The Faber-Manteuffel Theorem and its Consequences

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joint work with

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Optimal Krylov subspace methods

and low memory requirements?

- Consider a system of linear algebraic equations

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

$\mathbf{A} \in \mathbb{R}^{n \times n}$ is nonsingular, $b \in \mathbb{R}^n$.

- Given x_0, find an *optimal*

$$x_j \in x_0 + \mathcal{K}_j(\mathbf{A}, r_0)$$

so that the error is minimized in a given vector norm.

- What are necessary and sufficient conditions on $\mathbf{A}$ so that the optimal x_j can be computed using short recurrences? (only a constant number of vectors is needed)

Examples of optimal Krylov subspace methods

with short recurrences

CG [Hestenes, Stiefel 1952], MINRES, SYMMLQ [Paige, Saunders 1975]

- *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,

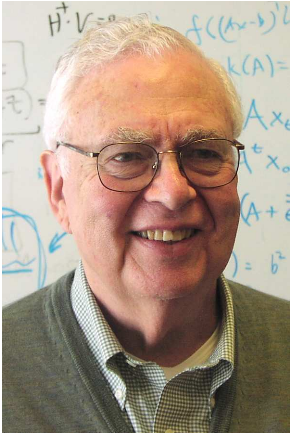
  $\| x - x_j \|$ in SYMMLQ - here $x_j \in x_0 + \mathbf{A}\mathcal{K}_j(\mathbf{A}, r_0)$.

- Generate orthogonal (or $\mathbf{A}$-orthogonal) Krylov subspace basis using a three-term recurrence,

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

- An important assumption: $\mathbf{A}$ is symmetric (MINRES, SYMMLQ) and positive 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 Symposium) held in Oxford in 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, $\| \cdot \|_{\mathbf{B}} = \langle \cdot, \cdot \rangle_{\mathbf{B}}^{1/2}$.
- Starting from x_0, compute

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

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

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

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

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

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

Optimal Krylov subspace method with short recurrences

The question about

> the existence of an optimal Krylov subspace method with short recurrences

can be reduced to the question:

> For which $\mathbf{A}$ is it possible to generate a $\mathbf{B}$-orthogonal basis of the Krylov subspace using short recurrences?

(for each initial starting vector)

Faber, Manteuffel 1984

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

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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

1. The Faber-Manteuffel theorem
2. Ideas of a new proof
3. Consequences
4. Other types of recurrences

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

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

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

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

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

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

In matrix notation:

$$v_1 = v\,,$$

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

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

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

Formulation of the problem

Optimal short recurrences (Definition - Liesen, 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.

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

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

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).

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

Given nonsingular $\mathbf{A}$ and nonnegative s, $s + 2 < d_{\min}(\mathbf{A})$.

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

if and only if

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

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

A new proof of the Faber-Manteuffel theorem

- Motivated by the paper [Liesen, 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."

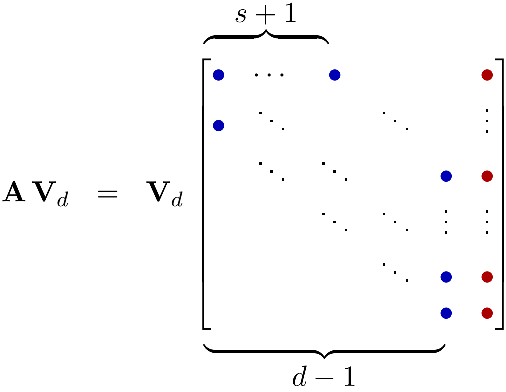
- In [Faber, Liesen, T. 2008] we give two new proofs of the Faber-Manteuffel theorem that use more elementary tools.

Extension of $\mathbf{A}\,\mathbf{V}_{d-1} = \mathbf{V}_d\,\mathbf{H}_{d,d-1}$

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

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

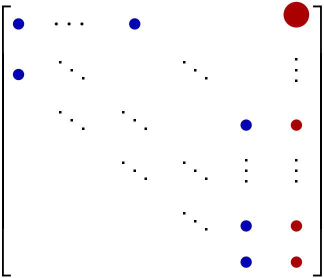
$$\mathbf{A}v_d = \sum_{i=1}^{d} h_{i,d}\, v_i\,.$$



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

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

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



$$\mathbf{G}$$

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

Faber-Manteuffel Theorem – 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) $\mathbf{A}^* = p(\mathbf{A})$

$\updownarrow$

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

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

  [Faber, Manteuffel 1984],

  [Khavinson, Świątek 2003]

  [Liesen, Strakoš 2008]

  1. $s = 1$ if and only if the eigenvalues of $\mathbf{A}$ lie on a line in $\mathbb{C}$.
  2. For $s > 1$, $\mathbf{A}$ has at most $3s - 2$ different eigenvalues.
- All classes of “interesting” matrices are known.

When is $\mathbf{A}$ orthogonally reducible
to $(s+2)$-band Hessenberg form?

The matrix representation of the Arnoldi algorithm can be extended by one column to

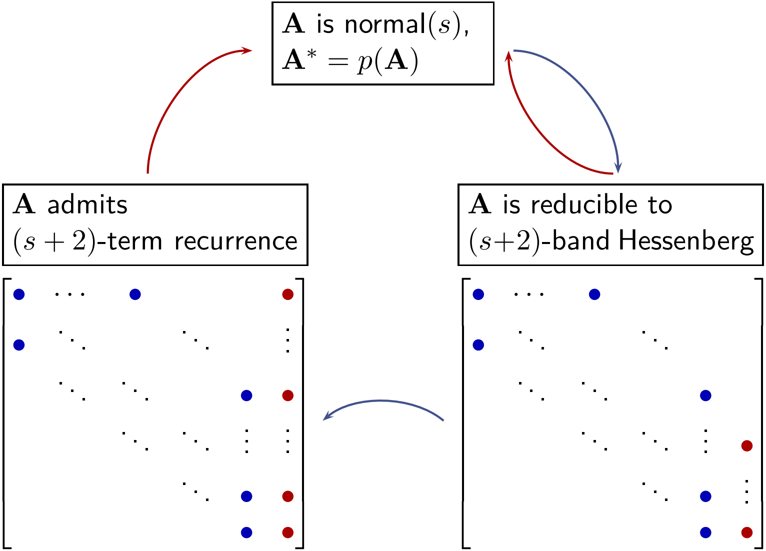
$$\mathbf{A}\,\mathbf{V}_d \;=\; \mathbf{V}_d\,\mathbf{H}_d$$

where $\mathbf{H}_d \in \mathbb{C}^{d\times d}$ is unreduced upper Hessenberg matrix.

We say that $\mathbf{A}$ is orthogonally reducible to $(s+2)$-band Hessenberg form if $\mathbf{H}_d$ is $(s+2)$-band Hessenberg matrix for each starting vector v_1.

What are necessary and sufficient conditions on $\mathbf{A}$ to be orthogonally reducible to $(s+2)$-band Hessenberg form?

When is $\mathbf{A}$ orthogonally reducible
to $(s+2)$-band Hessenberg form?



When is $\mathbf{A}$ orthogonally reducible

to $(s+2)$-band Hessenberg form?

Theorem [Liesen, Strakoš 2008]

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.

- $1 \iff 2$: [Faber, Manteuffel 1984].
- $2 \iff 3$: a simple proof in [Faber, Liesen, T. 2009].
- The subtle difference between 1. and 3. $\to$ source of confusions [Voevodin, Tyrtyshnikov 1981], [Liesen, Saylor 2005].

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

Faber-Manteuffel theorem

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 exists 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, Manteuffel 1984], [Liesen, 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).

- If $\mathbf{A}$ is diagonalizable and the eigenvalues are collinear, then there exists an HPD $\mathbf{B}$ such that $\mathbf{A}$ is $\mathbf{B}$-normal(1).
  [Liesen, Strakoš 2008] $\rightarrow$ complete parametrization of all $\mathbf{B}$'s.
- Find a preconditioner $\mathbf{P}$ so that $\mathbf{PA}$ is $\mathbf{B}$-normal(1) for some $\mathbf{B}$, e.g. [Concus, Golub 1976], [Widlund 1978], [Eisenstat 1983], [Bramble, Pasciak 1988], [Stoll, Wathen 2008].
- Saddle point matrix:

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

where $A_1 = A_1^T > 0$, $A_3 = A_3^T \geq 0$, A_2 full rank.

This matrix satisfies $\mathbf{B}_\gamma^{-1} \mathbf{A}^T \mathbf{B}_\gamma = \mathbf{A}$.

How to choose γ such that $\mathbf{B}_\gamma$ is positive definite?
[Fischer et al. 1998], [Benzi, Simoncini 2006], [Liesen, Parlett 2007].

Other types of recurrences

The existence of an optimal Krylov subspace method with short recurrences

For which $\mathbf{A}$ is it possible to generate an orthogonal basis of the Krylov subspace using short recurrences?

- We can use a different kind of recurrences than Arnoldi-like.
- For (shifted) unitary matrices: Isometric Arnoldi process [Gragg 1982; Jagels, Reichel 1994].
- Generalized by [Barth, Manteuffel 2000] to (ℓ, m)-recursion.
  A sufficient condition: $\mathbf{A}^*$ is a low degree rational func. of $\mathbf{A}$.
  Practical use: matrices with concyclic eigenvalues [Liesen 2007].
- [Barth, Manteuffel 2000]: Short multiple recursion for $\mathbf{A}$ such that $\Delta \equiv \mathbf{A}^* q_m(\mathbf{A}) - p_\ell(\mathbf{A})$ has low rank.
- [Beckermann, Reichel 2008]: GMRES-like algorithm with short recurrences for $\mathbf{A}$ such that $\Delta \equiv \mathbf{A}^* - \mathbf{A}$ is of low rank.
  Application: Path following methods.

Conclusions

- We characterized matrices for which it is possible to generate an orthogonal basis of Krylov subspaces via short recurrences.
- We presented ideas of a new proof of the Faber-Manteuffel theorem and studied its consequences.
- Practical case: If the eigenvalues of $\mathbf{A}$ are collinear or concyclic, then there exists an HPD matrix $\mathbf{B}$ such that $\mathbf{A}$ admits short recurrences for generating a $\mathbf{B}$-orthogonal basis.
- Examples: Find a preconditioner $\mathbf{P}$ so that short recurrences exist for $\mathbf{PA}$, saddle point matrices.

An interesting case to study:

- Short multiple recursion for $\mathbf{A}$ such that $\mathbf{A}^* q_m(\mathbf{A}) - p_\ell(\mathbf{A})$ has low rank. Practical cases? Algorithmic realizations?

Related papers

- V. Faber and T. Manteuffel, [Necessary and sufficient conditions for the existence of a conjugate gradient method, SIAM J. Numer. Anal., 21 (1984), pp. 352–362.]
- T. Barth and T. Manteuffel, [Multiple recursion conjugate gradient algorithms. I. Sufficient conditions, SIAM J. Matrix Anal. Appl., 21 (2000), pp. 768–796.]
- J. Liesen and Z. Strakoš, [On optimal short recurrences for generating orthogonal Krylov subspace bases, SIAM Review, 50, 2008, pp. 485-503].
- 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].
- V. Faber, J. Liesen and P. Tichý, [The Faber-Manteuffel Theorem for Linear Operators, SIAM J. Numer. Anal., 46 (2008), pp. 1323-1337.]
- V. Faber, J. Liesen, and P. Tichý, [On orthogonal reduction to Hessenberg form with small bandwidth, Numer. Algorithms, 51 (2009), pp. 133–142.]

Thank you for your attention!