a basis of  $\mathcal{K}_j(\mathbf{A}, v)$ ,  $j = 1, 2, \dots$**

- The trivial choice  $v, \mathbf{A}v, \dots, \mathbf{A}^{j-1}v$  is computationally infeasible (recall the Power Method).

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- 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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- generate orthogonal (or  $\mathbf{A}$ -orthogonal) Krylov subspace basis,
- *optimal* in the sense that they minimize some error norm:

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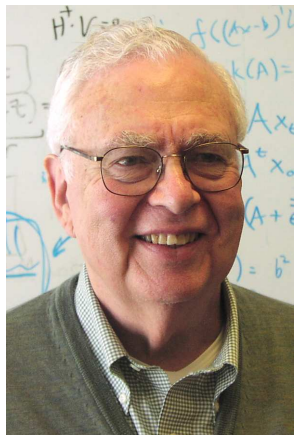
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- An important assumption on  $\mathbf{A}$ :  
 $\mathbf{A}$  is **symmetric** (MINRES, SYMMLQ) & **pos. definite** (CG).



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

$$x_{j+1} = x_j + \alpha_j p_j, \quad j = 0, 1, \dots,$$

$p_j$  is a direction vector,  $\alpha_j$  is a scalar (to be determined),

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

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- $\|x - x_{j+1}\|_{\mathbf{B}}$  is minimal iff

$$\alpha_j = \frac{\langle x - x_j, p_j \rangle_{\mathbf{B}}}{\langle p_j, p_j \rangle_{\mathbf{B}}} \quad \text{and} \quad \langle p_j, p_i \rangle_{\mathbf{B}} = 0.$$



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

## 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  $A$  there exists *no* short recurrence for generating orthogonal Krylov subspace bases.
- What are the details of this statement?

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# 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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**Input data:**

- $\mathbf{A} \in \mathbb{C}^{n \times n}$ , a nonsingular matrix.
- $v \in \mathbb{C}^n$ , an initial vector.

**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  $v_1, \dots, v_d$  of  $\mathcal{K}_d(\mathbf{A}, v)$  s.t.
  1.  $\text{span}\{v_1, \dots, v_j\} = \mathcal{K}_j(A, v)$ , for  $j = 1, \dots, d$ ,
  2.  $\langle v_i, v_j \rangle = 0$ , for  $i \neq j$ ,  $i, j = 1, \dots, d$ .

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### Arnoldi's method:

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

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

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



# Formulation of the problem

Arnoldi's method - matrix formulation

In matrix notation:

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

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

# Formulation of the problem

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

**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.

$$\mathbf{A} \mathbf{V}_{d-1} = \mathbf{V}_d$$

# Formulation of the problem

## Basic question

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

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In other words, **how can we characterize matrices  $\mathbf{A}$**  such that for any  $v$ , Arnoldi's method applied to  $\mathbf{A}$  and  $v$  generates an orthogonal basis via a short recurrence of length  $s + 2$ .

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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( $s$ )**.

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# 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

$\mathbf{A}$  is normal( $s$ ).



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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:

$$\mathbf{A} \mathbf{V}_{d-1} = \mathbf{V}_d$$

The diagram illustrates the matrix equation  $\mathbf{A} \mathbf{V}_{d-1} = \mathbf{V}_d$ . The matrix  $\mathbf{A}$  is represented by large square brackets. A horizontal brace above the top row is labeled  $s + 1$ . A horizontal brace below the bottom row is labeled  $d - 1$ . Blue dots are placed at the first and last elements of the top row, and at the last elements of the bottom row. Ellipses are used to indicate the continuation of the matrix structure.

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

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

$$\mathbf{A} \mathbf{V}_d = \mathbf{V}_d \begin{bmatrix} \underbrace{\quad s+1 \quad}_{\text{blue dots}} & & & & & \text{red dot} \\ \bullet & \dots & \bullet & & & \vdots \\ & \ddots & & \ddots & & \vdots \\ & & \ddots & & \ddots & \bullet & \text{red dot} \\ & & & \ddots & & \vdots & \vdots \\ & & & & \ddots & \bullet & \text{red dot} \\ & & & & & \bullet & \text{red dot} \end{bmatrix}$$

$\underbrace{\hspace{10em}}_{d-1}$

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- 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

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

$\mathbf{W}$  is unitary.



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$\mathbf{W}$  is unitary. If  $\mathbf{G}$  is chosen such that  $\tilde{\mathbf{H}}$  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  $w_1$ .

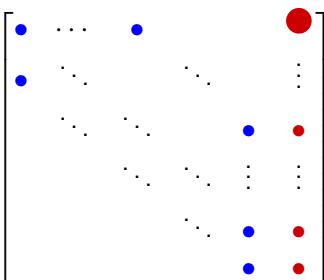
Up to the last column,  $\tilde{\mathbf{H}}$  has to be  $(s + 2)$ -band Hessenberg.

# 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  $h_{1,d} \neq 0$ .

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


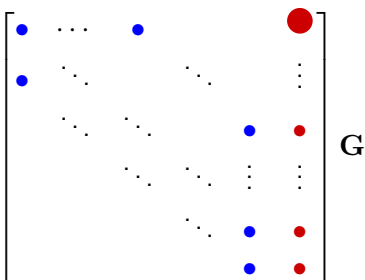
The diagram illustrates the matrix equation  $\mathbf{A} \mathbf{V} = \mathbf{V}$ . The matrix  $\mathbf{A}$  is represented by a large square bracket containing a grid of dots. The top row has a blue dot, followed by three dots, then a blue dot, and a large red dot in the top-right corner. The second row has a blue dot, followed by two dots, then a diagonal of two dots, and a vertical ellipsis. The third row has two dots, then a diagonal of two dots, then a blue dot, and a red dot. The fourth row has a diagonal of two dots, then a vertical ellipsis, and a red dot. The fifth row has a diagonal of two dots, then a blue dot, and a red dot. The sixth row has a blue dot and a red dot. The vector  $\mathbf{V}$  is represented by a column of dots, with a large red dot at the top and blue dots at the bottom.

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$$\mathbf{A}(\mathbf{V}\mathbf{G}) = (\mathbf{V}\mathbf{G})\mathbf{G}^*$$


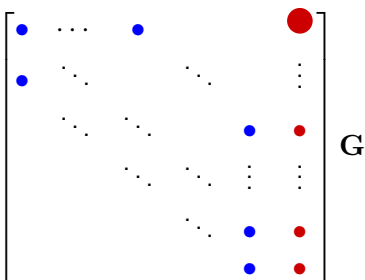
The diagram shows a matrix structure enclosed in large square brackets. The matrix is partitioned into several blocks. The top-left block contains a blue dot, followed by horizontal ellipses, and then another blue dot. The top-right block contains a large red dot. The middle-left block contains a blue dot. The middle-right block contains a vertical ellipsis. The bottom-left block contains a vertical ellipsis. The bottom-middle block contains a blue dot. The bottom-right block contains a red dot. The entire matrix is labeled  $\mathbf{G}$  to the right of the closing bracket.

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Find unitary  $\mathbf{G}$  (a product of Givens rotations) such that  $\tilde{\mathbf{H}}$  is unreduced upper Hessenberg, but  $\tilde{\mathbf{H}}$  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  $G_{7,8}$ .

$$\begin{bmatrix} \bullet & \bullet & \bullet & 0 & 0 & 0 & 0 & \bullet \\ \bullet & \bullet & \bullet & \bullet & 0 & 0 & 0 & \bullet \\ & \bullet & \bullet & \bullet & \bullet & 0 & 0 & \bullet \\ & & \bullet & \bullet & \bullet & 0 & & \bullet \\ & & & \bullet & \bullet & \bullet & & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \end{bmatrix} G_{7,8}$$

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$$G_{7,8}^* \begin{bmatrix} \bullet & \bullet & \bullet & 0 & 0 & 0 & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & 0 & 0 & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet & 0 & \bullet & \bullet \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \end{bmatrix}$$



# Idea of the second proof (3)

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

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

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$$G_{6,7}^* \begin{bmatrix} \bullet & \bullet & \bullet & 0 & 0 & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & 0 & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \end{bmatrix}$$



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

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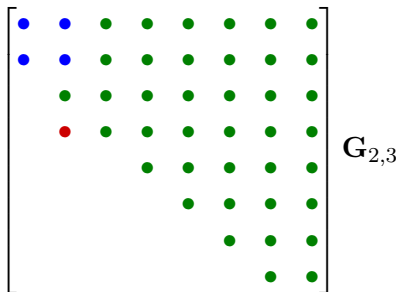
$$G_{3,4}^* \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \end{bmatrix}$$

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

Choose Givens rotation  $G_{7,8}$ .



The diagram shows an 8x8 matrix enclosed in large square brackets. The matrix contains dots representing non-zero entries. The dots are arranged in a staircase pattern from the top-left to the bottom-right. The first two columns have two blue dots each, located in the first and second rows. The remaining dots are green. The dot in the third row, second column is red. To the right of the matrix is the label  $G_{2,3}$ .

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Choose Givens rotation  $G_{7,8}$ .

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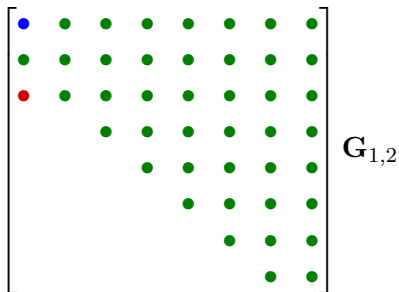


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The diagram shows an 8x8 matrix enclosed in large square brackets. The matrix contains dots representing its elements. The first row has a blue dot in the first column and green dots in the remaining seven columns. The second row has green dots in all eight columns. The third row has a red dot in the first column and green dots in the remaining seven columns. The fourth row has green dots in the second through eighth columns. The fifth row has green dots in the third through eighth columns. The sixth row has green dots in the fourth through eighth columns. The seventh row has green dots in the fifth through eighth columns. The eighth row has green dots in the sixth and seventh columns. To the right of the matrix is the label  $G_{1,2}$ .

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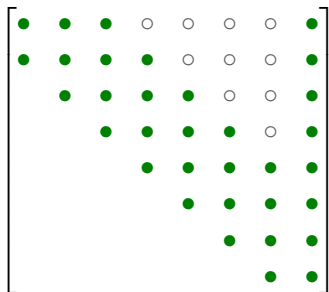
$$G_{1,2}^* \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet & \bullet & \bullet & \bullet \\ & & & & \bullet & \bullet & \bullet & \bullet \\ & & & & & \bullet & \bullet & \bullet \\ & & & & & & \bullet & \bullet \end{bmatrix}$$

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$$\mathbf{G} \equiv \mathbf{G}_{7,8} \mathbf{G}_{6,7} \dots \mathbf{G}_{1,2}, \quad \tilde{\mathbf{H}} \equiv \mathbf{G}^* \mathbf{H} \mathbf{G}.$$

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

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

# Summary

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

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



$\mathbf{A}$  is normal( $s$ )  
 $\mathbf{A}^* = p(\mathbf{A})$

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

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  - 1.  $s = 1$  if and only if the eigenvalues of  $\mathbf{A}$  lie on a line in  $\mathbb{C}$ .
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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
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