On short recurrences for generating orthogonal Krylov subspace bases

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joint work with

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Outline

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Krylov subspace methods

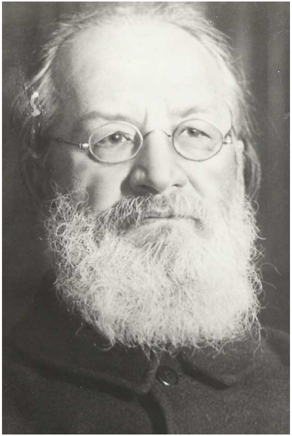
Given $\mathbf{A} \in \mathbb{R}^{n \times n}$, $v \in \mathbb{R}^n$. Define the j-dimensional Krylov subspace

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

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,
- named after Aleksei Nikolaevich Krylov (1863-1945), Russian navy general and scientist.

Krylov subspace methods



A. N. Krylov, 1931

1931 Krylov employs the sequence $v, \mathbf{A}v, \mathbf{A}^2v, \dots$ for determining the minimal polynomial of $\mathbf{A}$.

1952 First Krylov subspace methods (Hestenes/Stiefel, Lanczos), independently of Krylov's work.

1959 Term Krylov sequence (Householder/Bauer).

1980 Perception of *space* rather than *sequence*; term Krylov subspace (Parlett).

2000 Use of Krylov subspaces for solving $\mathbf{A}x = b$ considered among Top 10 algorithmic ideas of the 20th century (AIP/IEEE/SIAM).

Examples of Krylov subspace methods ideas

Projection onto the Krylov subspace

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

  find x_j such that

  $$x_j \in \mathcal{K}_j(\mathbf{A}, b), \qquad r_j \perp \mathbf{A}\mathcal{K}_j(\mathbf{A}, b).$$

- $\mathbf{A}y = \lambda y$,

  find (y_j, μ_j) such that

  $$\mathbf{A}\, y_j - \mu_j\, y_j \ \perp\ \mathcal{K}_j(\mathbf{A}, v).$$

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

Basis

- 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.
- Best of both worlds:
  Orthogonal basis computed by short recurrence.
- First such method for $\mathbf{A}x = b$:
  Conjugate gradient (CG) method of Hestenes and Stiefel.

The classical CG method of Hestenes and Stiefel

US Nat. Bureau of Standards Preprint No. 1659, March 10, 1952

In case the matrix A is <u>symmetric</u> and <u>positive definite</u>, the following formulas are used in the conjugate gradient method.

$$p_o = r_o = k - Ax_o \qquad (x_o \text{ arbitrary}) \tag{3:1a}$$

$$a_i = \frac{|r_i|^2}{(p_i, Ap_i)} \tag{3:1b}$$

$$x_{i+1} = x_i + a_i p_i \tag{3:1c}$$

$$\boxed{r_{i+1} = r_i - a_i A p_i} \tag{3:1d}$$

$$b_i = \frac{|r_{i+1}|^2}{|r_i|^2} \tag{3:1e}$$

$$\boxed{p_{i+1} = r_{i+1} + b_i p_i} . \tag{3:1f}$$

Properties of CG

If $\mathbf{A}$ is symmetric and positive definite,
the two coupled two-term recurrences yield

- $r_0, \ldots, r_{j-1}$, an orthogonal basis of $\mathcal{K}_j(\mathbf{A}, r_0)$,
- $p_0, \ldots, p_{j-1}$, an $\mathbf{A}$-orthogonal basis of $\mathcal{K}_j(\mathbf{A}, r_0)$.

Mathematically equivalent: One three-term recurrence

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

(Rutishauser implementation, 1959).

In the background of CG, one can see the Lanczos algorithm for computation of orthogonal basis.

MINRES and SYMMLQ

SIAM J. NUMER. ANAL.
Vol. 12, No. 4, September 1975

SOLUTION OF SPARSE INDEFINITE SYSTEMS OF LINEAR EQUATIONS*

C. C. PAIGE† AND M. A. SAUNDERS‡

Abstract. The method of conjugate gradients for solving systems of linear equations with a symmetric positive definite matrix A is given as a logical development of the Lanczos algorithm for tridiagonalizing A. This approach suggests numerical algorithms for solving such systems when A is symmetric but indefinite. These methods have advantages when A is large and sparse.

- CG is for symmetric positive definite $\mathbf{A}$.
- In 1975, Paige and Saunders derived MINRES and SYMMLQ, two short recurrence methods for symmetric indefinite $\mathbf{A}$.
- Similar to CG, both are based on three-term recurrences

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

for generating an orthogonal basis $r_0, \ldots, r_{j-1}$ of $\mathcal{K}_j(\mathbf{A}, r_0)$.

Observation

- Assumption: $\mathbf{A}$ is symmetric and positive definite (CG) or $\mathbf{A}$ is symmetric (MINRES, SYMMLQ).

- CG, MINRES, SYMMLQ are based on three-term recurrences

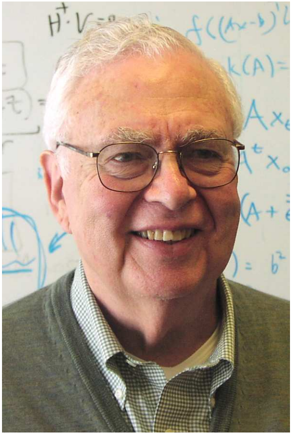
$$r_{j+1} = \gamma_j \mathbf{A} r_j - \alpha_j r_j - \beta_j r_{j-1} .$$

- These methods generate orthogonal (or $\mathbf{A}$-orthogonal) Krylov subspace basis.

- They are *optimal* in the sense that they minimize some norm of the error:

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

Gene Golub



G. H. Golub, 1932–2007

- By the end of the 1970s it was unknown if such methods existed also for general unsymmetric $\mathbf{A}$.
- Golub posed this fundamental question at 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 (1)

- We want to solve $\mathbf{A}x = b$ iteratively, starting from x_0.
- Step $j = 0, 1, \ldots$:

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

  p_j is a direction vector, α_j is a scalar (to be determined).
- This means

$$x_{j+1} \in x_0 + \mathrm{span}\{p_0, \ldots, p_j\} \,.$$

- This becomes a Krylov subspace method when

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

  $(r_0 = b - \mathbf{A}x_0)$.

What kind of method Golub had in mind (2)

- Error in step $j+1$:

$$x - x_{j+1} \;\in\; x - x_0 + \operatorname{span}\{p_0, \dots, p_j\}\,.$$

- CG-like descent method: error is minimized in some given inner product norm, $\|\cdot\|_{\mathbf{B}} = \langle \cdot, \cdot \rangle_{\mathbf{B}}^{1/2}$.
- $\|x - x_{j+1}\|_{\mathbf{B}}$ is minimal iff

$$x - x_{j+1} \;\perp_{\mathbf{B}}\; \operatorname{span}\{p_0, \dots, p_j\}\,.$$

- By construction, this is satisfied iff

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

  for $i = 0, \dots, j-1$.
- $p_0, \dots, p_j$ has to be a $\mathbf{B}$-orthogonal basis of $\mathcal{K}_{j+1}(\mathbf{A}, r_0)$.

Faber and Manteuffel, 1984

SIAM J. NUMER. ANAL.
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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

Our goal is to generate a $\mathbf{B}$-orthogonal basis of $\mathcal{K}_j(\mathbf{A}, v)$.

$\mathbf{B} \in \mathbb{C}^{n\times n}$, Hermitian positive definite (HPD),
defining the $\mathbf{B}$-inner product,

$$\langle x, y\rangle_{\mathbf{B}} \;\equiv\; y^*\mathbf{B}\, x\,.$$

If $\mathbf{B} \neq \mathbf{I}$, we can change the basis:

$$\langle x, y\rangle_{\mathbf{B}} \;=\; \langle \mathbf{B}^{1/2}x, \mathbf{B}^{1/2}y\rangle,$$

and consider the problem for $\hat{\mathbf{A}} \;\equiv\; \mathbf{B}^{1/2}\mathbf{A}\mathbf{B}^{-1/2}$ and $\hat{v} \;\equiv\; \mathbf{B}^{1/2}v$.

Without loss of generality, $\mathbf{B} = \mathbf{I}$.

Formulation of the problem

Input, Notation and Goal

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 $\mathbf{A}$,

  $\mathcal{K}_1(\mathbf{A}, v) \subset \ldots \subset \mathcal{K}_d(\mathbf{A}, v) = \mathcal{K}_{d+1}(\mathbf{A}, v) = \ldots = \mathcal{K}_n(\mathbf{A}, v)\,.$

  $\mathcal{K}_d(\mathbf{A}, v)$ is invariant under multiplication with $\mathbf{A}$.

Our goal:

- Generate an orthogonal basis $v_1, \ldots, v_d$ of $\mathcal{K}_d(\mathbf{A}, v)$,

  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 $i \neq j$, $i, j = 1, \ldots, d$.

Standard way for generating the orthogonal basis
(no normalization for convenience):

$$
\begin{aligned}
v_1 &= v\,, \\
v_2 &= \mathbf{A}v_1 - h_{1,1}\,v_1\,, \\
v_3 &= \mathbf{A}v_2 - h_{1,2}\,v_1 - h_{2,2}\,v_2\,, \\
&\vdots \\
v_{j+1} &= \mathbf{A}v_j - \sum_{i=1}^{j} h_{i,j}\,v_i\,, \qquad\qquad h_{i,j} = \frac{\langle \mathbf{A}v_j, v_i\rangle}{\langle v_i, v_i\rangle}\,. \\
&\vdots \\
v_d &= \mathbf{A}v_{d-1} - \sum_{i=1}^{d-1} h_{i,d-1}\,v_i\,.
\end{aligned}
$$

Formulation of the problem

Arnoldi's method - matrix formulation

In matrix notation:

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

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

The full recurrence in Arnoldi's method,

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

$(j = 1, \ldots, d-1)$ is an optimal $(s+2)$-term recurrence when

$$v_{j+1} = \mathbf{A}\, v_j \, - \sum_{\mathbf{i=j-s}}^{j} h_{i,j} v_i \,.$$

CG, MINRES, SYMMLQ: $s = 1 \rightarrow$ optimal 3-term recurrence,

$$v_{j+1} \; = \; \mathbf{A}\, v_j - h_{j,j}\, v_n - h_{j-1,j}\, v_{j-1} \,.$$

Why *optimal*?

1. Only the previous $s+1$ vectors are required.
2. Only one multiplication with $\mathbf{A}$ is performed.

Nonzero structure of the matrices $\mathbf{H}_{d,d-1}$:

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

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

$\mathbf{H}_{d,d-1}$ is $(s+2)$-band Hessenberg,

e.g. 3-band Hessenberg = tridiagonal.

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

(the first row spans $\overbrace{\bullet \;\cdots\; \bullet}^{s+1}$)

- $s \geq 0$ a nonnegative integer.
- Practical cases: s is a small positive integer.
- If $s + 2 = d_{\min}(\mathbf{A})$, the upper part of $\mathbf{H}_{d,d-1}$ is full

Interesting cases

$$0 \leq s < d_{\min}(\mathbf{A}) - 2\,.$$

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.

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

Formulation of the problem

Basic question

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

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

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

Outline

A sufficient condition

- $\mathbf{H}_{d,d-1}$ is at most $(s+2)$-band Hessenberg if

$$0 = h_{i,j} = \frac{\langle \mathbf{A} v_j, v_i \rangle}{\langle v_i, v_i \rangle} = \frac{\langle v_j, \mathbf{A}^* v_i \rangle}{\langle v_i, v_i \rangle},$$

  for $i < j - s$, $j = 1, \ldots, d-1$.

- Since $v_j \perp \mathcal{K}_{j-1}(\mathbf{A}, v)$,

  it would be sufficient if $\mathbf{A}^* v_i \in \mathcal{K}_{j-1}(\mathbf{A}, v)$,.

- If $\mathbf{A}^* = p_s(\mathbf{A})$ for a polynomial of degree s, then

$$\mathbf{A}^* v_i = p_s(\mathbf{A}) q_i(\mathbf{A}) v \in \mathcal{K}_{i+s}(\mathbf{A}, v) \subseteq \mathcal{K}_{j-1}(\mathbf{A}, v)$$

  for $i < j - s$.

- In other words:
  $\mathbf{A}^* = p_s(\mathbf{A}) \implies \mathbf{H}_{d,d-1}$ is at most $(s+2)$-band Hessenberg.

Normal(s) property

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).

$\mathbf{A}$ is normal means $\mathbf{A}^*\mathbf{A} = \mathbf{A}\mathbf{A}^*$, or,

$$\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^*, \quad \mathbf{U}^*\mathbf{U} = \mathbf{I}\,, \quad \mathbf{\Lambda} \text{ is diagonal}\,,$$

see [Elsner and Ikramov, 1997] for equivalent definitions of normality.

Let $\mathbf{A}$ be normal, i.e. $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^*$ and $\mathbf{A}^* = \mathbf{U}\mathbf{\Lambda}^*\mathbf{U}^*$. Then there exists the unique interpolating polynomial p such that

$$p(\lambda_i) = \overline{\lambda}_i, \qquad i = 1, \ldots, n, \qquad \text{i.e.} \qquad p(\mathbf{\Lambda}) = \mathbf{\Lambda}^*\,.$$

p is of degree at most $d_{\min}(\mathbf{A}) - 1$. Therefore

$$p(\mathbf{A}) = \mathbf{U}p(\mathbf{\Lambda})\mathbf{U}^* = \mathbf{U}\mathbf{\Lambda}^*\mathbf{U}^* = \mathbf{A}^*.$$

"normal(s)" can be understood as a grade of normality.

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).

- 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:

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

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

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

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

$$\mathbf{A}\,\mathbf{V}_d \quad = \quad \mathbf{V}_d \begin{array}{c} \begin{array}{cccccc} \multicolumn{3}{c}{\overbrace{\hspace{6em}}^{s+1}} & & & \end{array} \\ \left[\begin{array}{cccccc} {\color{blue}\bullet} & \cdots & {\color{blue}\bullet} & & & {\color{red}\bullet} \\ {\color{blue}\bullet} & \ddots & & \ddots & & \vdots \\ & \ddots & \ddots & & {\color{blue}\bullet} & {\color{red}\bullet} \\ & & \ddots & \ddots & \vdots & \vdots \\ & & & \ddots & {\color{blue}\bullet} & {\color{red}\bullet} \\ & & & & {\color{blue}\bullet} & {\color{red}\bullet} \end{array}\right] \\ \begin{array}{cccccc} \multicolumn{5}{c}{\underbrace{\hspace{12em}}_{d-1}} & \end{array} \end{array}$$

The Faber-Manteuffel theorem

The role of the matrix $\mathbf{B}$ defining scalar product

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

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

$$\mathbf{A}^+ \equiv \mathbf{B}^{-1} \mathbf{A}^* \mathbf{B} = p_s(\mathbf{A}),$$

where $\mathbf{A}^+$ the $\mathbf{B}$-adjoint of $\mathbf{A}$.

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).

Theorem. [Liesen and Strakoš, 2008]

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

1. $\mathbf{A}$ is diagonalizable ($\mathbf{A} = \mathbf{W}\boldsymbol{\Lambda}\mathbf{W}^{-1}$), 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 $\boldsymbol{\Lambda}$, and
3. $\boldsymbol{\Lambda}^* = p_s(\boldsymbol{\Lambda})$ for a polynomial p_s of (smallest possible) degree s.

- $s = 1$: If $\mathbf{A}$ is diagonalizable and $\boldsymbol{\Lambda}^* = p_1(\boldsymbol{\Lambda})$, then there exists $\mathbf{B}$ such that $\mathbf{A}$ is $\mathbf{B}$-normal(1).

The Faber-Manteuffel theorem

When is a matrix $\mathbf{B}$-normal(s)?

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

Theorem. [Faber and Manteuffel, 1984], [Khavinson and Świątek, 2003]

1. $s = 1$ if and only if the eigenvalues of $\mathbf{A}$ lie on a line in $\mathbb{C}$.
2. If the eigenvalues of $\mathbf{A}$ are *not* on a line, the shortest possible optimal recurrence $\mathbf{A}$ may admit has length at least $d_{\min}(\mathbf{A})/3 + 4$.

This results is connected with the question: How many roots can have the *harmonic polynomial** $p_s(z) - \overline{z}$?

Answer [Khavinson and Świątek, 2003]: with $s > 1$ it may have *at most* $3s - 2$ roots.

* A harmonic polynomial is a function of the form $p(z) + \overline{q(z)}$, where p and q are polynomials.

The previous results is very pessimistic:

Except for a few unimportant cases, the length of the optimal recurrence is either 3 or $d_{\min}(\mathbf{A}) - 1$.

The most interesting cases are

1. The Hermitian case ($\mathbf{A} = \mathbf{A}^*$)

$$\mathbf{A}^* = p_1(\mathbf{A}) \quad \text{for} \quad p_1(z) = z\,.$$

2. The skew-Hermitian case ($\mathbf{A} = -\mathbf{A}^*$):

$$\mathbf{A}^* = p_1(\mathbf{A}) \quad \text{for} \quad p_1(z) = -z\,.$$

We can try to find a HPD matrix $\mathbf{B} \in \mathbb{C}^{n \times n}$ such that

$$\mathbf{B}^{-1}\mathbf{A}^{*}\mathbf{B} = \pm\,\mathbf{A}.$$

Example: Saddle point matrix:

$$\mathbf{A} = \begin{bmatrix} A_1 & A_2^T \\ -A_2 & A_3 \end{bmatrix},$$

where $A_1 = A_1^T > 0$, $A_3 = A_3^T \geq 0$ has full rank $k \leq m$. Define

$$\mathbf{B} = \mathbf{B}(\gamma) = \begin{bmatrix} A_1 - \gamma I_m & A_2^T \\ A_2 & \gamma I_k - A_3 \end{bmatrix},$$

This matrix satisfies $\mathbf{B}^{-1}\mathbf{A}^{*}\mathbf{B} = \mathbf{A}$. How to choose γ such that $\mathbf{B}(\gamma)$ is positive definite? Conditions can be found in [Fischer et al., 1998], [Benzi and Simoncini, 2006], [Liesen and Parlett, 2007].

Summary

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

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

$$\Updownarrow$$

$\mathbf{A}$ is $\mathbf{B}$-normal(s)
$\mathbf{A}^+ = p(\mathbf{A})$

$$\updownarrow$$

the only interesting case
is $s = 1$,
collinear eigenvalues

Outline

The Faber-Manteuffel theorem

Historical remarks

1981 Golub posed the question

1984 V. Faber and T. Manteuffel, [Necessary and sufficient conditions for the existence of a conjugate gradient method, SIAM J. Numer. Anal. 21 , 352-362].

1981 V. V. Voevodin and E. E. Tyrtyshnikov, [On Generalization of Conjugate Direction Methods, Moscow State University Press, 3-9].

- Axelsson (1987), Greenbaum (1997) - sufficiency part

2005 J. Liesen and P. E. Saylor, [Orthogonal Hessenberg reduction and orthogonal Krylov subspace bases, SIAM J. Numer. Anal., 2005 , 42, 2148-2158].

2008 J. Liesen and Z. Strakoš, [On optimal short recurrences for generating orthogonal Krylov subspace bases, to appear in SIAM Review, 2008].

2008 V. Faber, J. Liesen and P. Tichý, [The Faber-Manteuffel Theorem for Linear Operators, to appear in SIAM Journal on Numerical Analysis, 2008].

Faber and Manteuffel, 1984

Necessary and sufficient conditions for the existence of a conjugate gradient method

- Their definition of "$\mathbf{A}$ admits an optimal s-term recurrence" (in the paper called $\mathbf{A} \in \mathrm{CG}(s)$) is not unique in the following sense:

$$\text{if } \mathbf{A} \in \mathrm{CG}(s), \text{ then also } \mathbf{A} \in \mathrm{CG}(s+1).$$

- The original version of the Faber-Manteuffel theorem:

  $\mathbf{A} \in \mathrm{CG}(s)$ if and only if
  $d_{\min}(\mathbf{A}) \leq s$ or $\mathbf{A}$ is normal and $n(\mathbf{A}) \leq s-2$.

  ($n(\mathbf{A})$ is the smallest polynomial degree such that $\mathbf{A}^* = p(\mathbf{A})$)

- This "non uniqueness" in the definition complicated understanding the theorem and led to some misunderstandings in later papers.

V. V. Voevodin and E. E. Tyrtyshnikov, 1981

On Generalization of Conjugate Direction Methods

A similar result was announced by V.V. Voevodin,

- V. V. Voevodin, [The problem of a non-selfadjoint generalization of the conjugate gradient method has been closed, U.S.S.R. Comput. Math. and Math. Phys., 1983, 23, 143–144].

Its proof (difficult to understand) appeared in

- V. V. Voevodin and E. E. Tyrtyshnikov, [On Generalization of Conjugate Direction Methods, Moscow State University Press, 3-9].

Two big differences:

- Assumptions: $\mathbf{A}$ is nonderogatory ($d_{\min}(\mathbf{A}) = n$),
- Characterization of necessity only for $3s + 2 \leq n$.
- Incorrect understanding of $(s + 2)$-term recurrence.

Faber and Manteuffel: $\mathbf{A}$ admits $(s+2)$-term recurrences if

$$
\mathbf{A}\,\mathbf{V}_d \;=\; \mathbf{V}_d
\begin{array}{l}
\overbrace{\hphantom{\bullet \quad \cdots \quad \bullet}}^{s+1} \\
\left[\begin{array}{cccccc}
\bullet & \cdots & \bullet & & & \bullet \\
\bullet & \ddots & & \ddots & & \vdots \\
 & \ddots & \ddots & & \bullet & \bullet \\
 & & \ddots & \ddots & \vdots & \vdots \\
 & & & \ddots & \bullet & \bullet \\
 & & & & \bullet & \bullet
\end{array}\right] \\
\underbrace{\hphantom{\bullet \quad \ddots \quad \ddots \quad \ddots \quad \bullet}}_{d-1}
\end{array}
$$

V. V. Voevodin and E. E. Tyrtyshnikov, 1981

On Generalization of Conjugate Direction Methods

Voevodin and Tyrtyshnikov: $\mathbf{A}$ admits $(s+2)$-term recurrences if

$$\mathbf{A}\,\mathbf{V}_d \;=\; \mathbf{V}_d \begin{array}{l} \overbrace{\hphantom{\bullet \quad \cdots \quad \bullet}}^{s+1} \\ \left[\begin{matrix} \bullet & \cdots & \bullet & & & \\ \bullet & \ddots & & \ddots & & \\ & \ddots & \ddots & & \bullet & \\ & & \ddots & \ddots & \vdots & \bullet \\ & & & \ddots & \bullet & \vdots \\ & & & & \bullet & \bullet \end{matrix}\right] \\ \underbrace{\hphantom{\bullet \quad \cdots \quad \bullet \quad \ddots \quad \ddots \quad \bullet}}_{d-1} \end{array}$$

i.e. $\mathbf{A}$ is orthogonally reduced to $(s+2)$-band Hessenberg form.

J. Liesen and P. E. Saylor, 2005

Orthogonal Hessenberg reduction and orthogonal Krylov subspace bases

They study necessary and sufficient conditions that $\mathbf{A}$ can be $\mathbf{B}$-orthogonally reduced to $(s+2)$-band upper Hessenberg form.

- A similar result to Voevodin and Tyrtyshnikov.
- The authors explain the difference between reducibility to $(s+2)$-band upper Hessenberg form and $(s+2)$-term recurrence.
- Assumption: $\mathbf{A}$ is nonderogatory.
- Complete characterization of necessity (not only for $3s+2 \leq n$).

J. Liesen and Z. Strakoš, 2008

On optimal short recurrences for generating orthogonal Krylov subspace bases

- Completely reworked the theory of short recurrences for generating orthogonal Krylov subspace bases; new, mathematically rigorous definitions of all important concepts have been given,
- unique definition of "$\mathbf{A}$ admits an optimal $(s+2)$-term recurrence",
- a stronger version of the Faber-Manteuffel theorem,
- characterization of the $\mathbf{B}$-normal(s) property,
- it is desirable to find an alternative, and possibly simpler proof.

Moreover ... (see the next slide)

J. Liesen and Z. Strakoš, 2008

On optimal short recurrences for generating orthogonal Krylov subspace bases

For simplicity assume that $\mathbf{B} = \mathbf{I}$.

Theorem. Let s be a nonnegative integer, $s + 2 < d_{\min}(\mathbf{A})$. Then the following three assertions are equivalent:

1. $\mathbf{A}$ admits an optimal $(s+2)$-term recurrence.
2. $\mathbf{A}$ is normal(s).
3. $\mathbf{A}$ is orthogonally reducible to $(s+2)$-band Hessenberg form.

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],
- in terms of linear operators on finite dimensional Hilbert spaces,
- two new proofs of the Faber-Manteuffel theorem,
- 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 $\mathbf{A}$ admits 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.
Let $\mathbf{G}$ be a $d \times d$ unitary matrix, $\mathbf{G}^*\mathbf{G} = \mathbf{I}$. Then

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

$\mathbf{W}$ 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 result of the 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 $\mathbf{A}$ admits an optimal $(s+2)$-term recurrence and $\mathbf{A}$ is not normal(s).

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

$$\mathbf{A}\,(\mathbf{VG}) \;=\; (\mathbf{VG})\,\mathbf{G}^{*} \begin{bmatrix} \bullet & \cdots & \bullet & & & \bullet \\ \bullet & \ddots & & \ddots & & \vdots \\ & \ddots & \ddots & & \bullet & \bullet \\ & & \ddots & \ddots & \vdots & \vdots \\ & & & \ddots & \bullet & \bullet \\ & & & & \bullet & \bullet \end{bmatrix} \mathbf{G}$$

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**.

Outline

Unitary matrices

Example

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

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

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

- The smallest degree of such polynomial is $n-1$ (n is the size of the matrix), i.e. $\mathbf{A}$ is normal$(n-1)$ [Liesen, 2007].

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

- 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 a $\mathbf{B}$-orthogonal basis via the (ℓ, m)-recursion of the form

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

- $(\ell, m) = (0, 1)$ if $\mathbf{A}$ is unitary,
  $(\ell, m) = (1, 1)$ if $\mathbf{A}$ is shifted unitary.
- A sufficient condition [Barth and Manteuffel, 2000]:
  $\mathbf{A}^+ = \mathbf{B}^{-1}\mathbf{A}^*\mathbf{B}$ is a rational function in $\mathbf{A}$,

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

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

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

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

$$\deg r = \max\{\deg p, \deg q\}.$$

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

- $d_p(\mathbf{A})$ ... normal degree of $\mathbf{A}$
  the smallest degree of a polynomial p that satisfies

  $$p(\lambda) = \overline{\lambda} \;\text{ for all eigenvalues }\; \lambda \;\text{ of }\; \mathbf{A}\,.$$

- $d_r(\mathbf{A})$ ... McMillan degree of $\mathbf{A}$
  the smallest McMillan degree of a rational function r that satisfies

  $$r(\lambda) = \overline{\lambda} \;\text{ for all eigenvalues }\; \lambda \;\text{ of }\; \mathbf{A}\,.$$

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

Collinear or concyclic eigenvalues

Are there any other matrices $\mathbf{A}$ whose adjoint $\mathbf{A}^+$ (for some $\mathbf{B}$) is a low degree rational function in $\mathbf{A}$?

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 $d_r(\mathbf{A}) > \frac{k}{5}$, $d_p(\mathbf{A}) > \frac{k}{3}$.

In other words, there is a HPD matrix $\mathbf{B}$ such that $\mathbf{A}^+ = r(\mathbf{A})$ with small $\deg r$ if and only if either $d_{\min}(\mathbf{A})$ is small, or $\mathbf{A}$ is diagonalizable with collinear or concyclic eigenvalues.

Summary

Generating of $\mathbf{B}$-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 $\mathbf{B}$-normal(s) $\mathbf{A}^+ = p(\mathbf{A})$	$\mathbf{A}$ is $\mathbf{B}$-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

Given $\mathbf{A}$.

- If eigenvalues of $\mathbf{A}$ are collinear or concyclic, then there exists a HPD matrix $\mathbf{B}$ such that $\mathbf{A}$ admits short recurrences for generating a $\mathbf{B}$-orthogonal basis.
- 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 $\mathbf{B}$,
  e.g. [Concus and Golub, 1978], [Widlund, 1978].

- T. Barth and T. Manteuffel, [Multiple recursion conjugate gradient algorithms. I. Sufficient conditions. SIAM J. Matrix Anal. Appl., 2000 , 21 , 768-79].

Generalized $\mathbf{B}$-normal(ℓ, m) **matrices** $\mathbf{A}$

are characterized through the existence of polynomials $p_\ell(\lambda)$ and $q_m(\lambda)$ of degree ℓ and m, respectively, such that

$$Q(\mathbf{A}) = \mathbf{A}^+ q_m(\mathbf{A}) - p_\ell(\mathbf{A}),$$

where $Q(\mathbf{A})$ is a matrix of a low rank s.

[Barth and Manteuffel, 2000]: It is possible to construct a $\mathbf{B}$-orthogonal basis of $\mathcal{K}_j(A, v)$ using short *multiple recursion*.

- B. Beckermann and L. Reichel, [The Arnoldi process and GMRES for nearly symmetric matrices, to appear in SIAM J. Matrix Anal. Appl., 2008].

Computation of an orthogonal basis of the Krylov space $\mathcal{K}_j(\mathbf{A}, v)$, where $\mathbf{A}$ is a matrix with a skew-symmetric part of low rank,

$$\mathbf{A} - \mathbf{A}^* = \sum_{k=1}^{s} f_k g_k^*, \qquad f_k, g_k \in \mathbb{R}^n, \qquad s \ll n\,.$$

- Efficient implementation of a GMRES-like algorithm - "Progressive GMRES".

- Application: Path following methods (Bratu problem).

Conclusions

- We considered two kinds of recurrences for generating a $\mathbf{B}$-orthogonal basis of Krylov subspaces.
- We characterized matrices for which these recurrences are short ($\mathbf{B}$-normal(s), $\mathbf{B}$-normal(ℓ, m) matrices).
- Practical cases: Eigenvalues of $\mathbf{A}$ are collinear or concyclic, $s = 1$, $(\ell, m) = (0, 1)$, $(\ell, m) = (1, 1)$.
- It is possible to generate a $\mathbf{B}$-orthogonal basis via short recurrences for low rank perturbations of $\mathbf{B}$-normal(ℓ, m) matrices.

Related papers

- J. Liesen and Z. Strakoš, [On optimal short recurrences for generating orthogonal Krylov subspace bases, to appear in SIAM Review, 2008].
  Completely reworked the theory of short recurrences for generating orthogonal Krylov subspace bases

- V. Faber, J. Liesen and P. Tichý, [The Faber-Manteuffel Theorem for Linear Operators, to appear in SIAM Journal on Numerical Analysis, 2008].
  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 can be found at

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