IDR versus other Krylov subspace solvers

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Outline

Krylov subspace methods

Hessenberg decompositions

Polynomial representations

IDR

IDR, IDR(s), and IDREig

IDR vs. other Krylov subspace methods

IDRStab and QMRIDR

Transferring techniques

Stay close to Arnoldi/Lanczos

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

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

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

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

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

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

- 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

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

satisfy

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

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

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

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

IDR: History repeating

	IDR		IDR(s)
1976	Idea by Sonneveld	2006	Sonneveld & van Gijzen
1979	First talk on IDR	2007	First presentation & report
1980	Proceedings	2008	SIAM paper (SISC)
1989	CGS	2008	IDR(s)BIO
1992	IDR $\rightsquigarrow$ BICGSTAB	2010	IDR(s)STAB(ℓ), IDREIG
1993	BICGSTAB2, BICGSTAB(ℓ)	2011	flexible & multi-shift QMRIDR
later	"acronym explosion" . . .	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):

$$\mathcal{G}_j = \mathcal{S}_j(P_j, \mathbf{A}, \widetilde{\mathbf{R}}_0) := \left\{ P_j(\mathbf{A})\mathbf{v} \mid \mathbf{v} \perp \mathcal{K}_j(\mathbf{A}^\mathsf{H}, \widetilde{\mathbf{R}}_0) \right\},$$
$$P_j(z) := \prod_{i=1}^{j} (\alpha_i z + \beta_i).$$

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 $\mathbf{G}_{s+1}$ of $\mathcal{K}_{s+1} \subset \mathcal{G}_0$,

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

“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 = \begin{pmatrix}
\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{pmatrix}, \quad
\begin{pmatrix}
\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 \\
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\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{pmatrix} = \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" ($k \geqslant 1$):

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

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

Initialization using Arnoldi's method:

$$\mathbf{G}_{21}^{(1)} = \mathbf{A}\mathbf{G}_{11}^{(1)} = (\mathbf{G}_{11}^{(1)}, \mathbf{g}_{\mathsf{tmp}})\underline{\mathbf{H}}_s^{(0)},$$
$$\mathbf{r}_{11}^{(1)} = \mathbf{r}_0 - \mathbf{G}_{21}^{(1)}\boldsymbol{\alpha}^{(1)} = (\mathbf{I} - \mathbf{G}_{21}^{(1)}(\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{G}_{21}^{(1)})^{-1}\widetilde{\mathbf{R}}_0^{\mathsf{H}})\mathbf{r}_0, \quad \mathbf{r}_{21}^{(1)} = \mathbf{A}\mathbf{r}_{11}^{(1)}.$$

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 $\rightsquigarrow \underline{\mathbf{H}}^{(j)}_{s-1} \in \mathbb{C}^{s\times(s-1)}$

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

$$\beta^{(j)}_i = (\widetilde{\mathbf{R}}_0^{\mathsf{H}} \mathbf{G}_{j,j-1})^{-1} \widetilde{\mathbf{R}}_0^{\mathsf{H}} (\mathbf{A}\widetilde{\mathbf{v}}_i)$$

$$\Rightarrow \quad (\mathbf{A}\widetilde{\mathbf{v}}_i) - \mathbf{G}_{j,j-1}\beta^{(j)}_i = \mathbf{A}(\widetilde{\mathbf{v}}_i - \mathbf{G}_{j-1,j-1}\beta^{(j)}_i) \in \mathcal{G}_j \cap \mathcal{S}$$

Every new vector in $\mathcal{G}_j \cap \mathcal{S}$ is orthonormalized with respect to the others.

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

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

All other blocks in column treated in same manner.

IDRSTAB

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

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

Here,

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

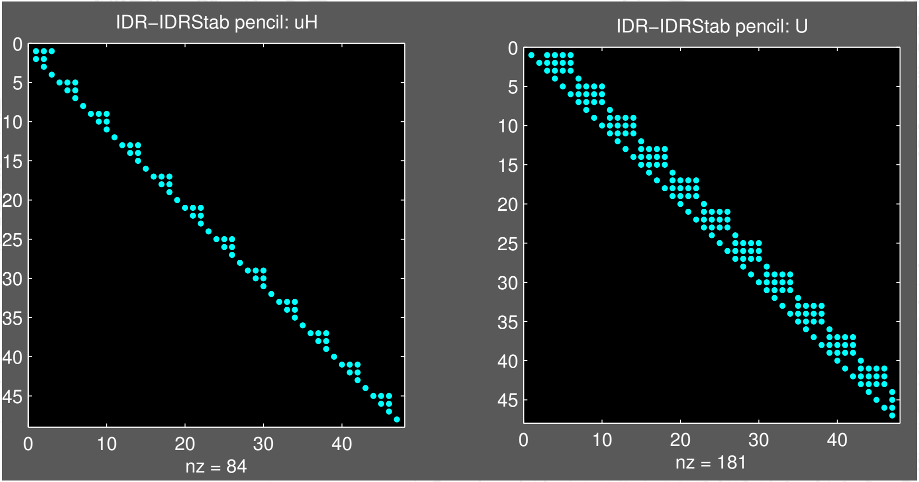
$\boldsymbol{\alpha}^{(j)}$ relating $\mathbf{r}_{j,j-1}^{(k)} = \mathbf{A}\mathbf{r}_{j-1,j-1}^{(k)}$ (old) and $\mathbf{r}_{j,j}^{(k)}$ (new) via $\mathbf{G}_{j+1,j}^{(k)} = \mathbf{A}\mathbf{G}_{j,j}^{(k)} \rightsquigarrow \mathbf{U}_k$.

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

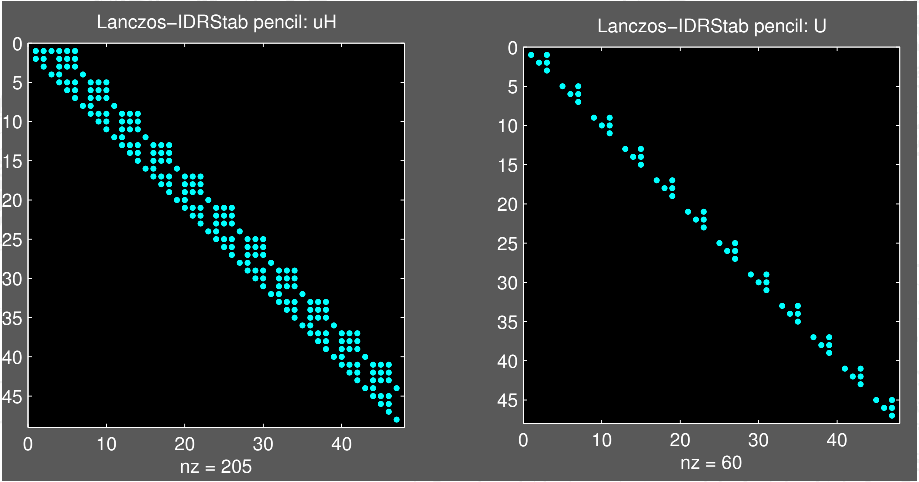
$$\mathbf{r}_{11}^{(k+1)} = \mathbf{r}_{1,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{r}_{i+1,\ell+1}^{(k)}\gamma_i^{(\ell)}, \quad \begin{cases} \mathbf{G}_{11}^{(k+1)} = \mathbf{G}_{1,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{G}_{i+1,\ell+1}^{(k)}\gamma_i^{(\ell)}, \\ \mathbf{G}_{21}^{(k+1)} = \mathbf{G}_{2,\ell+1}^{(k)}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

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

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

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,

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

Simplified residual bound (block-wise orthonormalization):

$$\|\mathbf{r}_k\| = \|\mathbf{r}_0 - \mathbf{A}\mathbf{x}_k\| \leqslant \|\mathbf{G}_{k+1}\| \cdot \left\|\underline{\mathbf{e}}_1\|\mathbf{r}_0\| - \underline{\mathbf{H}}_k\mathbf{z}_k\right\|$$

$$\leqslant \sqrt{\left\lceil \frac{k+1}{s+1} \right\rceil} \cdot \left\|\underline{\mathbf{e}}_1\|\mathbf{r}_0\| - \underline{\mathbf{H}}_k\mathbf{z}_k\right\|.$$

Implementation based on short recurrences possible.

QMRIDR

Other Krylov-paradigms possible, e.g., flexible QMRIDR:

$$P_j(\mathbf{A})\mathbf{v}_k = (\alpha_j \mathbf{A} + \beta_j \mathbf{I})\mathbf{v}_k \;\rightsquigarrow\; (\alpha_j \mathbf{A}\mathbf{P}_k^{-1} + \beta_j \mathbf{I})\mathbf{v}_k = \mathbf{A}\widetilde{\mathbf{v}}_k + \beta_j \mathbf{v}_k,$$

$$\widetilde{\mathbf{v}}_k := \mathbf{P}_k^{-1}\mathbf{v}_k\alpha_j, \quad \mathbf{A}\widetilde{\mathbf{V}}_k = \mathbf{G}_{k+1}\underline{\mathbf{H}}_k.$$

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

$$\mathbf{A}\widetilde{\mathbf{V}}_k \neq \mathbf{A}\mathbf{G}_k\widetilde{\mathbf{U}}_k$$

for every (upper triangular) $\widetilde{\mathbf{U}}_k$.

Computation of flexible MR iterate and flexible MR approximation:

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

Flexible IDR variants algorithmically very easy to implement.

QMRIDR

Multi-shift is a technique developed for shifted systems

$$(\mathbf{A}-\sigma\mathbf{I})\mathbf{x}^{(\sigma)} = \mathbf{r}_0, \quad \sigma \in \mathbb{C}.$$

We look for quasi-optimal approximations of the form

$$\mathbf{x}^{(\sigma)} \approx \underline{\mathbf{x}}_k^{(\sigma)} := \mathbf{V}_k \underline{\mathbf{z}}_k^{(\sigma)}.$$

Since $\mathbf{A}\mathbf{V}_k = \mathbf{A}\mathbf{G}_k\mathbf{U}_k = \mathbf{G}_{k+1}\underline{\mathbf{H}}_k$, and since we use $\mathbf{G}_{k+1}\underline{\mathbf{e}}_1\|\mathbf{r}_0\| = \mathbf{r}_0$,

$$\underline{\mathbf{r}}_k^{(\sigma)} = \mathbf{r}_0 - (\mathbf{A}-\sigma\mathbf{I})\underline{\mathbf{x}}_k^{(\sigma)} = \mathbf{G}_{k+1}\left(\underline{\mathbf{e}}_1\|\mathbf{r}_0\| - (\underline{\mathbf{H}}_k - \sigma\underline{\mathbf{U}}_k)\underline{\mathbf{z}}_k^{(\sigma)}\right).$$

Thus, $\underline{\mathbf{z}}_k^{(\sigma)}$ quasi-optimal:

$$\underline{\mathbf{z}}_k^{(\sigma)} := (\underline{\mathbf{H}}_k - \sigma\underline{\mathbf{U}}_k)^{\dagger}\underline{\mathbf{e}}_1\|\mathbf{r}_0\|.$$

Various extensions for IDRSTAB: Olaf Rendel, Z. ⇝ QMRIDRSTAB.

Optimality, cost, and stability

In (Sonneveld, 2010) a relation between IDR and GMRES for the case of random shadow vectors was pointed out.

Neglecting the influence of the STAB-part, i.e., focusing on Lanczos$(s, 1)$, the deviation of IDR from GMRES is described using stochastic arguments.

As a rule of thumb:

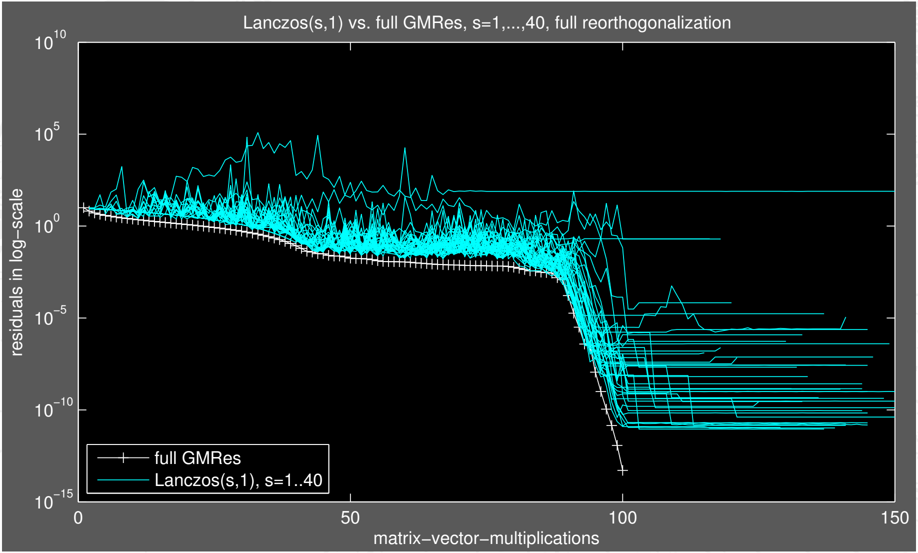
> *As s tends to infinity, the convergence curves of Lanczos$(s, 1)$ tend to the convergence curve of full GMRES.*

In practice, the first steps of IDR/QMRIDR and Arnoldi/GMRES coincide, as we ideally start IDR with these methods.

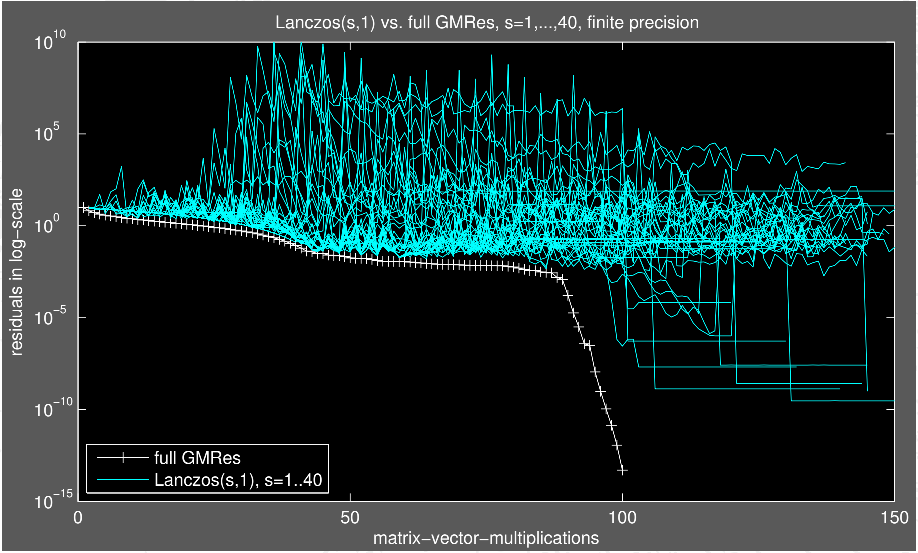
We present some examples that depict the relations in (Sonneveld, 2010), show additionally the effects of finite precision, and relate GMRES to QMR$(s, 1)$ and to QMRIDR(s).

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

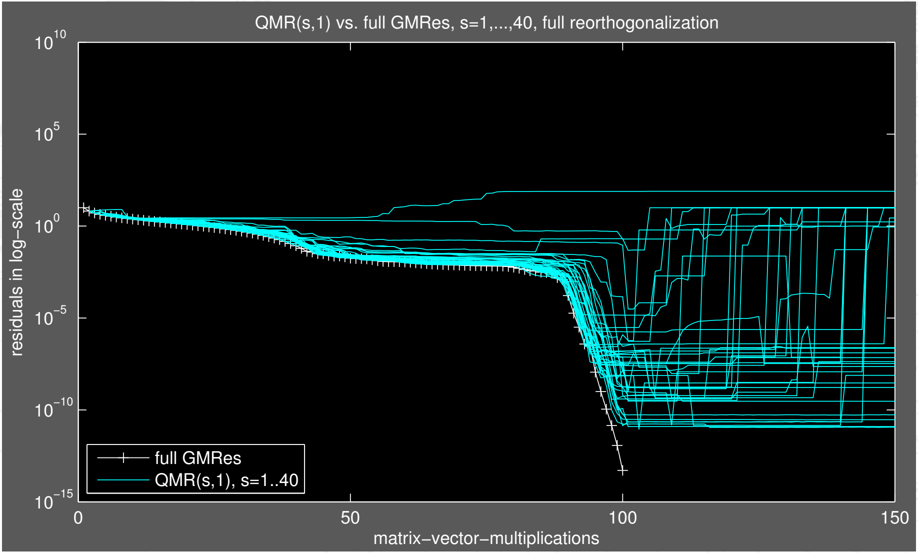
"Exact" Lanczos$(s, 1)$ versus full GMRES



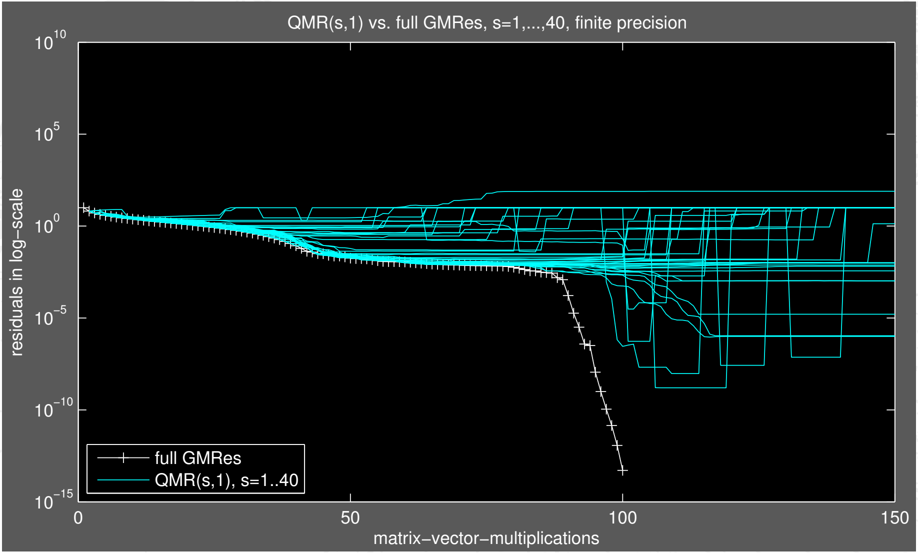
"Finite precision" Lanczos$(s, 1)$ versus full GMRES



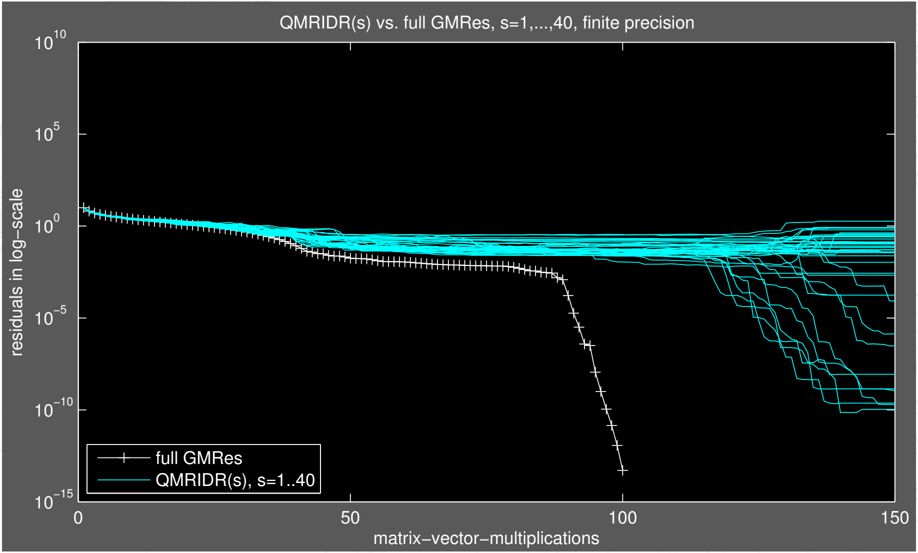
“Exact” QMR$(s, 1)$ versus full GMRES



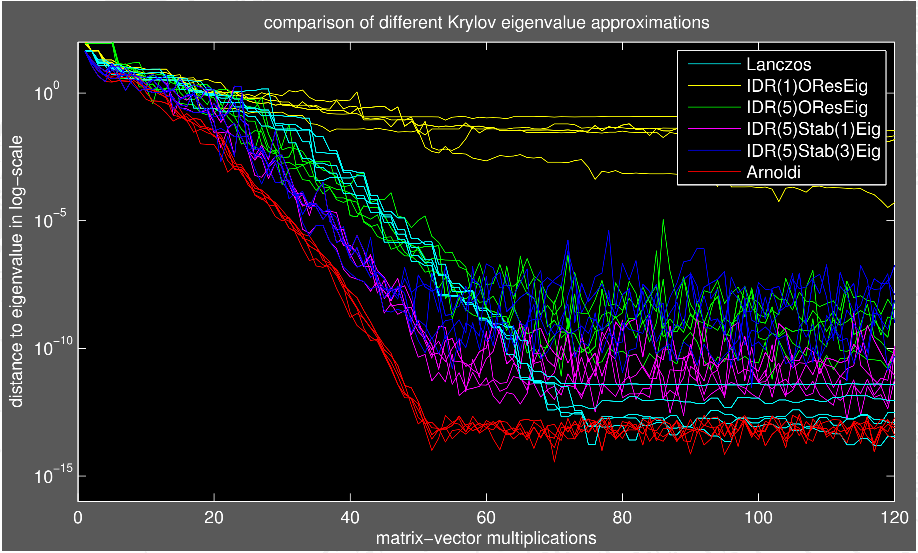
“Finite precision” QMR$(s, 1)$ versus full GMRes



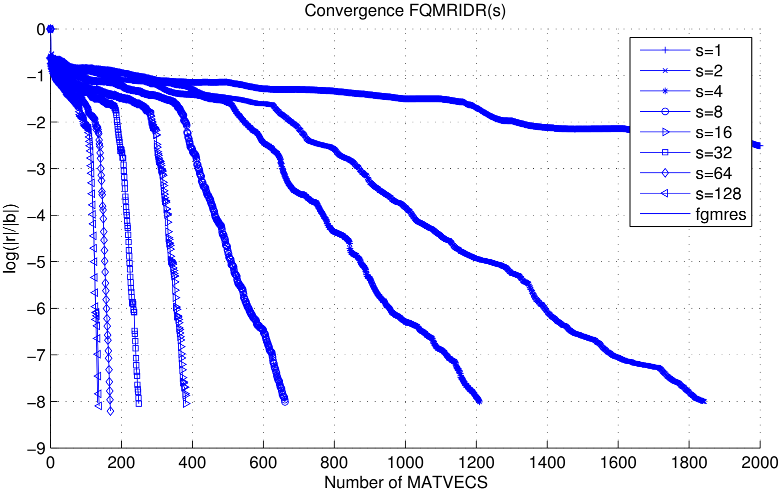
Finite precision QMRIDR(s) versus full GMRES



A comparison: IDR based eigenvalue solvers



Flexible QMRIDR(s)



Conclusion and Outlook

- The new implementations of IDR, i.e., IDRSTAB, QMRIDR, its combinations, and the eigensolver counterparts, are very promising.
- The new IDR implementations provide a “smooth” transition between Arnoldi/GMRES ($s \to \infty$) and Lanczos/QMR ($s \to 1$).
- The matrix generalization of Hessenberg decompositions to generalized Hessenberg decompositions and generalized Hessenberg relations allows for a simple application of standard Krylov subspace techniques.

- The dependence on the parameters (s, $\widetilde{\mathbf{R}}_0$, the STAB-part, ...) has to be analyzed carefully.
- An error analysis and a description of the finite precision behavior is desperately needed.

どうもありがとうございました。

Thank you very much for inviting me to 京都大学.

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.

An extended abstract can be found in the proceedings:

IDR versus other Krylov subspace solvers, Z., 2011.

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