IDR: A new generation of Krylov subspace methods?

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Outline

Krylov subspace methods

- Hessenberg decompositions
- Polynomial representations
- Perturbations

IDR

- IDR and IDR(s)
- IDREIG
- IDR(s)STAB(ℓ) and IDRSTABEIG
- (Flexible and multi-shift) QMRIDR
- Perturbations

Introduction

Krylov subspace methods: approximations

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

where

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

to solutions of linear systems

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

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

- $\mathbf{Q}_{k+1} = \left(\mathbf{Q}_k, \mathbf{q}_{k+1}\right) \in \mathbb{C}^{n\times(k+1)}$ collects basis vectors,
- $\underline{\mathbf{H}}_k \in \mathbb{C}^{(k+1)\times k}$ is unreduced extended Hessenberg.

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 $z_\nu^{(\nu-1)}$ $(\nu = 1,2,\ldots,n)$ ebenfalls in einer Matrix zusammenfassen, und zwar ist nach Gleichung (55) und (56)

(57) $$(z_1 z_2' z_3'' \cdots z_n^{(n-1)}) = \mathfrak{A} \cdot z' = z' \cdot \mathfrak{P},$$

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

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

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

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

Important Polynomials

Residuals of OR and MR approximation

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

with coefficient vectors

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

satisfy

$$\mathbf{r}_k := \mathbf{r}_0 - \mathbf{A}\mathbf{x}_k = \mathcal{R}_k(\mathbf{A})\mathbf{r}_0 \qquad \text{and} \qquad \underline{\mathbf{r}}_k := \mathbf{r}_0 - \mathbf{A}\underline{\mathbf{x}}_k = \underline{\mathcal{R}}_k(\mathbf{A})\mathbf{r}_0.$$

Residual polynomials $\mathcal{R}_k$, $\underline{\mathcal{R}}_k$ given by

$$\mathcal{R}_k(z) := \det\left(\mathbf{I}_k - z\mathbf{H}_k^{-1}\right) \qquad \text{and} \qquad \underline{\mathcal{R}}_k(z) := \det\left(\mathbf{I}_k - z\underline{\mathbf{H}}_k^{\dagger}\underline{\mathbf{I}}_k\right).$$

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

Perturbed OR methods

Setting changes when perturbations enter the stage, here, OR method.

In perturbed case

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

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).

Here,

$$\mathcal{R}_{\ell+1:k}(z) := \det\left(\mathbf{I}_{k-\ell} - z\mathbf{H}_{\ell+1:k}^{-1}\right).$$

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

IDR: History repeating

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

	IDR(s)
2006	Sonneveld & van Gijzen
2007	First presentation & report
2008	SIAM paper (SISC)
2008	IDR(s)BiO
2010	IDR(s)Stab(ℓ), IDREig
2011	flexible & multi-shift QMRIDR
later	"acronym explosion"?

- IDR and IDR based methods are old ($\rightsquigarrow$ my generation),
- IDR(s) is 5 years "old" ($\rightsquigarrow$ my son's generation).

IDR is based on Lanczos's method; IDR(s) is based on Lanczos($s, 1$).

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

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

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

$$\mathcal{G}_j = \mathcal{S}_j(P_j, \mathbf{A}, \widetilde{\mathbf{R}}_0) := \left\{ P_j(\mathbf{A}) v \mid v \perp \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \widetilde{\mathbf{R}}_0) \right\},$$

$$P_j(z) := \prod_{i=1}^{j} (\alpha_i z + \beta_i).$$

Image of shrinking space: Induced Dimension Reduction.

IDR(s)

IDR spaces nested:

$$\{\mathbf{o}\} = \mathcal{G}_{\text{jmax}} \subsetneq \cdots \subsetneq \mathcal{G}_{j+1} \subsetneq \mathcal{G}_j \subsetneq \mathcal{G}_{j-1} \subsetneq \cdots \subsetneq \mathcal{G}_2 \subsetneq \mathcal{G}_1 \subsetneq \mathcal{G}_0.$$

How many vectors in $\mathcal{G}_j \setminus \mathcal{G}_{j+1}$? In generic case, $s+1$.

Stable basis: Partially orthonormalize basis vectors $\mathbf{g}_k$, $1 \leqslant k \leqslant n$:

Arnoldi: compute orthonormal basis of $\mathcal{K}_{s+1} \subset \mathcal{G}_0$,

$$\mathbf{A}\mathbf{G}_s = \mathbf{G}_{s+1}\underline{\mathbf{H}}_s.$$

"Lanczos": perform intersection $\mathcal{G}_j \cap \mathcal{S}$, map, and orthonormalize,

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

$$\mathbf{g}_{k+1}\nu_{k+1} = (\alpha_j \mathbf{A} + \beta_j \mathbf{I})\mathbf{v}_k - \sum_{i=k-j(s+1)-1}^{k} \mathbf{g}_i \nu_i, \quad j = \left\lfloor \frac{k-1}{s+1} \right\rfloor.$$

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.

Structure of Sonneveld pencils:

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

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 $\mathbf{A}$.

Suppose $\mathbf{G}_{k+1}$ of full rank. Sonneveld pencil $(\mathbf{H}_k, \mathbf{U}_k)$ as oblique projection:

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

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

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

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

$$\mathbf{G}_{i,j}^{(k)} \in \mathbb{C}^{n \times s}, \quad \mathbf{r}_{i,j}^{(k)} \in \mathbb{C}^{n},$$

$$\mathbf{G}_{i+1,j}^{(k)} = \mathbf{A}\mathbf{G}_{i,j}^{(k)}, \quad \mathbf{r}_{i+1,j}^{(k)} = \mathbf{A}\mathbf{r}_{i,j}^{(k)},$$

$$\widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{G}_{ii}^{(k)} = \mathbf{O}_s, \quad \widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{r}_{ii}^{(k)} = \mathbf{o}_s,$$

$$(\mathbf{G}_{ii}^{(k)})^{\mathsf{H}} \mathbf{G}_{ii}^{(k)} = \mathbf{I}_s.$$

Initialization using Arnoldi's method:

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

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

IDRSTAB

Columnwise update (IDR part) such that diagonal blocks

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

All other blocks in column treated in same manner.

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

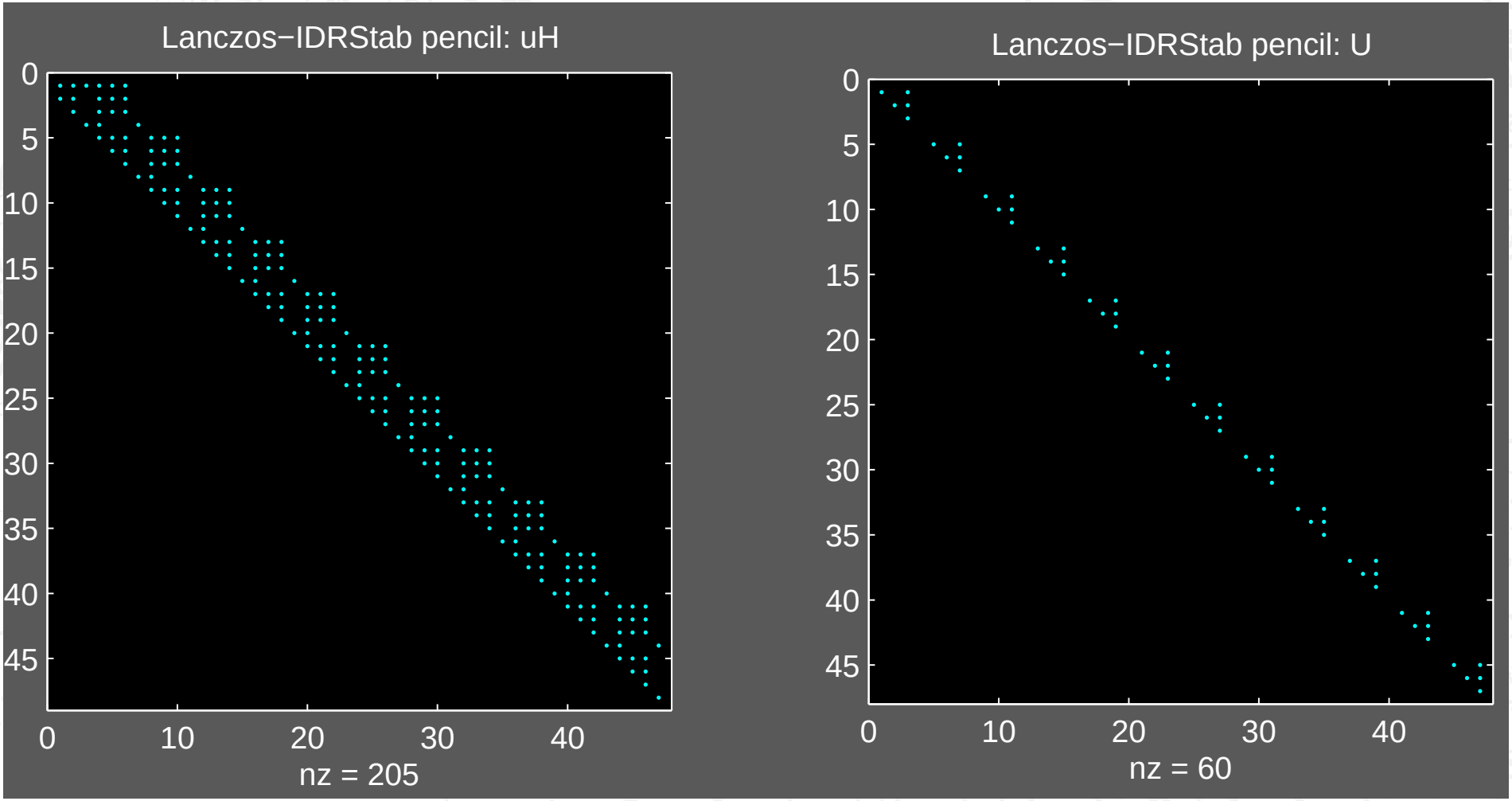
$$\mathbf{r}_{i,j}^{(k)} = \mathbf{r}_{i,j-1}^{(k)} - \mathbf{G}_{i+1,j}^{(k)} \boldsymbol{\alpha}^{(j)}, \quad \mathbf{r}_{j,j}^{(k)} = (\mathbf{I} - \mathbf{G}_{j+1,j}^{(k)} (\widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{G}_{j+1,j}^{(k)})^{-1} \widetilde{\mathbf{R}}_0^{\mathsf{H}}) \mathbf{r}_{j,j-1}^{(k)}.$$

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

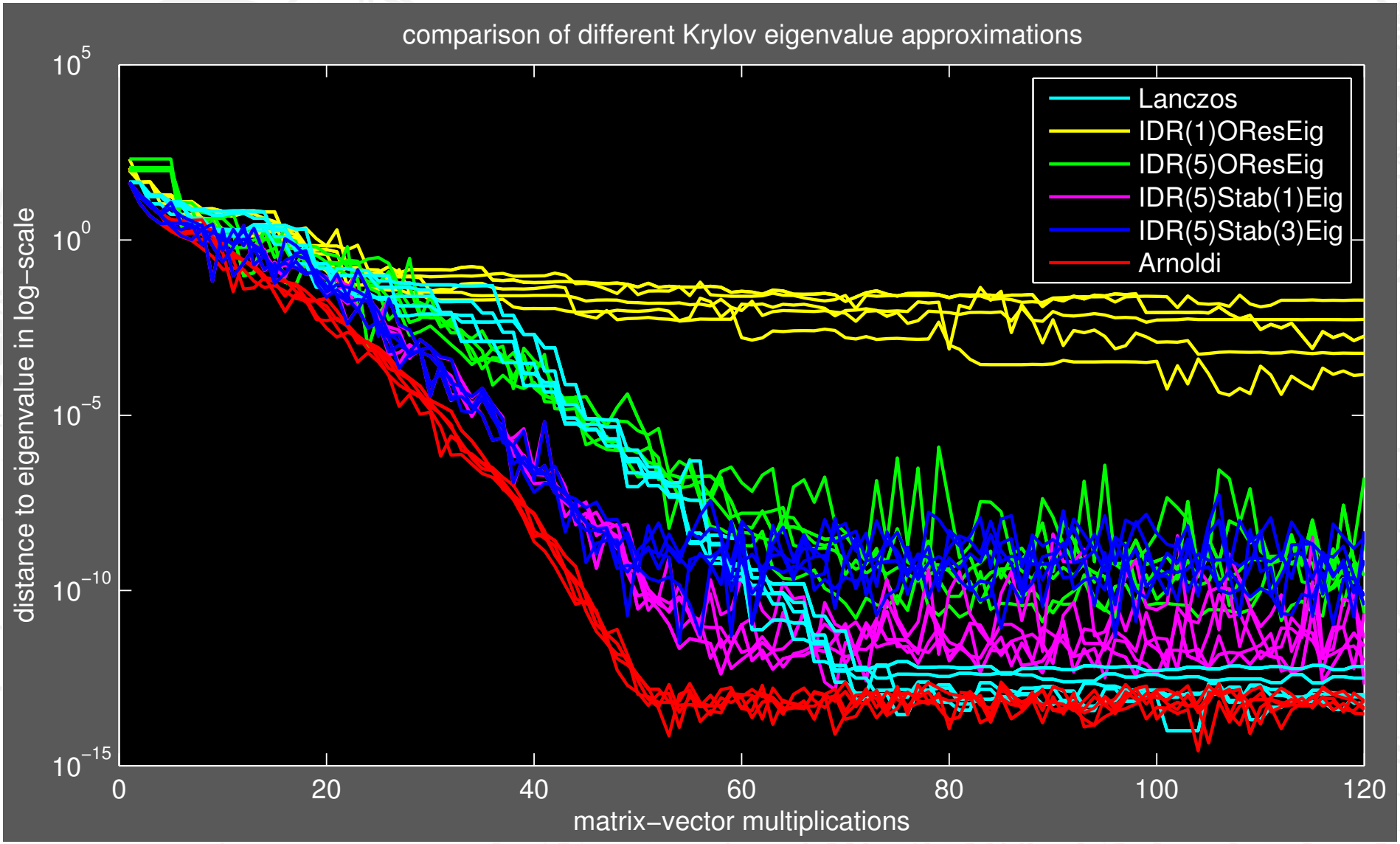
$$\mathbf{r}_{11}^{(k+1)} = \mathbf{r}_{1,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{r}_{i+1,\ell+1}^{(k)} \gamma_i^{(\ell)}, \quad \begin{cases} \mathbf{G}_{11}^{(k+1)} = \mathbf{G}_{1,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{G}_{i+1,\ell+1}^{(k)} \gamma_i^{(\ell)}, \\ \mathbf{G}_{21}^{(k+1)} = \mathbf{G}_{2,\ell+1}^{(k)}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

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

Structure of (undeflated) Lanczos-IDRSTAB pencil



A comparison: IDR based eigenvalue solvers



QMRIDR

MR methods: use extended Hessenberg matrix

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

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,

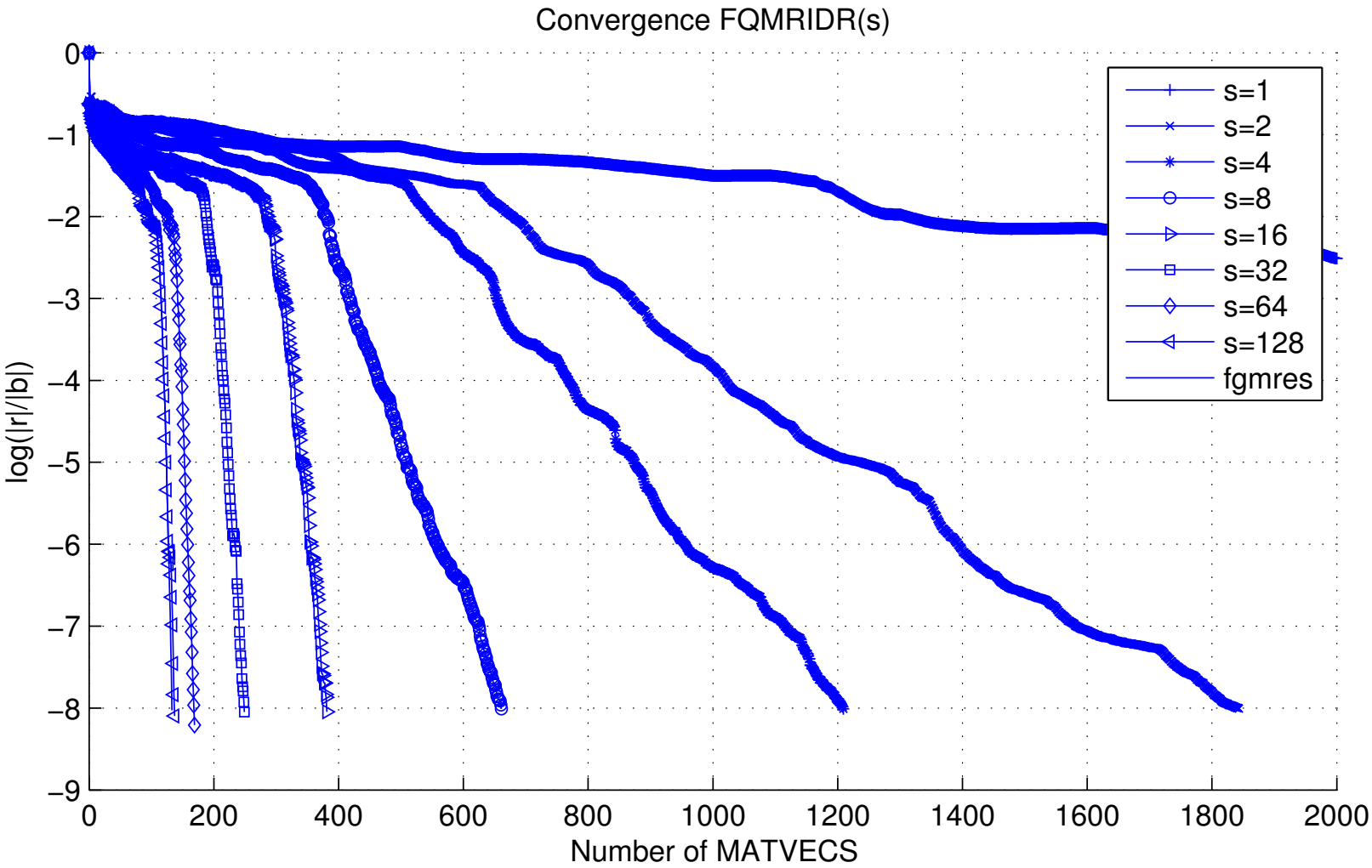
$$\underline{\mathbf{x}}_k := \mathbf{V}_k \underline{\mathbf{z}}_k = \mathbf{G}_k\mathbf{U}_k \underline{\mathbf{z}}_k, \quad \underline{\mathbf{z}}_k := \underline{\mathbf{H}}_k^{\dagger} \underline{\mathbf{e}}_1 \|\mathbf{r}_0\|.$$

Other Krylov-paradigms possible, e.g., flexible (& multi-shift) QMRIDR:

$$P_j(\mathbf{A})\mathbf{v}_k = (\alpha_j \mathbf{A} + \beta_j \mathbf{I})\mathbf{v}_k \rightsquigarrow (\alpha_j \mathbf{A}\mathbf{P}_j^{-1} + \beta_j \mathbf{I})\mathbf{v}_k = \mathbf{A}\widetilde{\mathbf{v}}_k + \beta_j \mathbf{v}_k,$$
$$\widetilde{\mathbf{v}}_k := \mathbf{P}_j^{-1}\mathbf{v}_k\alpha_j, \quad \mathbf{A}\widetilde{\mathbf{V}}_k = \mathbf{G}_{k+1}\underline{\mathbf{H}}_k \quad \text{(gen. Hessenberg relation)}.$$

Olaf Rendel, Gerard Sleijpen, Martin van Gijzen: $\rightsquigarrow$ QMRIDRStab.

Flexible QMRIDR(s)



Perturbations

IDR based on short recurrences, i.e., Lanczos based.

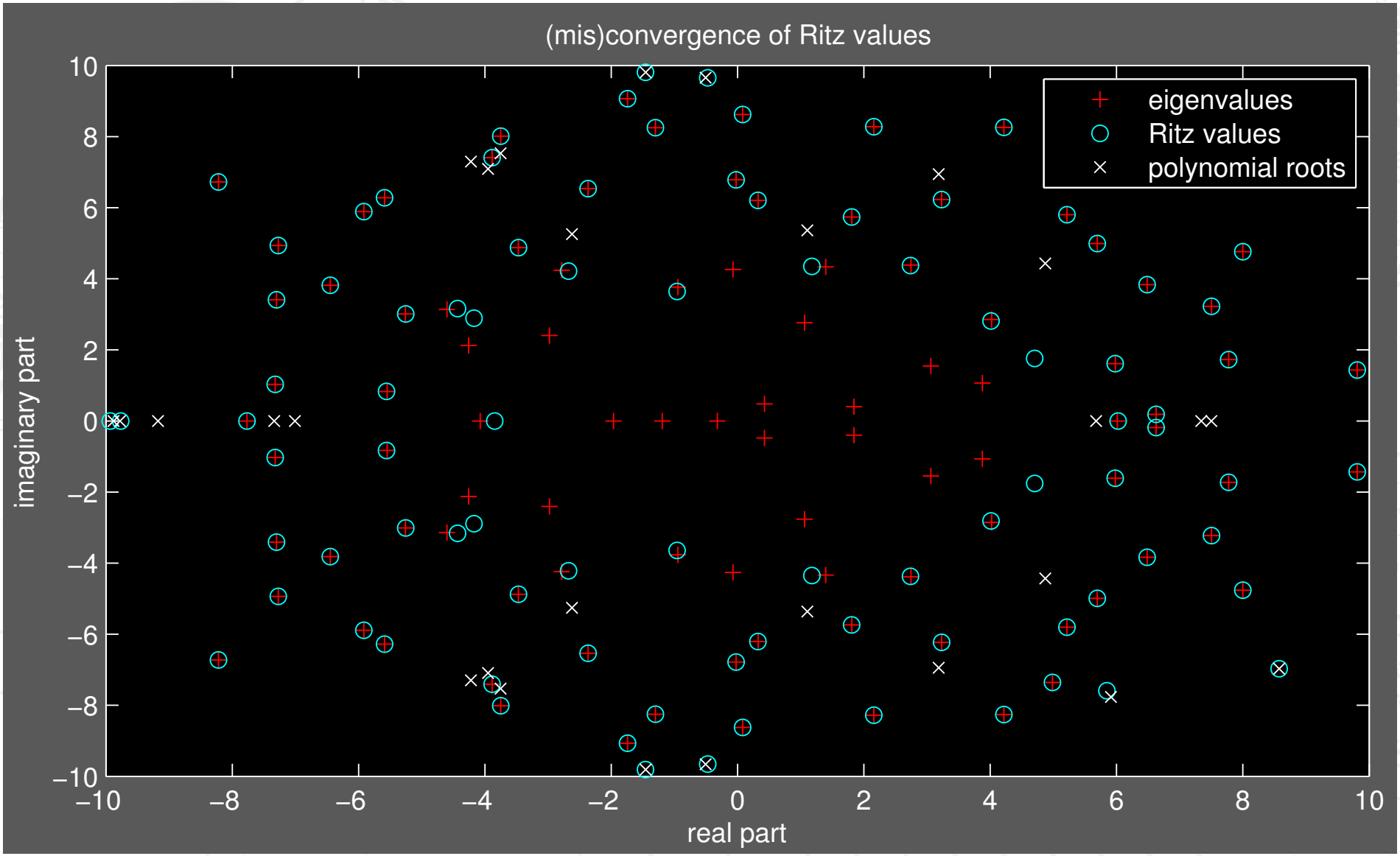
$\rightsquigarrow$ Behaviour in finite precision? Inexact methods? General perturbations?

Lanczos	IDR
deviation	deviation
multiple Ritz values	ghost polynomial roots
delay of convergence	delay of convergence
attainable accuracy: condition	attainable accuracy: worse than Lanczos
analysis by Chris Paige	thus far no error analysis available

But:

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

IDR(3)STAB(3): "Ghost polynomial roots"



Conclusion and Outview

- IDR is both old (original IDR, CGS, BiCGStab, BiCGStab2, BiCGStab(ℓ), ...) and new (IDR(s), IDRStab, QMRIDR, ...).
- IDR can be included in the framework of Krylov subspace methods using generalized Hessenberg decompositions.
- New developments double old developments at increased speed.
- IDR based methods bridge the gap between short- and long-term recurrences.
- IDR based methods offer more freedom in parameters (e.g., the choice of the additional polynomials).

ILAS related:

- The analysis & development of IDR based methods is a new branch of Krylov subspace methods.
- The pencils of IDR based methods are specially structured pencils (adapted backward stable algorithms; perturbation theory, ...).

Thank you for your attention!

In case of questions feel free to ask Anisa, Olaf & myself at any time.

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.