IDR – A New Class of Krylov Subspace Solvers: Benefits and Drawbacks

Jens-Peter M. Zemke zemke@tu-harburg.de

Institut für Numerische Simulation Technische Universität Hamburg-Harburg

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Outline

The basic idea behind IDR

History A sketch of IDR(s) Variants & Relatives

Points of View Polynomials Generalized Hessenberg Decompositions

Numerical Experiments

An Expected Deviation "Ghost" Polynomial Roots Enhanced Stability vs. Higher Cost

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 - Generalized Hessenberg Decompositions
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Spoiler:

- IDR marks the beginning of a new era in Krylov subspace methods,
- IDR(s) is closely related to ML(k)BiCGStab by Yeung and Chan.

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Let $f(\mathbf{x}) := \mathbf{b} - \mathbf{A}\mathbf{x}$, where $\mathbf{A} \in \mathbb{C}^{n \times n}$ and $\mathbf{b} \in \mathbb{C}^n$ are given. Then

$$\mathbf{F}_k := f(\mathbf{X}_k) := \begin{pmatrix} f(\mathbf{x}_0) & \cdots & f(\mathbf{x}_n) \end{pmatrix} \in \mathbb{C}^{n \times (n+1)}$$

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is rank deficient. For every solution $\hat{\mathbf{x}}$ of $\mathbf{A}\mathbf{x} = \mathbf{b}$,

 $\mathbf{F}_k = \mathbf{A}(\hat{\mathbf{x}}\mathbf{e}^{\mathsf{T}} - \mathbf{X}_k), \text{ where } \mathbf{e} := \text{ones}(n+1,1).$

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Thus, for $\mathbf{F}_k \mathbf{c}_k = \mathbf{o}_n$ and $\mathbf{e}^{\mathsf{T}} \mathbf{c}_k \neq 0$,

$$\mathbf{b}\mathbf{e}^{\mathsf{T}}\mathbf{c}_{k} = \mathbf{A}\hat{\mathbf{x}}\mathbf{e}^{\mathsf{T}}\mathbf{c}_{k} = \mathbf{A}\mathbf{X}_{k}\mathbf{c}_{k}$$

$$\Rightarrow \quad \hat{\mathbf{x}} = \frac{\mathbf{X}_k \mathbf{c}_k}{\mathbf{e}^{\mathsf{T}} \mathbf{c}_k}.$$

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Updating all columns of \mathbf{F}_k is ill-conditioned, as all columns converge to the same vector $\mathbf{f} := f(\hat{\mathbf{x}})$. Sonneveld updated only the last two columns:

 $\mathbf{F}_k := \begin{pmatrix} \mathbf{F}_{n-1}^{\mathsf{const}} & \mathbf{f}_{k-1} & \mathbf{f}_k \end{pmatrix}.$

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Therefore, with $\mathbf{A} := \nabla f(\hat{\mathbf{x}}),$

 $\mathbf{F}_{k} = \left(\mathbf{A}(\hat{\mathbf{x}}\mathbf{e}^{\mathsf{T}} - \mathbf{X}_{n-1}) + \mathbf{E}_{n-1} \quad \mathbf{A}(\hat{\mathbf{x}} - \mathbf{x}_{k-1}) + \mathbf{d}_{k-1} \quad \mathbf{A}(\hat{\mathbf{x}} - \mathbf{x}_{k}) + \mathbf{d}_{k}\right),$

where E_{n-1} is a constant matrix and the vectors d_k converge to zero.

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$$\begin{split} \| \mathbf{r}_0 \|_2 &= 7.416198487, \\ \| \mathbf{r}_1 \|_2 &= 31.28897569, \\ \| \mathbf{r}_2 \|_2 &= 3.838120391, \\ \| \mathbf{r}_4 \|_2 &= 1.035754508, \\ \| \mathbf{r}_6 \|_2 &= 0.983756197, \\ \| \mathbf{r}_6 \|_2 &= 0.520741201, \\ \| \mathbf{r}_7 \|_2 &= 0.983648677, \\ \| \mathbf{r}_8 \|_2 &= 0.520741201, \\ \| \mathbf{r}_9 \|_2 &= 0.520740892, \\ \| \mathbf{r}_{10} \|_2 &= \| \mathbf{r}_{2n} \|_2 &= 0. \end{split}$$

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He analyzed this startling behavior: the first IDR method was born.

To analyze, he realized that c_k is of interest up to a scalar non-zero factor. He considered the case that $c_{n-1} + c_n = 1$, i.e., that the sum of the last two elements is scaled to be one. He sets $c_{n-1} := \gamma_k$ and thus $c_n = 1 - \gamma_k$.

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Now, for $\mathbf{c}_{n-1}^{(k)}$, we have to solve the overdetermined consistent linear system

$$\mathbf{F}_{n-1}\mathbf{c}_{n-1}^{(k)} = -\mathbf{f}_k - \gamma_k(\mathbf{f}_k - \mathbf{f}_{k-1}).$$

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As $\mathbf{F}_{n-1} \in \mathbb{C}^{n \times (n-1)}$, there exists a non-zero vector $\mathbf{p} \in \mathbb{C}^n$ in the left null space of \mathbf{F}_{n-1} . With this vector,

$$0 = \mathbf{p}^{\mathsf{H}} \mathbf{F}_{n-1} \mathbf{c}_{n-1}^{(k)} = \mathbf{p}^{\mathsf{H}} (-\mathbf{f}_k - \gamma_k (\mathbf{f}_k - \mathbf{f}_{k-1})),$$

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i.e., γ_k is uniquely (in case of no breakdown) determined by

$$\mathbf{y}_k := -rac{\mathbf{p}^{\mathsf{H}} \mathbf{f}_k}{\mathbf{p}^{\mathsf{H}} (\mathbf{f}_k - \mathbf{f}_{k-1})}$$

The vector $\mathbf{c}_{n-1}^{(k)}$ is then (because of the consistency of the given overdetermined system) given by

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The new residual $\mathbf{f}_{k+1} = \mathbf{o}_n - \mathbf{A}\mathbf{x}_{k+1}$ satisfies

$$\mathbf{f}_{k+1} = -\frac{\mathbf{A}(\mathbf{X}_{n-1}\mathbf{c}_{n-1}^{(k)} + \mathbf{x}_{k} + \gamma_{k}(\mathbf{x}_{k} - \mathbf{x}_{k-1}))}{\mathbf{e}^{\mathsf{T}}\mathbf{c}_{n-1}^{(k)} + 1}$$

= $\frac{(\mathbf{E}_{n-1} - \mathbf{F}_{n-1})\mathbf{c}_{n-1}^{(k)} - \mathbf{f}_{k} - \gamma_{k}(\mathbf{f}_{k} - \mathbf{f}_{k-1})}{\mathbf{e}^{\mathsf{T}}\mathbf{c}_{n-1}^{(k)} + 1} = \frac{\mathbf{E}_{n-1}\mathbf{c}_{n-1}^{(k)}}{\mathbf{e}^{\mathsf{T}}\mathbf{c}_{n-1}^{(k)} + 1}$
= $\frac{\mathbf{E}_{n-1}\mathbf{F}_{n-1}^{\dagger}(\mathbf{f}_{k} + \gamma_{k}(\mathbf{f}_{k} - \mathbf{f}_{k-1}))}{\mathbf{e}^{\mathsf{T}}\mathbf{F}_{n-1}^{\dagger}(\mathbf{f}_{k} + \gamma_{k}(\mathbf{f}_{k} - \mathbf{f}_{k-1})) - 1} = \rho_{k}\mathbf{B}(\mathbf{f}_{k} + \gamma_{k}(\mathbf{f}_{k} - \mathbf{f}_{k-1}))$

The basic idea behind IDR

The origin of IDR: poor man's secant method

As the method usually converges, the vector \mathbf{c}_k in the null space of $\mathbf{F}_n^{(k)}$ will not change much, thus the scaling will not change much, thus for $k \gg 1$

$$\boldsymbol{\rho}_{k} := \frac{1}{\mathbf{e}^{\mathsf{T}} \mathbf{F}_{n-1}^{\dagger}(\mathbf{f}_{k} + \gamma_{k}(\mathbf{f}_{k} - \mathbf{f}_{k-1})) - 1} = \frac{1}{\mathbf{e}^{\mathsf{T}} \mathbf{c}_{k}} \approx \text{const} \neq 0.$$

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The finite termination property of the resulting three-term recurrence

$$\mathbf{f}_{k+1} = \rho_k \mathbf{B}(\mathbf{f}_k + \gamma_k(\mathbf{f}_k - \mathbf{f}_{k-1}))$$

can thus not depend on the scaling, but only on the way γ_k and thus \mathbf{f}_k is computed. For this reason, Sonneveld considered the case $\rho_k = 1$ for all k.

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Do we need the information that the matrix $\mathbf{B} \in \mathbb{C}^{n \times n}$ is defined by

$$\mathbf{B} := \mathbf{E}_{n-1} \mathbf{F}_{n-1}^{\dagger}?$$

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We could use any $\mathbf{B} \in \mathbb{C}^{n \times n}$ without spoiling the finite termination property!

The origin of IDR: primitive IDR

Sonneveld first made experiments and then gave a rigorous proof. It is easy to see that apart from the first two (arbitrarily chosen) residuals the constructed residuals are in the **B** image of the space $S := \mathbf{p}^{\perp}$.

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The same argument proves that in general (observe that the first two residuals f_0, f_1 are usually not in S) for $k \ge 1$

$$\mathbf{f}_{2k}, \mathbf{f}_{2k+1} \in \mathcal{G}_{k} := \bigcap_{j=1}^{k} \mathbf{B}^{j}(\mathcal{S}) = \left(\stackrel{k}{\underset{j=1}{+}} \mathbf{B}^{-j\mathsf{H}} \{\mathbf{p}\} \right)^{\perp} = \left(\mathcal{K}_{k}(\mathbf{B}^{-\mathsf{H}}, \mathbf{B}^{-\mathsf{H}}, \mathbf{p}) \right)$$

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Sonneveld proved that the dimensions of the spaces constructed are shrinking. This is the essence of the first IDR Theorem. He did not use the description as an orthogonal complement of a Krylov subspace as it is done here. We remark that generically $\dim(\mathcal{K}_n(\mathbf{B}^{-H}, \mathbf{B}^{-H}\mathbf{p})) = n$.
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Using the Krylov subspace point of view and the explicit orthogonalization against **p** before multiplication with **B**, we see that indeed $\mathbf{f}_{2n} = \mathbf{B}\mathbf{o}_n = \mathbf{o}_n$.

The three-term recurrence

 $\mathbf{f}_{k+1} = \mathbf{B}(\mathbf{f}_k + \gamma_k(\mathbf{f}_k - \mathbf{f}_{k-1})), \quad \text{where} \quad \gamma_k = \frac{\mathbf{p}^{\mathsf{rr}} \mathbf{f}_k}{\mathbf{p}^{\mathsf{H}}(\mathbf{f}_{k-1} - \mathbf{f}_k)},$

is an "implementation" of the Induced Dimension Reduction (IDR) Theorem. The vectors constructed live in spaces of shrinking dimensions. Methods like this are called "IDR Algorithms".

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Another implementation by Sonneveld can be used to solve "genuine" linear systems. The idea is to rewrite the linear system to Richardson iteration form,

$$\mathbf{A}\mathbf{x} = \mathbf{b} \implies \mathbf{x} = (\mathbf{I} - \mathbf{A})\mathbf{x} + \mathbf{b} =: \mathbf{B}\mathbf{x} + \mathbf{b}.$$

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The classical Richardson iteration with a starting guess \mathbf{x}_0 is then given by

$$\mathbf{x}_{k+1} = (\mathbf{I} - \mathbf{A})\mathbf{x}_k + \mathbf{b}.$$

With $\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$, the Richardson iteration is carried out as follows:

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In a Richardson-type IDR Algorithm, the second equation is replaced by the update

$$\mathbf{r}_{k+1} = (\mathbf{I} - \mathbf{A})(\mathbf{r}_k + \gamma_k(\mathbf{r}_k - \mathbf{r}_{k-1})), \quad \gamma_k = \frac{\mathbf{p}^{\mathsf{H}}\mathbf{r}_k}{\mathbf{p}^{\mathsf{H}}(\mathbf{r}_{k-1} - \mathbf{r}_k)}.$$

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In a Richardson-type IDR Algorithm, the second equation is replaced by the update

$$\mathbf{r}_{k+1} = (\mathbf{I} - \mathbf{A})(\mathbf{r}_k + \gamma_k(\mathbf{r}_k - \mathbf{r}_{k-1})), \quad \gamma_k = \frac{\mathbf{p}^{\mathsf{m}} \mathbf{r}_k}{\mathbf{p}^{\mathsf{H}}(\mathbf{r}_{k-1} - \mathbf{r}_k)}$$

The update of the iterates has to be modified accordingly,

$$-\mathbf{A}(\mathbf{x}_{k+1} - \mathbf{x}_k) = \mathbf{r}_{k+1} - \mathbf{r}_k = (\mathbf{I} - \mathbf{A})(\mathbf{r}_k + \gamma_k(\mathbf{r}_k - \mathbf{r}_{k-1})) - \mathbf{r}_k$$

= $(\mathbf{I} - \mathbf{A})(\mathbf{r}_k - \gamma_k \mathbf{A}(\mathbf{x}_k - \mathbf{x}_{k-1})) - \mathbf{r}_k$
= $-\mathbf{A}(\mathbf{r}_k + \gamma_k(\mathbf{I} - \mathbf{A})(\mathbf{x}_k - \mathbf{x}_{k-1}))$
 $\Leftrightarrow \mathbf{x}_{k+1} - \mathbf{x}_k = \mathbf{r}_k + \gamma_k(\mathbf{I} - \mathbf{A})(\mathbf{x}_k - \mathbf{x}_{k-1})$
= $\mathbf{r}_k + \gamma_k(\mathbf{x}_k - \mathbf{x}_{k-1} + \mathbf{r}_k - \mathbf{r}_{k-1}).$

Sonneveld terms the outcome the Primitive IDR Algorithm (Sonneveld, 2006):

$$\mathbf{r}_{0} = \mathbf{b} - \mathbf{A}\mathbf{x}_{0}$$
$$\mathbf{x}_{1} = \mathbf{x}_{0} + \mathbf{r}_{0}$$
$$\mathbf{r}_{1} = \mathbf{r}_{0} - \mathbf{A}\mathbf{r}_{0}$$
For $k = 1, 2, \dots$ do
$$\gamma_{k} = \mathbf{p}^{\mathsf{T}}\mathbf{r}_{k}/\mathbf{p}^{\mathsf{T}}(\mathbf{r}_{k-1} - \mathbf{r}_{k})$$
$$\mathbf{s}_{k} = \mathbf{r}_{k} + \gamma_{k}(\mathbf{r}_{k} - \mathbf{r}_{k-1})$$
$$\mathbf{x}_{k+1} = \mathbf{x}_{k} + \gamma_{k}(\mathbf{x}_{k} - \mathbf{x}_{k-1}) + \mathbf{s}_{k}$$
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 $\begin{aligned} \mathbf{x}_{\text{old}} &= \mathbf{x}_{0} \\ \mathbf{r}_{\text{old}} &= \mathbf{b} - \mathbf{A}\mathbf{x}_{\text{old}} \\ \mathbf{x}_{\text{new}} &= \mathbf{x}_{\text{old}} + \mathbf{r}_{\text{old}} \\ \mathbf{r}_{\text{new}} &= \mathbf{r}_{\text{old}} - \mathbf{A}\mathbf{r}_{\text{old}} \end{aligned}$

While "not converged" do

$$\begin{split} \gamma &= \mathbf{p}^{\mathsf{T}} \mathbf{r}_{\mathsf{new}} / \mathbf{p}^{\mathsf{T}} (\mathbf{r}_{\mathsf{old}} - \mathbf{r}_{\mathsf{new}}) \\ \mathbf{s} &= \mathbf{r}_{\mathsf{new}} + \gamma (\mathbf{r}_{\mathsf{new}} - \mathbf{r}_{\mathsf{old}}) \\ \mathbf{x}_{\mathsf{tmp}} &= \mathbf{x}_{\mathsf{new}} + \gamma (\mathbf{x}_{\mathsf{new}} - \mathbf{x}_{\mathsf{old}}) + \mathbf{s} \\ \mathbf{r}_{\mathsf{tmp}} &= \mathbf{s} - \mathbf{As} \\ \mathbf{x}_{\mathsf{old}} &= \mathbf{x}_{\mathsf{new}}, \ \mathbf{x}_{\mathsf{new}} = \mathbf{x}_{\mathsf{tmp}} \\ \mathbf{r}_{\mathsf{old}} &= \mathbf{r}_{\mathsf{new}}, \ \mathbf{r}_{\mathsf{new}} = \mathbf{r}_{\mathsf{tmp}} \end{split}$$

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 \mathbf{S}_k

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done

On the next slide we compare Richardson iteration (red) and PIA (blue).

Impressions of "finite termination" and acceleration in finite precision:



Sonneveld never did use PIA, as he considered it to be too unstable, instead he went on with a corresponding acceleration of the Gauß-Seidel method. In (Sonneveld, 2008) he terms this method Accelerated Gauß-Seidel (AGS) and refers to it as "[t]he very first IDR-algorithm [..]", see page 6, Ibid.

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In September 1979 Sonneveld did attend the IUTAM Symposium on Approximation Methods for Navier-Stokes Problems in Paderborn, Germany. At this symposium he presented a new variant of IDR based on a variable splitting $I - \omega_j A$, where ω_j is fixed for two steps and otherwise could be chosen freely, but non-zero.

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This algorithm with minimization of every second residual is included in the proceedings from 1980 (Wesseling and Sonneveld, 1980). The connection to Krylov methods, e.g., BiCG/Lanczos, is also given there.

The origin of IDR: classical IDR

A numerical comparison of Richardson iteration, original IDR, and PIA.



IDR(s) is a Krylov subspace method based on two building blocks:

- Multiplication by polynomials in A. (IDR(s): linear, IDR(s)Stab(l): higher degree)
- Oblique projection perpendicular to $\mathbf{P} \in \mathbb{C}^{n \times s}$.

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The prototype IDR(s) method constructs spaces G_j as follows:

- Define $\mathcal{G}_0 := \mathcal{K}(\mathbf{A}, \mathbf{r}_0) = \text{span} \{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \ldots\}.$
- ► Iterate $\mathcal{G}_j := (\mathbf{I} \omega_j \mathbf{A})(\mathcal{G}_{j-1} \cap \mathcal{S}), \quad j = 1, 2, \dots, \quad \mathbb{C} \ni \omega_j \neq 0$

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Only sufficiently many vectors in each space are constructed.

IDR is Lanczos times something

It turns out that:

IDR(s) is a transpose-free variant of a Lanczos process with one right-hand side and s left-hand sides.

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 $\mathbf{r}_{j(s+1)+k}^{\mathsf{IDR}} = \Omega_j(\mathbf{A})\rho_{js+k}(\mathbf{A})\mathbf{r}_0, \quad 1 \leq k \leq s$

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Reminder: Residual polynomials are polynomials that

- satisfy $\mathbf{r}_k = \rho_k(\mathbf{A})\mathbf{r}_0$ and
- are normalized by the condition $\rho_k(0) = 1$.

IDR @ Oxford

Outline

The basic line a behind IDR History A sketch of IDR(s) Variants & Relatives

Points of View

Polynomials Generalized Hessenberg Decompositions

Numerical Experiments

An Expected Deviation "Ghost" Polynomial Roots Enhanced Stability vs. Higher Cost

Krylov subspace: try thinking in polynomials

 $IDR/IDR(s)/IDR(s)Stab(\ell)$ are classes of Krylov subspace methods, they construct approximations from Krylov subspaces

 $\mathcal{K}_k(\mathbf{A},\mathbf{r}_0) := \text{span} \{\mathbf{r}_0,\mathbf{A}\mathbf{r}_0,\ldots,\mathbf{A}^{k-1}\mathbf{r}_0\}.$

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Krylov subspaces are isomorphic (up to a certain degree) to polynomial spaces,

$$\mathbf{x} \in \mathcal{K}_k \quad \Leftrightarrow \quad \mathbf{x} = \sum_{j=0}^{k-1} \mathbf{A}^j \mathbf{r}_0 c_j = p_{k-1}(\mathbf{A}) \mathbf{r}_0, \quad p_{k-1}(z) = \sum_{j=0}^{k-1} c_j z^j.$$

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Residual polynomials arise because

$$\mathbf{r}_k := \mathbf{r}_0 - \mathbf{A}\mathbf{x}_k = (\mathbf{I} - \mathbf{A}p_{k-1}(\mathbf{A}))\mathbf{r}_0 =: \rho_k(\mathbf{A})\mathbf{r}_0.$$

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Denote $\Omega_k(\mathbf{A}) := \prod_{\ell=1}^k (\mathbf{I} - \omega_\ell \mathbf{A})$. It can easily be proven that $(\mathcal{S} := \mathbf{P}^{\perp})$

 $\mathcal{G}_0 = \mathcal{K}(A,r_0), \quad \text{where } \mathcal{K}(A,r_0) \text{ denotes the } \textit{full Krylov subspace},$

$$\mathcal{G}_{j} = \bigcap_{k=0}^{j-1} \Omega_{k}(\mathbf{A})^{-1} \Omega_{j}(\mathbf{A})(\mathcal{S}) = \left(\stackrel{j-1}{+} \Omega_{j}(\mathbf{A})^{-\mathsf{H}} \Omega_{k}(\mathbf{A})^{\mathsf{H}} \{\mathbf{P}\} \right)^{\perp}$$
$$= \left(\Omega_{j}(\mathbf{A})^{-\mathsf{H}} \mathcal{K}_{j}(\mathbf{A}^{\mathsf{H}}, \mathbf{P}) \right)^{\perp} = \Omega_{j}(\mathbf{A}) \left(\mathcal{K}_{j}(\mathbf{A}^{\mathsf{H}}, \mathbf{P}) \right)^{\perp}$$

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This has to be compared with Theorem 4.2 in (Sleijpen et al., 2008) and with Theorem 4.1 in (Simoncini and Szyld, 2009) (similar result; slightly different method of proof).



 $\begin{array}{ll} \text{Recall that} \quad \mathcal{G}_0 := \mathcal{K}(\mathbf{A}, \mathbf{r}_0), \quad \mathcal{G}_j := (\mathbf{I} - \omega_j \mathbf{A})(\mathcal{G}_{j-1} \cap \mathcal{S}), \quad j = 1, 2, \dots \\ \text{The first equality} \end{array}$

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- the last s + 1 vectors are in the $\mathbf{I} \omega_j \mathbf{A}$ image of $S = \mathbf{P}^{\perp}$,
- the last vectors are I − ω_jA images of linear combinations of previously obtained images (I − ω_j−1A) · · · (I − ω_kA) of S = P[⊥].

The second equality

i-1 $\Omega_k(\mathbf{A})^{-1}\Omega_j(\mathbf{A})(\mathcal{S}) = \begin{pmatrix} j^{-1} \\ + \\ k=0 \end{pmatrix} \Omega_j(\mathbf{A})^{-\mathsf{H}}\Omega_k(\mathbf{A})^{\mathsf{H}}\{\mathbf{P}\} \Big)^{\perp}$ k=0

The second equality

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and

 $\mathbf{B}\mathbf{P}^{\perp} = (\mathbf{B}^{-\mathsf{H}}\mathbf{P})^{\perp}$

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and

$$\mathcal{U}^{\perp} \cap \mathcal{V}^{\perp} = (\mathcal{U} \cup \mathcal{V})^{\perp} = (\mathcal{U} + \mathcal{V})^{\perp}.$$

The second relations are basic linear algebra. The first relation follows from

$$\mathbf{P}^{\perp} = \left\{ \mathbf{v} \in \mathbb{C}^n \mid \mathbf{P}^{\mathsf{H}} \mathbf{v} = \mathbf{o}_n \right\} \quad \Rightarrow \quad \mathbf{B} \mathbf{P}^{\perp} = \left\{ \mathbf{B} \mathbf{v} \in \mathbb{C}^n \mid \mathbf{P}^{\mathsf{H}} \mathbf{v} = \mathbf{o}_n \right\}$$

since, for invertible B,

$$\mathbf{y} \in \mathbf{B}\mathbf{P}^{\perp} \iff \left\{\mathbf{y} = \mathbf{B}\mathbf{v} \land \mathbf{P}^{\mathsf{H}}\mathbf{v} = \mathbf{o}_{n}\right\} \iff \mathbf{P}^{\mathsf{H}}\mathbf{v} = \mathbf{P}^{\mathsf{H}}\mathbf{B}^{-1}\mathbf{y} = (\mathbf{B}^{-\mathsf{H}}\mathbf{P})^{\mathsf{H}}\mathbf{y} = \mathbf{o}_{n}$$

The third and fourth equality

$$\begin{pmatrix} j^{j-1} \\ + \\ k=0 \end{pmatrix} \Omega_{j}(\mathbf{A})^{-\mathsf{H}} \Omega_{k}(\mathbf{A})^{\mathsf{H}} \{\mathbf{P}\} \end{pmatrix}^{\perp} = \left(\Omega_{j}(\mathbf{A})^{-\mathsf{H}} \mathcal{K}_{j}(\mathbf{A}^{\mathsf{H}}, \mathbf{P})\right)^{\perp}$$
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$$= \Omega_{j}(\mathbf{A}) \left(\mathcal{K}_{j}(\mathbf{A}^{\mathsf{H}}, \mathbf{P})\right)^{\perp}$$

are satisfied

- since the polynomials $\Omega_k(\mathbf{A})$, $0 \leq k < j$ form a basis of the space of polynomials of degree less j, and
- by the property proved on the last slide, respectively.

The third and fourth equality

$$\begin{pmatrix} j^{-1} \\ + \\ k=0 \end{pmatrix}^{\perp} \Omega_{j}(\mathbf{A})^{-\mathsf{H}} \Omega_{k}(\mathbf{A})^{\mathsf{H}} \{\mathbf{P}\} \end{pmatrix}^{\perp} = \left(\Omega_{j}(\mathbf{A})^{-\mathsf{H}} \mathcal{K}_{j}(\mathbf{A}^{\mathsf{H}}, \mathbf{P})\right)$$
$$= \Omega_{j}(\mathbf{A}) \left(\mathcal{K}_{j}(\mathbf{A}^{\mathsf{H}}, \mathbf{P})\right)^{\perp}$$

are satisfied

- since the polynomials Ω_k(A), 0 ≤ k < j form a basis of the space of polynomials of degree less j, and</p>
- by the property proved on the last slide, respectively.

This is of interest in round-off error analysis (Lanczos): "Local orthogonality" is preserved, the inner products with the oldest basis vectors, i.e., those that are the columns of **P**, are "small".

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"Classical" Krylov subspace methods generate

- ▶ "basis" matrices $\mathbf{Q}_{k+1} = (\mathbf{Q}_k, \mathbf{q}_{k+1}) \in \mathbb{C}^{n \times (k+1)}$ and
- unreduced extended Hessenberg matrices $\underline{\mathbf{H}}_k \in \mathbb{C}^{(k+1) \times k}$

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IDR based Krylov subspace methods additionally generate upper triangular matrices $\mathbf{U}_k \in \mathbb{C}^{k \times k}$ such that we obtain a generalized Hessenberg decomposition

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IDR based methods include BiCGStab (rewritten version of IDR), and CGS.

Points of View Generalized 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 $\frac{1}{2} e^{-\alpha_1}$ (v = 1,2,...,n) ebenfalle in einer Matrix susammenfassen, und zwar ist nach Gleichung (55) und (56) (57) $(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\cdots,\frac{1}{2},\frac{1}{\alpha_1}) \in \mathfrak{A} \cdot \frac{1}{2}^{(2)} \frac{1}{2}^{(2)} \mathbb{P}$, worin die Matrix \mathbb{P} zur Abkürsung gesetzt ist für (52) $\mathbb{P} = \begin{pmatrix} \alpha_{\alpha_1} & \alpha_{\alpha_2} & \cdots & \alpha_{\alpha_n-\alpha_n} \\ \alpha_{\alpha_1} & \alpha_{\alpha_1} & \cdots & \alpha_{\alpha_n-\alpha_n} \\ 0 & 1 & \cdots & \alpha_{\alpha_n-\alpha_n} \\ 0 & 0 & \cdots & 1 & \alpha_{\alpha_n-\alpha_n} \end{pmatrix}$

Hessenberg decomposition, Eqn. (57),

Hessenberg matrix, Eqn. (58).

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

IDR: Sonneveld pencil and Sonneveld matrix

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The upper triangular matrix $\mathbf{Y}_n \mathbf{D}_{\omega}^{(n)}$ could be inverted, which results in the Sonneveld matrix, a full unreduced Hessenberg matrix.

Understanding IDR: Purification

We know the eigenvalues \approx roots of kernel polynomials $1/\omega_j$. We are only interested in the other eigenvalues.

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We get rid of the infinite eigenvalues using a change of basis (Gauß/Schur).

Understanding IDR: Gaussian elimination

The deflated purified IDR(*s*)ORes pencil, after the elimination step $(\mathbf{Y}_n^{\circ}\mathbf{G}_n, \mathbf{U}_n\mathbf{D}_{\omega}^{(n)})$, can be depicted by



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Using Laplace expansion of the determinant of $_{z}\mathbf{U}_{n}\mathbf{D}_{\omega}^{(n)} - \mathbf{Y}_{n}^{\circ}\mathbf{G}_{n}$ we can get rid of the trivial constant factors corresponding to infinite eigenvalues. This amounts to a deflation.

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Let *D* denote an deflation operator that removes every (s + 1)th column and row from the matrix the operator is applied to.

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The block-diagonal matrix $D(\mathbf{U}_n \mathbf{D}_{\omega}^{(n)})$ has invertible upper triangular blocks and can be inverted to expose the underlying Lanczos process.

Points of View

Generalized Hessenberg Decompositions

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IDR: a Lanczos process with multiple left-hand sides

Inverting the block-diagonal matrix $D(\mathbf{U}_n \mathbf{D}_{\omega}^{(n)}))$ gives an algebraic eigenvalue problem with a block-tridiagonal unreduced upper Hessenberg matrix

$$\mathbf{L}_{n} := D(\mathbf{Y}_{n}^{\circ}\mathbf{G}_{n}) \cdot D(\mathbf{U}_{n}\mathbf{D}_{n}^{(n)}))^{-1} = \begin{bmatrix} \circ + \times \times \times \times \circ \circ \circ \\ \circ \circ + \times \times \times \times \times \\ \circ \circ \circ + \times \times \times \times \\ \circ \circ \circ + \times \times \times \times \\ \circ \circ \circ + \times \times \times \times \\ \bullet & \circ \circ + \times \times \times \times \\ \bullet & \circ \circ + \times \times \times \times \\ \bullet & \circ & \circ + \times \times \times \\ \bullet & \circ & \circ + \times \times \times \\ \bullet & \circ & \circ + \times \times \times \\ \bullet & \circ & \circ + \times \times \times \\ \bullet & \circ & \circ & \circ \\ \bullet & \circ & \circ \\ \bullet & \circ & \circ & \circ \\ \bullet & \circ & \circ \\ \bullet & \circ & \circ & \circ \\ \bullet & \circ$$

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Points of View

Generalized Hessenberg Decompositions

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Points of View

Generalized Hessenberg Decompositions

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This matrix (in the extended version) satisfies

$$\mathbf{A}\mathbf{Q}_n=\mathbf{Q}_{n+1}\underline{\mathbf{L}}_n$$

where the reduced residuals \mathbf{q}_{js+k} , $k = 0, \dots, s-1, j = 0, 1, \dots$, are given by

$$\Omega_j(\mathbf{A})\mathbf{q}_{js+k}=\mathbf{r}_{j(s+1)+k}.$$

Outline

History A sketch of IDR(s) Variants & Relatives Points of View Polynomials Generalized Hessenberg Decompositio

Numerical Experiments

An Expected Deviation "Ghost" Polynomial Roots Enhanced Stability vs. Higher Cost

At least we might expect some deviation, as IDR is based on short term recurrences.

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In the following plots we depict (known) behavior of Lanczos algorithms and compare if to the (yet to be analyzed) behavior of IDR algorithms.

In a recent report, Collignon, Sleijpen and van Gijzen show that IDR can be interpreted as a sort of preconditioning based on deflation; the preconditioned matrix has the polynomial roots as eigenvalues.



Numerical Experiments An Expected Deviatio

Lanczos' method in finite precision



The theory of the Lanczos method in case of non-selfadjoint matrices is still less satisfactory. Some of the conclusions carry over, and the behavior in finite precision shows some similarities.

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As there does not exist the **best** Lanczos method, we have chosen one of the more stable ones, namely the variant described in (Bai, 1994).
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We note that we can observe multiple copies, but this time the approximation quality is reduced after a couple of steps, all Ritz values computed after certain steps show worse behavior than before.

Lanczos' method in finite precision



IDR, IDR(1), and BiCGStab



IDR, IDR(1), and BiCGStab



Numerical Experiments An Expected Deviation

Understanding IDR: 600 steps for s = 2



"Ghost" Polynomial Roots



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- Experiments by Seiji Fujino indicate that IDR(s) applied to SPD matrices is comparable to CG, both with the best available preconditioners, yet IDR(s) is a general purpose solver.
- ▶ Using real values for the polynomial roots gives bad results. To use real arithmetic, $IDR(s)Stab(\ell)$ can be used, e.g., $\ell = 2, 4, 8$. Unfortunately, in this case $(\ell + 1) \cdot s$ vectors have to be stored.

Conclusion and Outview

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- What about "continous" IDR?

Thank you for your attention!

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