On optimal short recurrences for generating orthogonal Krylov subspace bases

Jörg Liesen

based on joint work with

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Vance Faber (BD Biosciences, Seattle),

Beresford Parlett (Berkeley), and Paul Saylor (Illinois)

Overview

1. Introduction: Krylov subspace methods
2. Optimal short recurrences
3. Characterization and examples

Introduction: Krylov subspace methods (1)

- Methods that are based on *projection onto the Krylov subspaces*

$$\mathcal{K}_n(A, v_1) \equiv \text{span}\{v_1, Av_1, \ldots, A^{n-1}v_1\}, \quad n = 1, 2, \ldots,$$

  where A is a given square matrix and v_1 is the initial vector.

- Must generate bases of $\mathcal{K}_n(A, v_1)$, $n = 1, 2, \ldots$.
- Trivial choice: $v_1, Av_1, \ldots, A^{n-1}v_1$.
  This is computationally infeasible (recall the Power Method).

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  This 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 $Ax = b$:
  Conjugate gradient (CG) method of Hestenes and Stiefel (1952).

Introduction: Krylov subspace methods (2)

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

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

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

(3:1c) $$x_{i+1} = x_i + a_i p_i$$

(3:1d) $$r_{i+1} = r_i - a_i A p_i$$

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

(3:1f) $$p_{i+1} = r_{i+1} + b_i p_i .$$

The classical CG method of Hestenes and Stiefel

(US National Bureau of Standards Preprint No. 1659, March 10, 1952)

The residual vectors $r_0, r_1, \ldots, r_{n-1}$ are generated by a short recurrence and form an orthogonal basis of $\mathcal{K}_n(A, r_0)$.

Introduction: Krylov subspace methods (3)

- CG is for symmetric positive definite A.
- (Paige and Saunders, 1975):
  Short recurrence & orthogonal basis methods for symmetric A.

SIAM J. NUMER. ANAL.
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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.

Introduction: Krylov subspace methods (4)

- By the end of the 1970s it was unknown if such methods existed also for general unsymmetric A.
- *Gene Golub posed this fundamental question* at Gatlinburg VIII (now Householder VIII) held in Oxford from July 5 to 11, 1981:

SIGNUM
NEWSLETTER

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It is not uncommon for speakers to pose an open problem to their audience during their talk. What is unprecedented is for such a proposition to be backed by some stake money. Perhaps a new era in numerical analysis sponsorship began at Gatlinburg VIII when three of the participants offered prize money for the solution of problems which they posed during the meeting. I list the challenges below so that you can make a bid for glory (or cash) by solving them.

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 does this mean?

Introduction: Krylov subspace methods (5)

- We want to solve $Ax = b$ iteratively, starting from x_0.
- Step $n = 1, 2, \ldots$: $x_n = x_{n-1} + \alpha_{n-1} p_{n-1}$,
  direction vector p_{n-1}, scalar α_{n-1} (both to be determined).
- Krylov subspace method:
  $\mathrm{span}\{p_0, \ldots, p_{n-1}\} = \mathcal{K}_n(A, v_1) \quad (v_1 = r_0 = b - Ax_0)$.
- CG-like descent method:
  Error is minimized in some given inner product norm, $\| \cdot \|_B = \langle \cdot, \cdot \rangle_B^{1/2}$.

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- CG-like descent method:
  Error is minimized in some given inner product norm, $\|\cdot\|_B = \langle \cdot, \cdot \rangle_B^{1/2}$.
- $\|x - x_n\|_B$ is minimal iff $x - x_n \perp_B \mathrm{span}\{p_0, \ldots, p_{n-1}\}$.
- By construction, this is satisfied iff

$$\alpha_{n-1} = \frac{\langle x - x_{n-1}, p_{n-1} \rangle_B}{\langle p_{n-1}, p_{n-1} \rangle_B} \quad \text{and} \quad \langle p_{n-1}, p_j \rangle_B = 0, \;\; j = 0, \ldots, n-2,$$

i.e. $p_0, \ldots, p_{n-1}$ *must be a* B*-orthogonal basis of* $\mathcal{K}_n(A, v_1)$.

Introduction: Krylov subspace methods (6)

- Faber and Manteuffel answered Golub's question in 1984:
  For a general matrix A there exists *no* CG-like descent method (related results by Voevodin and Tyrtyshnikov in the early 1980s).

SIAM J. NUMER. ANAL.
Vol. 21, No. 2, April 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 $B^*=-B$.

What are the details of this result?

Optimal short recurrences (1)

Notation:

- Matrix $A \in \mathbb{C}^{N \times N}$, nonsingular.
- Matrix $B \in \mathbb{C}^{N \times N}$, Hermitian positive definite (HPD), defining the B-inner product, $\langle x, y \rangle_B \equiv y^* B x$.
- Initial vector $v_1 \in \mathbb{C}^N$.
- $d = d(A, v_1)$, the grade of v_1 with respect to A,

$$\mathcal{K}_1(A, v_1) \subset \ldots \subset \mathcal{K}_d(A, v_1) = \mathcal{K}_{d+1}(A, v_1) = \ldots = \mathcal{K}_N(A, v_1)\,.$$

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Our goal:
Generate a B-orthogonal basis $v_1, \ldots, v_d$ of $\mathcal{K}_d(A, v_1)$.

1. $\text{span}\{v_1, \ldots, v_n\} = \mathcal{K}_n(A, v_1), \quad \text{for} \quad n = 1, \ldots, d,$
2. $\langle v_j, v_k \rangle_B = 0, \quad \text{for} \quad j \neq k, \quad j, k = 1, \ldots, d.$

Optimal short recurrences (2)

- Standard way for generating the B-orthogonal basis: Arnoldi's method.

$$\begin{aligned} v_{n+1} &= Av_n - \sum_{m=1}^{n} h_{m,n} v_m \,, \quad n = 1, \ldots, d-1 \,, \\ h_{m,n} &= \frac{\langle Av_n, v_m \rangle_B}{\langle v_m, v_m \rangle_B} \,, \quad d = \dim \mathcal{K}_N(A, v_1) \,. \end{aligned}$$

(No normalization for convenience.)

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\end{aligned}
$$

(No normalization for convenience.)

- Rewritten in matrix notation: $AV_{d-1} = V_d H_{d,d-1}$, where

matrix of size $d \times (d-1)$

$$
V_d \equiv [v_1, \ldots, v_d], \qquad H_{d,d-1} \equiv \begin{bmatrix} h_{1,1} & \cdots & h_{1,d-1} \\ 1 & \ddots & \vdots \\ & \ddots & h_{d-1,d-1} \\ & & 1 \end{bmatrix}
$$

$$
V_d^* B V_d \ \text{ is diagonal} \,, \quad d = \dim \mathcal{K}_N(A, v_1) \,.
$$

Optimal short recurrences (3)

- The *full recurrence* in Arnoldi's method,

$$v_{n+1} = Av_n - \sum_{m=1}^{n} h_{m,n} v_m \,, \quad n = 1, \ldots, d-1 \,,$$

is an *optimal* $(s+2)$*-term recurrence* when

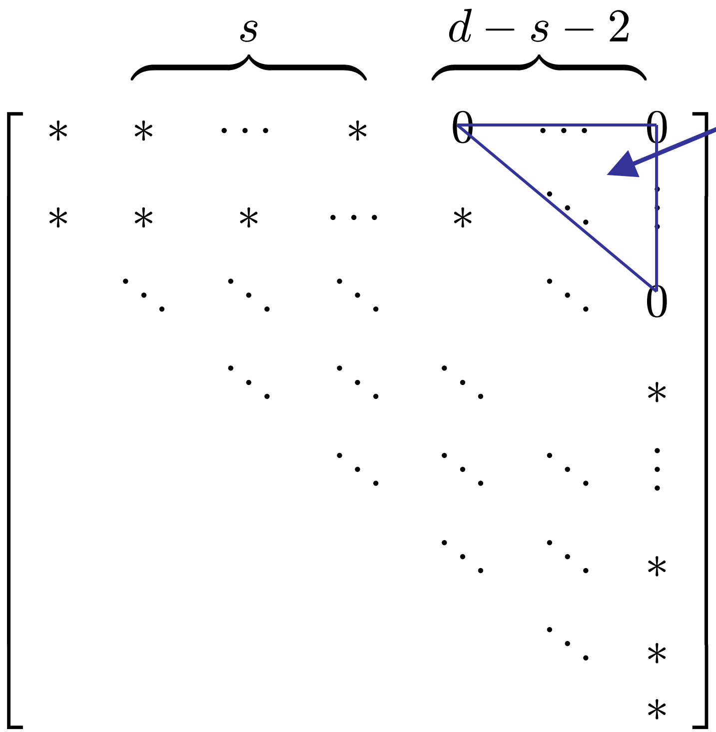
$$v_{n+1} = Av_n - \sum_{m=n-s}^{n} h_{m,n} v_m \,, \quad n = 1, \ldots, d-1 \,.$$

- For $s = 1$: Optimal 3-term recurrence,

$$v_{n+1} \; = \; Av_n - h_{n,n} v_n - h_{n-1,n} v_{n-1}$$

- Why *optimal*?
  1. Only one multiplication with A is performed.
  2. Only the previous $s+1$ vectors are required.

Optimal short recurrences (4)



largest upper triangle that is zero

Optimal $(s+2)$-term recurrence:
$H_{d,d-1}$ *is* $(s+2)$*-band Hessenberg*

(e.g. 3-band Hessenberg = tridiagonal)

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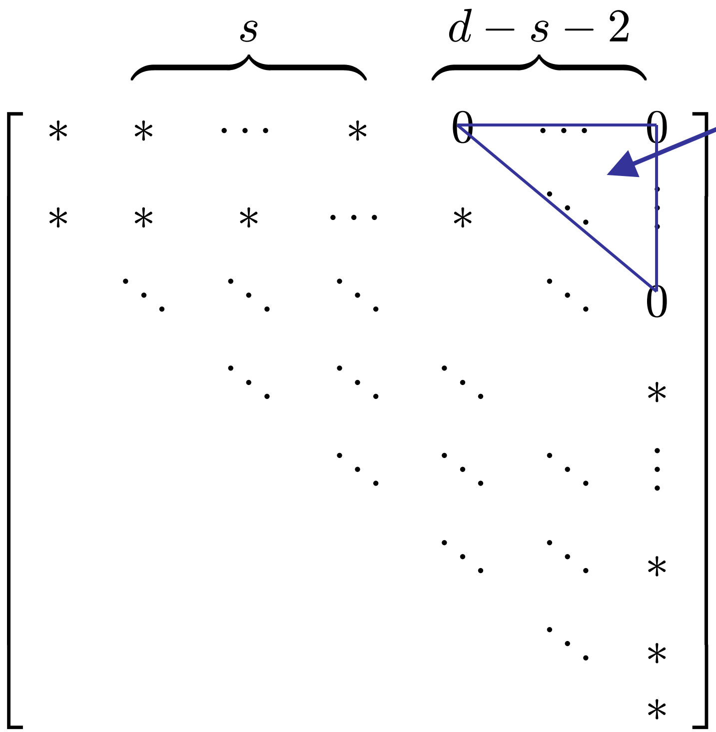

Optimal $(s+2)$-term recurrence:
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Definition (L. and Strakoš, 2007)

Given A, B as above and a nonnegative integer s with $s+2 \leq d_{\min}(A)$.
($d_{\min}(A)$ = degree of A's minimal polynomial.)

Then A *admits for* B *an optimal* $(s+2)$*-term recurrence*, if

- for any v_1 the matrix $H_{d,d-1}$ is at most $(s+2)$-band Hessenberg, and
- for at least one v_1 the matrix $H_{d,d-1}$ is $(s+2)$-band Hessenberg.

Optimal short recurrences (5)

- $H_{d,d-1}$ is at most $(s+2)$-band Hessenberg if

$$h_{m,n} = \frac{\langle Av_n, v_m \rangle_B}{\langle v_m, v_m \rangle_B} = 0 \,, \quad \text{for} \quad n > m + s \,, \quad n = 1, \ldots, d-1 \,.$$

- Therefore: $h_{m,n} = 0 \iff 0 = \langle Av_n, v_m \rangle_B = \langle v_n, A^+ v_m \rangle_B$, where $A^+ \equiv B^{-1} A^* B$ is the *B-adjoint of A*.

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- If $A^+ = p_s(A)$ for a polynomial of degree s, then $A^+ v_m \in \mathcal{K}_{m+s}(A, v_1)$.
- Then for $n > m+s$: $v_n \perp_B A^+ v_m \Leftrightarrow h_{m,n} = 0$.
- Hence: If $A^+ = p_s(A)$, then $H_{d,d-1}$ is at most $(s+2)$-band Hessenberg.
- The condition $A^+ = p_s(A)$ is *essential* in this context.

Optimal short recurrences (6)

Definition

If $A^+ = p_s(A)$, where p_s is a polynomial of the smallest possible degree s, then A is called B-normal(s).

Theorem (Faber and Manteuffel, 1984)
For A, B as above, and a nonnegative integer s with $s + 2 < d_{\min}(A)$:
A admits for the given B an optimal $(s + 2)$-term recurrence if and only if A is B-normal(s).

- This is a (generalized) characterization of normality.
- 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).
- In (Faber, L., Tichý, 2007) we give *two new proofs*,
  both using only "elementary" tools.

Optimal short recurrences (7)

In (Faber, L., Tichý, 2007) we explain why necessity is so difficult to prove:

- Assumption: For any v_1,

$$(1) \qquad A\,[v_1, \ldots, v_{d-1}] \;=\; [v_1, \ldots, v_{d-1}, v_d]\, H_{d,d-1},$$

where $H_{d,d-1}$ is $(s+2)$-band Hessenberg. To prove: A is B-normal(s).

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- By construction, $Av_d \in \mathcal{K}_d(A,v_1)$, i.e. $\quad Av_d \;=\; \sum_{j=1}^{d} h_{j,d} v_j$.

  Adding this in (1) gives

$$(2) \qquad A\,[v_1,\ldots,v_{d-1},v_d] \;=\; [v_1,\ldots,v_{d-1},v_d]\,H_{d,d}.$$

  But we don't know whether $H_{d,d}$ is $(s+2)$-band Hessenberg.

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  But we don't know whether $H_{d,d}$ is $(s+2)$-band Hessenberg.

- $H_{d,d}$ is the matrix representation of $A : \mathcal{K}_d(A, v_1) \to \mathcal{K}_d(A, v_1)$ with respect to the orthonormal basis $v_1, \ldots, v_d$.
- Problem: *Prove something about the linear operator A, without complete knowledge of the structure of its matrix representation.*

Characterization and examples (1)

- In practice A is given and we ask:
  Does there exist an HPD B such that A is B-normal(s) with small s?
- Standard example: $A = A^*$ and $B = I$, then $A^+ = p_1(A)$ for $p_1(z) = z$.

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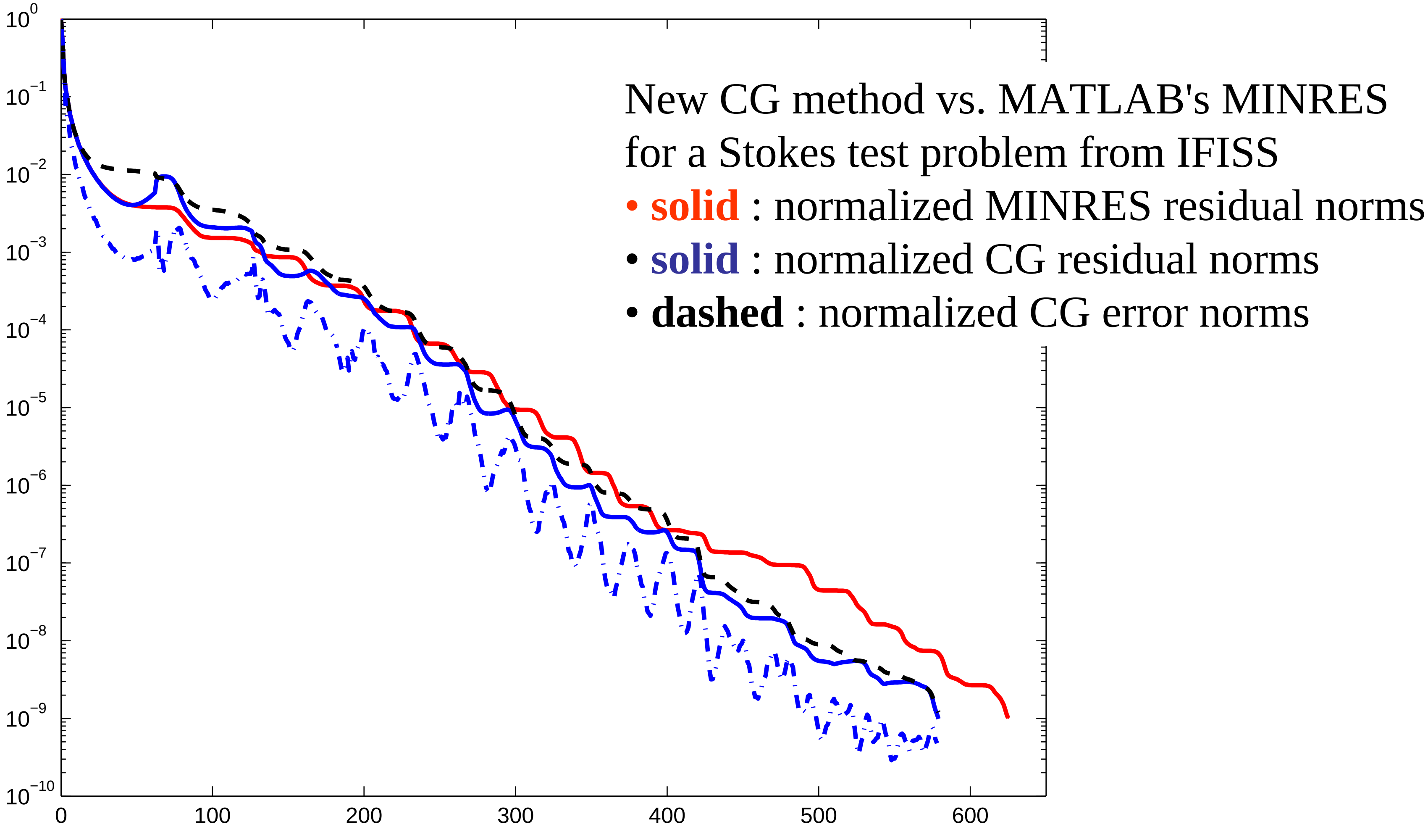
- Standard example: $A = A^*$ and $B = I$, then $A^+ = p_1(A)$ for $p_1(z) = z$.
- More interesting example: Saddle point matrices.

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

  where $A_1 = A_1^T > 0$, $A_3 = A_3^T \geq 0$, and $A_2 \in \mathbb{R}^{k \times m}$ has full rank k.
- A is a standard saddle point matrix with negated second block row.
- Transformation: symmetric indefinite into nonsymmetric positive real.
- **Theorem** (L. and Parlett, 2007)
  $B = B^T > 0$ holds if $\|A_2\|^2 < (\lambda_{\min}(A_1) - \gamma)\,(\gamma - \lambda_{\max}(A_3))$,
  and in this case A is B-normal(1).
  (Generalization of (Fischer et al., 1998); (Benzi and Simoncini, 2006).)

Characterization and examples (2)

- In (L. and Parlett, 2007) a corresponding 3-term CG method is constructed and analyzed. This method appears to be competitive with MINRES:



Characterization and examples (3)

General characterization:

Theorem. (L. and Strakoš, 2007)
A is B-normal(s) if and only if

1. A *is diagonalizable* with the eigendecomposition $A = W\Lambda W^{-1}$, and
2. $B = (WDW^*)^{-1}$, where D is HPD and block diagonal with blocks corresponding to those of Λ, and
3. $\Lambda^* = p_s(\Lambda)$ for a polynomial p_s of (smallest possible) degree s.

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3. $\Lambda^* = p_s(\Lambda)$ for a polynomial p_s of (smallest possible) degree s.

- Every $A = W\Lambda W^{-1}$ is B-normal(s) for *some* HPD B and *some* s, but no optimal short recurrence in the nondiagonalizable case.
- s is the smallest degree of a polynomial p_s for which $p_s(\Lambda) = \Lambda^*$.

Characterization and examples (4)

Theorem. (Faber and Manteuffel, 1984; Khavinson and Świątek, 2003)

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

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

$\Longrightarrow$ Overabundant supply of Krylov subspace methods for general A.

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Options for $Ax = b$ in case the eigenvalues of A are not collinear:

- Orthogonality but full recurrence (GMRES).
- Short recurrence but no orthogonality (BiCG, QMR, etc.).
- "Preconditioners" P so that PA is B-normal(1) for some B, e.g. (Concus and Golub, 1978) and (Widlund, 1978).
- *Special types of recurrences (Isometric Arnoldi).*

Characterization and examples (5)

- (Gragg, 1982) discovered the *isometric Arnoldi process*:
  Orthogonal Krylov subspace bases for unitary A can be generated by a (non-optimal) 3-term recurrence of the form

$$v_{n+1} \; = \; Av_n - \beta_{n,1} A v_{n-1} - \beta_{n,2} v_n$$

  (stable implementation is in form of two coupled 2-term recurrences).

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- Generalized in (Barth and Manteuffel, 2000):
  If $A^+ = r(A)$ for $r = p/q$, where p and q have degrees s and t,
  a B-orthogonal Krylov subspace can be generated by a (non-optimal) recurrence of length at most $t + s + 2$.

- In case A is unitary: $A^* = A^{-1}$, hence $p(z) = 1$, $q(z) = z$.

Characterization and examples (5)

- Are thre any other matrices A whose adjoint A^+ (for some B) is a low degree rational function in A?
- **Theorem** (L., 2007)
  There is an HPD B such that $A^+ = r(A)$ with *small* $\deg r \equiv \max\{\deg p,\ \deg q\}$ if and only if either $d_{\min}(A)$ is small,
  or A is diagonalizable with collinear or concyclic eigenvalues.

More precisely:
For diagonalizable A with $n \geq 4$ distinct eigenvalues that are neither collinear nor concyclic,

$$d_r(A) > \frac{n}{5}, \qquad d_p(A) > \frac{n}{3}, \qquad \text{and} \qquad 1 \leq \frac{d_p(A)}{d_r(A)} < 5.$$

Concluding remarks

- Completely reworked the theory of short recurrences for generating orthogonal Krylov subspace bases; new, mathematically rigorous definitions of all important concepts have been given.
- In particular, here we discussed:

  new proofs of the fundamental theorem of Faber and Manteuffel,
  a new 3-term CG method for saddle point matrices,
  the existence of alternative (isometric Arnoldi style) recurrences.

- Visit `http://www.math.tu-berlin.de/~liesen` for the related papers:

J.L. and P. Saylor, *Orthogonal Hessenberg reduction and orthogonal Krylov subspace bases*, SINUM 42 (2005).

J.L. and Z. Strakoš, *On optimal short recurrences for generating orthogonal Krylov subspace bases*, to appear in SIREV.

J.L., *When is the adjoint of a matrix a low degree rational function in the matrix?*, to appear in SIMAX.

V. Faber, J.L. and P. Tichý, *The Faber-Manteuffel Theorem for linear operators*, submitted.

J.L. and B. N. Parlett, *On nonsymmetric saddle point matrices that allow conjugate gradient iterations*, submitted.