On the genealogy of the IDR family

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Outline

The origin of transpose-free methods . . .

“ Instead of iterating with $\mathbf{A}$ and $\mathbf{A}^T$ n times, we can also iterate with $\mathbf{A}$ alone $2n$ times. [..] The transposed matrix is not used here at all. E. C. Bouwer of the Douglas Aircraft Co. points out to the author that from the machine viewpoint a uniform iteration scheme of $2n$ iterations is preferable to a divided scheme of $n + n$ iterations. [..] In case of a symmetric matrix it is evident that after n iterations the basic scalars should be formed, instead of continuing with n more iterations. ”

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— Cornelius Lanczos, footnote on page 263 in (Lanczos, 1950), referring to his progressive algorithm based on Hankel determinants.

The origin of IDR: poor man's secant method

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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 $\mathbf{A}\mathbf{x} = \mathbf{b}$,

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

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

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

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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:

$$\mathbf{F}_k := \left(\mathbf{F}_{n-1}^{\text{const}} \quad \mathbf{f}_{k-1} \quad \mathbf{f}_k\right).$$

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

$$\mathbf{F}_k = \begin{pmatrix} \mathbf{A}(\hat{\mathbf{x}}\mathbf{e}^{\mathsf{T}} - \mathbf{X}_{n-1}) + \mathbf{E}_{n-1} & \mathbf{A}(\hat{\mathbf{x}} - \mathbf{x}_{k-1}) + \mathbf{d}_{k-1} & \mathbf{A}(\hat{\mathbf{x}} - \mathbf{x}_k) + \mathbf{d}_k \end{pmatrix},$$

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

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$$\begin{aligned}
\|\mathbf{r}_0\|_2 &= 7.416198487, & \|\mathbf{r}_1\|_2 &= 31.28897569,\\
\|\mathbf{r}_2\|_2 &= 3.838120391, & \|\mathbf{r}_3\|_2 &= 3.944190988,\\
\|\mathbf{r}_4\|_2 &= 1.035754508, & \|\mathbf{r}_5\|_2 &= 1.035728492,\\
\|\mathbf{r}_6\|_2 &= 0.983756197, & \|\mathbf{r}_7\|_2 &= 0.983648677,\\
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\end{aligned}$$

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

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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

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

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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

$$\gamma_k := -\frac{\mathbf{p}^{\mathsf{H}}\mathbf{f}_k}{\mathbf{p}^{\mathsf{H}}(\mathbf{f}_k - \mathbf{f}_{k-1})}.$$

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

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

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

$$\begin{aligned}
\mathbf{f}_{k+1} &= -\frac{\mathbf{A}(\mathbf{X}_{n-1}\mathbf{c}_{n-1}^{(k)} + \mathbf{x}_k + \gamma_k(\mathbf{x}_k - \mathbf{x}_{k-1}))}{\mathbf{e}^{\mathsf{T}}\mathbf{c}_{n-1}^{(k)} + 1} \\
&= \frac{(\mathbf{E}_{n-1} - \mathbf{F}_{n-1})\mathbf{c}_{n-1}^{(k)} - \mathbf{f}_k - \gamma_k(\mathbf{f}_k - \mathbf{f}_{k-1})}{\mathbf{e}^{\mathsf{T}}\mathbf{c}_{n-1}^{(k)} + 1} = \frac{\mathbf{E}_{n-1}\mathbf{c}_{n-1}^{(k)}}{\mathbf{e}^{\mathsf{T}}\mathbf{c}_{n-1}^{(k)} + 1} \\
&= \frac{\mathbf{E}_{n-1}\mathbf{F}_{n-1}^{\dagger}(\mathbf{f}_k + \gamma_k(\mathbf{f}_k - \mathbf{f}_{k-1}))}{\mathbf{e}^{\mathsf{T}}\mathbf{F}_{n-1}^{\dagger}(\mathbf{f}_k + \gamma_k(\mathbf{f}_k - \mathbf{f}_{k-1})) - 1} = \rho_k\mathbf{B}(\mathbf{f}_k + \gamma_k(\mathbf{f}_k - \mathbf{f}_{k-1}))
\end{aligned}$$

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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 $k \gg 1$

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

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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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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 γ_k,

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

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

is "immune" to changes in $\mathbf{B}$ in direction of $\mathbf{p}$, as the γ_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 $k \geqslant 1$

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

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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 $\dim(\mathcal{K}_n(\mathbf{B}^{-\mathsf{H}}, \mathbf{B}^{-\mathsf{H}}\mathbf{p})) = n$.

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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 $\mathbf{f}_{2n} = \mathbf{B}\mathbf{o}_n = \mathbf{o}_n$.

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The three-term recurrence

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

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

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

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

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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

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

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:

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

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

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

The update of the iterates has to be modified accordingly,

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

The origin of IDR: primitive IDR

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 $k = 1, 2, \ldots$ 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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$$\mathbf{x}_{\text{old}} = \mathbf{x}_0$$
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$$\mathbf{x}_{\text{new}} = \mathbf{x}_{\text{old}} + \mathbf{r}_{\text{old}}$$
$$\mathbf{r}_{\text{new}} = \mathbf{r}_{\text{old}} - \mathbf{A}\mathbf{r}_{\text{old}}$$

While “not converged” do

$$\gamma = \mathbf{p}^{\mathsf{T}}\mathbf{r}_{\text{new}} / \mathbf{p}^{\mathsf{T}}(\mathbf{r}_{\text{old}} - \mathbf{r}_{\text{new}})$$
$$\mathbf{s} = \mathbf{r}_{\text{new}} + \gamma(\mathbf{r}_{\text{new}} - \mathbf{r}_{\text{old}})$$
$$\mathbf{x}_{\text{tmp}} = \mathbf{x}_{\text{new}} + \gamma(\mathbf{x}_{\text{new}} - \mathbf{x}_{\text{old}}) + \mathbf{s}$$
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$$\mathbf{x}_{\text{old}} = \mathbf{x}_{\text{new}},\ \mathbf{x}_{\text{new}} = \mathbf{x}_{\text{tmp}}$$
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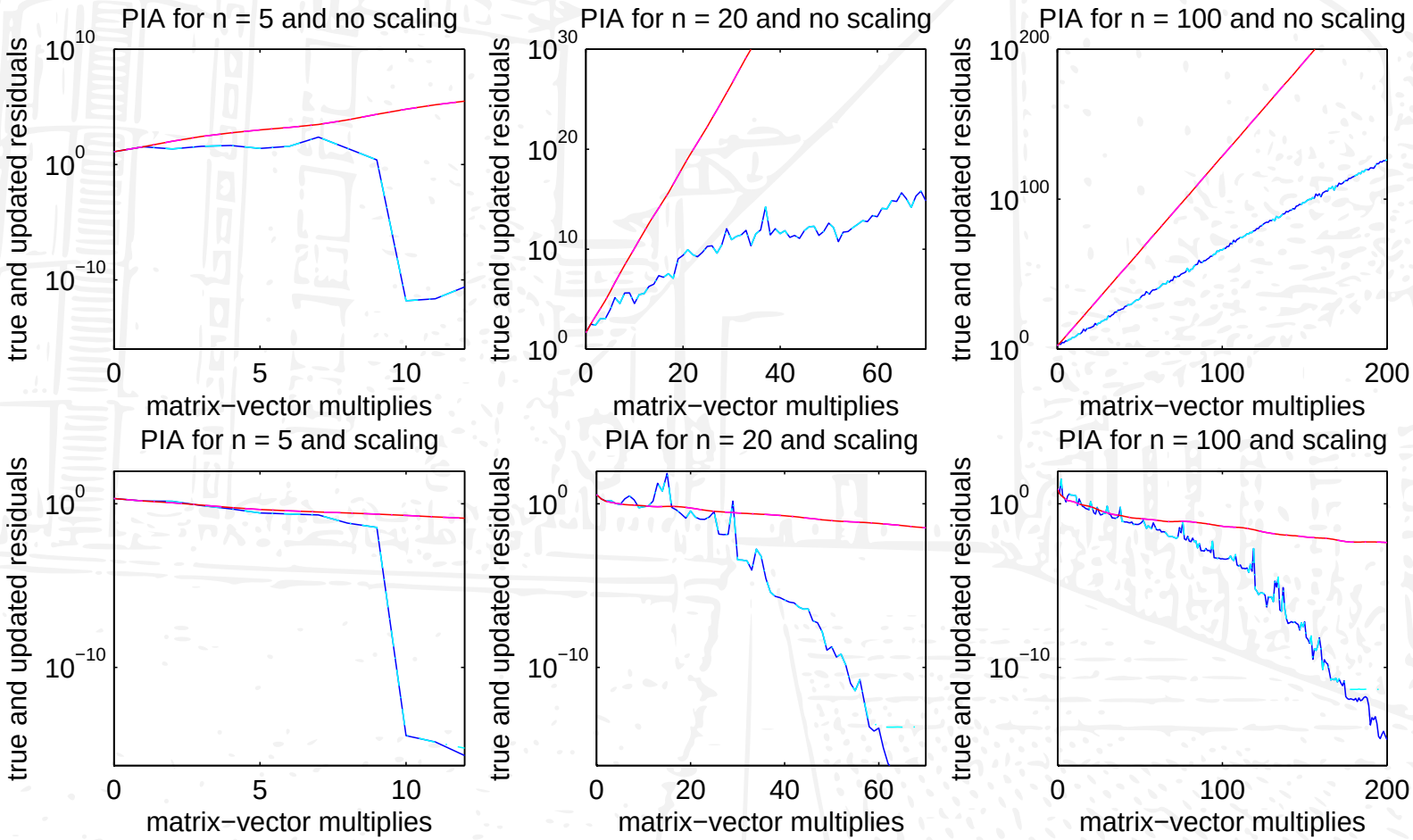
done

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:



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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 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

$\gamma_0 = 0$, $\mathbf{f}_0 = \mathbf{A}\mathbf{x}_0 - \mathbf{b}$, $\Delta\mathbf{g}_0 = \mathbf{o}_n$, $\Delta\mathbf{y}_0 = \mathbf{o}_n$
For $k = 1, \ldots$ do
  $\mathbf{s}_k = \mathbf{f}_{k-1} + \gamma_{k-1}\Delta\mathbf{g}_{k-1}$
  $\mathbf{t}_k = \mathbf{A}\mathbf{s}_k$
  if $k = 1$ or k is even
    $\omega_k = (\mathbf{t}_k^{\mathsf{H}}\mathbf{s}_k)/(\mathbf{t}_k^{\mathsf{H}}\mathbf{t}_k)$
  else
    $\omega_k = \omega_{k-1}$
  end
  $\Delta\mathbf{x}_k = \gamma_{k-1}\Delta\mathbf{y}_{k-1} - \omega_k\mathbf{s}_k$
  $\Delta\mathbf{f}_k = \gamma_{k-1}\Delta\mathbf{g}_{k-1} - \omega_k\mathbf{t}_k$
  $\mathbf{x}_k = \mathbf{x}_{k-1} + \Delta\mathbf{x}_k$
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  if k is even
    $\Delta\mathbf{y}_k = \Delta\mathbf{y}_{k-1}$
    $\Delta\mathbf{g}_k = \Delta\mathbf{g}_{k-1}$
  else
    $\Delta\mathbf{y}_k = \Delta\mathbf{x}_k$
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This is the original IDR Algorithm from page 551 of (Wesseling and Sonneveld, 1980).

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It uses OrthoRes(1) in the first step and a residual (these are the $-\mathbf{f}_{2j}$) minimization every second step.

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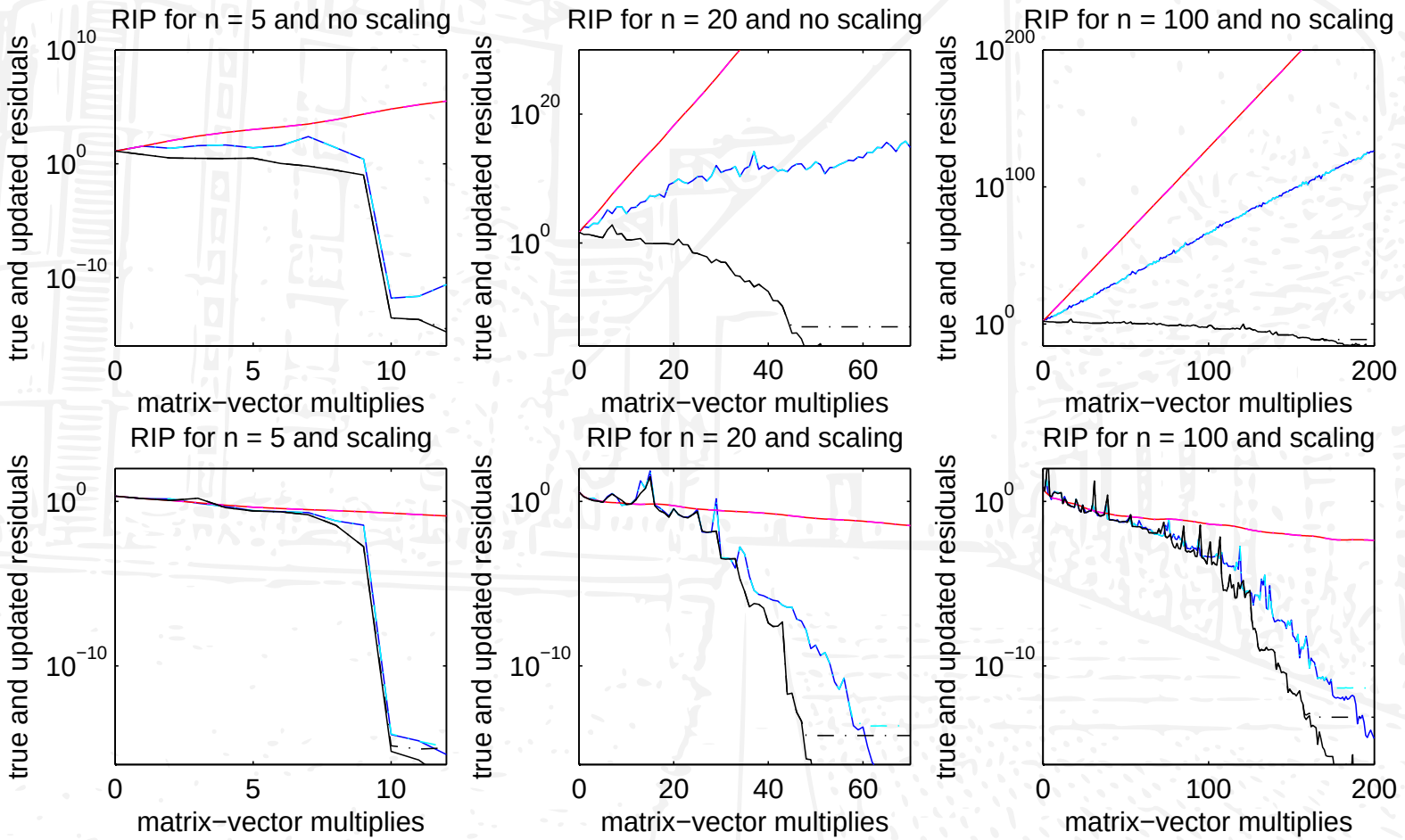
The finite termination property follows from a generalization of the IDR Theorem based on commutativity of the linear polynomials $\mathbf{I} - \omega_j\mathbf{A}$.

The origin of IDR: classical IDR

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



Evolution: CGS and BiCGStab

IDR was presented at a Symposium on CFD. The Numerical Linear Algebra community missed it completely. This changed, when Sonneveld gained more understanding of Krylov subspace methods and developed “better variants” of IDR.

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The analysis of IDR from the Krylov subspace point of view was based on the orthogonality properties of the residual polynomials. This immediately leads to the observation that all IDR methods construct residual polynomials that are products of auxiliary polynomials with the Lanczos polynomials.

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CGS was based on choosing the auxiliary polynomial equal to the Lanczos polynomial. This has two advantages: It is at hand and the contraction is enhanced in case of contraction.

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If only a moderate backward error reduction is of interest and BiCG converges quite well, CGS is a better choice. But many problems are not of this type, and for these one might want to use a transpose-free method.

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Sonneveld thought about rewriting the IDR Algorithm from (Wesseling and Sonneveld, 1980) and discussed this during a weekend with Henk van der Vorst. The resulting BiCGStab (van der Vorst and Sonneveld, 1990; van der Vorst, 1992) is mathematically equivalent to IDR. In the title of the report CGS was explicitely mentioned and Sonneveld was one of the authors . . .

Evolution: CGS and BiCGStab

> *Early ideas by Sonneveld (1984) for improvements in the bi-Conjugate Gradient (Bi-CG) method, for the solution of unsymmetric linear systems, intrigued me for a long time. Sonneveld had a brilliant idea for doubling the speed of convergence of Bi-CG for virtually the same computational costs: CGS. He also published a rather obscure method under the name of IDR. I doubt whether that paper got more than two or three citations altogether. The eventual understanding of that method and the reformulation of it, so that rounding errors had much less bad influence on its speed of convergence, led to the so frequently cited Bi-CGSTAB paper (1992).*

— Henk van der Vorst on IDR and CGS by Peter Sonneveld, see in-cites, September 2001, `http://www.in-cites.com/papers/dr-henk-van-der-vorst.html`.

Evolution: LTPM

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- BiCGStab2 (Gutknecht, 1993),
- BiCGStab(ℓ) (Sleijpen and Fokkema, 1993),
- GCGS (Fokkema et al., 1996), includes CGS2 and shifted CGS,
- GPBiCG (Zhang, 1997) = BiCG$\times$MR2 (Gutknecht, 1997),
- ML(k)BiCGStab (Yeung and Chan, 2000),
- BiCG$\times$MR2_2$\times$2 (Röllin and Gutknecht, 2002),
- GPBiCG(m,l) (Fujino, 2002),
- BiCGSafe (Fujino et al., 2005), ...

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- QMRS (Freund and Szeto, 1991; Freund and Szeto, 1992a; Freund and Szeto, 1992b),
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- general smoothing techniques: (Zhou and Walker, 1994).

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It was even considered to implement algorithms based on the (two-sided) Lanczos process via "transpose-free implementations" (Chan et al., 1991; Chan et al., 1998). These are called

- squared Lanczos,
- TFiBiCG, and
- TFiQMR.

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"Look-ahead for (Bi)CG"S was considered in (Brezinski and Redivo Zaglia, 1994), the resulting algorithm is called BSMRZS; look-ahead for BiCGStab (and related LTPM) was considered in (Brezinski and Redivo-Zaglia, 1995). In (Gutknecht and Ressel, 2000) look-ahead for general LTPM based on three-term recurrences was considered.

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Stability in finite precision was investigated by very few people.

Of all "new" methods, only ML(k)BiCGStab differs substantially from the others: This method is based on s left starting vectors (shadow vectors) and one right starting vector (zeroth residual).

The origin of IDR(s): ancestors

ML(k)BiCGStab was largely neglected by the Numerical Linear Algebra community. The main reason is the very technical paper, where the appendix contained the derivation of the computation of the scalars. Currently, Man-Chung Yeung is reconsidering ML(k)BiCGStab and developing variants that exploit the freedom inherent in the method (Yeung, 2009).

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Without knowing anything about ML(k)BiCGStab in 2006 the IDR idea was reconsidered. Peter Sonneveld together with Martin van Gijzen developed a new variant of IDR based on multiple shadow vectors: IDR(s) ($\approx$ IDR(s)ORes).

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ML(k)BiCGStab was largely neglected by the Numerical Linear Algebra community. The main reason is the very technical paper, where the appendix contained the derivation of the computation of the scalars. Currently, Man-Chung Yeung is reconsidering ML(k)BiCGStab and developing variants that exploit the freedom inherent in the method (Yeung, 2009).

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The following is an excerpt of an e-mail and a copy of slide 36 of the after dinner talk by Peter Sonneveld at the Thirty-fourth Woudschoten Conference.

The origin of IDR(s): rebirth of IDR

```
Date: Wed, 17 May 2006 14:02:27 +0200 (CEST)
From: Jens-Peter M. Zemke <zemke@xxxxxxxxxxxxx>
To:  <p.sonneveld@xxxxxxxxxxxxxx>
Cc: Jens-Peter M. Zemke <zemke@xxxxxxxxxxxxx>
Subject: A question about IDR

[..] entitled
   "The method of induced dimension reduction, an
    iterative solver for non-symmetric linear systems"
with the annotation "Publication in preparation".

My question is: What happended to this paper?

More precisely formulated:
   - Did it evolve into the CGS paper?
or [..]
```

The origin of IDR(s): rebirth of IDR

Zemke, and a short monologue

- 2006: Jens-Peter Zemke, from Hamburg, mails: What happened to IDR?
- Have to read carefully the 1980 version of the theorem, and the ancient history.
- Theorem used a space $\mathcal{S}$, not just $\boldsymbol{p}^{\perp}$.
- Serendipity moment: Why didn't I use more vectors $\boldsymbol{p}$, say s instead of 1???
- Because it costs $s+1$ matvecs per $\mathcal{G}_j$-space.
- But maybe there is more dimension reduction per $\mathcal{G}_j$
- .... Never thought about, must try... and call it IDR(s)

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IDR(s)ORes is based on oblique projections and $s+1$ consecutive multiplications with the same linear factor $\mathbf{I} - \omega_j\mathbf{A}$.

Understanding IDR: Hessenberg decompositions

Essential features of Krylov subspace methods can be described by a Hessenberg decomposition

$$\mathbf{A}\mathbf{Q}_n = \mathbf{Q}_{n+1}\underline{\mathbf{H}}_n = \mathbf{Q}_n\mathbf{H}_n + \mathbf{q}_{n+1}h_{n+1,n}\mathbf{e}_n^T. \tag{1}$$

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The matrix $\mathbf{H}_n$ of the perturbed variant will, in general, still be unreduced.

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In case of IDR, we have to consider generalized Hessenberg decompositions

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Generalized Hessenberg decompositions correspond to a skew projection of the pencil $(\mathbf{A}, \mathbf{I})$ to the pencil $(\mathbf{H}_n, \mathbf{U}_n)$ as long as $\mathbf{Q}_{n+1}$ has full rank.

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These approaches extend easily to generalized Hessenberg decompositions.

Understanding IDR: OrthoRes-type methods

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IDR: The underlying Hessenberg decomposition

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Here, $n > s$, and the index of the scalar ω_j is defined by

$$j := \left\lfloor \frac{n}{s+1} \right\rfloor,$$

compare with the so-called “index functions” (Yeung/Boley, 2005).

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$$\begin{aligned}\mathbf{v}_{n-1} &:= \mathbf{r}_{n-1} - \nabla\mathbf{R}_{n-s:n-1}\mathbf{c}_n = \mathbf{R}_{n-s-1:n-1}\mathbf{y}_n \\ &= (1-\gamma_s^{(n)})\,\mathbf{r}_{n-1} + \textstyle\sum_{\ell=1}^{s-1}(\gamma_{s-\ell+1}^{(n)} - \gamma_{s-\ell}^{(n)})\,\mathbf{r}_{n-\ell-1} + \gamma_1^{(n)}\,\mathbf{r}_{n-s-1}\,, \\ \mathbf{r}_n &:= (\mathbf{I}-\omega_j\mathbf{A})\,\mathbf{v}_{n-1}\,.\end{aligned} \tag{7}$$

Here, $n > s$, and the index of the scalar ω_j is defined by

$$j := \left\lfloor \frac{n}{s+1} \right\rfloor,$$

compare with the so-called “index functions” (Yeung/Boley, 2005).

Removing $\mathbf{v}_{n-1}$ from the recurrence we obtain the generalized Hessenberg decomposition

$$\mathbf{A}\mathbf{R}_n\mathbf{Y}_n\mathbf{D}_\omega = \mathbf{R}_{n+1}\underline{\mathbf{Y}}_n^\circ. \tag{8}$$

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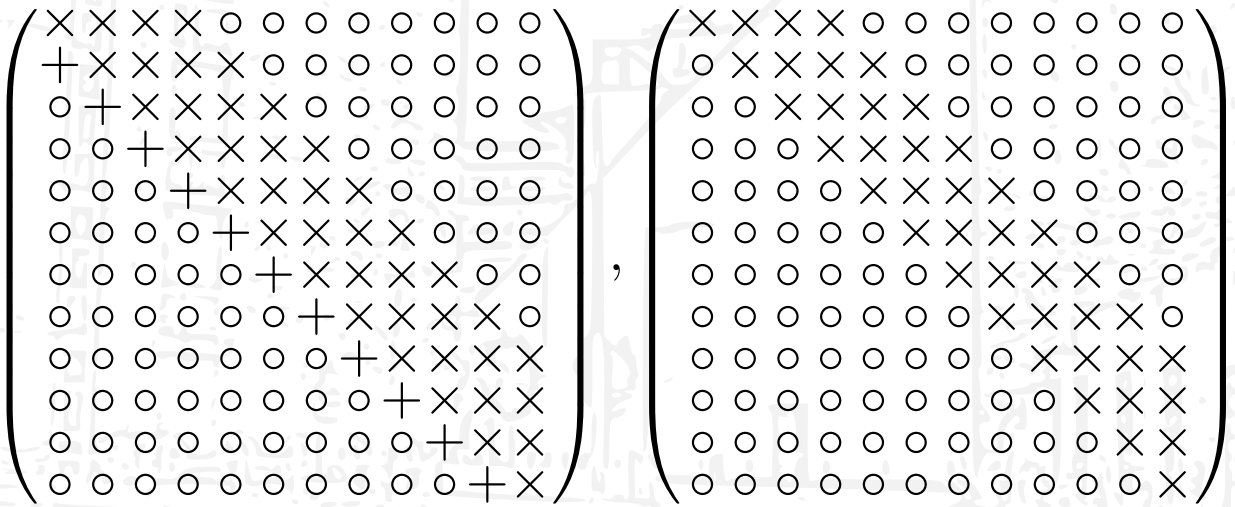
IDR: Sonneveld pencil and Sonneveld matrix

The IDR(s)ORes pencil, the so-called Sonneveld pencil $(\mathbf{Y}_n^\circ, \mathbf{Y}_n \mathbf{D}_\omega^{(n)})$, can be depicted by



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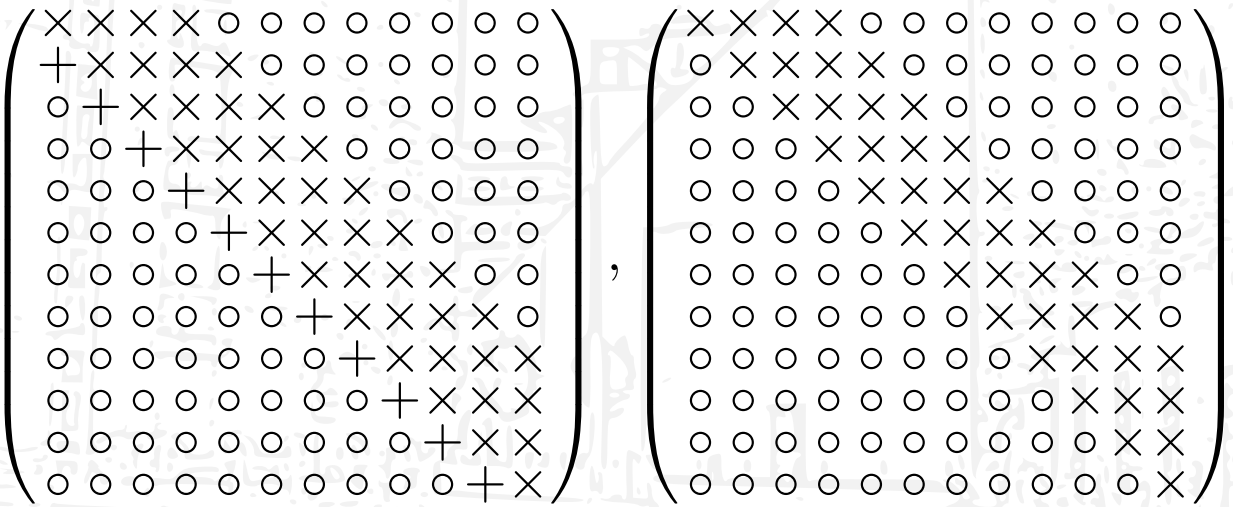

The upper triangular matrix $\mathbf{Y}_n\mathbf{D}_\omega^{(n)}$ could be inverted, which results in the Sonneveld matrix, a full unreduced Hessenberg matrix.

Understanding IDR: Purification

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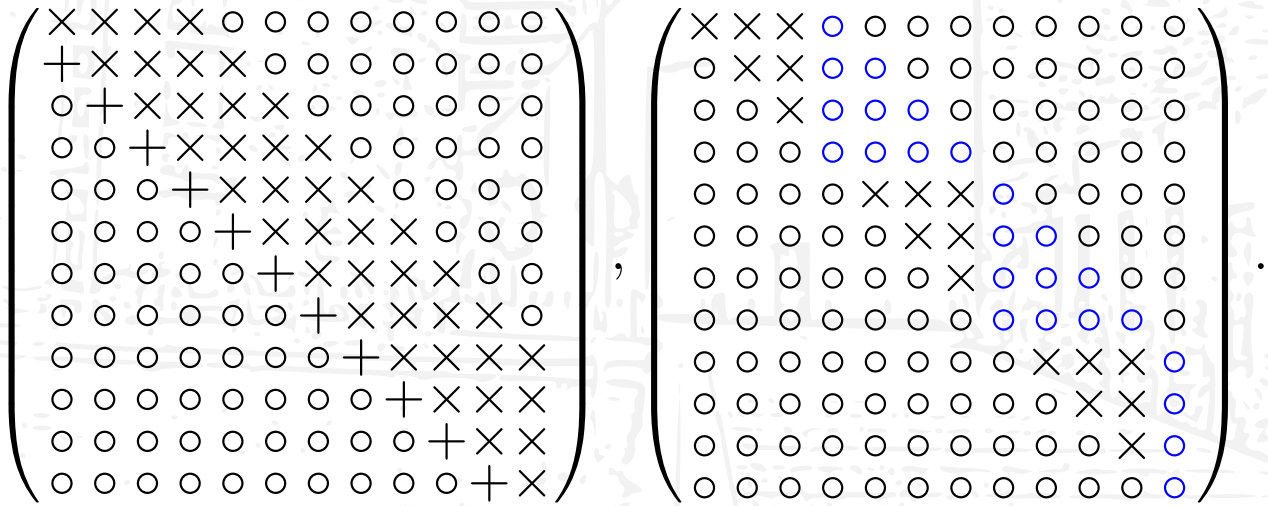

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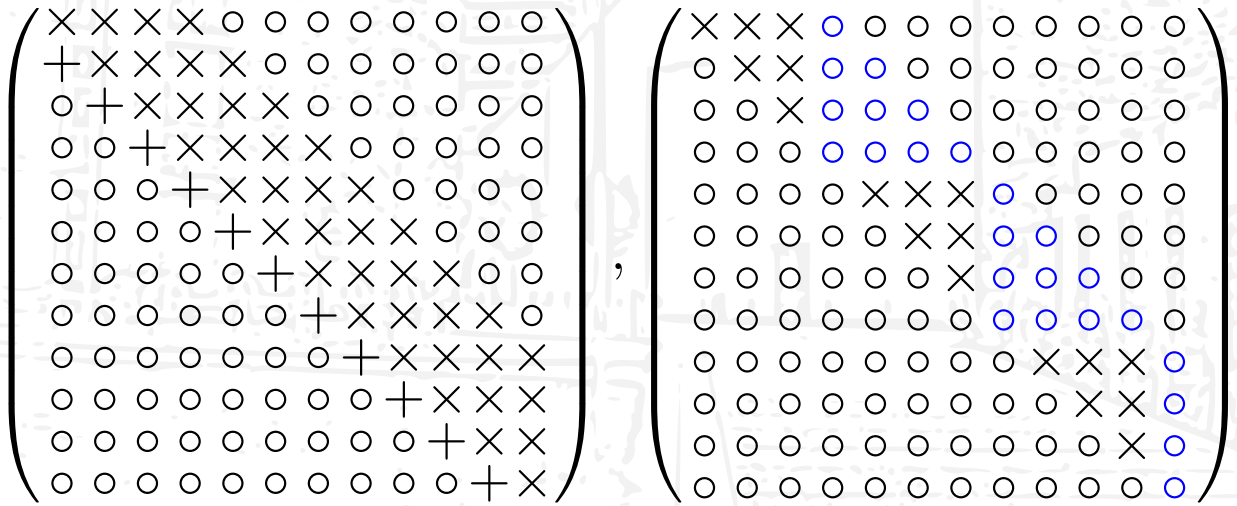
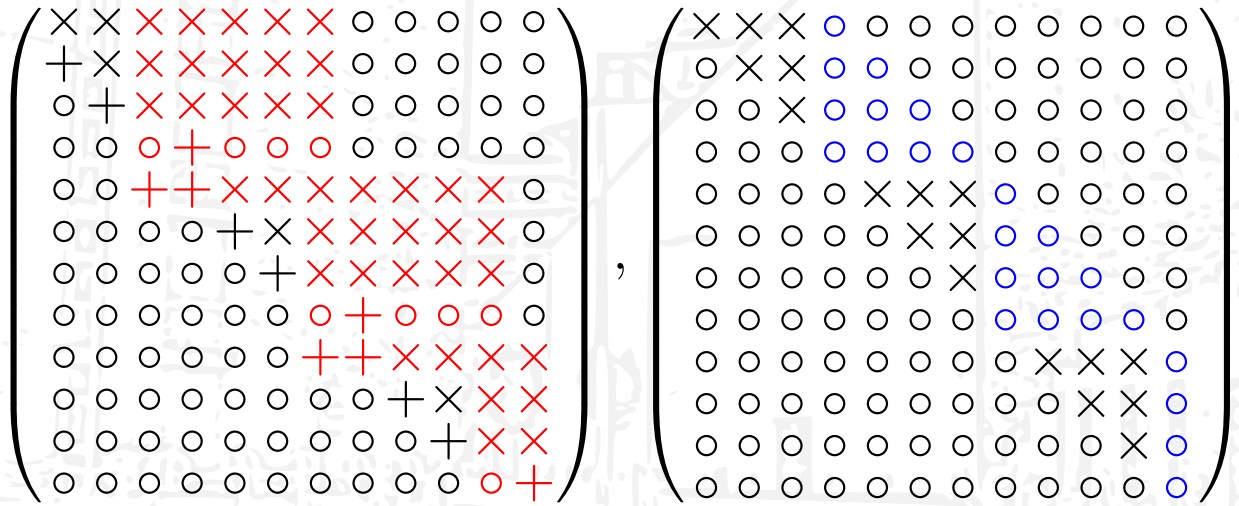


We get rid of the infinite eigenvalues using a change of basis (Gauß/Schur).

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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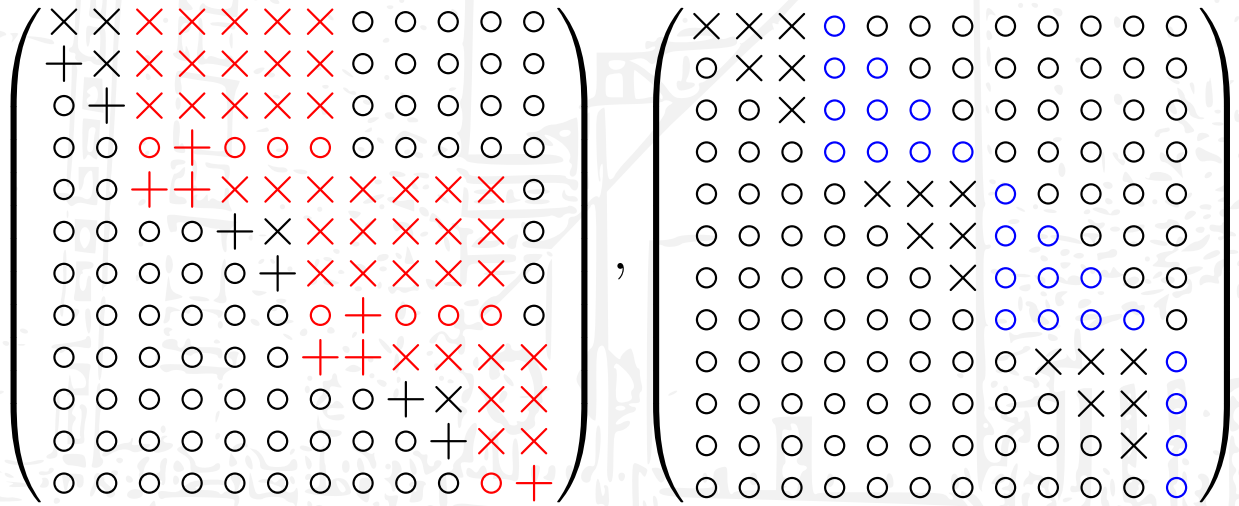

Using Laplace expansion of the determinant of $z\mathbf{U}_n\mathbf{D}_\omega^{(n)} - \mathbf{Y}_n^\circ\mathbf{G}_n$ we can get rid of the trivial constant factors corresponding to infinite eigenvalues. This amounts to a deflation.

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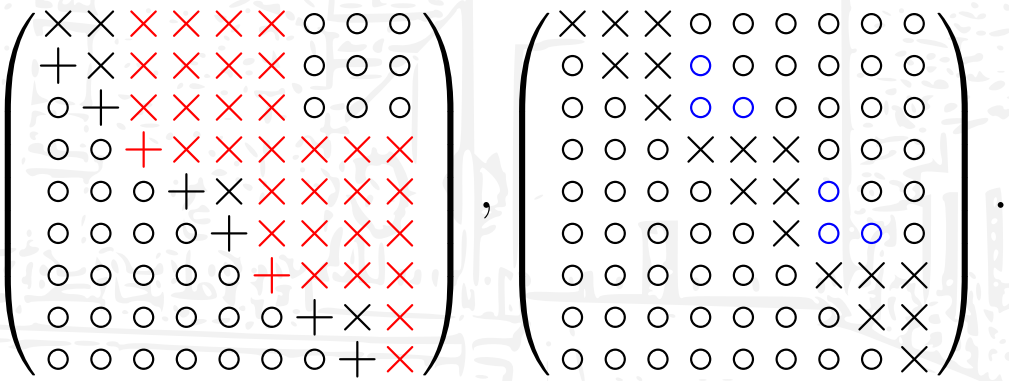
The deflated purified IDR(s)ORes pencil, after the deflation step $(D(\mathbf{Y}_n^\circ \mathbf{G}_n), D(\mathbf{U}_n \mathbf{D}_\omega^{(n)}))$, can be depicted by



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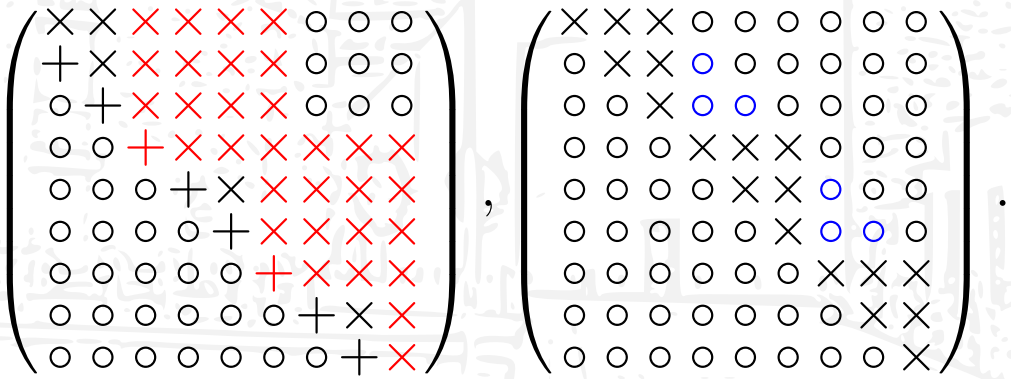

The block-diagonal matrix $D(\mathbf{U}_n \mathbf{D}_\omega^{(n)})$ has invertible upper triangular blocks and can be inverted to expose the underlying Lanczos process.

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

$$\mathbf{L}_n := D(\mathbf{Y}_n^\circ\mathbf{G}_n)\cdot D(\mathbf{U}_n\mathbf{D}_\omega^{(n)}))^{-1} = \begin{pmatrix} \times & \times & \times & \times & \times & \times & \circ & \circ & \circ \\ + & \times & \times & \times & \times & \times & \circ & \circ & \circ \\ \circ & + & \times & \times & \times & \times & \circ & \circ & \circ \\ \circ & \circ & + & \times & \times & \times & \times & \times & \times \\ \circ & \circ & \circ & + & \times & \times & \times & \times & \times \\ \circ & \circ & \circ & \circ & + & \times & \times & \times & \times \\ \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times \\ \circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times \\ \circ & \circ & \circ & \circ & \circ & \circ & \circ & + & \times \end{pmatrix}.$$

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This is the matrix of the underlying BiORes$(s,1)$ process.

This matrix (in the extended version) satisfies

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

where the reduced residuals $\mathbf{q}_{js+k}$, $k = 0,\ldots,s-1$, $j = 0,1,\ldots$, with $\Omega_0(z) \equiv 1$ and $\Omega_j(z) = \prod_{k=1}^{j}(1-\omega_k z)$ are given by

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

IDR: a Lanczos process with multiple left-hand sides

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This can more easily be proven using the representations ($\mathcal{S} := \mathbf{P}^{\perp}$)

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

$$\mathcal{G}_j = \bigcap_{k=0}^{j-1} \Omega_k(\mathbf{A})^{-1}\Omega_j(\mathbf{A})(\mathcal{S}) = \left(\mathop{+}_{k=0}^{j-1} \Omega_j(\mathbf{A})^{-\mathsf{H}}\Omega_k(\mathbf{A})^{\mathsf{H}}\{\mathbf{P}\}\right)^{\perp}$$

$$= \left(\Omega_j(\mathbf{A})^{-\mathsf{H}}\mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \mathbf{P})\right)^{\perp} = \Omega_j(\mathbf{A})\left(\mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \mathbf{P})\right)^{\perp}$$

of the Sonneveld spaces.

IDR: a Lanczos process with multiple left-hand sides

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 first equality

$$\mathcal{G}_j = \bigcap_{k=0}^{j-1} \Omega_k(\mathbf{A})^{-1}\Omega_j(\mathbf{A})(\mathcal{S}) = \bigcap_{k=1}^{j} (\mathbf{I} - \omega_j\mathbf{A}) \cdots (\mathbf{I} - \omega_k\mathbf{A})(\mathcal{S})$$

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follows from the observations that

- the first $s+1$ residuals obviously are in $\mathcal{G}_0 := \mathcal{K}(\mathbf{A}, \mathbf{r}_0)$,
- the next $s+1$ residuals (or any other vectors in $\mathcal{G}_1$) are in the $\mathbf{I} - \omega_1\mathbf{A}$ image of $\mathcal{S} = \mathbf{P}^{\perp}$,
- the last $s+1$ residuals are in the $\mathbf{I} - \omega_j\mathbf{A}$ image of $\mathcal{S} = \mathbf{P}^{\perp}$,
- the last residuals are $\mathbf{I} - \omega_j\mathbf{A}$ images of linear combinations of previously obtained images $(\mathbf{I} - \omega_{j-1}\mathbf{A}) \cdots (\mathbf{I} - \omega_k\mathbf{A})$ of $\mathcal{S} = \mathbf{P}^{\perp}$.

IDR: a Lanczos process with multiple left-hand sides

The second equality

$$\bigcap_{k=0}^{j-1} \Omega_k(\mathbf{A})^{-1}\Omega_j(\mathbf{A})(\mathcal{S}) = \left(\mathop{+}_{k=0}^{j-1} \Omega_j(\mathbf{A})^{-\mathsf{H}}\Omega_k(\mathbf{A})^{\mathsf{H}}\{\mathbf{P}\}\right)^{\perp}$$

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

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

since, for invertible $\mathbf{B}$,

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

IDR: a Lanczos process with multiple left-hand sides

The third and fourth equality

$$\left(\mathop{+}_{k=0}^{j-1} \Omega_j(\mathbf{A})^{-\mathsf{H}} \Omega_k(\mathbf{A})^{\mathsf{H}} \{\mathbf{P}\} \right)^{\perp} = \left(\Omega_j(\mathbf{A})^{-\mathsf{H}} \mathcal{K}_j(\mathbf{A}^{\mathsf{H}}, \mathbf{P}) \right)^{\perp}$$

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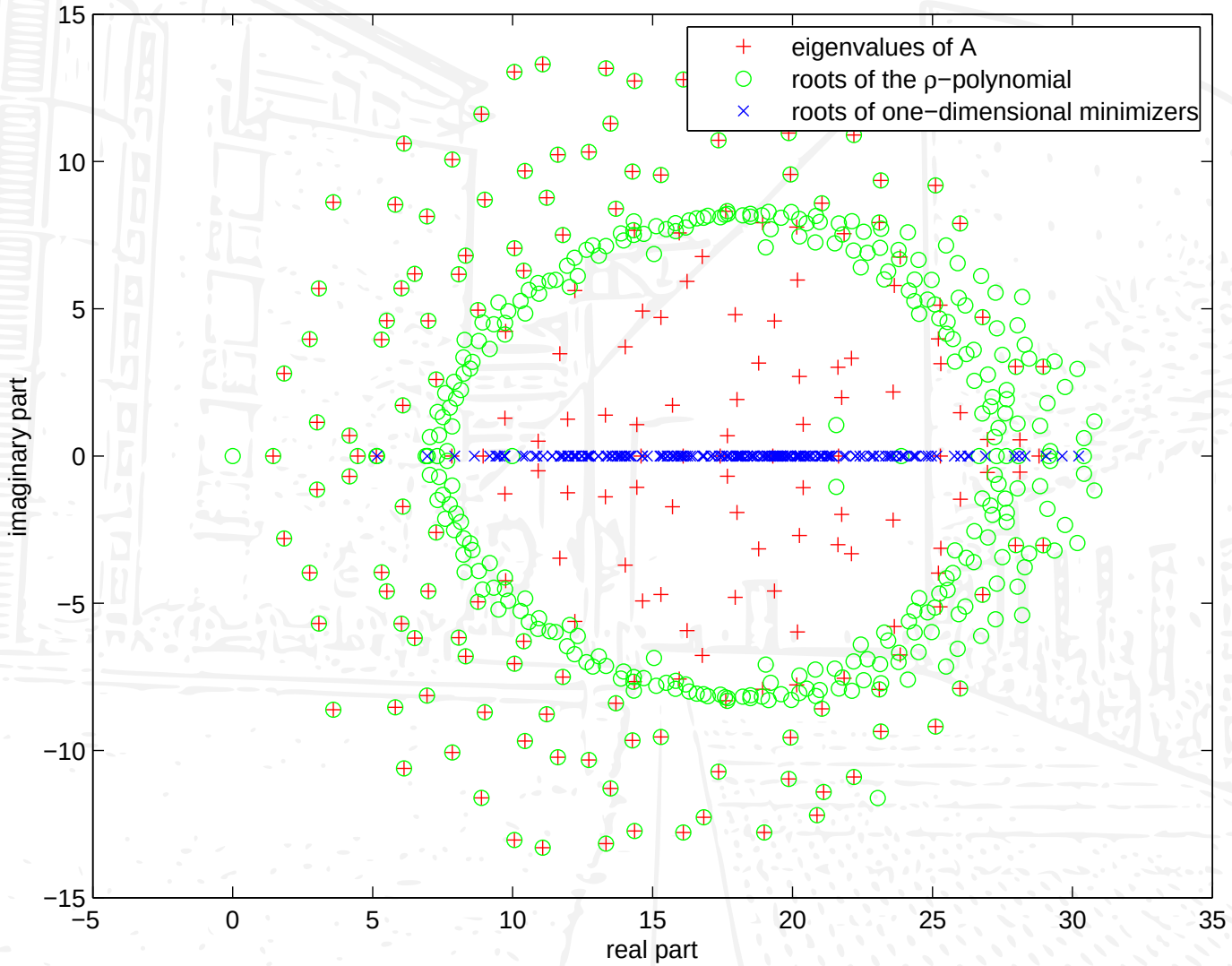
are satisfied

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

Understanding IDR: 600 steps for $s = 2$



IDR: recent developments

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The analysis should carry over to the new developments in IDR methods. The recent developments in the IDR family and some current trends are summarized on the next slides.

These can be grouped into

- incorporation of higher degree polynomials: like BiCGStab2, BiCGStab(ℓ), GCGS (CGS2, shifted CGS) and GPBiCG,
- a better understanding of the IDR Theorem: construction of better IDR algorithms,
- choices of ω_j: eigenvalue estimates, classical splitting methods,
- changing the shadow space: sparsification, (non-)overlapping Schwarz.

IDR: recent developments

The residuals computed first in a complete cycle are uniquely defined. Based on the analysis of a possible breakdown of IDR(s), Sonneveld and van Gijzen came up with their new implementation IDR(s)BiO (van Gijzen and Sonneveld, 2008) of the IDR Theorem.

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The new vectors $\mathbf{v}_n$ and $\mathbf{r}_{n+1}$ are in this general setting given by the updates

$$\mathbf{v}_n = \mathbf{r}_n - \sum_{i=1}^{s} \mathbf{g}_{n-i}\gamma_i =: \mathbf{r}_n - \mathbf{G}_n\mathbf{c}_n, \quad \text{and thus,}$$

$$\mathbf{r}_{n+1} = (\mathbf{I} - \omega\mathbf{A})\mathbf{v}_n = \mathbf{r}_n - \omega\mathbf{A}\mathbf{v}_n - \sum_{i=1}^{s} \mathbf{g}_{n-i}\gamma_i,$$

where $\mathbf{c}_n$ is determined such that $\mathbf{P}^{\mathsf{H}}\mathbf{v}_n = \mathbf{o}$.

IDR: recent developments

As basis vectors $\mathbf{g}_{n+k}$ they compute as before updates of residuals which are in $\mathcal{G}_j \cap \mathcal{S}$. The update vectors $\mathbf{u}_n$ of the iterates $\mathbf{x}_n$ are stored in $\mathbf{U}_n$, "prototypes" of these are given by

$$\widetilde{\mathbf{x}}_{n+1} = \mathbf{x}_n + \widetilde{\mathbf{u}}_n = \mathbf{x}_n + \omega \mathbf{v}_n - \sum_{i=1}^{s} \mathbf{u}_{n-i}\gamma_i =: \mathbf{x}_n + \omega \mathbf{v}_n - \mathbf{U}_n \mathbf{c}_n.$$

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If we had computed all these, we could use a basis transformation to ensure a simple structure of the update formulas and the systems to be solved. In order to not destroy the nested structure and to obtain an explicit formula, these transformations should be triangular, e.g., QR- or LR-like.

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Sonneveld and van Gijzen impose the bi-orthogonality conditions

$$\mathbf{g}_{n+k} \perp \mathbf{p}_1, \ldots, \mathbf{p}_{k-1},$$
$$\mathbf{r}_{n+k+1} \perp \mathbf{p}_1, \ldots, \mathbf{p}_k.$$

IDR: recent developments

The triangular basis transformations result in the general update formulas

$$\mathbf{v}_{n+k} = \mathbf{r}_{n+k} - \mathbf{G}_{n+k}\mathbf{c}_{n+k}, \quad (\mathbf{c}_{n+k} \text{ is determined by orthogonality to } \mathbf{P})$$

$$\widetilde{\mathbf{u}}_{n+k} = \mathbf{U}_{n+k}\mathbf{c}_{n+k} + \omega\mathbf{v}_{n+k}, \qquad \mathbf{u}_{n+k} = \widetilde{\mathbf{u}}_{n+k} - \sum_{i=1}^{k-1} \mathbf{u}_{n+i}\alpha_i,$$

$$\widetilde{\mathbf{g}}_{n+k} = \mathbf{A}\widetilde{\mathbf{u}}_{n+k}, \qquad \mathbf{g}_{n+k} = \widetilde{\mathbf{g}}_{n+k} - \sum_{i=1}^{k-1} \mathbf{g}_{n+i}\alpha_i = \mathbf{A}\mathbf{u}_{n+k},$$

$$\mathbf{r}_{n+k+1} = \mathbf{r}_{n+k} - \sum_{i=1}^{k} \mathbf{g}_{n+i}\beta_i, \qquad \mathbf{x}_{n+k+1} = \mathbf{x}_{n+k} + \sum_{i=1}^{k} \mathbf{u}_{n+i}\beta_i.$$

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In the approach by Sonneveld and van Gijzen, the vector $\widetilde{\mathbf{g}}_{n+k}$ is orthogonalized against the vectors $\mathbf{p}_i$, $1 \leqslant i < k$ using the α_i, $1 \leqslant i < k$, the vector $\mathbf{r}_{n+k+1}$ is orthogonal to $\mathbf{p}_1, \ldots, \mathbf{p}_k$ by choice of the β_i, $1 \leqslant i \leqslant k$.

IDR: recent developments

This (modified) Gram-Schmidt-like approach results in the kth inner step in nested systems of the form (indices omitted)

$$\begin{pmatrix} \mu_{11} & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots & \ddots & \vdots \\ \mu_{k-1,1} & \cdots & \mu_{k-1,k-1} & 0 & \cdots & 0 \\ \mu_{k,1} & \cdots & \mu_{k,k-1} & \mu_{kk} & \ddots & \vdots \\ \vdots & \ddots & \vdots & \vdots & \ddots & 0 \\ \mu_{s1} & \cdots & \mu_{s,k-1} & \mu_{sk} & \cdots & \mu_{ss} \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \gamma_k \\ \vdots \\ \gamma_s \end{pmatrix} = \underbrace{(\mathbf{P}^{\mathsf{H}}\mathbf{G})}_{=:\mathbf{M}} \mathbf{c} = \mathbf{P}^{\mathsf{H}}\mathbf{r} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \phi_k \\ \vdots \\ \phi_s \end{pmatrix},$$

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i.e., $\mathbf{r} \perp \mathbf{p}_1, \ldots, \mathbf{p}_{k-1}$ and $\mathbf{g}_{-k} \perp \mathbf{p}_1, \ldots, \mathbf{p}_{k-1}$, and thus we only have to solve

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Initially, $\mathbf{M} := \mathbf{I}_s$. The resulting IDR($s$)BiO is cheaper and seems more stable.

IDR: recent developments

Recently, the relations between IDR(s) and BiCGStab(ℓ) and combinations of both methods have been investigated.

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- In (Tanio and Sugihara, 2009) the authors derive the algorithm GBiCGStab(s,L), which is similar to IDR(s)Stab(ℓ). In their own words: “Our algorithm is to theirs what the Gauss-Seidel iteration is to the Jacobi iteration.” A predecessor of GBiCGStab(s,L) seems to be the method called GIDR(s,L) in (Tanio and Sugihara, 2008).

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- In (Sleijpen and Abe, 2010) the ideas behind BiCGStab2 by Gutknecht and GPBiCG by Zhang are considered. The resulting algorithms IDR(s)Stab2 and GIDR(s) seem to be less efficient when compared with IDR(s)Stab(ℓ).

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The relation of IDR to Petrov-Galërkin with a rational Krylov space motived the method IDR-Ritz (Simoncini and Szyld, 2009).

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The minimization used in IDR(s)ORes and IDR(s)BiO results in values ω_j which are in the field of values of $\mathbf{A}^{-\mathsf{H}}$, thus Simoncini and Szyld suggest to use a few steps of Arnoldi to compute some Ritz values, which are then used in some ordering as $1/\omega_j$ values.

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For real nonsymmetric matrices this typically results in an algorithm based on complex arithmetic in place of real arithmetic.

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Last but not least: Certain old ideas have been reactivated. Sonneveld presented the hitherto unpublished Accelerated Gauß-Seidel (AGS) method at the Kyoto Forum on Krylov Subspace Methods in 2008.

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These approaches result in a “tight packing” of preconditioning and Krylov subspace methods, compare with PIA. In most of these methods the ω_j are fixed by the splitting chosen.

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The choice of the shadow vectors has been analyzed experimentally by Seiji Fujino (non-overlapping Schwarz-like to save computational costs), Man-Chung Yeung (sparse $\pm 1, 0$-random vectors).

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- variable preconditioning?

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Conclusion

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My personal overall conclusion:

The IDR(s)-approach to LTPM by Sonneveld is more easy to follow (compared to other “multiple Lanczos” approaches).

. . . und zu guter Letzt:

Thank you for your attention

—

Vielen Dank für die Aufmerksamkeit,
Frohe Weihnachten!

(und für einige hier: Eine schöne Weihnachtsfeier!)

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