A quick and dirty introduction to IDR

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UNIVERSITY OF BATH

Outline

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- Internal guidelines
- Krylov subspace methods
- Hessenberg decompositions
- Polynomial representations
- Perturbations

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I am trying to motivate why the method of Induced Dimension Reduction (IDR) and its generalization IDR(s) are worth considering when looking for iterative solvers for your type of problem, e.g.,

- (large sparse) linear systems: $\mathbf{A}\mathbf{x} = \mathbf{r}_0$, $\mathbf{A} \in \mathbb{C}^{n\times n}$, $\mathbf{r}_0 \in \mathbb{C}^n$, or
- (large sparse) eigenvalue problems: $\mathbf{A}\mathbf{v} = \mathbf{v}\lambda$.

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My personal interest lies in the error analysis of perturbed Krylov subspace methods and their convergence properties. These perturbations are

- always caused by finite precision,
- sometimes caused deliberately, e.g., in inexact methods.

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- mostly restricted to the simplest method, the symmetric Lanczos method,
- based on tools from a variety of areas that do not seem to be related to Krylov subspace methods at all,
- either for very specific implementations or does offer very little insight.

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- and many, many more . . .

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In passing, I will note some aspects not to be found in the literature and outline some paths of possible generalizations.

Background

Large linear systems are solved by projection onto smaller subspaces,

$$\mathbf{A}\mathbf{x} = \mathbf{r}_0, \quad \mathbf{x}_k := \mathbf{Q}_k\mathbf{z}_k, \quad \hat{\mathbf{Q}}_k^{\mathsf{H}}\mathbf{A}\mathbf{x} = (\hat{\mathbf{Q}}_k^{\mathsf{H}}\mathbf{A}\mathbf{Q}_k)\mathbf{z}_k = \hat{\mathbf{Q}}_k^{\mathsf{H}}\mathbf{r}_0.$$

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- Bubnov-Galërkin: $\hat{\mathbf{Q}}_k = \mathbf{Q}_k$, $\mathbf{Q}_k^{\mathsf{H}}\mathbf{Q}_k = \mathbf{I}_k$ (orthonormal basis),
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Subspaces of increasing dimension. As starting vector use $\mathbf{r}_0$, e.g.,

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Compute residual: $\mathbf{r}_1 := \mathbf{r}_0 - \mathbf{A}\mathbf{x}_1 = \mathbf{Q}_1\mathbf{e}_1\|\mathbf{r}_0\| - \mathbf{A}\mathbf{Q}_1\mathbf{z}_1.$

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Expand space:

$$\mathcal{K}_2 := \text{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0\} = \text{span}\{\mathbf{q}_1, \mathbf{q}_2\}.$$

Krylov subspaces

Natural generalization of this simple idea: Krylov subspaces. Obtained by multiplication of last basis vector by $\mathbf{A}$,

$$\mathcal{K}_k := \text{span}\,\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \ldots, \mathbf{A}^{k-1}\mathbf{r}_0\} = \text{span}\,\{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_k\}.$$

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

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

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Residual polynomials arise because

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Krylov subspace methods

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- long-term (Hessenberg, Arnoldi),
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Arnoldi: Example of a long-term method building an orthonormal basis.

$$
\begin{array}{l}
\mathbf{r} = \mathbf{r}_0,\ \mathbf{q} = \mathbf{r}/\|\mathbf{r}\| \\
\mathbf{Q} = \mathbf{q},\ \underline{\mathbf{H}} = () \\
\text{for } k = 1, \dots \\
\qquad \mathbf{r} = \mathbf{A}\mathbf{q} \\
\qquad \mathbf{c} = \mathbf{Q}^{\mathsf{H}}\mathbf{r} \\
\qquad \mathbf{r} = \mathbf{r} - \mathbf{Q}\mathbf{c} \\
\qquad \underline{\mathbf{H}} = \left(\underline{\mathbf{H}}, \mathbf{c}; \mathbf{o}^{\mathsf{T}}, \|\mathbf{r}\|\right) \\
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Hessenberg decompositions

The construction of basis vectors is resembled in the structure of the arising Hessenberg decomposition

$$\mathbf{A}\mathbf{Q}_k = \mathbf{Q}_{k+1}\underline{\mathbf{H}}_k,$$

where

- $\mathbf{Q}_{k+1} = \left(\mathbf{Q}_k, \mathbf{q}_{k+1}\right) \in \mathbb{C}^{n\times(k+1)}$ collects the basis vectors,
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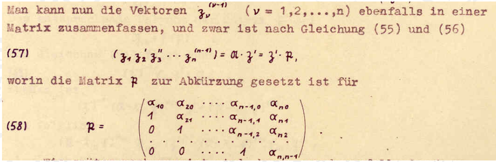
Aspects of perturbed Krylov subspace methods can be captured with perturbed Hessenberg decompositions

$$\mathbf{A}\mathbf{Q}_k + \mathbf{F}_k = \mathbf{Q}_{k+1}\underline{\mathbf{H}}_k,$$

where $\mathbf{F}_k \in \mathbb{C}^{n\times k}$ accounts for the perturbations.

Karl Hessenberg & “his” matrix + decomposition

Behandlung linearer Eigenwertaufgaben mit Hilfe der Hamilton-Cayleyschen Gleichung, Karl Hessenberg, 1. Bericht der Reihe „Numerische Verfahren“, July, 23rd 1940, page 23:



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

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

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

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

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

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

Important Polynomials

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The residuals of the OR approximation $\mathbf{x}_k := \mathbf{Q}_k\mathbf{z}_k$ and the MR approximation $\underline{\mathbf{x}}_k := \mathbf{Q}_k\underline{\mathbf{z}}_k$ with coefficient vectors

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

satisfy

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

with residual polynomials $\mathcal{R}_k$ and $\underline{\mathcal{R}}_k$ given by

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

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

The convergence of OR and MR depends on the Ritz and harmonic Ritz values, respectively.

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under the assumption that all trailing square Hessenberg matrices are regular, the polynomial representation for the OR residuals changes to

$$\mathbf{r}_k = \mathcal{R}_k(\mathbf{A})\mathbf{r}_0 - \sum_{\ell=1}^{k} z_{\ell k}\mathcal{R}_{\ell+1:k}(\mathbf{A})\mathbf{f}_\ell + \mathbf{F}_k\mathbf{z}_k,$$

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We can expect convergence when $\mathbf{F}_k\mathbf{z}_k$ remains bounded (inexact methods) and all $\mathcal{R}_{\ell+1:k}(\mathbf{A})$ are “small”.

Outline

Birth of a method

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This recurrence (almost) always results in the zero vector after $2n$ steps, where $\mathbf{A} \in \mathbb{C}^{n\times n}$ and $\mathbf{r}_0 \in \mathbb{C}^n$, $\mathbf{r}_1 = \mathbf{A}\mathbf{r}_0$, and $\mathbf{p} \in \mathbb{C}^n$ are arbitrarily chosen.

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More precisely,

$$\mathbf{r}_{2j}, \mathbf{r}_{2j+1} \in \mathcal{G}_j, \quad j = 0, 1, \ldots$$

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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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The update of the iterates has to be modified accordingly,

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

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

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$$\mathbf{r}_1 = \mathbf{r}_0 - \mathbf{A}\mathbf{r}_0$$

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

$$\gamma_k = \mathbf{p}^\mathsf{T}\mathbf{r}_k / \mathbf{p}^\mathsf{T}(\mathbf{r}_{k-1} - \mathbf{r}_k)$$
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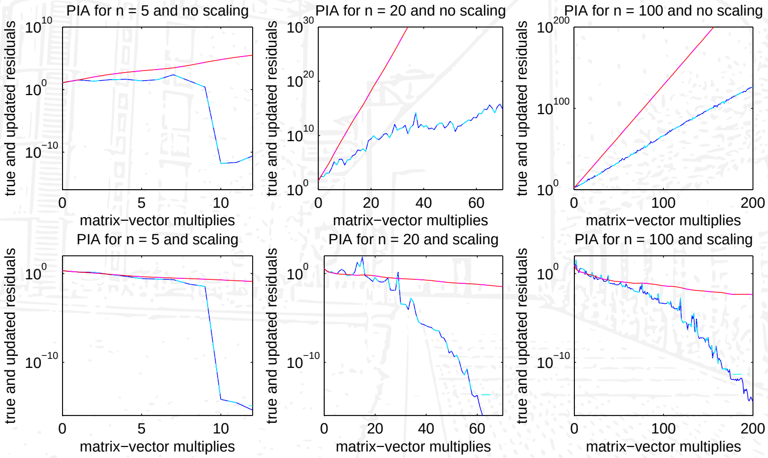
On the next slide we compare Richardson iteration (red) and PIA (blue).

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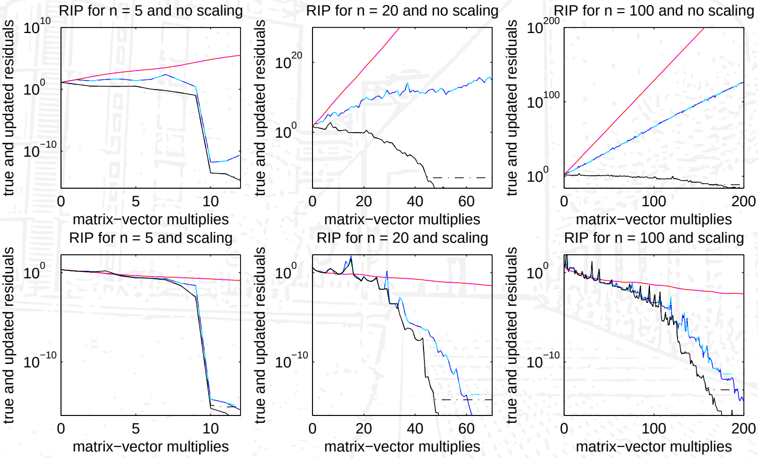
This algorithm with minimization of every second residual is included in the proceedings from 1980 (Wesseling and Sonneveld, 1980). The connection to Krylov methods, e.g., BiCG/Lanczos, is also given there.

The origin of IDR: classical IDR

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



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In short: BiCGStab is (almost mathematically equivalent to) IDR.

IDR(s)

IDR can be generalized: instead of using one hyperplane $(\operatorname{span}\{\mathbf{p}\})^{\perp}$, one uses the intersection of s hyperplanes. This makes the dimension reduction step less frequent but the reduction a larger one.

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In the context of Krylov subspace methods, IDR(s) can be thought of as a two-sided Lanczos method. There is a predecessor to such a method, namely, ML(k)BiCGStab by Man-Chung Yeung and Tony Chan.

Building blocks of IDR(s)

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

- Multiplication by polynomials in $\mathbf{A}$.
  (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 $\mathcal{G}_j$ as follows:

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Only sufficiently many vectors in each space are constructed.

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$$\mathbf{r}^{\text{IDR}}_{j(s+1)+k} = \Omega_j(\mathbf{A})\rho_{js+k}(\mathbf{A})\mathbf{r}_0, \quad 1 \leqslant k \leqslant s$$
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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 $\rho_k(0) = 1$.

Generalized Hessenberg decomposition

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\mathbf{r}_k := \mathbf{r}_0 - \mathbf{A}\mathbf{x}_k &= \mathbf{r}_0 - \mathbf{A}\mathbf{Q}_k\mathbf{U}_k\mathbf{z}_k = \mathbf{r}_0 - \mathbf{Q}_{k+1}\underline{\mathbf{H}}_k\mathbf{z}_k \\
&= \mathbf{Q}_k(\mathbf{e}_1\|\mathbf{r}_0\| - \mathbf{H}_k\mathbf{z}_k) - \mathbf{q}_{k+1}h_{k+1,k}\mathbf{e}_k^{\mathsf{T}}\mathbf{z}_k \\
&= \mathcal{R}_k(\mathbf{A})\mathbf{r}_0, \quad \mathcal{R}_k(z) := \det\left(\mathbf{I}_k - z\mathbf{U}_k\mathbf{H}_k^{-1}\right).
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$$\begin{aligned}\mathbf{r}_k := \mathbf{r}_0 - \mathbf{A}\mathbf{x}_k = \mathbf{r}_0 - \mathbf{A}\mathbf{Q}_k\mathbf{U}_k\mathbf{z}_k &= \mathbf{r}_0 - \mathbf{Q}_{k+1}\underline{\mathbf{H}}_k\mathbf{z}_k \\ &= \mathbf{Q}_k(\mathbf{e}_1\|\mathbf{r}_0\| - \mathbf{H}_k\mathbf{z}_k) - \mathbf{q}_{k+1}h_{k+1,k}\mathbf{e}_k^{\mathsf{T}}\mathbf{z}_k \\ &= \mathcal{R}_k(\mathbf{A})\mathbf{r}_0, \quad \mathcal{R}_k(z) := \det\left(\mathbf{I}_k - z\mathbf{U}_k\mathbf{H}_k^{-1}\right).\end{aligned}$$

Tacitly assuming $\|\mathbf{q}_{k+1}\| = 1$, we have $\|\mathbf{r}_k\| = |h_{k+1,k}z_k|$.

IDR: Sonneveld pencil and Sonneveld matrix

We consider the prototype IDR(s) by Sonneveld/van Gijzen (IDR(s)ORes).

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\end{array}\right).
$$

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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\begin{pmatrix}
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The purified IDR(s)ORes pencil $(\mathbf{Y}_n^\circ, \mathbf{U}_n\mathbf{D}_\omega^{(n)})$, that has only the remaining eigenvalues and some infinite ones as eigenvalues, can be depicted by

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\end{pmatrix}.
$$

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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\end{pmatrix}.
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$$
\begin{pmatrix}
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\end{pmatrix}.
$$

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.

Understanding IDR: Deflation

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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\end{pmatrix}.$$

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

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This matrix (in the extended version) satisfies

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

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

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

IDREig

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Suppose that $\mathbf{Q}_{k+1}$ has full rank. The pencil $(\mathbf{H}_k, \mathbf{U}_k)$ arises as a oblique projection of $(\mathbf{A}, \mathbf{I}_n)$, as

$$\begin{aligned} \widehat{\mathbf{Q}}_k^{\mathsf{H}}(\mathbf{A}, \mathbf{I}_n)\mathbf{Q}_k\mathbf{U}_k &= \widehat{\mathbf{Q}}_k^{\mathsf{H}}(\mathbf{A}\mathbf{Q}_k\mathbf{U}_k, \mathbf{Q}_k\mathbf{U}_k) \\ &= \widehat{\mathbf{Q}}_k^{\mathsf{H}}(\mathbf{Q}_{k+1}\underline{\mathbf{H}}_k, \mathbf{Q}_k\mathbf{U}_k) = (\underline{\mathbf{I}}_k^{\mathsf{T}}\underline{\mathbf{H}}_k, \mathbf{U}_k) = (\mathbf{H}_k, \mathbf{U}_k), \end{aligned} \tag{1}$$

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One uses a deflated pencil that only gives the Ritz values. The theory was developed by Martin Gutknecht and Z. (2010), currently we investigate how to select parameters (s, ω_j, $\mathbf{P}$) to obtain good eigenpair approximations (this is ongoing joint work with Olaf Rendel and Anisa Rizvanolli).

IDRStab

Recently, IDR(s) was generalized by combining ideas from IDR(s) with the higher dimensional minimization underlying BiCGStab(ℓ).

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IDRStab and the eigenvalue approximations of the resulting Sonneveld pencils are currently analyzed („Studienarbeit“ of Anisa Rizvanolli).

QMRIDR

MR methods use the extended Hessenberg matrix to compute the coefficients of the vector in the Krylov subspace, i.e.,

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

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The implementation has many parameters that we should select “optimal”. Extensive numerical tests are currently done by Olaf Rendel. As an example we show the convergence curves (the true residuals) for the matrix `add20` from Matrix Market.

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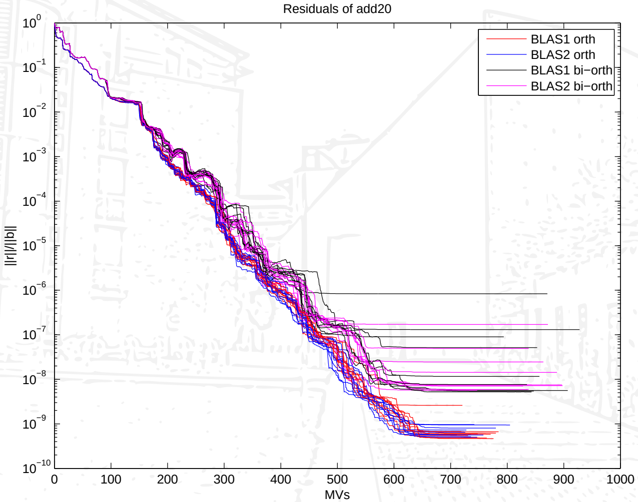
Ongoing joint work with Olaf Rendel, Gerard Sleijpen, and Martin van Gijzen.

QMRIDR: add20



$s = 8$; ω_j local minimization; next by maximal last; various orthogonalizations

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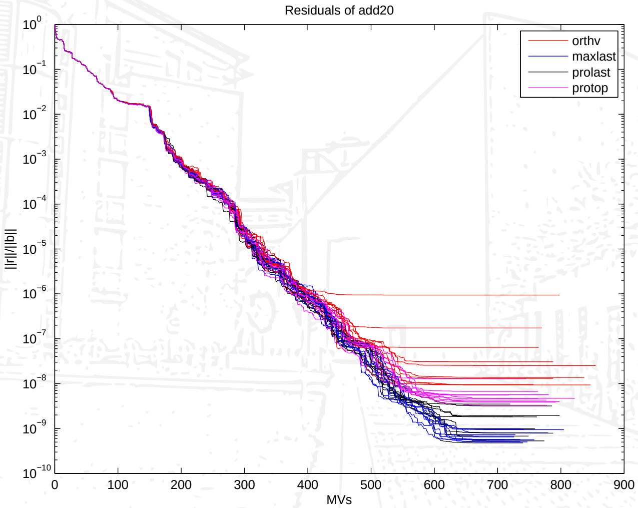

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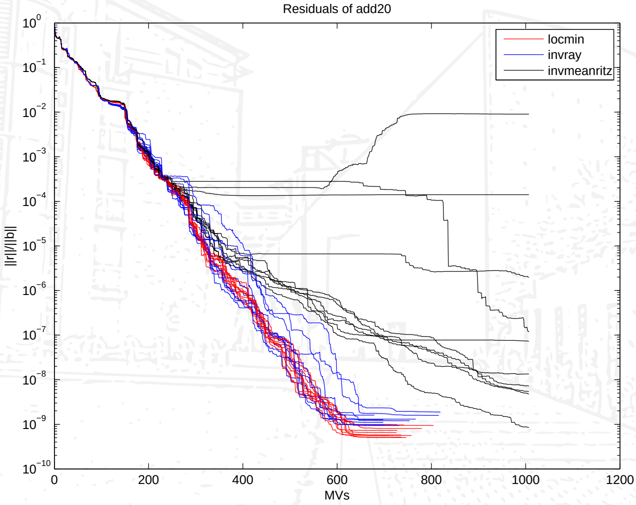

$s = 8$; ω_j various strategies; GS expansion; stable basis vectors

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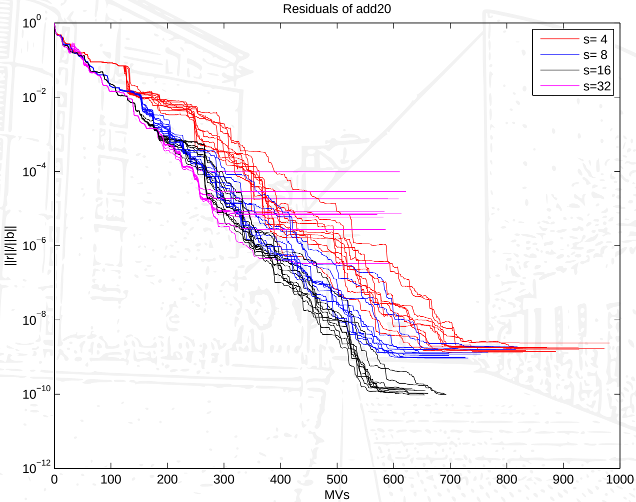
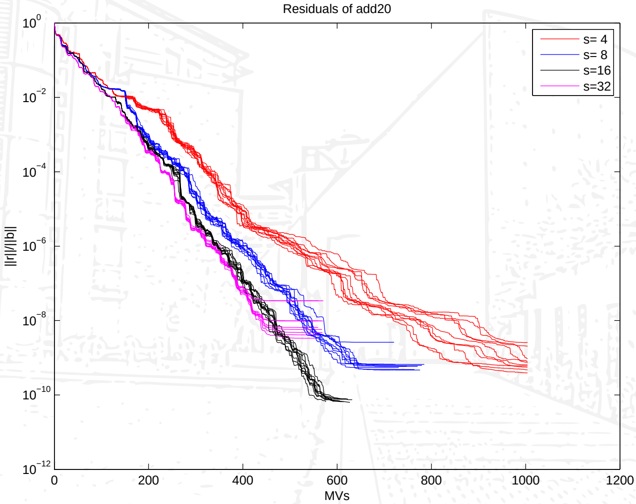


various s; ω_j inverse Rayleigh; stable expansion; GS expansion

QMRIDR: add20



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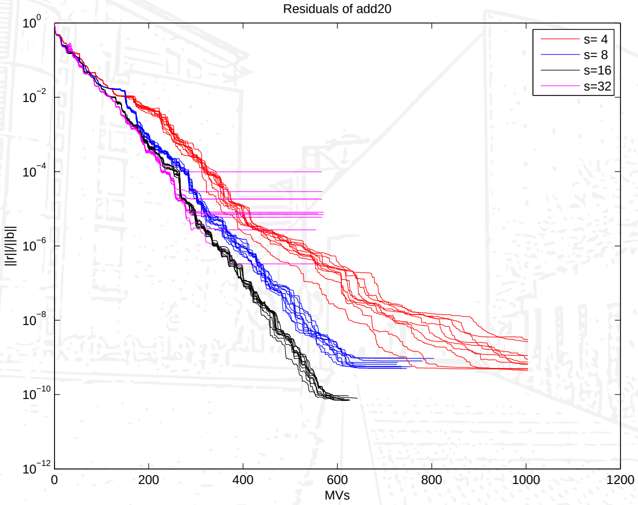

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- What about inexact IDR/IDREig/IDRStab/QMRIDR?

Thank you for your attention!

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