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

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## Outline

## The basic idea behind IDR

History
A sketch of $\operatorname{IDR}(s)$
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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- Is $\operatorname{IDR} / \mathrm{IDR}(s)$ really new? Are parts of it new?


## Spoiler:

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


## The origin of IDR: poor man's secant method

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

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\mathbf{F}_{k}:=f\left(\mathbf{X}_{k}\right):=\left(\begin{array}{lll}
f\left(\mathbf{x}_{0}\right) & \cdots & \left.f\left(\mathbf{x}_{n}\right)\right)
\end{array}\right) \in \mathbb{C}^{n \times(n+1)}
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is rank deficient. For every solution $\hat{\mathbf{x}}$ of $\mathbf{A x}=\mathbf{b}$,

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\mathbf{F}_{k}=\mathbf{A}\left(\hat{\mathbf{x}} \mathbf{e}^{\top}-\mathbf{X}_{k}\right), \quad \text { where } \quad \mathbf{e}:=\operatorname{ones}(n+1,1) .
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Thus, for $\mathbf{F}_{k} \mathbf{c}_{k}=\mathbf{o}_{n}$ and $\mathbf{e}^{\top} \mathbf{c}_{k} \neq 0$,

$$
\mathbf{b e}^{\top} \mathbf{c}_{k}=\mathbf{A} \hat{\mathbf{x}}^{\top} \mathbf{c}_{k}=\mathbf{A} \mathbf{X}_{k} \mathbf{c}_{k} \Rightarrow \hat{\mathbf{x}}=\frac{\mathbf{X}_{k} \mathbf{c}_{k}}{\mathbf{e}^{\top} \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:

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\mathbf{F}_{k}:=\left(\begin{array}{lll}
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Therefore, with $\mathbf{A}:=\nabla f(\hat{\mathbf{x}})$,

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

where $\mathbf{E}_{n-1}$ is a constant matrix and the vectors $\mathbf{d}_{k}$ converge to zero.

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\begin{array}{ll}
\left\|\mathbf{r}_{0}\right\|_{2}=7.416198487, & \left\|\mathbf{r}_{1}\right\|_{2}=31.28897569 \\
\left\|\mathbf{r}_{2}\right\|_{2}=3.838120391, & \left\|\mathbf{r}_{3}\right\|_{2}=3.944190988 \\
\left\|\mathbf{r}_{4}\right\|_{2}=1.035754508, & \left\|\mathbf{r}_{5}\right\|_{2}=1.035728492 \\
\left\|\mathbf{r}_{6}\right\|_{2}=0.983756197, & \left\|\mathbf{r}_{7}\right\|_{2}=0.983648677 \\
\left\|\mathbf{r}_{8}\right\|_{2}=0.520741201, & \left\|\mathbf{r}_{9}\right\|_{2}=0.520740892 \\
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He analyzed this startling behavior: the first IDR method was born.

## The origin of IDR: poor man's secant method

To analyze, he realized that $\mathbf{c}_{k}$ 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

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\mathbf{F}_{n-1} \mathbf{c}_{n-1}^{(k)}=-\mathbf{f}_{k}-\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right) .
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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,

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0=\mathbf{p}^{\mathrm{H}} \mathbf{F}_{n-1} \mathbf{c}_{n-1}^{(k)}=\mathbf{p}^{\mathrm{H}}\left(-\mathbf{f}_{k}-\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)\right)
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i.e., $\gamma_{k}$ is uniquely (in case of no breakdown) determined by

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\gamma_{k}:=-\frac{\mathbf{p}^{\mathrm{H}} \mathbf{f}_{k}}{\mathbf{p}^{\mathrm{H}}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)} .
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The vector $\mathbf{c}_{n-1}^{(k)}$ is then (because of the consistency of the given overdetermined system) given by

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\mathbf{c}_{n-1}^{(k)}:=-\mathbf{F}_{n-1}^{\dagger}\left(\mathbf{f}_{k}+\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)\right) .
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The new residual $\mathbf{f}_{k+1}=\mathbf{o}_{n}-\mathbf{A} \mathbf{x}_{k+1}$ satisfies

$$
\begin{aligned}
\mathbf{f}_{k+1} & =-\frac{\mathbf{A}\left(\mathbf{X}_{n-1} \mathbf{c}_{n-1}^{(k)}+\mathbf{x}_{k}+\gamma_{k}\left(\mathbf{x}_{k}-\mathbf{x}_{k-1}\right)\right)}{\mathbf{e}^{\top} \mathbf{c}_{n-1}^{(k)}+1} \\
& =\frac{\left(\mathbf{E}_{n-1}-\mathbf{F}_{n-1}\right) \mathbf{c}_{n-1}^{(k)}-\mathbf{f}_{k}-\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)}{\mathbf{e}^{\top} \mathbf{c}_{n-1}^{(k)}+1}=\frac{\mathbf{E}_{n-1} \mathbf{c}_{n-1}^{(k)}}{\mathbf{e}^{\top} \mathbf{c}_{n-1}^{(k)}+1} \\
& =\frac{\mathbf{E}_{n-1} \mathbf{F}_{n-1}^{\dagger}\left(\mathbf{f}_{k}+\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)\right)}{\mathbf{e}^{\top} \mathbf{F}_{n-1}^{\dagger}\left(\mathbf{f}_{k}+\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)\right)-1}=\rho_{k} \mathbf{B}\left(\mathbf{f}_{k}+\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)\right)
\end{aligned}
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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 $k \gg 1$

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\rho_{k}:=\frac{1}{\mathbf{e}^{\top} \mathbf{F}_{n-1}^{\dagger}\left(\mathbf{f}_{k}+\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)\right)-1}=\frac{1}{\mathbf{e}^{\top} \mathbf{c}_{k}} \approx \text { const } \neq 0 .
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The finite termination property of the resulting three-term recurrence

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\mathbf{f}_{k+1}=\rho_{k} \mathbf{B}\left(\mathbf{f}_{k}+\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)\right)
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can thus not depend on the scaling, but only on the way $\gamma_{k}$ 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

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\mathbf{B}:=\mathbf{E}_{n-1} \mathbf{F}_{n-1}^{\dagger} ?
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The right kernel of $\mathbf{F}_{n-1}^{\dagger}$ is the left kernel of $\mathbf{F}_{n-1}$, i.e., it is spanned by the vector $\mathbf{p}$ used in the computation of $\gamma_{k}$,

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The simplified (i.e., scaled) three-term recurrence

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is "immune" to changes in $\mathbf{B}$ in direction of $\mathbf{p}$, as the $\gamma_{k}$ are chosen to construct vectors orthogonal to $\mathbf{p}$.

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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 $\mathbf{B}$ image of the space $\mathcal{S}:=\mathbf{p}^{\perp}$.

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The same argument proves that in general (observe that the first two residuals $\mathbf{f}_{0}, \mathbf{f}_{1}$ are usually not in $\mathcal{S}$ ) for $k \geqslant 1$

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

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Using the Krylov subspace point of view and the explicit orthogonalization against $\mathbf{p}$ before multiplication with $\mathbf{B}$, we see that indeed $\mathbf{f}_{2 n}=\mathbf{B} \mathbf{o}_{n}=\mathbf{o}_{n}$.

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$$

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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The three-term recurrence

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\mathbf{f}_{k+1}=\mathbf{B}\left(\mathbf{f}_{k}+\gamma_{k}\left(\mathbf{f}_{k}-\mathbf{f}_{k-1}\right)\right), \quad \text { where } \quad \gamma_{k}=\frac{\mathbf{p}^{\mathrm{H}} \mathbf{f}_{k}}{\mathbf{p}^{\mathrm{H}}\left(\mathbf{f}_{k-1}-\mathbf{f}_{k}\right)},
$$

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".

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 x}=\mathbf{b} \quad \Rightarrow \mathbf{x}=(\mathbf{I}-\mathbf{A}) \mathbf{x}+\mathbf{b}=: \mathbf{B} \mathbf{x}+\mathbf{b} .
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## The origin of IDR: primitive IDR

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$$

The classical Richardson iteration with a starting guess $\mathbf{x}_{0}$ is then given by

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

## The origin of IDR: primitive IDR

With $\mathbf{r}_{0}:=\mathbf{b}-\mathbf{A} \mathbf{x}_{0}$, the Richardson iteration is carried out as follows:

$$
\mathbf{x}_{k+1}=\mathbf{x}_{k}+\mathbf{r}_{k}, \quad \mathbf{r}_{k+1}=(\mathbf{I}-\mathbf{A}) \mathbf{r}_{k}
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In a Richardson-type IDR Algorithm, the second equation is replaced by the update

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\mathbf{r}_{k+1}=(\mathbf{I}-\mathbf{A})\left(\mathbf{r}_{k}+\gamma_{k}\left(\mathbf{r}_{k}-\mathbf{r}_{k-1}\right)\right), \quad \gamma_{k}=\frac{\mathbf{p}^{\mathrm{H}} \mathbf{r}_{k}}{\mathbf{p}^{\mathrm{H}}\left(\mathbf{r}_{k-1}-\mathbf{r}_{k}\right)} .
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$$

The update of the iterates has to be modified accordingly,

$$
\begin{aligned}
-\mathbf{A}\left(\mathbf{x}_{k+1}-\mathbf{x}_{k}\right) & =\mathbf{r}_{k+1}-\mathbf{r}_{k}=(\mathbf{I}-\mathbf{A})\left(\mathbf{r}_{k}+\gamma_{k}\left(\mathbf{r}_{k}-\mathbf{r}_{k-1}\right)\right)-\mathbf{r}_{k} \\
& =(\mathbf{I}-\mathbf{A})\left(\mathbf{r}_{k}-\gamma_{k} \mathbf{A}\left(\mathbf{x}_{k}-\mathbf{x}_{k-1}\right)\right)-\mathbf{r}_{k} \\
& =-\mathbf{A}\left(\mathbf{r}_{k}+\gamma_{k}(\mathbf{I}-\mathbf{A})\left(\mathbf{x}_{k}-\mathbf{x}_{k-1}\right)\right) \\
\Leftrightarrow \quad \mathbf{x}_{k+1}-\mathbf{x}_{k} & =\mathbf{r}_{k}+\gamma_{k}(\mathbf{I}-\mathbf{A})\left(\mathbf{x}_{k}-\mathbf{x}_{k-1}\right) \\
& =\mathbf{r}_{k}+\gamma_{k}\left(\mathbf{x}_{k}-\mathbf{x}_{k-1}+\mathbf{r}_{k}-\mathbf{r}_{k-1}\right)
\end{aligned}
$$

## The origin of IDR: primitive IDR

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

$$
\begin{aligned}
& \mathbf{r}_{0}=\mathbf{b}-\mathbf{A} \mathbf{x}_{0} \\
& \mathbf{x}_{1}=\mathbf{x}_{0}+\mathbf{r}_{0} \\
& \mathbf{r}_{1}=\mathbf{r}_{0}-\mathbf{A} \mathbf{r}_{0}
\end{aligned}
$$

For $k=1,2, \ldots$ do

$$
\begin{aligned}
& \gamma_{k}=\mathbf{p}^{\top} \mathbf{r}_{k} / \mathbf{p}^{\top}\left(\mathbf{r}_{k-1}-\mathbf{r}_{k}\right) \\
& \mathbf{s}_{k}=\mathbf{r}_{k}+\gamma_{k}\left(\mathbf{r}_{k}-\mathbf{r}_{k-1}\right) \\
& \mathbf{x}_{k+1}=\mathbf{x}_{k}+\gamma_{k}\left(\mathbf{x}_{k}-\mathbf{x}_{k-1}\right)+\mathbf{s}_{k} \\
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& \mathbf{x}_{\text {old }}=\mathbf{x}_{0} \\
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& \mathbf{x}_{\text {new }}=\mathbf{x}_{\text {old }}+\mathbf{r}_{\text {old }} \\
& \mathbf{r}_{\text {new }}=\mathbf{r}_{\text {old }}-\mathbf{A} \mathbf{r}_{\text {old }}
\end{aligned}
$$

While "not converged" do

$$
\begin{aligned}
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$$

done

$$
\begin{aligned}
& \gamma=\mathbf{p}^{\top} \mathbf{r}_{\text {new }} / \mathbf{p}^{\top}\left(\mathbf{r}_{\text {old }}-\mathbf{r}_{\text {new }}\right) \\
& \mathbf{s}=\mathbf{r}_{\text {new }}+\gamma\left(\mathbf{r}_{\text {new }}-\mathbf{r}_{\text {old }}\right) \\
& \mathbf{x}_{\text {tmp }}=\mathbf{x}_{\text {new }}+\gamma\left(\mathbf{x}_{\text {new }}-\mathbf{x}_{\text {old }}\right)+\mathbf{s} \\
& \mathbf{r}_{\text {tmp }}=\mathbf{s}-\mathbf{A s} \\
& \mathbf{x}_{\text {old }}=\mathbf{x}_{\text {new }}, \mathbf{x}_{\text {new }}=\mathbf{x}_{\text {tmp }} \\
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& \text { For } k=1,2, \ldots \text { do } \\
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$$

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

## The origin of IDR: primitive IDR

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



## The origin of IDR: primitive IDR

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 $\mathbf{I}-\omega_{j} \mathbf{A}$, where $\omega_{j}$ 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.








## Building blocks of IDR(s)

$\operatorname{IDR}(s)$ is a Krylov subspace method based on two building blocks:

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


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The prototype $\operatorname{IDR}(s)$ method constructs spaces $\mathcal{G}_{j}$ as follows:

- Define $\mathcal{G}_{0}:=\mathcal{K}\left(\mathbf{A}, \mathbf{r}_{0}\right)=\operatorname{span}\left\{\mathbf{r}_{0}, \mathbf{A r}_{0}, \mathbf{A}^{2} \mathbf{r}_{0}, \ldots\right\}$.
- Iterate $\mathcal{G}_{j}:=\left(\mathbf{I}-\omega_{j} \mathbf{A}\right)\left(\mathcal{G}_{j-1} \cap \mathcal{S}\right), \quad j=1,2, \ldots, \quad \mathbb{C} \ni \omega_{j} \neq 0$


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Only sufficiently many vectors in each space are constructed.

## IDR is Lanczos times something

It turns out that:

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- $\operatorname{IDR}(s)$ is a Lanczos-type product method, i.e., most residuals can be written as

$$
\mathbf{r}_{j(s+1)+k}^{\mathrm{IDR}}=\Omega_{j}(\mathbf{A}) \rho_{j s+k}(\mathbf{A}) \mathbf{r}_{0}, \quad 1 \leqslant k \leqslant s
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where $\rho_{j s+k}$ are residual polynomials of the Lanczos process.

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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 $\rho_{k}(0)=1$.


## Outline

The basic 雷a bénino HDR
History
A sketch of IDR ( $s$ )
Variants \& Relatives

## Points of View

Polynomials
Generalized Hessenberg Decompositions
Numetral Experments
An Expected Deviation
"Ghost" Polynomial Roots
Enhanced Stability vs. Higher Cost

## Krylov subspace: try thinking in polynomials

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

$$
\mathcal{K}_{k}\left(\mathbf{A}, \mathbf{r}_{0}\right):=\operatorname{span}\left\{\mathbf{r}_{0}, \mathbf{A} \mathbf{r}_{0}, \ldots, \mathbf{A}^{k-1} \mathbf{r}_{0}\right\} .
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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

$$
\mathbf{r}_{k}:=\mathbf{r}_{0}-\mathbf{A} \mathbf{x}_{k}=\left(\mathbf{I}-\mathbf{A} p_{k-1}(\mathbf{A})\right) \mathbf{r}_{0}=: \rho_{k}(\mathbf{A}) \mathbf{r}_{0}
$$

## IDR: a Lanczos process with multiple left-hand sides

The derivation and the theoretical properties of IDR are easy to describe using the language of polynomials.

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Denote $\Omega_{k}(\mathbf{A}):=\prod_{\ell=1}^{k}\left(\mathbf{I}-\omega_{\ell} \mathbf{A}\right)$. It can easily be proven that $\left(\mathcal{S}:=\mathbf{P}^{\perp}\right)$
$\mathcal{G}_{0}=\mathcal{K}\left(\mathbf{A}, \mathbf{r}_{0}\right)$, where $\mathcal{K}\left(\mathbf{A}, \mathbf{r}_{0}\right)$ denotes the full Krylov subspace,
$\mathcal{G}_{j}=\bigcap_{k=0}^{j-1} \Omega_{k}(\mathbf{A})^{-1} \Omega_{j}(\mathbf{A})(\mathcal{S})=\left({ }_{k=0}^{j-1} \Omega_{j}(\mathbf{A})^{-\mathrm{H}} \Omega_{k}(\mathbf{A})^{\mathrm{H}}\{\mathbf{P}\}\right)^{\perp}$ $=\left(\Omega_{j}(\mathbf{A})^{-\mathrm{H}} \mathcal{K}_{j}\left(\mathbf{A}^{\mathrm{H}}, \mathbf{P}\right)\right)^{\perp}=\Omega_{j}(\mathbf{A})\left(\mathcal{K}_{j}\left(\mathbf{A}^{\mathrm{H}}, \mathbf{P}\right)\right)^{\perp}$.

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\begin{aligned}
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& =\left(\Omega_{j}(\mathbf{A})^{-\mathrm{H}} \mathcal{K}_{j}\left(\mathbf{A}^{\mathrm{H}}, \mathbf{P}\right)\right)^{\perp}=\Omega_{j}(\mathbf{A})\left(\mathcal{K}_{j}\left(\mathbf{A}^{\mathrm{H}}, \mathbf{P}\right)\right)^{\perp} .
\end{aligned}
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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).

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- the next $s+1$ vectors in $\mathcal{G}_{2}$ are in the $\mathbf{I}-\omega_{2} \mathbf{A}$ image of $\mathcal{S}=\mathbf{P}^{\perp}$,


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Recall that $\quad \mathcal{G}_{0}:=\mathcal{K}\left(\mathbf{A}, \mathbf{r}_{0}\right), \quad \mathcal{G}_{j}:=\left(\mathbf{I}-\omega_{j} \mathbf{A}\right)\left(\mathcal{G}_{j-1} \cap \mathcal{S}\right), \quad j=1,2, \ldots$ The first equality

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follows from the observations that:

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- the last $s+1$ vectors are in the $\mathbf{I}-\omega_{j} \mathbf{A}$ image of $\mathcal{S}=\mathbf{P}^{\perp}$,
- the last vectors are $\mathbf{I}-\omega_{j} \mathbf{A}$ images of linear combinations of previously obtained images $\left(\mathbf{I}-\omega_{j-1} \mathbf{A}\right) \cdots\left(\mathbf{I}-\omega_{k} \mathbf{A}\right)$ of $\mathcal{S}=\mathbf{P}^{\perp}$.


## IDR: a Lanczos process with multiple left-hand sides

## The second equality

$$
\bigcap_{k=0}^{j-1} \Omega_{k}(\mathbf{A})^{-1} \Omega_{j}(\mathbf{A})(\mathcal{S})=\left(\begin{array}{c}
+\underset{k=0}{j-1} \\
+ \\
j
\end{array}(\mathbf{A})^{-\mathrm{H}} \Omega_{k}(\mathbf{A})^{\mathrm{H}}\{\mathbf{P}\}\right)^{\perp}
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is based on

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

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

since, for invertible B,

$$
\mathbf{y} \in \mathbf{B P}^{\perp} \Leftrightarrow\left\{\mathbf{y}=\mathbf{B} \mathbf{v} \wedge \mathbf{P}^{\mathrm{H}} \mathbf{v}=\mathbf{o}_{n}\right\} \Leftrightarrow \mathbf{P}^{\mathrm{H}} \mathbf{v}=\mathbf{P}^{\mathrm{H}} \mathbf{B}^{-1} \mathbf{y}=\left(\mathbf{B}^{-\mathrm{H}} \mathbf{P}\right)^{\mathrm{H}} \mathbf{y}=\mathbf{o}_{n} .
$$

## IDR: a Lanczos process with multiple left-hand sides

The third and fourth equality

$$
\begin{aligned}
& \stackrel{c}{k=0}+\frac{1}{+}_{\left.\rho_{j}(\mathbf{A})^{-\mathrm{H}} \Omega_{k}(\mathbf{A})^{\mathrm{H}}\{\mathbf{P}\}\right)^{\perp}}=\left(\Omega_{j}(\mathbf{A})^{-\mathrm{H}} \mathcal{K}_{j}\left(\mathbf{A}^{\mathrm{H}}, \mathbf{P}\right)\right)^{\perp} \\
&=\Omega_{j}(\mathbf{A})\left(\mathcal{K}_{j}\left(\mathbf{A}^{\mathrm{H}}, \mathbf{P}\right)\right)^{\perp}
\end{aligned}
$$

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j-1 \\
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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 $\mathbf{P}$, are "small".

## Hessenberg decompositions: basic linear algebra

The implementation and (round-off error) analysis of IDR is more closely related to so-called generalized Hessenberg decompositions.

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"Classical" Krylov subspace methods generate

- "basis" matrices $\mathbf{Q}_{k+1}=\left(\mathbf{Q}_{k}, \mathbf{q}_{k+1}\right) \in \mathbb{C}^{n \times(k+1)}$ 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.

## 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:


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

Karl Hessenberg (* September 8th, 1904, $\dagger$ 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.

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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 $\left(\mathbf{Y}_{n}^{\circ} \mathbf{G}_{n}, \mathbf{U}_{n} \mathbf{D}_{\omega}^{(n)}\right)$, 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 $D\left(\mathbf{U}_{n} \mathbf{D}_{\omega}^{(n)}\right)$ has invertible upper triangular blocks and can be inverted to expose the underlying Lanczos process.

## IDR: a Lanczos process with multiple left-hand sides

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

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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 $\mathbf{q}_{j s+k}, k=0, \ldots, s-1, j=0,1, \ldots$, are given by

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

## Outline

The basid iequa befind MLR
History
A sketch of IDR(s)
Variants \& Relatives

Polynomials
GeneralizedHessenberg Decompositions

## Numerical Experiments

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

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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.

## Lanczos' method in finite precision

comparison of 29 steps of symbolic and floating point Lanczos


## Lanczos' method in finite precision

Floating point Lanczos characteristics


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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).

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



## 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 $\operatorname{IDR}(s)$ is a general purpose solver.
- Using real values for the polynomial roots gives bad results. To use real arithmetic, $\operatorname{IDR}(s) \operatorname{Stab}(\ell)$ 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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