On short recurrences for generating orthogonal Krylov subspace bases

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

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

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

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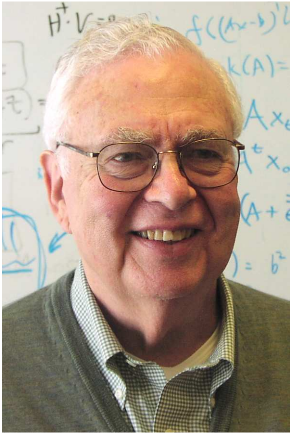
- An important assumption on $\mathbf{A}$:
  $\mathbf{A}$ is symmetric (MINRES, SYMMLQ) & pos. definite (CG).

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

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

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

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- $p_0, \dots, p_j$ 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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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. $\mathrm{span}\{v_1, \ldots, v_j\} = \mathcal{K}_j(A, v),$ for $j = 1, \ldots, d$,
  2. $\langle v_i, v_j \rangle = 0,$ for $i \neq j, \quad i, j = 1, \ldots, d$.

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

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

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

Formulation of the problem

Arnoldi's algorithm - matrix formulation

In matrix notation:

$$v_1 = v\,,$$

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

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

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$(s+2)$-term recurrence: $\quad v_{j+1} = \mathbf{A}\,v_j - \sum_{\mathbf{i=j-s}}^{j} h_{i,j} v_i\,.$

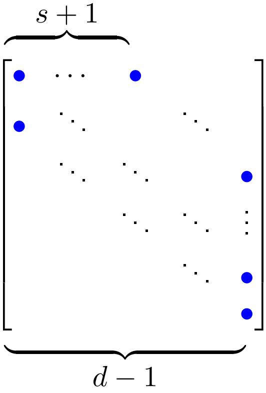
Formulation of the problem

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.

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



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

Sufficient and necessary conditions on $\mathbf{A}$?

Outline

The Faber-Manteuffel theorem

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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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, $s + 2 < d_{\min}(\mathbf{A})$:

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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).

Outline

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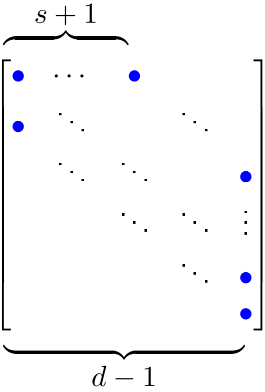
- We give two new proofs of the Faber-Manteuffel theorem that use more elementary tools,
- first proof - improved version of the Faber-Manteuffel proof,
- second proof - completely new proof based on orthogonal transformations of upper Hessenberg matrices.

Idea of the second proof

Optimal $(s+2)$-term recurrence

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



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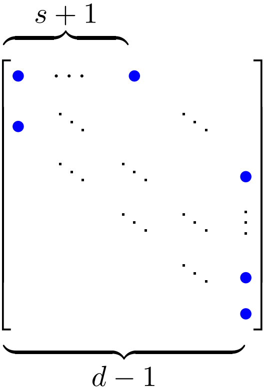


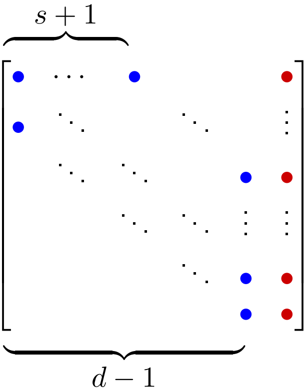
Since $\mathcal{K}_d(\mathbf{A}, v)$ is invariant, $\mathbf{A}v_d \in \mathcal{K}_d(\mathbf{A}, v)$ and

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

Idea of the second proof

Matrix representation of $\mathbf{A}$ in $\mathbf{V}_d$

$$\mathbf{A}\,\mathbf{V}_d \;=\; \mathbf{V}_d$$



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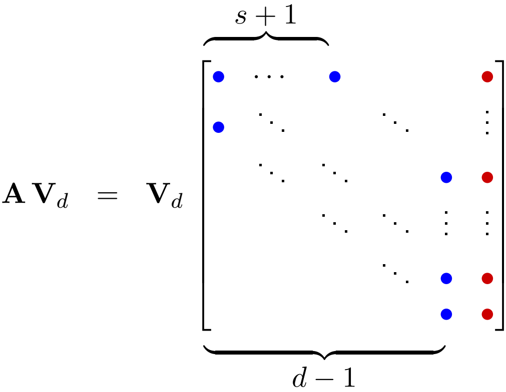

Prove something about the linear operator $\mathbf{A}$, without complete knowledge of the structure of its matrix representation.

Idea of the second proof

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 algorithm 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

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

$$\mathbf{A}\ \mathbf{V} \quad = \quad \mathbf{V} \begin{bmatrix} \bullet & \cdots & \bullet & & & \bullet \\ \bullet & \ddots & & \ddots & & \vdots \\ & \ddots & \ddots & & \bullet & \bullet \\ & & \ddots & \ddots & \vdots & \vdots \\ & & & \ddots & \bullet & \bullet \\ & & & & \bullet & \bullet \end{bmatrix}$$

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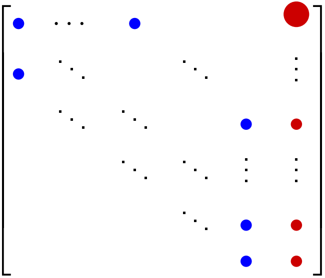

$$\mathbf{G}$$

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**.

Summary

Generating an orthogonal basis of $\mathcal{K}_d(\mathbf{A}, v)$ via Arnoldi-type recurrence

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

$$\Updownarrow$$

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

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

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  [Faber and Manteuffel, 1984],
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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.

Outline

Unitary matrices

Example

- Consider a unitary matrix $\mathbf{A}$ with different eigenvalues.

  $\mathbf{A}$ is normal $\implies$ $\mathbf{A}^*$ is a polynomial in $\mathbf{A}$

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- Using Faber-Manteuffel theorem: generating orthogonal Krylov subspace bases for unitary matrices via the Arnoldi process would require a full recurrence.

Unitary matrices

Isometric Arnoldi process

- Gragg (1982) discovered the *isometric Arnoldi process*: Orthogonal Krylov subspace bases for unitary $\mathbf{A}$ can be generated by a 3-term recurrence of the form

$$v_{j+1} = \beta_{j,j}\mathbf{A}v_j - \beta_{j-1,j}\mathbf{A}v_{j-1} - \sigma_{j,j}v_{j-1}$$

  (stable implementation - two coupled 2-term recurrences).

- Used for solving unitary eigenvalue problems and linear systems with shifted unitary matrices [Jagels and Reichel, 1994].

- This short recurrence is not of the "Arnoldi-type".

Generalization: (ℓ, m)-recursion

Barth and Manteuffel, 2000

Generate an orthogonal basis via the (ℓ, m)-recursion of the form

$$v_{j+1} = \sum_{i=j-m}^{j} \beta_{i,j}\, \mathbf{A}\, v_i \;-\; \sum_{i=j-\ell}^{j} \sigma_{i,j}\, v_i \,, \tag{1}$$

- $(\ell, m) = (0, 1)$ if $\mathbf{A}$ is unitary,
  $(\ell, m) = (1, 1)$ if $\mathbf{A}$ is shifted unitary.

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- A sufficient condition [Barth and Manteuffel, 2000]:
  $\mathbf{A}^*$ is a rational function in $\mathbf{A}$,

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

  where $r = p/q$, p and q have degrees ℓ and m.

  Example: Unitary matrices, $\mathbf{A}^* = \mathbf{A}^{-1}$, i.e. $r = 1/z$.

  Matrices $\mathbf{A}$ such that $\mathbf{A}^* = r(\mathbf{A})$ are called normal(ℓ, m).

Degree of a rational function, degrees of normality

normal degree of $\mathbf{A}$, McMillan degree of $\mathbf{A}$

Definition. McMillan degree of a rational function $r = p/q$ where p and q are relatively prime is defined as

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Definition. Let $\mathbf{A}$ be a diagonalizable matrix.

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When is $\mathbf{A}$ a low degree rational function in $\mathbf{A}$?

Collinear or concyclic eigenvalues

Application of results from rational interpolation theory:

Theorem. [Liesen, 2007] Let $\mathbf{A}$ be a diagonalizable matrix with $k \geq 4$ distinct eigenvalues.

- If the eigenvalues are collinear, then $d_r(\mathbf{A}) = d_p(\mathbf{A}) = 1$.
- If the eigenvalues are concyclic, then $d_r(\mathbf{A}) = 1$, $d_p(\mathbf{A}) = k - 1$.
- In all other cases $d_r(\mathbf{A}) > \frac{k}{5}$, $d_p(\mathbf{A}) > \frac{k}{3}$.

Summary

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

Arnoldi-type recurrence $(s+2)$-term	Barth-Manteuffel (ℓ, m)-recursion
$\Updownarrow$	$\Uparrow$
$\mathbf{A}$ is normal(s) $\mathbf{A}^* = p(\mathbf{A})$	$\mathbf{A}$ is normal(ℓ, m) $\mathbf{A}^* = r(\mathbf{A})$
$\updownarrow$	$\updownarrow$
the only interesting case is $s = 1$, collinear eigenvalues	the only interesting cases are $(0, 1)$ or $(1, 1)$ concyclic eigenvalues

Outline

The role of the matrix $\mathbf{B}$

Generating a $\mathbf{B}$-orthogonal basis

Let $\mathbf{B} \in \mathbb{C}^{n\times n}$ be a Hermitian positive definite (HPD), defining the $\mathbf{B}$-inner product, $\langle x, y\rangle_{\mathbf{B}} \equiv y^*\mathbf{B}x$.

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$\mathbf{B}$-normal(s) matrices: there exist a polynomial p_s of the smallest possible degree s such that

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Theorem. [Faber and Manteuffel, 1984], [Liesen and Strakoš, 2008]
For $\mathbf{A}$, $\mathbf{B}$ as above, and an integer $s \geq 0$ with $s + 2 < d_{\min}(\mathbf{A})$:

$\mathbf{A}$ admits for the given $\mathbf{B}$ an optimal $(s+2)$-term recurrence if and only if $\mathbf{A}$ is $\mathbf{B}$-normal(s).

The role of the matrix $\mathbf{B}$

Characterization of $\mathbf{B}$-normal(s) matrices

Theorem. [Liesen and Strakoš, 2008]

$\mathbf{A}$ is $\mathbf{B}$-normal(s) if and only if

1. $\mathbf{A}$ is diagonalizable ($\mathbf{A} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^{-1}$), and
2. $\mathbf{B} = (\mathbf{W}\mathbf{D}\mathbf{W}^*)^{-1}$, where $\mathbf{D}$ is HPD and block diagonal with blocks corresponding to those of $\mathbf{\Lambda}$, and
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The only interesting case: $\mathbf{B}$-normal(1) matrices

- If $\mathbf{A}$ is diagonalizable and the eigenvalues are collinear, then there exists $\mathbf{B}$ such that $\mathbf{A}$ is $\mathbf{B}$-normal(1).
- Find a preconditioner $\mathbf{P}$ so that $\mathbf{PA}$ is $\mathbf{B}$-normal(1) for some $\mathbf{B}$, e.g. [Concus and Golub, 1978], [Widlund, 1978].

Conclusions

We characterized matrices for which it is possible to generate an orthogonal basis of Krylov subspaces using short recurrences (normal(s), normal(ℓ, m)).

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- Find a preconditioner $\mathbf{P}$ so that $\mathbf{PA}$ is $\mathbf{B}$-normal(1) ($\mathbf{B}$-normal$(0,1)$, $\mathbf{B}$-normal$(1,1)$) for some $\mathbf{B}$.

Related papers

- J. Liesen and Z. Strakoš, [On optimal short recurrences for generating orthogonal Krylov subspace bases, SIAM Review, 50, 2008, pp. 485-503].
  The 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 Journal on Numerical Analysis, Volume 46, 2008, pp. 1323-1337.]
  New proofs of the fundamental theorem of Faber and Manteuffel.
- J. Liesen, [When is the adjoint of a matrix a low degree rational function in the matrix? SIAM J. Matrix Anal. Appl., 2007 , 29 , 1171-1180].
  A nice application of results from rational approximation theory.

More details

More details can be found at

http://www.cs.cas.cz/~tichy
http://www.math.tu-berlin.de/~liesen
http://www.cs.cas.cz/~strakos

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Thank you for your attention!