Tuning IDR to fit your applications

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joint work with Olaf Rendel & Anisa Rizvanolli

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Outline

Krylov subspace methods

Hessenberg decompositions

Polynomial representations

IDR

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IDRStab and QMRIDR

Tuning IDR

General comments

Shadow vectors

Stabilizing polynomials

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Outline

Introduction

Krylov subspace methods: approximations

$$\left.\begin{array}{l}\mathbf{x}_k,\underline{\mathbf{x}}_k,\\ \mathbf{y}_k,\underline{\mathbf{y}}_k\end{array}\right\} \in \mathcal{K}_k(\mathbf{A},\mathbf{q}) := \text{span}\,\{\mathbf{q},\mathbf{A}\mathbf{q},\ldots,\mathbf{A}^{k-1}\mathbf{q}\} = \{p(\mathbf{A})\mathbf{q} \mid p \in \mathbb{P}_{k-1}\},$$

where

$$\mathbb{P}_{k-1} := \Big\{\sum_{j=0}^{k-1} \alpha_j z^j \mid \alpha_j \in \mathbb{C},\ 0 \leqslant j < k\Big\},$$

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to solutions of linear systems

$$\mathbf{A}\mathbf{x} = \mathbf{r}_0 \ (= \mathbf{b} - \mathbf{A}\mathbf{x}_0), \qquad \mathbf{A} \in \mathbb{C}^{n \times n}, \quad \mathbf{b}, \mathbf{x}_0 \in \mathbb{C}^n,$$

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and (partial) eigenproblems

$$\mathbf{A}\mathbf{v} = \mathbf{v}\lambda, \qquad \mathbf{A} \in \mathbb{C}^{n \times n}.$$

Hessenberg decompositions

Construction of basis vectors resembled in structure of arising Hessenberg decomposition

$$\mathbf{A}\mathbf{Q}_k = \mathbf{Q}_{k+1}\underline{\mathbf{H}}_k,$$

where

- $\mathbf{Q}_{k+1} = (\mathbf{Q}_k, \mathbf{q}_{k+1}) \in \mathbb{C}^{n\times(k+1)}$ collects basis vectors,
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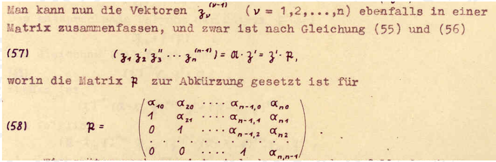
Aspects of perturbed Krylov subspace methods: captured with perturbed Hessenberg decompositions

$$\mathbf{A}\mathbf{Q}_k + \mathbf{F}_k = \mathbf{Q}_{k+1}\underline{\mathbf{H}}_k,$$

$\mathbf{F}_k \in \mathbb{C}^{n\times k}$ accounts for perturbations (finite precision & inexact methods).

Karl Hessenberg & “his” matrix + decomposition

"‘Behandlung linearer Eigenwertaufgaben mit Hilfe der Hamilton-Cayleyschen Gleichung"’, Karl Hessenberg, 1. Bericht der Reihe "‘Numerische Verfahren"’, July, 23rd 1940, page 23:



Man kann nun die Vektoren $\mathfrak{z}_\nu^{(\nu-1)}$ $(\nu = 1,2,\dots,n)$ ebenfalls in einer Matrix zusammenfassen, und zwar ist nach Gleichung (55) und (56)

$$(57) \qquad (\mathfrak{z}_1\,\mathfrak{z}_2'\,\mathfrak{z}_3''\cdots\mathfrak{z}_n^{(n-1)}) = \mathfrak{A}\cdot\mathfrak{Z}' = \mathfrak{Z}'\cdot\mathfrak{P},$$

worin die Matrix $\mathfrak{P}$ zur Abkürzung gesetzt ist für

$$(58) \qquad \mathfrak{P} = \begin{pmatrix} \alpha_{10} & \alpha_{20} & \cdots & \alpha_{n-1,0} & \alpha_{n0} \\ 1 & \alpha_{21} & \cdots & \alpha_{n-1,1} & \alpha_{n1} \\ 0 & 1 & \cdots & \alpha_{n-1,2} & \alpha_{n2} \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & \alpha_{n,n-1} \end{pmatrix}.$$

- Hessenberg decomposition, Eqn. (57),
- Hessenberg matrix, Eqn. (58).

Karl Hessenberg (* September 8th, 1904, † February 22nd, 1959)

Important Polynomials

Residuals of OR and MR approximation

$$\mathbf{x}_k := \mathbf{Q}_k \mathbf{z}_k \quad \text{and} \quad \underline{\mathbf{x}}_k := \mathbf{Q}_k \underline{\mathbf{z}}_k$$

with coefficient vectors

$$\mathbf{z}_k := \mathbf{H}_k^{-1} \mathbf{e}_1 \|\mathbf{r}_0\| \quad \text{and} \quad \underline{\mathbf{z}}_k := \underline{\mathbf{H}}_k^{\dagger} \underline{\mathbf{e}}_1 \|\mathbf{r}_0\|$$

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Convergence of OR and MR depends on (harmonic) Ritz values.

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polynomial representation

$$\mathbf{r}_k = \mathcal{R}_k(\mathbf{A})\mathbf{r}_0 - \sum_{\ell=1}^{k} z_{\ell k}\mathcal{R}_{\ell+1:k}(\mathbf{A})\mathbf{f}_\ell + \mathbf{F}_k\mathbf{z}_k$$

(all trailing square Hessenberg matrices are assumed to be regular).

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Convergence: $\mathbf{F}_k\mathbf{z}_k$ bounded (inexact methods) & $\mathcal{R}_{\ell+1:k}(\mathbf{A})$ “small”.

Outline

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1976	Idea by Sonneveld
1979	First talk on IDR
1980	Proceedings
1989	CGS
1992	IDR $\rightsquigarrow$ BiCGStab
1993	BiCGStab2, BiCGStab(ℓ)
later	“acronym explosion” ...

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IDR(s) is a Krylov subspace method $\rightsquigarrow$ all techniques from 90's applicable!

IDR(s)

IDR spaces:

$$\mathcal{G}_0 := \mathcal{K}(\mathbf{A}, \mathbf{q}), \qquad \text{(full Krylov subspace)}$$
$$\mathcal{G}_j := (\alpha_j \mathbf{A} + \beta_j \mathbf{I})(\mathcal{G}_{j-1} \cap \mathcal{S}), \quad j \geqslant 1, \quad \alpha_j, \beta_j \in \mathbb{C}, \quad \alpha_j \neq 0,$$

where

$$\operatorname{codim}(\mathcal{S}) = s, \quad \text{e.g.,} \quad \mathcal{S} = \operatorname{span}\{\widetilde{\mathbf{R}}_0\}^\perp, \quad \widetilde{\mathbf{R}}_0 \in \mathbb{C}^{n \times s}.$$

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Interpreted as Sonneveld spaces (Sleijpen, Sonneveld, van Gijzen 2010):

$$\mathcal{G}_j = \mathcal{S}_j(P_j, \mathbf{A}, \widetilde{\mathbf{R}}_0) := \left\{ P_j(\mathbf{A})\mathbf{v} \mid \mathbf{v} \perp \mathcal{K}_j(\mathbf{A}^\mathsf{H}, \widetilde{\mathbf{R}}_0) \right\},$$
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Image of shrinking space: Induced Dimension Reduction.

IDR(s)

IDR spaces nested:

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$$\mathbf{v}_k = \sum_{i=k-s}^{k} \mathbf{g}_i \gamma_i, \quad \widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{v}_k = \mathbf{o}_s, \quad k \geqslant s+1,$$

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IDR(s)

Generalized Hessenberg decomposition:

$$\mathbf{A}\mathbf{V}_k = \mathbf{A}\mathbf{G}_k\mathbf{U}_k = \mathbf{G}_{k+1}\underline{\mathbf{H}}_k,$$

where $\mathbf{U}_k \in \mathbb{C}^{k\times k}$ upper triangular.

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Structure of Sonneveld pencils:

$$\mathbf{H}_k = \left(\begin{array}{cccccccccccc}
\times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
+ & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & + & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & + & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & + & \times & \times & \times & \times & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & + & \times
\end{array}\right), \quad
\left(\begin{array}{cccccccccccc}
\times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \times & \times & \times & \times & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \times & \times & \times & \times & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \times & \times & \times & \times & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \times & \times & \times & \times & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \times & \times & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \times & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \times
\end{array}\right) = \mathbf{U}_k$$

IDREIG

Eigenvalues of Sonneveld pencil $(\mathbf{H}_k, \mathbf{U}_k)$ are roots of residual polynomials. Those distinct from roots of

$$P_j(z) = \prod_{i=1}^{j} (\alpha_i z + \beta_i), \quad \text{i.e.,} \quad z_i = -\frac{\beta_i}{\alpha_i}, \quad 1 \leqslant i \leqslant j$$

converge to eigenvalues of $\mathbf{A}$.

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$$\begin{aligned} \widehat{\mathbf{G}}_k^{\mathsf{H}}(\mathbf{A}, \mathbf{I}_n)\mathbf{G}_k\mathbf{U}_k &= \widehat{\mathbf{G}}_k^{\mathsf{H}}(\mathbf{A}\mathbf{G}_k\mathbf{U}_k, \mathbf{G}_k\mathbf{U}_k) \\ &= \widehat{\mathbf{G}}_k^{\mathsf{H}}(\mathbf{G}_{k+1}\underline{\mathbf{H}}_k, \mathbf{G}_k\mathbf{U}_k) = (\underline{\mathbf{I}}_k^{\mathsf{T}}\underline{\mathbf{H}}_k, \mathbf{U}_k) = (\mathbf{H}_k, \mathbf{U}_k), \end{aligned} \tag{1}$$

here, $\widehat{\mathbf{G}}_k^{\mathsf{H}} := \underline{\mathbf{I}}_k^{\mathsf{T}}\mathbf{G}_{k+1}^{\dagger}$.

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Use deflated pencil for Lanczos Ritz values (Gutknecht, Z. (2010): IDREig).

IDREIG

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Use deflated pencil for Lanczos Ritz values (Gutknecht, Z. (2010): IDREIG). First: IDR(s)ORES, Olaf Rendel: IDR(s)BIO, Anisa Rizvanolli: IDR(s)STAB(ℓ).

IDRSTAB

IDR(s)STAB(ℓ) (Tanio & Sugihara; Sleijpen & van Gijzen): combine ideas of IDR(s) and BiCGSTAB(ℓ).

IDRSTAB

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IDRSTAB (Sleijpen's implementation) recursively computes "(extended) Hessenberg matrices of basis matrices and residuals" ($k \geqslant 1$):

$$
\begin{array}{llll}
\mathbf{G}_{11}^{(k)}, \mathbf{r}_{11}^{(k)} & \mathbf{G}_{12}^{(k)}, \mathbf{r}_{12}^{(k)} & \cdots & \mathbf{G}_{1,\ell+1}^{(k)}, \quad \mathbf{r}_{1,\ell+1}^{(k)} \\
\mathbf{G}_{21}^{(k)}, \mathbf{r}_{21}^{(k)} & \mathbf{G}_{22}^{(k)}, \mathbf{r}_{22}^{(k)} & \cdots & \mathbf{G}_{2,\ell+1}^{(k)}, \quad \mathbf{r}_{2,\ell+1}^{(k)} \\
 & \mathbf{G}_{32}^{(k)}, \mathbf{r}_{32}^{(k)} & \ddots & \vdots \\
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 & & & \mathbf{G}_{\ell+2,\ell+1}^{(k)}
\end{array}
$$

$$
\begin{aligned}
\mathbf{G}_{i,j}^{(k)} &\in \mathbb{C}^{n\times s}, & \mathbf{r}_{i,j}^{(k)} &\in \mathbb{C}^{n}, \\
\mathbf{G}_{i+1,j}^{(k)} &= \mathbf{A}\mathbf{G}_{i,j}^{(k)}, & \mathbf{r}_{i+1,j}^{(k)} &= \mathbf{A}\mathbf{r}_{i,j}^{(k)}, \\
\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{G}_{ii}^{(k)} &= \mathbf{O}_s, & \widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{r}_{ii}^{(k)} &= \mathbf{o}_s, \\
(\mathbf{G}_{ii}^{(k)})^{\mathsf{H}}\mathbf{G}_{ii}^{(k)} &= \mathbf{I}_s.
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$$

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\end{aligned}
$$

Initialization using Arnoldi's method:

$$
\mathbf{G}_{21}^{(1)} = \mathbf{A}\mathbf{G}_{11}^{(1)} = (\mathbf{G}_{11}^{(1)}, \mathbf{g}_{\mathsf{tmp}})\underline{\mathbf{H}}_s^{(0)},
$$

$$
\mathbf{r}_{11}^{(1)} = \mathbf{r}_0 - \mathbf{G}_{21}^{(1)}\boldsymbol{\alpha}^{(1)} = (\mathbf{I} - \mathbf{G}_{21}^{(1)}(\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{G}_{21}^{(1)})^{-1}\widetilde{\mathbf{R}}_0^{\mathsf{H}})\mathbf{r}_0, \quad \mathbf{r}_{21}^{(1)} = \mathbf{A}\mathbf{r}_{11}^{(1)}.
$$

IDRSTAB

Columnwise update (IDR part) such that diagonal blocks

- form basis of $\mathcal{G}_j \setminus \mathcal{G}_{j+1}$ with expansion $\mathcal{G}_j = \mathbf{A}(\mathcal{G}_{j-1} \cap \mathcal{S}) \rightsquigarrow \beta^{(j)} \in \mathbb{C}^{s \times s}$,
- are orthonormalized $\rightsquigarrow \underline{\mathbf{H}}_{s-1}^{(j)} \in \mathbb{C}^{s \times (s-1)}$

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In particular, with $\widetilde{\mathbf{v}}_i \in \mathcal{G}_{j-1} \cap \mathcal{S}$,

$$
\begin{aligned}
\boldsymbol{\beta}_i^{(j)} &= (\widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{G}_{j,j-1})^{-1} \widetilde{\mathbf{R}}_0^{\mathsf{H}} (\mathbf{A}\widetilde{\mathbf{v}}_i) \\
\Rightarrow \quad (\mathbf{A}\widetilde{\mathbf{v}}_i) - \mathbf{G}_{j,j-1}\boldsymbol{\beta}_i^{(j)} &= \mathbf{A}(\widetilde{\mathbf{v}}_i - \mathbf{G}_{j-1,j-1}\boldsymbol{\beta}_i^{(j)}) \in \mathcal{G}_j \cap \mathcal{S}
\end{aligned}
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Every new vector in $\mathcal{G}_j \cap \mathcal{S}$ is orthonormalized with respect to the others.

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Thus, for the IDR-IDRSTAB pencil relating (STAB-purified) diagonal blocks,

- $\beta^{(j)} \in \mathbb{C}^{s \times s}$ couples $\mathbf{G}_{jj}$ and $\mathbf{G}_{j,j-1} = \mathbf{A}\mathbf{G}_{j-1,j-1} \rightsquigarrow \mathbf{U}_k$,
- $\underline{\mathbf{H}}_{s-1}^{(j)} \in \mathbb{C}^{s \times (s-1)}$ couples result with others in same block $\rightsquigarrow \underline{\mathbf{H}}_k$.

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All other blocks in column treated in same manner.

IDRSTAB

Residual updates en détail ($i \leqslant j$, $\mathbf{r}_{j+1,j}^{(k)} = \mathbf{A}\mathbf{r}_{j,j}^{(k)}$):

$$\mathbf{r}_{i,j}^{(k)} = \mathbf{r}_{i,j-1}^{(k)} - \mathbf{G}_{i+1,j}^{(k)}\alpha^{(j)}, \quad \mathbf{r}_{j,j}^{(k)} = (\mathbf{I} - \mathbf{G}_{j+1,j}^{(k)}(\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{G}_{j+1,j}^{(k)})^{-1}\widetilde{\mathbf{R}}_0^{\mathsf{H}})\mathbf{r}_{j,j-1}^{(k)}.$$

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$$\alpha^{(j)} := (\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{G}_{j+1,j}^{(k)})^{-1}\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{r}_{j,j-1}^{(k)},$$

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$\alpha^{(j)}$ relating $\mathbf{r}_{j,j-1}^{(k)} = \mathbf{A}\mathbf{r}_{j-1,j-1}^{(k)}$ (old) and $\mathbf{r}_{j,j}^{(k)}$ (new) via $\mathbf{G}_{j+1,j}^{(k)} = \mathbf{A}\mathbf{G}_{j,j}^{(k)} \rightsquigarrow \mathbf{U}_k$.

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New cycle (STAB part, $\mathbf{r}_{21}^{(k+1)} = \mathbf{A}\mathbf{r}_{11}^{(k+1)}$, $\gamma^{(\ell)} \in \mathbb{C}^s$ such that $\|\mathbf{r}_{11}^{(k+1)}\| = \min$):

$$\mathbf{r}_{11}^{(k+1)} = \mathbf{r}_{1,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{r}_{i+1,\ell+1}^{(k)}\gamma_i^{(\ell)}, \quad \begin{cases} \mathbf{G}_{11}^{(k+1)} = \mathbf{G}_{1,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{G}_{i+1,\ell+1}^{(k)}\gamma_i^{(\ell)}, \\ \mathbf{G}_{21}^{(k+1)} = \mathbf{G}_{2,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{G}_{i+2,\ell+1}^{(k)}\gamma_i^{(\ell)}. \end{cases}$$

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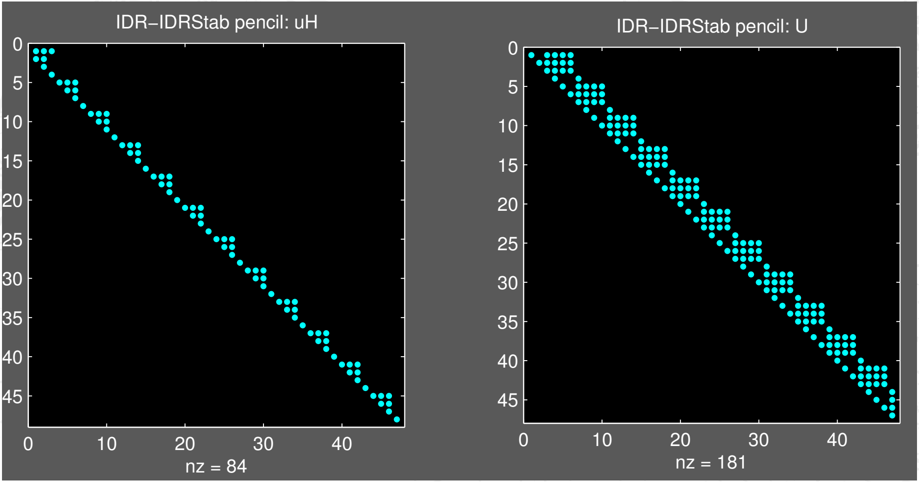
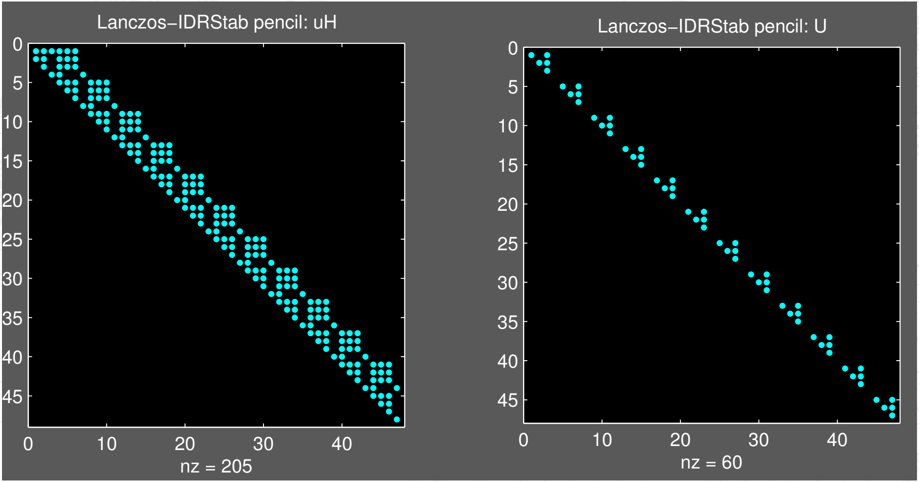
Anisa Rizvanolli: $\rightsquigarrow$ Lanczos-IDRSTAB pencil for eigenvalues, IDRSTABEIG.

Structure of (STAB-purified) IDR-IDRSTAB pencil



Structure of (undeflated) Lanczos-IDRSTAB pencil



QMRIDR

MR methods: use extended Hessenberg matrix

$$\underline{\mathbf{x}}_k := \mathbf{Q}_k \underline{\mathbf{z}}_k, \quad \underline{\mathbf{z}}_k := \underline{\mathbf{H}}_k^{\dagger} \underline{\mathbf{e}}_1 \|\mathbf{r}_0\|.$$

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IDR based: generalized Hessenberg decomposition,

$$\mathbf{A}\mathbf{V}_k = \mathbf{A}\mathbf{G}_k\mathbf{U}_k = \mathbf{G}_{k+1}\underline{\mathbf{H}}_k.$$

Thus,

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Simplified residual bound (block-wise orthonormalization):

$$\begin{aligned} \|\mathbf{r}_k\| = \|\mathbf{r}_0 - \mathbf{A}\mathbf{x}_k\| &\leqslant \|\mathbf{G}_{k+1}\| \cdot \left\| \underline{\mathbf{e}}_1 \|\mathbf{r}_0\| - \underline{\mathbf{H}}_k \mathbf{z}_k \right\| \\ &\leqslant \sqrt{\left\lceil \frac{k+1}{s+1} \right\rceil} \cdot \left\| \underline{\mathbf{e}}_1 \|\mathbf{r}_0\| - \underline{\mathbf{H}}_k \mathbf{z}_k \right\|. \end{aligned}$$

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$$\mathbf{x}_k := \mathbf{V}_k \mathbf{z}_k = \mathbf{G}_k \mathbf{U}_k \mathbf{z}_k, \quad \mathbf{z}_k := \underline{\mathbf{H}}_k^{\dagger} \underline{\mathbf{e}}_1 \|\mathbf{r}_0\|.$$

Simplified residual bound (block-wise orthonormalization):

$$\begin{aligned}\|\mathbf{r}_k\| = \|\mathbf{r}_0 - \mathbf{A}\mathbf{x}_k\| &\leqslant \|\mathbf{G}_{k+1}\| \cdot \left\|\underline{\mathbf{e}}_1 \|\mathbf{r}_0\| - \underline{\mathbf{H}}_k \mathbf{z}_k\right\| \\ &\leqslant \sqrt{\left\lceil \frac{k+1}{s+1} \right\rceil} \cdot \left\|\underline{\mathbf{e}}_1 \|\mathbf{r}_0\| - \underline{\mathbf{H}}_k \mathbf{z}_k\right\|.\end{aligned}$$

Implementation based on short recurrences possible.

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Generalized Hessenberg relation, generically no longer generalized Hessenberg decomposition, as generically

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Computation of flexible MR iterate and flexible MR approximation:

$$\underline{\mathbf{z}}_k := \underline{\mathbf{H}}_k^{\dagger}\underline{\mathbf{e}}_1\|\mathbf{r}_0\|, \quad \underline{\mathbf{x}}_k := \widetilde{\mathbf{V}}_k\underline{\mathbf{z}}_k.$$

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Flexible IDR variants algorithmically very easy to implement.

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Various extensions for IDRSTAB: Olaf Rendel, Z. $\rightsquigarrow$ QMRIDRSTAB.

Outline

Lanczos$(s, 1) \rightsquigarrow$ the idea behind IDR(s)

Excerpt from (Sleijpen and van der Vorst, 1995, p. 204):

> *"[..], we expect to recover the convergence behavior of the incorporated Bi-CG process (in the BiCGstab methods) if we compute the iteration coefficients as accurately as possible. Therefore, we want to avoid all additional perturbations that might be introduced by an unfortunate choice of the polynomial process that is carried out on top of the Bi-CG process."*

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Noted in (van Gijzen et al., 2011):

> *"[..] numerical experiments indicate that the "local closeness" of this Lanczos process to an unperturbed one is the driving force behind IDR based methods."*

Natural & good choices

Variety of approaches to chose the shadow vectors $\widetilde{\mathbf{R}}_0$:

- problem dependent,
- Recycle old information, e.g., use space spanned by previous solutions to similar problems (Newton's method; Optimization; Design Processes),
- Use (previously computed) (left) eigenvector information in IDR eigenvalue solvers,
- In PDE problems adapt shadow space to match geometrical structure (Substructuring; (Non-)Overlapping Schwarz).

Natural & good choices

Variety of approaches to chose the shadow vectors $\widetilde{\mathbf{R}}_0$:

- problem dependent,
- computer dependent,

- In general use orthonormalized basis vectors; this ensures enhanced numerical stability,
- In parallel implementations use shadow vectors adapted to the topology, i.e., non-overlapping shadow vectors,
- For better Lanczos$(s, 1)$ coefficients use higher precision,
- For faster evaluation use sparse and/or integer (e.g., with elements $0, \pm 1$) shadow vectors.

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Variety of approaches to chose the shadow vectors $\widetilde{\mathbf{R}}_0$:

- problem dependent,
- computer dependent,
- independent.

If nothing is known about the matrix $\mathbf{A}$ and the computer architecture, in some sense the best choice seems to be an orthonormalized set of random vectors, cf. (Sonneveld, 2010).

This is the choice we used in our experiments.

Thinking locally or acting globally

Questions concerning the STAB-part:

- How do we choose the degrees of the polynomials?
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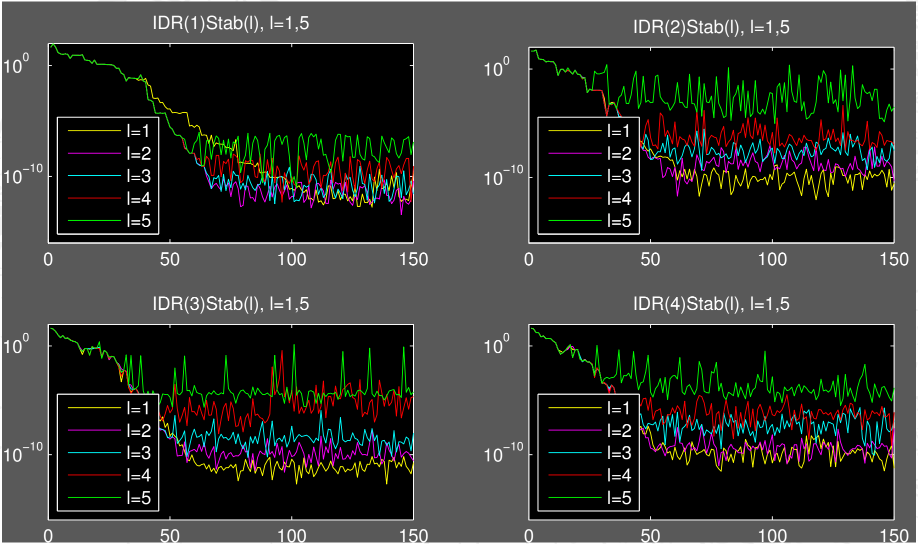
We advocate to use a moderate degree ($\ell \in \{1, 2, 3, 4\}$) for eigenvalues.

Dependence of the Ritz value convergence on ℓ



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This may slow down convergence, a cure is to ensure that the coefficients of the Lanczos$(s, 1)$ process are computed more accurately, allowing an increase in norm $\rightsquigarrow$ "vanilla variant" (Sleijpen and van der Vorst, 1995).

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Convergence depends on the interpolation of the function $z \mapsto z^{-1}$ on the spectrum using the Ritz values. We investigate various choices for the polynomial roots based on inclusion/exclusion regions for the spectrum and placement of poles.

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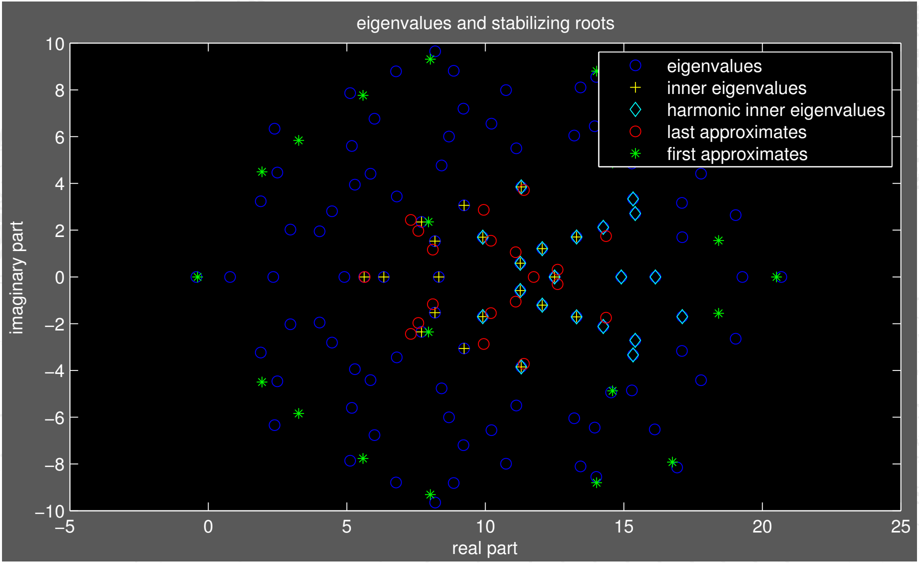
In the experiments we always used matrices $\mathbf{A} \in \mathbb{R}^{100\times 100}$:

- a shifted random matrix,
- a Grcar matrix,
- a Frank matrix,
- a randomly perturbed Poisson matrix, $\tau = \texttt{eps} = 2^{-52} \approx 2.2204 \cdot 10^{-16}$,
- a randomly perturbed Poisson matrix, $\tau = \sqrt[4]{\texttt{eps}} \approx 1.2207 \cdot 10^{-4}$.

Various choices for stabilizer roots: Example 1



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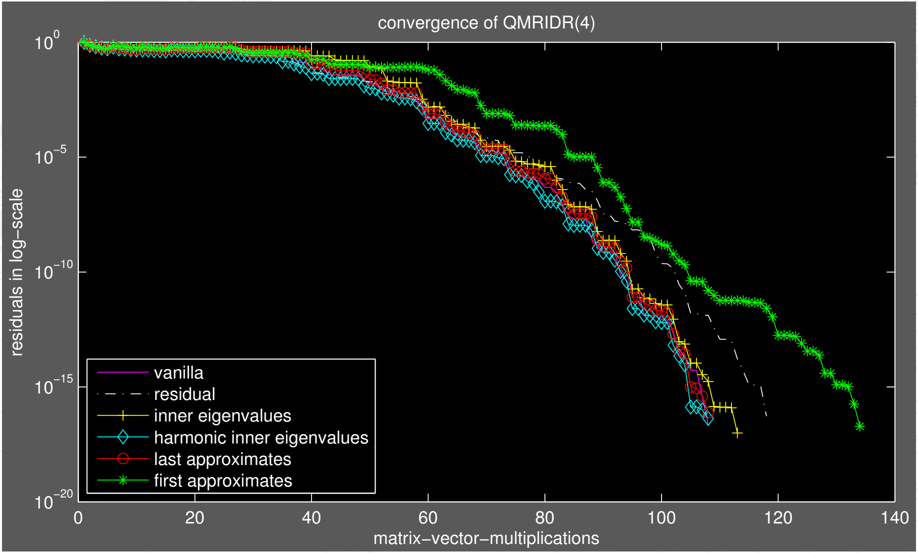
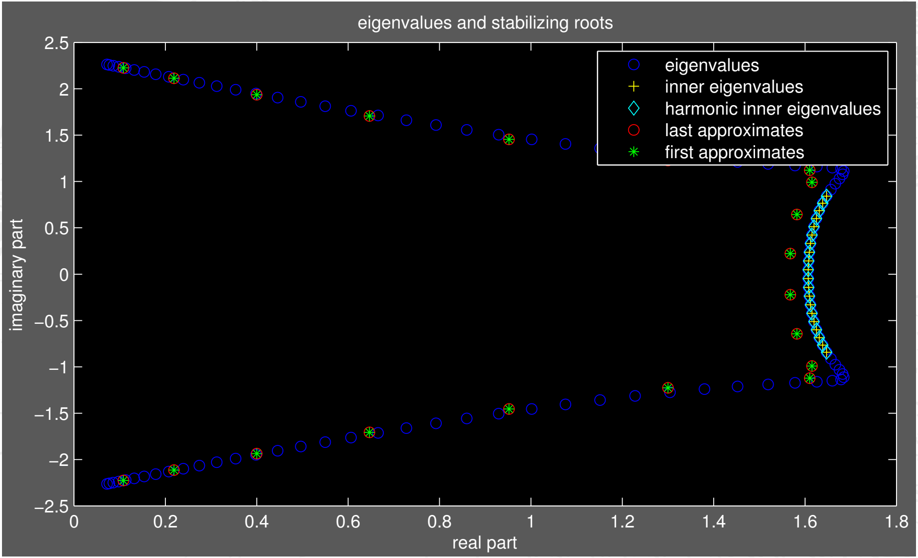


Various choices for stabilizer roots: Example 2



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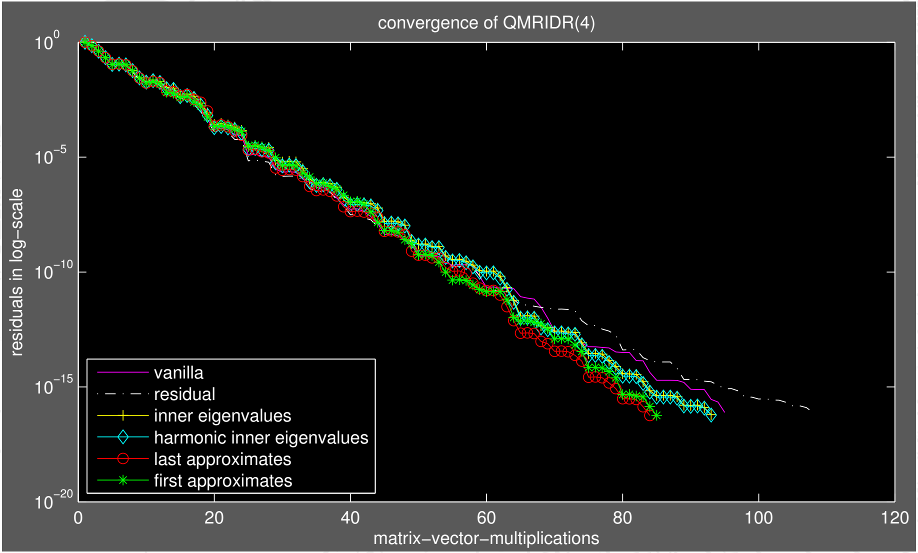
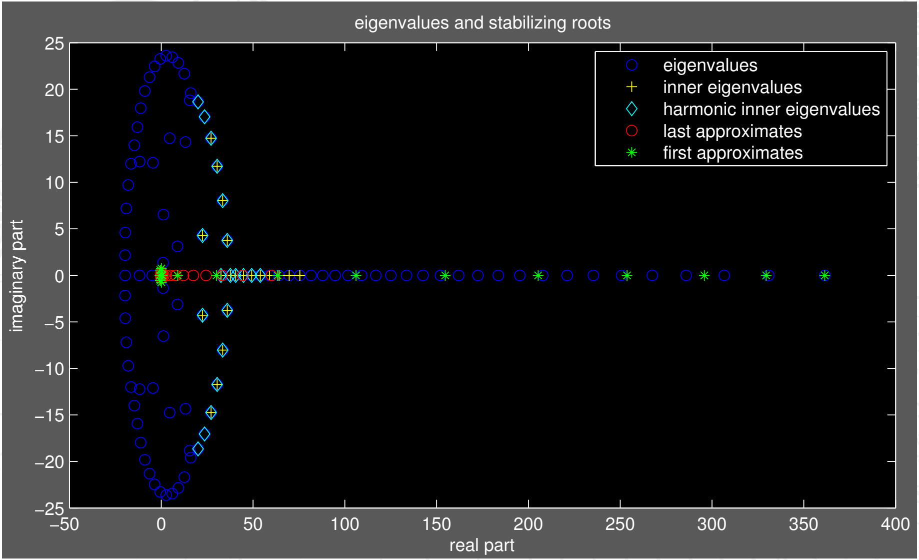


Various choices for stabilizer roots: Example 3



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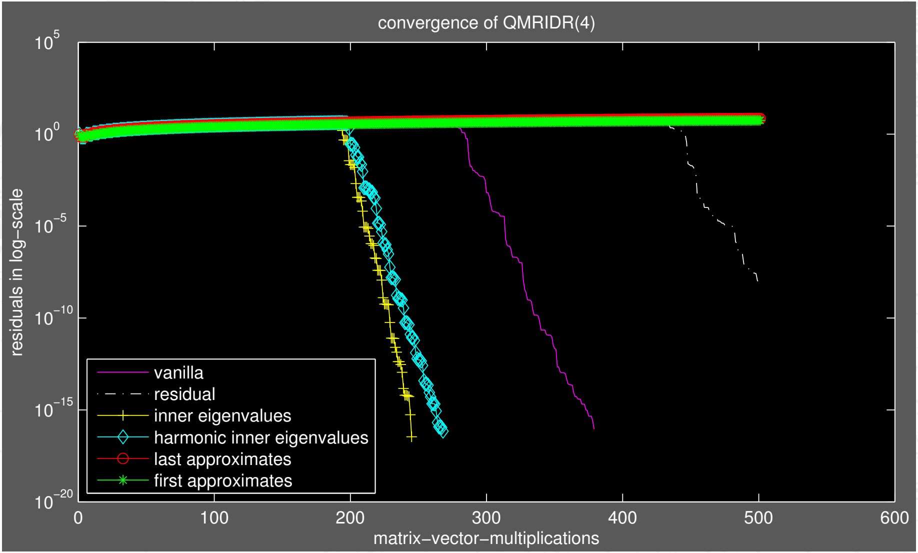
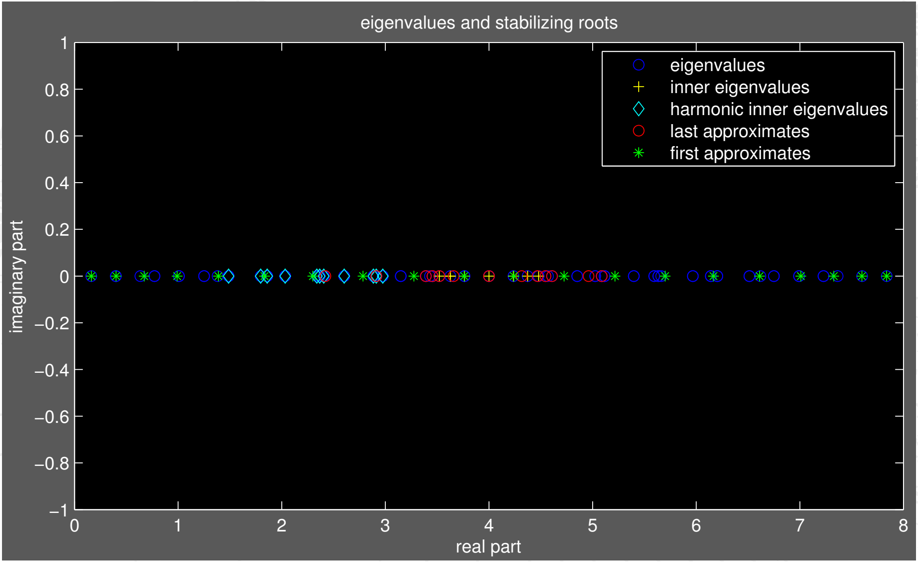


Various choices for stabilizer roots: Example 4



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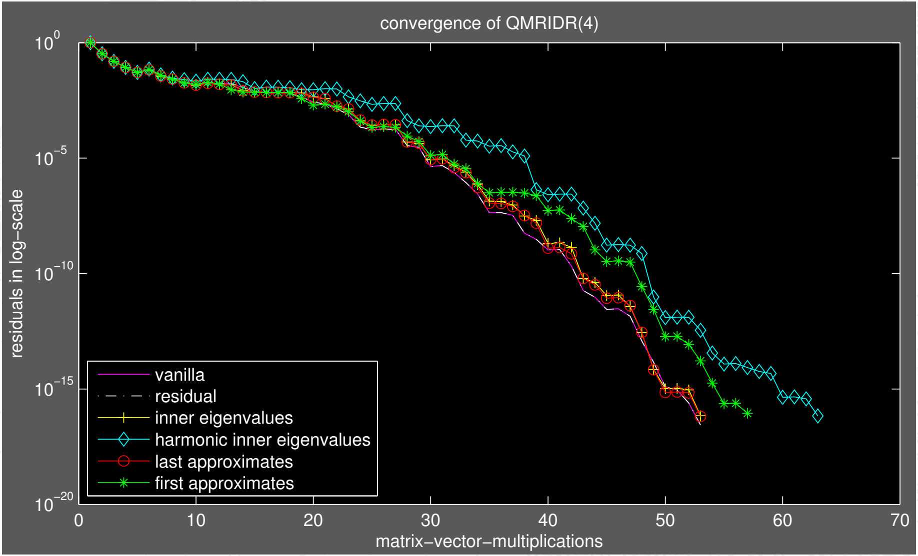

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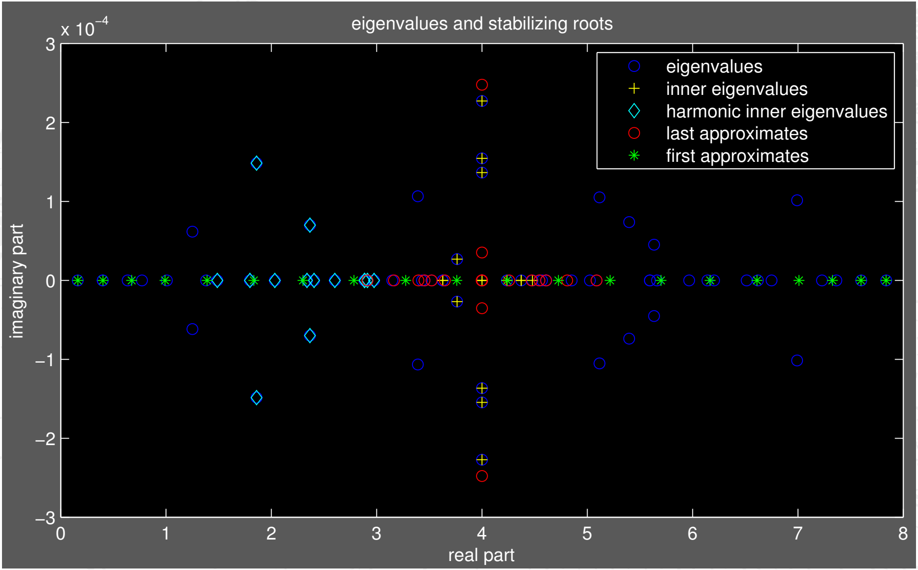

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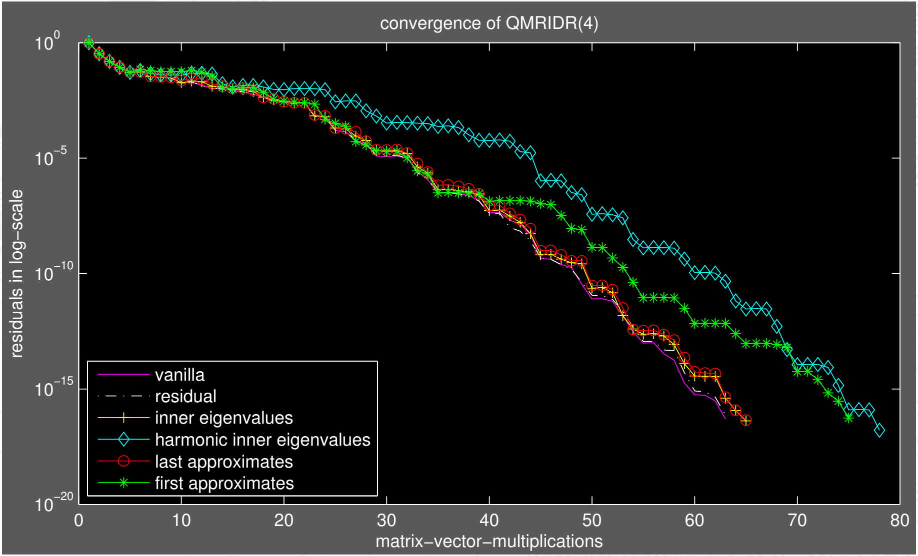

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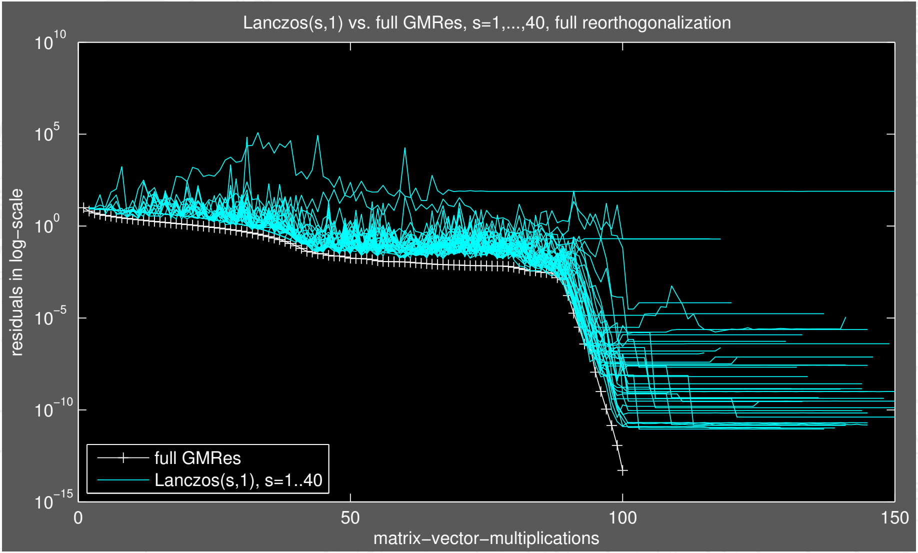
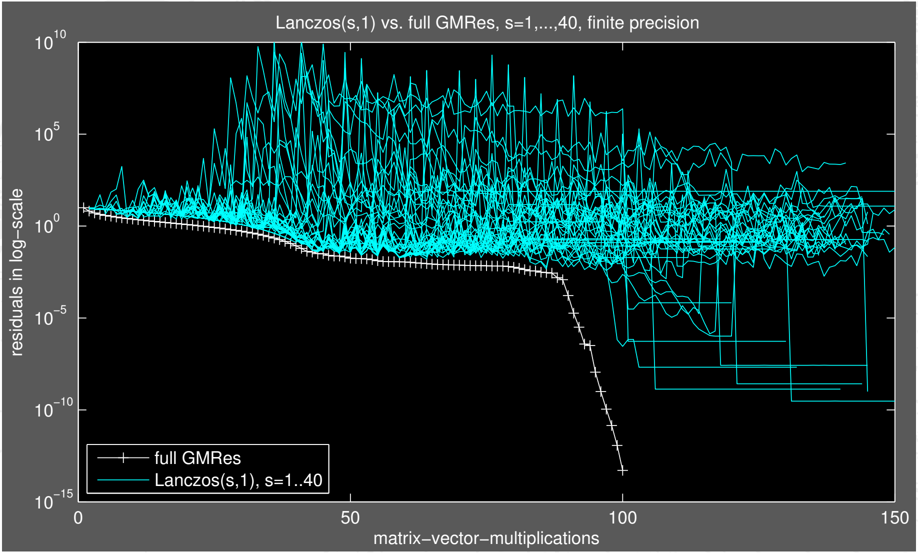
We remark that the prototype IDR algorithm suffered from instability for large values of s. We only consider new, stable implementations.

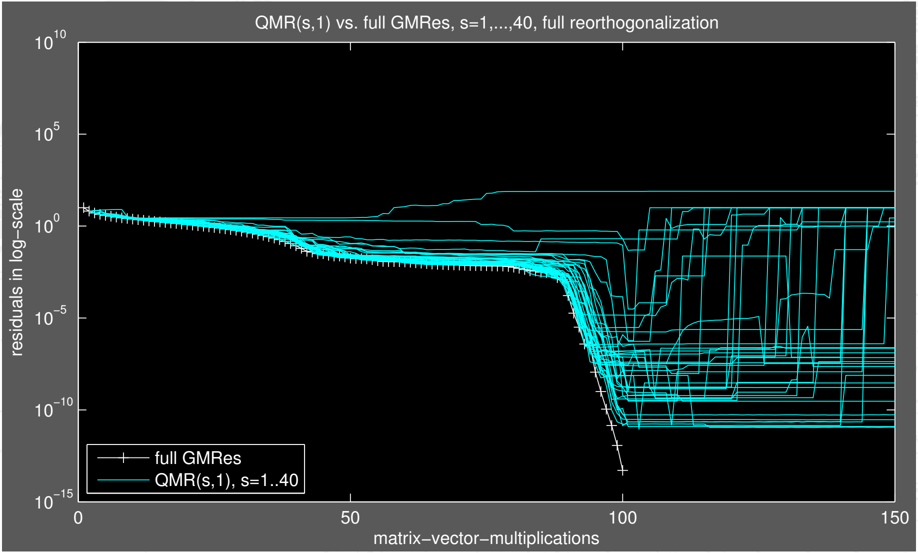
"Exact" Lanczos$(s, 1)$ versus full GMRES



"Finite precision" Lanczos$(s, 1)$ versus full GMRES



"Exact" QMR$(s, 1)$ versus full GMRES



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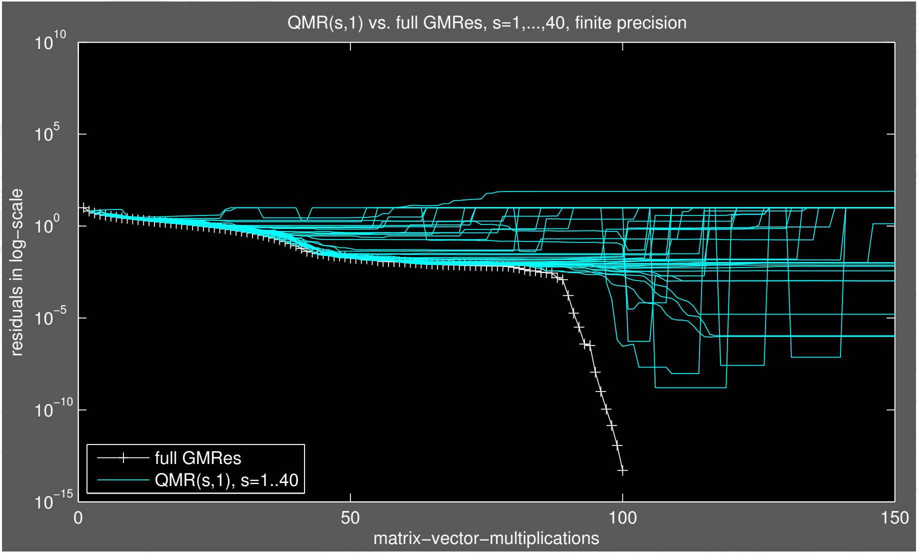
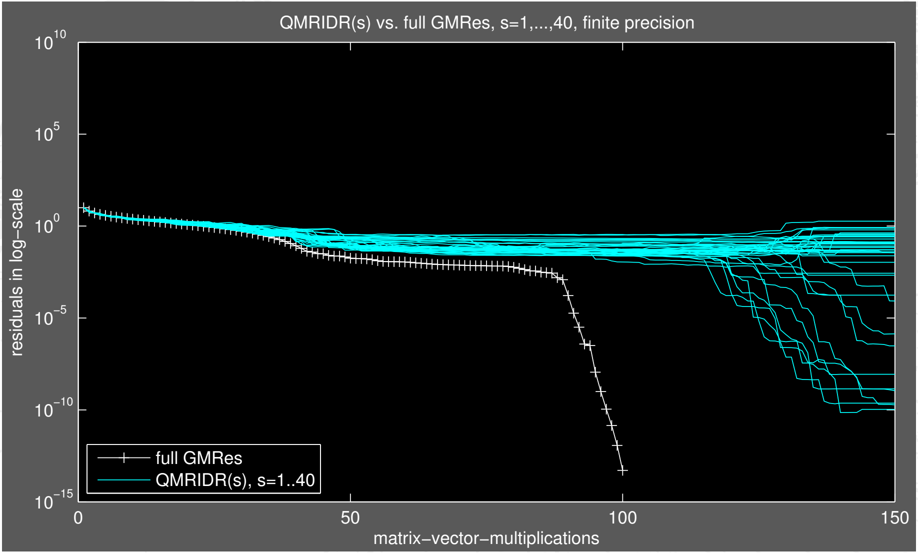
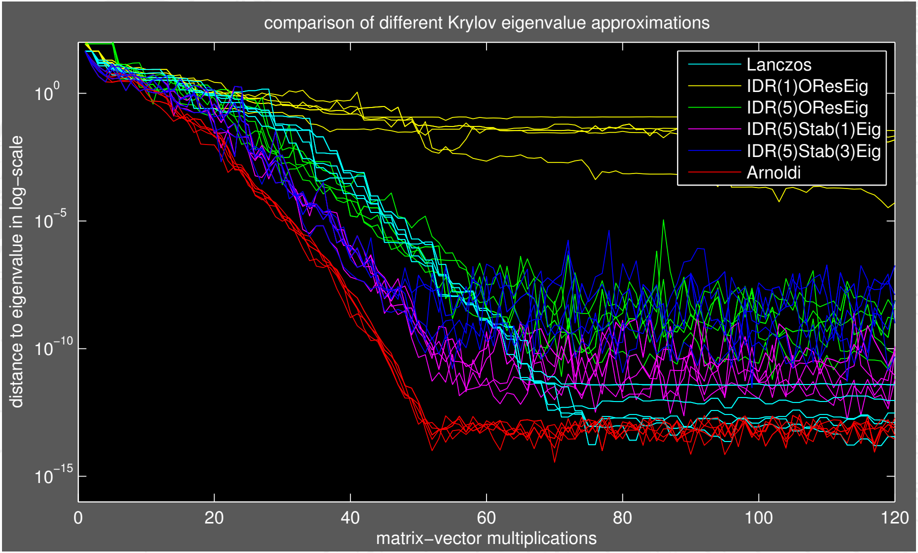


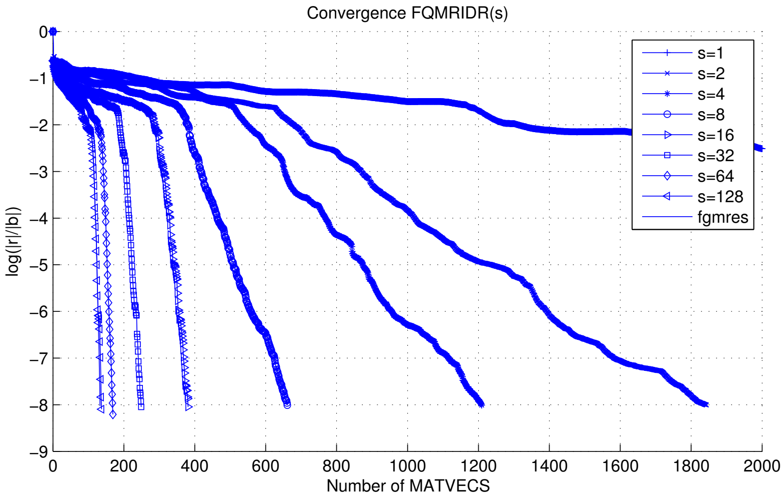
Finite precision QMRIDR(s) versus full GMRES



A comparison: IDR based eigenvalue solvers



Flexible QMRIDR(s)



Perturbations

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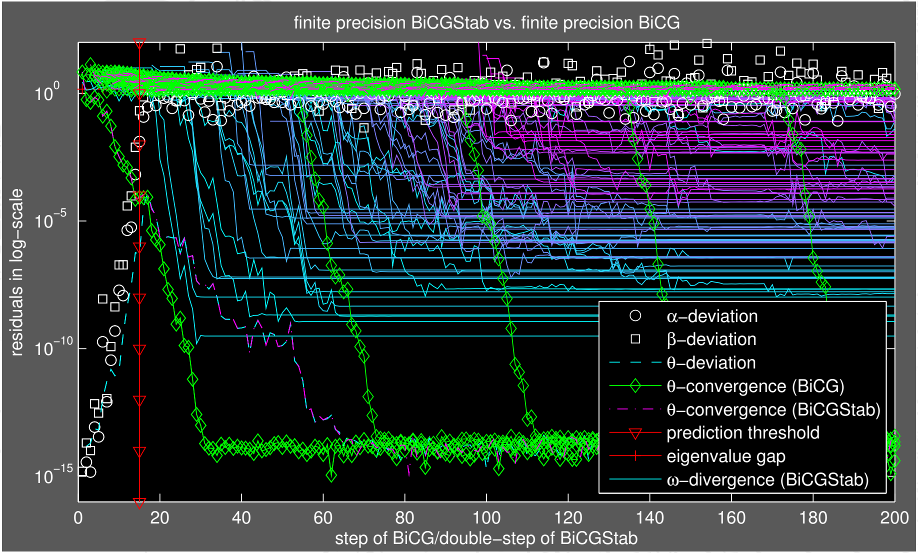
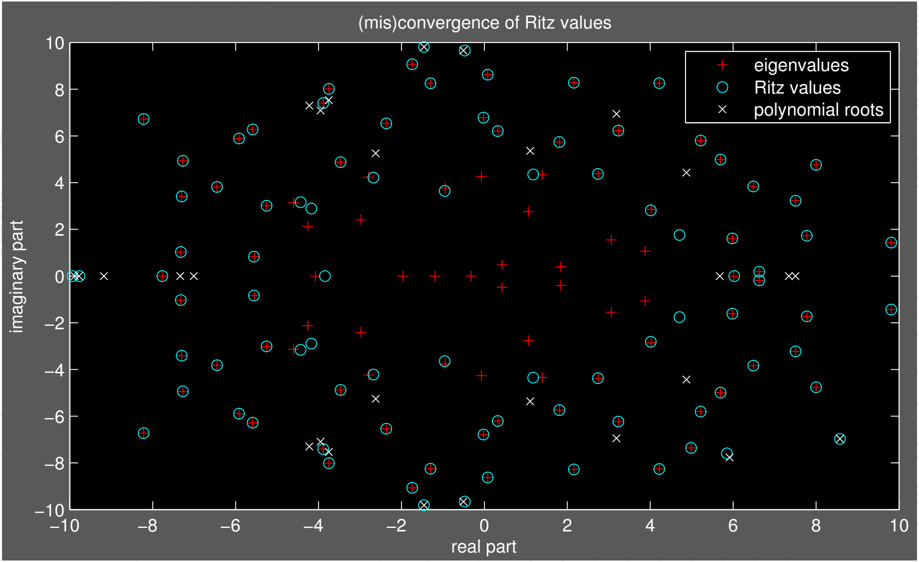
But:

- IDR transpose-free,
- easy to implement,
- more stable (for large values of s),
- often close to “optimal” methods (for large values of s).

BiCGStab vs. BiCG



IDR(3)STAB(3): “Ghost polynomial roots”



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- Knowledge should be used carefully in the parameter selection process, but accelerating the convergence should definitely be tried.
- An error analysis and a description of the finite precision behavior is desperately needed.
- The next logical step, the development of IDR algorithms that allow to change the old stabilizing polynomials on the fly, cures some of the peculiarities current implementations suffer from.

どうも有難う御座いました。

Thank you very much for inviting me to 同志社大学.

This talk is partially based on the following technical reports:

Eigenvalue computations based on IDR, Martin H. Gutknecht and Z., Bericht 145, Institut für Numerische Simulation, TUHH, 2010,

Flexible and multi-shift induced dimension reduction algorithms for solving large sparse linear systems, Martin B. van Gijzen, Gerard L.G. Sleijpen, and Z., Bericht 156, Institut für Numerische Simulation, TUHH, 2011.

Additional material can be found in the proceedings:

Tuning IDR to fit your applications, Olaf Rendel and Z., 2011.

Sleijpen, G. L. and van der Vorst, H. A. (1995).
Maintaining convergence properties of BiCGstab methods in finite precision arithmetic.
Numer. Algorithms, 10(3-4):203–223.

Sonneveld, P. (2010).
On the convergence behaviour of IDR(s).
Technical Report 10-08, Department of Applied Mathematical Analysis, Delft University of Technology, Delft.

van Gijzen, M. B., Sleijpen, G. L., and Zemke, J.-P. M. (2011).
Flexible and multi-shift induced dimension reduction algorithms for solving large sparse linear systems.
Bericht 156, TUHH, Institute of Numerical Simulation.
Online available at
`http://doku.b.tu-harburg.de/volltexte/2011/1114/`.