Abstract Perturbed Krylov Methods

Just another point of view?

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Outline

1. Getting started
   - the name of the game
   - a few examples
   - basic notations
   - HESSENBERG structure

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2. The results ...
   - “basis” transformations
   - eigenvalue problems
   - linear systems: (Q)OR
   - linear systems: (Q)MR

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   - general comments
   - finite precision issues
   - inexact KRYLOV methods

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We aim at 1a (possibly 3 and 4a), not 2.

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Selected definitions for “abstract”

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2. to consider apart from application to or association with a particular instance

Merriam-Webster Online: abstract (adjective)

1. a : disassociated from any specific instance
2. expressing a quality apart from an object
3. a : dealing with a subject in its abstract aspects

perturbed KRYLOV methods

We consider perturbed KRYLOV subspace methods that can be written in the form

$$AQ_k = Q_{k+1}\underline{C}_k - F_k, \tag{1a}$$

$$Q_{k+1}\underline{C}_k = Q_k C_k + M_k, \tag{1b}$$

$$M_k = q_{k+1} c_{k+1,k} e_k^T. \tag{1c}$$

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\end{aligned}
$$

We refer to the set of equations (1) as a *perturbed* KRYLOV *decomposition*.

the main actors

In the perturbed KRYLOV decomposition:

- $A \in \mathbb{C}^{n \times n}$ is the system matrix from

$$Ax = b \qquad \text{or} \qquad Av = v\lambda$$

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- $\underline{C}_k \in \mathbb{C}^{(k+1) \times k}$ is extended upper HESSENBERG
- $F_k \in \mathbb{C}^{n \times k}$ is zero or captures perturbations (due to finite precision, inexact methods, both, . . .)

crucial assumptions

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- “measurable”: the perturbation terms F_k

We treat the system matrix A, the starting vector q_1 and the perturbation terms $\{f_l\}_{l=1}^{k}$ as input data and express everything else based on the *computed* C_k.

Outline

ARNOLDI

In the ARNOLDI method:

- $A \in \mathbb{C}^{n\times n}$ is a general matrix
- $Q_k \in \mathbb{C}^{n\times k}$ has orthonormal columns
- $C_k \in \mathbb{C}^{k\times k}$ is unreduced HESSENBERG

ARNOLDI

In the finite precision ARNOLDI method:

- $A \in \mathbb{C}^{n\times n}$ is a general matrix
- $Q_k \in \mathbb{C}^{n\times k}$ has “approximately” orthonormal columns
- $C_k \in \mathbb{C}^{k\times k}$ is unreduced HESSENBERG
- $F_k \in \mathbb{C}^{n\times k}$ is “small”

(ask Miro about the details : -)

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In the inexact ARNOLDI method:

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In the LANCZOS method:

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- $C_k \in \mathbb{C}^{k\times k}$ is unreduced tridiagonal

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- $A \quad \in \mathbb{C}^{n \times n}$ is a general matrix
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The error terms may grow unbounded ...

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The error terms may grow unbounded . . .

power method

In the power method:

- $A \in \mathbb{C}^{n\times n}$ is a general matrix
- $Q_k \in \mathbb{C}^{n\times k}$ has nearly dependent columns
- $C_k \in \mathbb{C}^{k\times k}$ is nilpotent unreduced HESSENBERG

Columns of Q_k may be dependent from the beginning.

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- $F_k \in \mathbb{C}^{n\times k}$ is “small” compared to Q_k

Columns of Q_k may be dependent from the beginning.

a rather silly method

Consider any $v \neq 0$ such that $Av = v\lambda$ with $\lambda \neq 0$

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Set

$$C_k \equiv \begin{pmatrix} o_{k-1}^T & 0 \\ \lambda I_{k-1} & \lambda e_{k-1} \end{pmatrix} \quad (2)$$

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Then $AQ_k = Q_k C_k$.

Outline

eigenmatrices et al.

JORDAN form, eigenmatrices:

$$AV = VJ_\Lambda, \qquad C_k S_k = S_k J_\Theta. \tag{3}$$

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JORDAN matrices (, boxes) and blocks:

$$J_\Lambda = \oplus J_\lambda, \quad J_\lambda = \oplus J_{\lambda\iota}, \qquad J_\Theta = \oplus J_\theta. \tag{5}$$

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partial eigenmatrices:

$$V = \oplus V_\lambda, \quad V_\lambda = \oplus V_{\lambda\iota}, \qquad S_k = \oplus S_\theta. \tag{6}$$

characteristic matrix et al.

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$$ {}^{z}A \equiv zI - A, \qquad {}^{z}C_k \equiv zI_k - C_k. \tag{7} $$

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$$ \chi_{C_k}(z) \equiv \det({}^{z}C_k), \quad \chi_{C_{i:j}}(z) \equiv \det({}^{z}C_{i:j}). \tag{9} $$

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reduced characteristic polynomial:

$$ \chi_{C_k}(z) = (z - \theta)^{\alpha}\omega(z). \tag{10} $$

Outline

HESSENBERG eigenvalue-eigenmatrix relations

Definition (off-diagonal products)

We denote the products of off-diagonal elements by

$$c_{i:j} \equiv \prod_{\ell=i}^{j} c_{\ell+1,\ell}. \tag{11}$$

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Definition (polynomial vectors ν and $\check{\nu}$)

We define vectors of (scaled) characteristic polynomials by

$$\nu(z) \equiv \left(\frac{\chi_{C_{l+1:k}}(z)}{c_{l:k-1}} \right)_{l=1}^{k}, \qquad \check{\nu}(z) \equiv \left(\frac{\chi_{C_{l-1}}(z)}{c_{1:l-1}} \right)_{l=1}^{k}. \tag{12}$$

HESSENBERG eigenvalue-eigenmatrix relations

Definition (matrices of derivatives)

We define rectangular matrices collecting the derivatives by

$$\mathcal{S}_{\alpha-1}(\theta) \equiv \left[\nu(\theta), \nu'(\theta), \frac{\nu''(\theta)}{2}, \dots, \frac{\nu^{(\alpha-1)}(\theta)}{(\alpha-1)!}\right] \tag{13}$$

$$\check{\mathcal{S}}_{\alpha-1}(\theta) \equiv \left[\frac{\check{\nu}^{(\alpha-1)}(\theta)}{(\alpha-1)!}, \dots, \frac{\check{\nu}''(\theta)}{2}, \check{\nu}'(\theta), \check{\nu}(\theta)\right] \tag{14}$$

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Observation

These matrices gather complete left and right JORDAN chains.

HESSENBERG eigenvalue-eigenmatrix relations

Theorem (HEER)

HESSENBERG *eigenmatrices satisfy*

$$\frac{P^{(\alpha-1)}(\theta)}{(\alpha-1)!} = S_\theta\, \omega(J_\theta)\, \check{S}_\theta^T = c_{1:k-1}\, \mathcal{S}_{\alpha-1}(\theta)\, \check{\mathcal{S}}_{\alpha-1}(\theta)^T. \qquad (15)$$

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Proof.

Proof based on comparison of TAYLOR expansions of the adjugate $P(z)$ as inverse divided by determinant and the polynomial expression for the adjugate in terms of characteristic polynomials of submatrices (Zemke 2004, submitted to LAA). □

HESSENBERG eigenvalue-eigenmatrix relations

Lemma (HEER)

We can choose the partial eigenmatrices such that

$$e_1^T \check{S}_\theta = e_\alpha^T (\omega(J_\theta))^{-T}, \tag{16a}$$

$$S_\theta^T e_l = c_{1:l-1} \chi_{C_{l+1:k}}(J_\theta)^T e_1. \tag{16b}$$

Tailored to diagonalizable C_k:

$$\check{s}_{lj} s_{\ell j} = \frac{\chi_{C_{1:l-1}}(\theta_j) c_{l:\ell-1} \chi_{C_{\ell+1:k}}(\theta_j)}{\chi'_{C_k}(\theta_j)} \quad \forall\, l \leqslant \ell. \tag{17}$$

Outline

basic definitions

Definition (basis polynomials)

We define the (trailing) basis polynomials by

$$\mathcal{B}_k(z) \equiv \frac{\chi_{C_k}(z)}{c_{1:k}} = \check{\nu}_{k+1}(z), \tag{18}$$

$$\mathcal{B}_{l+1:k}(z) \equiv \frac{\chi_{C_{l+1:k}}(z)}{c_{l+1:k}} = \frac{c_{l+1,l}}{c_{k+1,k}}\nu_l(z), \quad \forall\, l = 1, \ldots, k. \tag{19}$$

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Observation

The trailing basis polynomials are the basis polynomials of the trailing submatrices $C_{l+1:k}$.

“basis” vectors

Theorem (the “basis” vectors)

The “basis” vectors of a KRYLOV *method are given by*

$$q_{k+1} = \mathcal{B}_k(A)q_1 \quad . \tag{20}$$

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$$q_{k+1} = \mathcal{B}_k(A)q_1 + \sum_{l=1}^{k} \mathcal{B}_{l+1:k}(A)\frac{f_l}{c_{l+1,l}}. \qquad (20)$$

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Observation

The perturbed "basis" vectors can be interpreted as an additive overlay of exact "basis" vectors.

a rough sketch of a short proof

Proof.

Introduce variable z:

$$M_k = Q_k(zI - C_k) + (zI - A)Q_k + F_k$$

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HEER: $\operatorname{adj}({}^zC_k)e_1 = c_{1:k-1}\nu(z)$.

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HEER: $\operatorname{adj}({}^zC_k)e_1 = c_{1:k-1}\nu(z)$. Insert A into

$$c_{k+1,k}q_{k+1} = \frac{q_1 \chi_{C_k}(z)}{c_{1:k-1}} + (zI - A)Q_k\nu(z) + F_k\nu(z). \qquad \square$$

a closer & deeper look

Theorem (the "basis" vectors revisited)

Let C_k be diagonalizable and suppose that $\lambda \neq \theta_j$ for all j:

$$\left(\sum_{j=1}^{k} \frac{c_{1:k}}{\chi'_{C_k}(\theta_j)(\lambda - \theta_j)} \right) \hat{v}^H q_{k+1} = \hat{v}^H q_1$$

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$$+ \sum_{l=1}^{k} \left(\sum_{j=1}^{k} \frac{c_{1:l}\chi_{C_{l+1:k}}(\theta_j)}{\chi'_{C_k}(\theta_j)(\lambda - \theta_j)}\right) \frac{\hat{v}^H f_l}{c_{l+1,l}}.$$

a closer & deeper look

Theorem (the “basis” vectors revisited)

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$$\left(\sum_{j=1}^{k} \frac{c_{1:k}}{\chi'_{C_k}(\theta_j)(\lambda - \theta_j)} \right) \hat{v}^H q_{k+1} = \hat{v}^H q_1 + \sum_{l=1}^{k} \left(\sum_{j=1}^{k} \frac{c_{1:l}\chi_{C_{l+1:k}}(\theta_j)}{\chi'_{C_k}(\theta_j)(\lambda - \theta_j)} \right) \frac{\hat{v}^H f_l}{c_{l+1,l}}.$$

Remark

Generalization to the non-diagonalizable case exists.

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eigenvalues, JORDAN block, partial eigenmatrix

Unreduced HESSENBERG matrices C_k are non-derogatory.

Notations

In the following,

The matrices are such that

$$C_k S_\theta = S_\theta J_\theta, \quad \text{where} \quad J_\theta \in \mathbb{C}^{\alpha \times \alpha}. \tag{21}$$

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In the following,

(generic) eigenvalue: denoted by $\theta = \theta^{(k)}$,

The matrices are such that

$$C_k S_\theta = S_\theta J_\theta, \quad \text{where} \quad J_\theta \in \mathbb{C}^{\alpha \times \alpha}. \tag{21}$$

eigenvalues, JORDAN block, partial eigenmatrix

Unreduced HESSENBERG matrices C_k are non-derogatory.

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partial eigenmatrix: $S_\theta = S_\theta^{(k)}$.

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RITZ pairs, RITZ residuals

Definition (RITZ pair)

Define RITZ pair by

$$(J_\theta, Y_\theta \equiv Q_k S_\theta). \tag{22}$$

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Observation

A backward expression for the RITZ residual is given by

$$AY_\theta - Y_\theta J_\theta = q_{k+1} c_{k+1,k} e_k^T S_\theta - F_k S_\theta. \tag{23}$$

RITZ residuals (generic case)

Theorem (generic RITZ residuals)

The RITZ *residual for an (arbitrarily chosen)* RITZ *pair:*

$$AY_\theta - Y_\theta J_\theta = \left(\frac{\chi_{C_k}(A)}{c_{1:k}}\right) q_1 e_k^T S_\theta + \sum_{l=1}^{k} \left(\frac{\chi_{C_{l+1:k}}(A)}{c_{l:k-1}}\right) f_l e_k^T S_\theta - f_l e_l^T S_\theta. \quad (24)$$

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Proof.

Backward expression and Theorem on the "basis" vectors. □

RITZ residuals (special case)

Use (unique) choice for the partial eigenmatrix S_θ (HEER):

Theorem (special RITZ residuals)

The RITZ *residual for the special partial eigenmatrix from HEER is given by*

$$AY_\theta - Y_\theta J_\theta = \chi_{C_k}(A) q_1 e_1^T + \sum_{l=1}^{k} c_{1:l-1} \left(\chi_{C_{l+1:k}}(A) f_l e_1^T - f_l e_1^T \chi_{C_{l+1:k}}(J_\theta) \right). \quad (25)$$

bivariate adjugate polynomials

Definition (bivariate adjugate polynomials)

We define the bivariate adjugate polynomials by

$$\mathcal{A}_k(\theta, z) \equiv \begin{cases} \left(\chi_{C_k}(\theta) - \chi_{C_k}(z)\right)(\theta - z)^{-1}, & z \neq \theta, \\ \chi'_{C_k}(z), & z = \theta. \end{cases} \quad (26)$$

Trailing bivariate adjugate polynomials $\mathcal{A}_{l+1:k}$ are defined using $C_{l+1:k}$ in place of C_k, $l = 1, \ldots, k$.

bivariate adjugate polynomials

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Trailing bivariate adjugate polynomials $\mathcal{A}_{l+1:k}$ are defined using $C_{l+1:k}$ in place of C_k, $l = 1, \ldots, k$.

Observation

Even with an eigenvalue θ: $\mathcal{A}_k(\theta, C_k) = \mathrm{adj}(\theta I_k - C_k) = P(\theta)$.

RITZ vectors

Theorem (the RITZ vectors)

The RITZ *vectors of a* KRYLOV *method are given by*

$$\operatorname{vec}(Y_\theta) = \begin{pmatrix} \mathcal{A}_k(\theta, A) \\ \mathcal{A}_k'(\theta, A) \\ \vdots \\ \frac{\mathcal{A}_k^{(\alpha-1)}(\theta, A)}{(\alpha-1)!} \end{pmatrix} q_1 \quad . \tag{27}$$

(derivation with respect to “shift” θ)

RITZ vectors

Theorem (the RITZ vectors)

The RITZ vectors of a perturbed KRYLOV method are given by

$$\operatorname{vec}(Y_\theta) = \begin{pmatrix} \mathcal{A}_k(\theta, A) \\ \mathcal{A}_k'(\theta, A) \\ \vdots \\ \frac{\mathcal{A}_k^{(\alpha-1)}(\theta, A)}{(\alpha-1)!} \end{pmatrix} q_1 + \sum_{l=1}^{k} c_{1:l-1} \begin{pmatrix} \mathcal{A}_{l+1:k}(\theta, A) \\ \mathcal{A}_{l+1:k}'(\theta, A) \\ \vdots \\ \frac{\mathcal{A}_{l+1:k}^{(\alpha-1)}(\theta, A)}{(\alpha-1)!} \end{pmatrix} f_l. \quad (27)$$

(derivation with respect to "shift" θ)

sketch of proof: basics

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sketch of proof: basics

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- The adjugate of a matrix is defined as matrix of cofactors.
- The adjugate is linked to eigenvectors and, more general, principal vectors.
- The adjugate is linked to the inverse and the determinant.

The problem: the definition of the bivariate adjugate polynomials given here is not “adequate”, we need another form.

sketch of proof: HESSENBERG basics

To derive this peculiar form we use the first adjugate identity:

Lemma (first (HESSENBERG) adjugate identity)

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First adjugate identity:

$$(z-\theta)\mathrm{adj}({}^{z}A)\mathrm{adj}({}^{\theta}A) = \det({}^{z}A)\mathrm{adj}({}^{\theta}A) - \det({}^{\theta}A)\mathrm{adj}({}^{z}A). \qquad (28)$$

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Specialized to HESSENBERG *matrices:*

$$(z-\theta)\sum_{j=1}^{k}\chi_{C_{1:j-1}}(z)\chi_{C_{j+1:k}}(\theta) = \chi_{C_k}(z) - \chi_{C_k}(\theta). \quad (29)$$

sketch of proof: gluing results together

The last line implies the following representations ($\ell \geqslant 0$):

$$\mathcal{A}^{(\ell)}_{l+1:k}(\theta, z) = \sum_{j=l+1}^{k} \chi_{C_{l+1:j-1}}(z)\chi^{(\ell)}_{C_{j+1:k}}(\theta) \quad \forall\, l = 0, 1, \ldots, k. \quad (30)$$

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This together with

are the building blocks for the proof.

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This together with

- the special choice of the partial eigenmatrix S_θ
- the representation of the "basis" vectors

are the building blocks for the proof.

Outline

(Q)OR: the approach

Suppose that C_k is invertible and that $q_1 = r_0/\|r_0\|$. Let z_k denote the solution to the linear system of equations

$$C_k z_k = e_1\|r_0\|. \tag{31}$$

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Define the kth (Q)OR iterate x_k by

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and the kth (true) (Q)OR residual by

$$r_k = r_0 - A x_k. \tag{33}$$

a backward expression for the (Q)OR residual

Observation

A backward expression for the (Q)OR residual is given by

$$r_k = r_0 - Ax_k = (Q_k C_k - AQ_k) C_k^{-1} e_1 \|r_0\|$$

a backward expression for the (Q)OR residual

Observation

A backward expression for the (Q)OR residual is given by

$$r_k = r_0 - Ax_k = (Q_k C_k - AQ_k)C_k^{-1} e_1 \|r_0\|$$

$$= (-q_{k+1} c_{k+1,k} e_k^T + F_k) z_k$$

a backward expression for the (Q)OR residual

Observation

A backward expression for the (Q)OR residual is given by

$$
\begin{aligned}
r_k = r_0 - Ax_k &= (Q_k C_k - AQ_k) C_k^{-1} e_1 \|r_0\| \\
&= (-q_{k+1} c_{k+1,k} e_k^T + F_k) z_k \\
&= -q_{k+1} c_{k+1,k} z_{kk} + \sum_{l=1}^{k} f_l z_{lk}
\end{aligned}
$$

adjugate, inverse, determinant

Express the inverse of C_k as adjugate by determinant:

$$\frac{-z_{lk}}{\|r_0\|} = e_l^T(-C_k)^{-1}e_1$$

adjugate, inverse, determinant

Express the inverse of C_k as adjugate by determinant:

$$\frac{-z_{lk}}{\|r_0\|} = e_l^T(-C_k)^{-1}e_1 = \frac{e_l^T \operatorname{adj}(-C_k)e_1}{\det(-C_k)}$$

adjugate, inverse, determinant

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$$\frac{-z_{lk}}{\|r_0\|} = e_l^T(-C_k)^{-1}e_1 = \frac{e_l^T \operatorname{adj}(-C_k)e_1}{\det(-C_k)} = \frac{c_{1:l-1}\chi_{C_{l+1:k}}(0)}{\chi_{C_k}(0)}.$$

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Utilize

$$r_k = q_{k+1}c_{k+1,k}(-z_{kk}) - \sum_{l=1}^{k} f_l(-z_{lk}). \tag{34}$$

(Q)OR: the residuals

This backward expression plus Theorem on the "basis" vectors:

Theorem (the (Q)OR residual vectors)

The residual vectors of a (Q)OR KRYLOV *method are given by*

$$r_k = \frac{\chi_{C_k}(A)}{\chi_{C_k}(0)} r_0 \quad . \tag{35}$$

(Q)OR: the residuals

This backward expression plus Theorem on the “basis” vectors:

Theorem (the (Q)OR residual vectors)

The residual vectors of a perturbed (Q)OR KRYLOV *method are given by*

$$r_k = \frac{\chi_{C_k}(A)}{\chi_{C_k}(0)} r_0 + \|r_0\| \sum_{l=1}^{k} c_{1:l-1} \frac{\chi_{C_{l+1:k}}(A) - \chi_{C_{l+1:k}}(0)}{\chi_{C_k}(0)} f_l. \quad (35)$$

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The perturbation terms remind of adjugate polynomials . . .

adjugate, inverse, interpolation (I)

Definition (univariate adjugate polynomials)

We define univariate adjugate polynomials by

$$\mathcal{A}_k(z) = (-1)^k(\chi_{C_k}(0) - \chi_{C_k}(z))z^{-1}$$

By Cayley-Hamilton: $\mathcal{A}_k(C_k) = \mathrm{adj}(C_k)$

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Observation

Univariate and bivariate adjugate polynomials are related by

$$\mathcal{A}_k(z) = (-1)^{k+1}\mathcal{A}_k(z, 0) = (-1)^{k+1}\mathcal{A}_k(0, z)$$

adjugate, inverse, interpolation (II)

Notations

We define and denote the LAGRANGE interpolation of the inverse by

$$\mathcal{L}_k[z^{-1}](z) = \frac{\mathcal{A}_k(z)}{\det(C_k)} = \left(1 - \frac{\chi_{C_k}(z)}{\chi_{C_k}(0)}\right) z^{-1}$$

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Notations

We define and denote the LAGRANGE interpolation of a perturbed identity by

$$\mathcal{L}_k^0[1 - \delta_{z0}](z) = \mathcal{L}_k[z^{-1}](z)z = \frac{\chi_{C_k}(0) - \chi_{C_k}(z)}{\chi_{C_k}(0)}.$$

trailing {adjugate, inverse, interpolation}

We expand all notations to the trailing submatrices $C_{l+1:k}$.

trailing {adjugate, inverse, interpolation}

We expand all notations to the trailing submatrices $C_{l+1:k}$. Then,

$$c_{1:l-1}\frac{\chi_{C_{l+1:k}}(0)-\chi_{C_{l+1:k}}(A)}{\chi_{C_k}(0)} = \tag{36}$$

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We expand all notations to the trailing submatrices $C_{l+1:k}$. Then,

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trailing {adjugate, inverse, interpolation}

We expand all notations to the trailing submatrices $C_{l+1:k}$. Then,

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trailing {adjugate, inverse, interpolation}

We expand all notations to the trailing submatrices $C_{l+1:k}$. Then,

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(Q)OR: the residuals

Theorem (the (Q)OR residual vectors)

Suppose that all submatrices $C_{l+1:k}$ are nonsingular. Then the residual vectors can be written as

$$r_k = \frac{\chi_{C_k}(A)}{\chi_{C_k}(0)} r_0 - \sum_{l=1}^{k} z_{lk} \mathcal{L}^0_{l+1:k}[1 - \delta_{z0}](A) f_l. \qquad (37)$$

This occurs frequently, consider e.g. CG for HPD A.

(Q)OR: the errors, regular A

What about the error vectors?

(Q)OR: the errors, regular A

What about the error vectors?

Theorem (the (Q)OR error vectors, regular A)

Suppose that A is invertible and let $x = A^{-1}r_0$ denote the unique solution of the linear system $Ax = r_0$.
Then the error vectors are given by

$$(x - x_k) = \frac{\chi_{C_k}(A)}{\chi_{C_k}(0)}(x - 0) + \|r_0\| \sum_{l=1}^{k} c_{1:l-1} \frac{\mathcal{A}_{l+1:k}(0, A)}{\chi_{C_k}(0)} f_l. \quad (38)$$

(Q)OR: the errors, regular A

What about invertible submatrices?

(Q)OR: the errors, regular A

What about invertible submatrices?

Theorem (the (Q)OR error vectors, regular A and $C_{l+1:k}$)

Suppose that all trailing submatrices $C_{l+1:k}$ are nonsingular. Then the error vectors can be written as

$$(x - x_k) = \frac{\chi_{C_k}(A)}{\chi_{C_k}(0)}(x - 0) - \sum_{l=1}^{k} z_{lk} \mathcal{L}_{l+1:k}[z^{-1}](A) f_l. \qquad (39)$$

(Q)OR: the errors, singular A

What about singular A?

(Q)OR: the errors, singular A

What about singular A?

Theorem (the (Q)OR error vectors, singular A)

When A is singular, with $x \equiv A^D r_0$, where A^D denotes the DRAZIN *inverse of A,*

$$(x - AA^D x_k) = \frac{\chi_{C_k}(A)}{\chi_{C_k}(0)}(x - 0) + \|r_0\| \sum_{l=1}^{k} c_{1:l-1} \frac{\mathcal{A}_{l+1:k}(0, A)}{\chi_{C_k}(0)} AA^D f_l. \quad (40)$$

(Q)OR: the errors, singular A

What about invertible submatrices?

(Q)OR: the errors, singular A

What about invertible submatrices?

Theorem (the (Q)OR error vectors, singular A, regular $C_{l+1:k}$)

When A is singular, with $x \equiv A^D r_0$,

$$(x - AA^D x_k) = \frac{\chi_{C_k}(A)}{\chi_{C_k}(0)}(x - 0) - \sum_{l=1}^{k} z_{lk} \mathcal{L}_{l+1:k}[z^{-1}](A) AA^D f_l. \quad (41)$$

(Q)OR: the iterates

The iterates x_k can be composed like the RITZ vectors.

(Q)OR: the iterates

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Theorem (the (Q)OR iterates)

$$x_k = \mathcal{L}_k[z^{-1}](A)r_0 - \|r_0\| \sum_{l=1}^{k} c_{1:l-1} \frac{\mathcal{A}_{l+1:k}(0, A)}{\chi_{C_k}(0)} f_l. \qquad (42)$$

(Q)OR: the iterates

The case of invertible $C_{l+1:k}$:

(Q)OR: the iterates

The case of invertible $C_{l+1:k}$:

Theorem (the (Q)OR iterates, regular $C_{l+1:k}$)

Suppose that all $C_{l+1:k}$ are regular.
Then

$$x_k = \mathcal{L}_k[z^{-1}](A)r_0 + \sum_{l=1}^{k} z_{lk}\mathcal{L}_{l+1:k}[z^{-1}](A)f_l. \qquad (43)$$

(Q)OR: the iterates

The case of invertible $C_{l+1:k}$:

Theorem (the (Q)OR iterates, regular $C_{l+1:k}$)

Suppose that all $C_{l+1:k}$ are regular.
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$$x_k = \mathcal{L}_k[z^{-1}](A)r_0 + \sum_{l=1}^{k} z_{lk}\mathcal{L}_{l+1:k}[z^{-1}](A)f_l. \tag{43}$$

Observation

This is a linear combination of $k+1$ approximations from distinct KRYLOV subspaces, spanned by the same matrix A, *but* distinct starting vectors.

Outline

(Q)MR: the approach

Let $\underline{z}_k$ denote the minimal-norm solution of the least-squares problem

$$\|\underline{C}_k \underline{z}_k - \underline{e}_1 \|r_0\|\| = \min . \tag{44}$$

(Q)MR: the approach

Let $\underline{z}_k$ denote the minimal-norm solution of the least-squares problem

$$\|\underline{C}_k \underline{z}_k - \underline{e}_1 \|r_0\|\| = \min . \tag{44}$$

Define the kth (Q)MR iterate $\underline{x}_k$ by

$$\underline{x}_k = Q_k \underline{z}_k \tag{45}$$

(Q)MR: the approach

Let $\underline{z}_k$ denote the minimal-norm solution of the least-squares problem

$$\|\underline{C}_k \underline{z}_k - \underline{e}_1 \|r_0\|\| = \min\,. \tag{44}$$

Define the kth (Q)MR iterate $\underline{x}_k$ by

$$\underline{x}_k = Q_k \underline{z}_k \tag{45}$$

and the kth quasi-residual by

$$\mathfrak{r}_k = \underline{e}_1 \|r_0\| - \underline{C}_k \underline{z}_k = (\underline{I}_k - \underline{C}_k \underline{C}_k^{\dagger}) \underline{e}_1 \|r_0\|. \tag{46}$$

(Q)MR: a backward expression for the residual

Observation

The residual $\underline{r}_k$ of the (Q)MR iterates has the following backward expression:

$$\underline{r}_k = r_0 - A\underline{x}_k = Q_{k+1}\underline{e}_1\|r_0\| - AQ_k\underline{z}_k \tag{47}$$

$$= Q_{k+1}(\underline{e}_1\|r_0\| - \underline{C}_k\underline{z}_k) + F_k\underline{z}_k = Q_{k+1}\mathfrak{r}_k + \sum_{l=1}^{k} f_l\underline{z}_{lk}. \tag{48}$$

(Q)MR: a backward expression for the residual

Observation

The residual $\underline{r}_k$ of the (Q)MR iterates has the following backward expression:

$$\underline{r}_k = r_0 - A\underline{x}_k = Q_{k+1}\underline{e}_1\|r_0\| - AQ_k\underline{z}_k \tag{47}$$

$$= Q_{k+1}(\underline{e}_1\|r_0\| - \underline{C}_k\underline{z}_k) + F_k\underline{z}_k = Q_{k+1}\mathfrak{r}_k + \sum_{l=1}^{k} f_l \underline{z}_{lk}. \tag{48}$$

Observation

To express the residual $\underline{r}_k$ as polynomial in A, we "only" need "polynomial" expressions for $\mathfrak{r}_k$ and $\underline{z}_k$.

(Q)MR: HESSENBERG rewritings

Definition (the scalar vectors μ, $\check{\mu}$ and $\hat{\mu}$)

We define pairs of vectors $\mu^j, \check{\mu}^j \in \mathbb{C}^j$ and $\hat{\mu}^j \equiv \overline{\check{\mu}}^j \in \mathbb{C}^j$:

$$\mu \equiv \left(\frac{(-1)^{l+1} \det(C_{l+1:j})}{c_{l:j-1}} \right)_{l=1}^{j}, \tag{49}$$

$$\check{\mu} \equiv \left(\frac{(-1)^{j-l} \det(C_{l-1})}{c_{1:l-1}} \right)_{l=1}^{j}. \tag{50}$$

(Q)MR: HESSENBERG rewritings

Lemma (MOORE-PENROSE inverse of extended HESSENBERG)

The MOORE-PENROSE *inverse of the extended* HESSENBERG *matrix $\underline{C}_k$ is given by*

$$\underline{C}_k^\dagger = \frac{\sum_{j=1}^{k} |c_{j+1:k}|^2 \begin{pmatrix} \overline{\det(C_j)}\mathrm{adj}(C_j) & \overline{c_{1:j}}\mathrm{adj}(C_j)\hat{\underline{\mu}}^j & O_{j,k-j} \\ O_{k-j,j} & o_{k-j} & O_{k-j} \end{pmatrix}}{\sum_{j=0}^{k} |c_{j+1:k}|^2 |\det(C_j)|^2}. \tag{51}$$

(Q)MR: HESSENBERG rewritings

Lemma (the minimal norm solution)

The minimal norm solution $\underline{z}_k$ is given by

$$\frac{\underline{z}_k}{\|r_0\|} = \frac{\sum_{j=1}^{k} |c_{j+1:k}|^2 \begin{pmatrix} \overline{\det(C_j)} c_{1:j-1} \mu^j \\ o_{k-j} \end{pmatrix}}{\sum_{j=0}^{k} |c_{j+1:k}|^2 |\det(C_j)|^2} \tag{52}$$

$$= (-1)^{k+1} \frac{\begin{pmatrix} o_k & \operatorname{adj}(C_{k+1}^{\triangle}) \end{pmatrix} \operatorname{adj}(C_{k+1}^H) e_{k+1}}{\sum_{j=0}^{k} |c_{j+1:k}|^2 |\det(C_j)|^2}. \tag{53}$$

(Q)MR: HESSENBERG rewritings

Lemma ((Q)MR and (Q)OR)

Suppose all leading C_j are regular. Then the relation between the kth (Q)MR solution $\underline{z}_k$ and all prior (Q)OR solutions z_j is given by

$$\underline{z}_k = \frac{\sum_{j=0}^{k} |\det(C_j)|^2 |c_{j+1:k}|^2 \begin{pmatrix} z_j \\ o_{k-j} \end{pmatrix}}{\sum_{j=0}^{k} |\det(C_j)|^2 |c_{j+1:k}|^2}, \qquad (54)$$

where z_0 is the empty matrix with dimensions 0×1.

(Q)MR: HESSENBERG rewritings

Lemma (the quasi-residual)

The quasi-residual $\mathfrak{r}_k$ is given by

$$\frac{\mathfrak{r}_k}{\|r_0\|} = c_{1:k} \left(\frac{(-1)^{l-1}\overline{c_{l:k} \det(C_{l-1})}}{\sum_{j=0}^{k} |c_{j+1:k}|^2 |\det(C_j)|^2} \right)_{l=1}^{k+1} . \tag{55}$$

(Q)MR: the residuals, errors and iterates

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This is currently work in progress.

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- on the (Q)OR iterates to understand the “delay”.

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We have proven

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Based on the behavior of the solution vectors z_k and/or the LAGRANGE interpolations we can allow the perturbation vectors f_l to grow (in certain directions).

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- (Q)MR case has to be investigated more thoroughly.

that’s all . . .

Děkuji.