IDR versus other Krylov subspace solvers

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joint work with Olaf Rendel & Anisa Rizvanolli

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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



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Introduction

Krylov subspace methods: approximations

$$\begin{array}{l} \mathbf{x}_{k}, \mathbf{x}_{k}, \\ \mathbf{y}_{k}, \mathbf{y}_{k} \end{array} \right\} \in \mathcal{K}_{k}(\mathbf{A}, \mathbf{q}) := \operatorname{span} \left\{ \mathbf{q}, \mathbf{A}\mathbf{q}, \dots, \mathbf{A}^{k-1}\mathbf{q} \right\} = \left\{ p(\mathbf{A})\mathbf{q} \mid p \in \mathbb{P}_{k-1} \right\}, \\ \text{where} \\ \mathbb{P}_{k-1} := \left\{ \sum_{j=0}^{k-1} \alpha_{j} z^{j} \mid \alpha_{j} \in \mathbb{C}, \ 0 \leq j < k \right\}, \end{array}$$

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to solutions of linear systems

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

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 $\overline{i=0}$

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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

Q_{k+1} = (**Q**_k, **q**_{k+1}) ∈ C^{n×(k+1)} collects basis vectors,
 H_k ∈ C^{(k+1)×k} is unreduced extended Hessenberg.

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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).

Krylov subspace methods Hessenberg decomposition

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 $\frac{1}{2} \int_{0}^{n-n} (y = 1, 2, ..., n)$ ebenfalle in einer Matrix susammenfassen, und zwar ist nach Gleichung (55) und (56) (57) $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \cdots, \frac{1}{2}, \frac{n}{n}) \neq \alpha \cdot \frac{1}{2} \in \frac{1}{2}, \frac{1}{p},$ worin die Matrix P zur Abkürsung gesetzt ist für (52) $P = \begin{pmatrix} \alpha_{ne} & \alpha_{1e} & \cdots & \alpha_{n-e}, \alpha_{ne}, \\ \alpha_{ne} & \alpha_{1e} & \cdots & \alpha_{n-e}, \alpha_{ne}, \\ 0 & 4 & \cdots & \alpha_{n-e}, \alpha_{ne}, \\ 0 & 0 & \cdots & 4 & \alpha_{ne}, \end{pmatrix}$

Hessenberg decomposition, Eqn. (57),

Hessenberg matrix, Eqn. (58).

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

Residuals of OR and MR approximation

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

with coefficient vectors

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

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

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 $\underline{\mathcal{R}}_k(z) := \det(\mathbf{I}_k - z \underline{\mathbf{H}}_k^{\dagger} \underline{\mathbf{I}}_k).$

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

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IDR: History repeating

IDR

- 1976 Idea by Sonneveld
- 1979 First talk on IDR
- 1980 Proceedings
- 1989 CGS
- 1992 IDR ~ BICGSTAB
- 1993 BICGSTAB2, BICGSTAB (ℓ)
- later "acronym explosion" ...

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- 2007 First presentation & report
- 2008 SIAM paper (SISC)
- 2008 IDR(s)BIO
- 2010 $IDR(s)STAB(\ell)$, IDREIG
- 2011 flexible & multi-shift QMRIDR
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- IDR and IDR based methods are old (~> my generation),
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IDR(s) is a Krylov subspace method $\sim all$ techniques from 90's applicable!

JDR(s)

IDR spaces:

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

where

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

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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 spaces nested:

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

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

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$$\mathbf{g}_{k+1} \nu_{k+1} = (\alpha_{j}\mathbf{A} + \beta_{j}\mathbf{I})\mathbf{v}_{k} - \sum_{i=k-j(s+1)-1}^{k} \mathbf{g}_{i} \nu_{i}, \quad j = \left\lfloor \frac{k-1}{s+1} \right\rfloor$$

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:



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

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

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Suppose \mathbf{G}_{k+1} of full rank. Sonneveld pencil $(\mathbf{H}_k, \mathbf{U}_k)$ as oblique projection: $\widehat{\mathbf{G}}_k^{\mathsf{H}}(\mathbf{A}, \mathbf{I}_n) \mathbf{G}_k \mathbf{U}_k = \widehat{\mathbf{G}}_k^{\mathsf{H}}(\mathbf{A}\mathbf{G}_k \mathbf{U}_k, \mathbf{G}_k \mathbf{U}_k)$ $= \widehat{\mathbf{G}}_k^{\mathsf{H}}(\mathbf{G}_{k+1} \mathbf{H}_k, \mathbf{G}_k \mathbf{U}_k) = (\mathbf{I}_k^{\mathsf{T}} \mathbf{H}_k, \mathbf{U}_k) = (\mathbf{H}_k, \mathbf{U}_k),$

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(1)

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

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Initialization using Arnoldi's method:

$$\begin{split} \mathbf{G}_{21}^{(1)} &= \mathbf{A}\mathbf{G}_{11}^{(1)} = (\mathbf{G}_{11}^{(1)}, \mathbf{g}_{\text{tmp}})\underline{\mathbf{H}}_{s}^{(0)}, \\ \mathbf{r}_{11}^{(1)} &= \mathbf{r}_{0} - \mathbf{G}_{21}^{(1)} \boldsymbol{\alpha}^{(1)} = (\mathbf{I} - \mathbf{G}_{21}^{(1)} (\widetilde{\mathbf{R}}_{0}^{\mathsf{H}} \mathbf{G}_{21}^{(1)})^{-1} \widetilde{\mathbf{R}}_{0}^{\mathsf{H}}) \mathbf{r}_{0}, \quad \mathbf{r}_{21}^{(1)} = \mathbf{A}\mathbf{r}_{11}^{(1)}. \end{split}$$

Columnwise update (IDR part) such that diagonal blocks

form basis of G_j \ G_{j+1} with expansion G_j = A(G_{j-1} ∩ S) → β^(j) ∈ C^{s×s},
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In particular, with $\widetilde{\mathbf{v}}_i \in \mathcal{G}_{j-1} \cap \mathcal{S}$,

 $\begin{aligned} \boldsymbol{\beta}_{i}^{(j)} &= (\widetilde{\mathbf{R}}_{0}^{\mathsf{H}}\mathbf{G}_{j,j-1})^{-1}\widetilde{\mathbf{R}}_{0}^{\mathsf{H}}(\mathbf{A}\widetilde{\mathbf{v}}_{i}) \\ \Rightarrow & (\mathbf{A}\widetilde{\mathbf{v}}_{i}) - \mathbf{G}_{j,j-1}\boldsymbol{\beta}_{i}^{(j)} = \mathbf{A}(\widetilde{\mathbf{v}}_{i} - \mathbf{G}_{j-1,j-1}\boldsymbol{\beta}_{i}^{(j)}) \in \mathcal{G}_{j} \cap \boldsymbol{\mathcal{S}} \end{aligned}$

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

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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 $\mathbf{G}_{j,j-1} = \mathbf{A}\mathbf{G}_{j-1,j-1} \rightsquigarrow \mathbf{U}_k$,
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All other blocks in column treated in same manner.

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

$$\mathbf{r}_{i,j}^{(k)} = \mathbf{r}_{i,j-1}^{(k)} - \mathbf{G}_{i+1,j}^{(k)} \boldsymbol{\alpha}^{(j)}, \quad \mathbf{r}_{j,j}^{(k)} = (\mathbf{I} - \mathbf{G}_{j+1,j}^{(k)} (\widetilde{\mathbf{R}}_{0}^{\mathsf{H}} \mathbf{G}_{j+1,j}^{(k)})^{-1} \widetilde{\mathbf{R}}_{0}^{\mathsf{H}}) \mathbf{r}_{j,j-1}^{(k)}$$

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Here,

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

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Anisa Rizvanolli: ~> Lanczos-IDRSTAB pencil for eigenvalues, IDRSTABEIG.

IDR vs. other Krylov subspace methods

RSTAB and QMRIDR

Structure of (STAB-purified) IDR-IDRSTAB pencil



IDR vs. other Krylov subspace methods IDRS

RSTAB and QMRIDR

Structure of (undeflated) Lanczos-IDRSTAB pencil



Jens

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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Simplified residual bound (block-wise orthonormalization):

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Implementation based on short recurrences possible.

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Computation of flexible MR iterate and flexible MR approximation:

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Flexible IDR variants algorithmically very easy to implement.

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

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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).

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:

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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.

Stay close to Arnoldi/Lanczos

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


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



Stay close to Arnoldi/Lanczos

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



tay close to Arnoldi/Lanczos

"Finite precision" QMR(s, 1) versus full GMRES



tay close to Arnoldi/Lanczos

Finite precision QMRIDR(s) versus full GMRES



Stay close to Arnoldi/Lanczos

A comparison: IDR based eigenvalue solvers



ГUHH

Flexible QMRIDR(s)



Conclusion and Outlook

The new implementations of IDR, i.e., IDRSTAB, QMRIDR, its combinations, and the eigensolver counterparts, are very promising.

Conclusion

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- The new IDR implementations provide a "smooth" transition between Arnoldi/GMRES ($s \rightarrow \infty$) and Lanczos/QMR ($s \rightarrow 1$).

Conclusion

- The new implementations of IDR, i.e., IDRSTAB, QMRIDR, its combinations, and the eigensolver counterparts, are very promising.
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- The matrix generalization of Hessenberg decompositions to generalized Hessenberg decompositions and generalized Hessenberg relations allows for a simple application of standard Krylov subspace techniques.

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- ► The dependence on the parameters (*s*, **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.