On the behavior of IDR(s) algorithms in finite precision

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Outline

Krylov methods in finite precision

... an introduction

IDR and IDR(s) 1976–1980: IDR 2006–2010: IDR(s)

IDR: two close relatives

IDR and Lanczos IDR and Lanczos-type product methods

Numerical experiments

Many pictures — less mathematics

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In this talk we consider the IDR methods by Peter Sonneveld (Sonneveld, 2006; Sonneveld, 2008; Wesseling and Sonneveld, 1980) and their generalizations, the IDR(*s*) methods, starting with the first IDR(*s*) algorithm (Sonneveld and van Gijzen, 2008).

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IDR and IDR(s) are Krylov subspace methods. The mth Krylov subspace \mathcal{K}_m is defined for a given square matrix A and a starting vector q as follows,

 $\mathcal{K}_m(\mathbf{A},\mathbf{q}) := \operatorname{span} \{\mathbf{q}, \mathbf{A}\mathbf{q}, \dots, \mathbf{A}^{m-1}\mathbf{q}\}.$

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IDR and IDR(s) are Krylov subspace methods. The *m*th Krylov subspace \mathcal{K}_m is defined for a given square matrix A and a starting vector \mathbf{q} as follows,

$$\mathcal{K}_m(\mathbf{A},\mathbf{q}) := \operatorname{span} \{\mathbf{q},\mathbf{A}\mathbf{q},\ldots,\mathbf{A}^{m-1}\mathbf{q}\}.$$

There is a natural isomorphism

$$\mathbf{v} \in \mathcal{K}_m \quad \Leftrightarrow \quad \mathbf{v} = \nu(\mathbf{A})\mathbf{q}$$

between vectors v in a Krylov subspace and polynomials $\nu \in \mathcal{P}_{m-1}$ (as long as the Krylov subspace \mathcal{K}_m has full dimension $\dim(\mathcal{K}_m) = m$).

(1)

Fukuoka, 2010/02/09

The origin of Krylov subspace methods

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The Krylov matrices $\mathbf{K}_m := (\mathbf{q}, \mathbf{A}\mathbf{q}, \mathbf{A}^2\mathbf{q}, \dots, \mathbf{A}^{m-1}\mathbf{q})$ satisfy the matrix recurrence $(\mathbf{q}, \mathbf{A}\mathbf{K}_m) = \mathbf{K}_{m+1}.$

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The *m*th Krylov matrix spans a basis of the *m*th Krylov space \mathcal{K}_m iff *m* is less or equal to the grade of **q**. We assume here that this is always the case.

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Suppose we choose upper triangular basis transformations $\mathbf{K}_m =: \mathbf{Q}_m \mathbf{R}_m$,

$$\left(\mathbf{q}, \mathbf{A}\mathbf{Q}_m\mathbf{R}_m\right) = \mathbf{Q}_{m+1}\mathbf{R}_{m+1} \quad \Rightarrow \quad \left(\mathbf{q}, \mathbf{A}\mathbf{Q}_m\right) = \mathbf{Q}_{m+1}\mathbf{R}_{m+1} \begin{pmatrix} 1 & \mathbf{o}^\mathsf{T} \\ \mathbf{o} & \mathbf{R}_m \end{pmatrix}^{-1}.$$
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Next we strip off the first column on both sides.

(1)

The connection to Hessenberg decompositions

The matrix $\underline{\mathbf{C}}_m \in \mathbb{C}^{(m+1) \times m}$ defined by

$$\mathbf{\underline{C}}_{m} := \mathbf{R}_{m+1} \begin{pmatrix} 1 & \mathbf{o}^{\mathsf{T}} \\ \mathbf{o} & \mathbf{R}_{m} \end{pmatrix}$$

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We end up with a Hessenberg decomposition

$$\mathbf{A}\mathbf{Q}_m = \mathbf{Q}_{m+1}\underline{\mathbf{C}}_m =: \mathbf{Q}_m\mathbf{C}_m + \mathbf{q}_{m+1}\mathbf{c}_{m+1,m}\mathbf{e}_m^{\mathsf{I}},$$

where C_m is unreduced Hessenberg and measures the "ratio" of the basis transformations.

(3)

(4)

Classification of Krylov methods: Matrix based

There are three well-known approaches based on such Hessenberg decompositions (with $\|\mathbf{r}_0\|_2 \mathbf{q}_1 = \mathbf{r}_0$), namely,

QOR: approximate $\mathbf{x} = \mathbf{A}^{-1}\mathbf{r}_0$ by $\mathbf{x}_m := \mathbf{Q}_m \mathbf{C}_m^{-1} \mathbf{e}_1 \|\mathbf{r}_0\|_2$, QMR: approximate $\mathbf{x} = \mathbf{A}^{-1}\mathbf{r}_0$ by $\underline{\mathbf{x}}_m := \mathbf{Q}_m \underline{\mathbf{C}}_m^{\dagger} \underline{\mathbf{e}}_1 \|\mathbf{r}_0\|_2$, Ritz-Galërkin: approximate part of $\mathbf{J} = \mathbf{V}^{-1}\mathbf{A}\mathbf{V}$ by $\mathbf{J}_m := \mathbf{S}_m^{-1}\mathbf{C}_m\mathbf{S}_m$ and part of \mathbf{V} by $\mathbf{V}_m := \mathbf{Q}_m\mathbf{S}_m$, where $\mathbf{C}_m\mathbf{S}_m = \mathbf{S}_m\mathbf{J}_m$.

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It turns out to be helpful to look at the corresponding polynomial description: Krylov subspace methods compute elements from the polynomial Krylov subspace \mathcal{K}_m .

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In finite precision the recurrence will only approximately be satisfied,

$$\mathbf{A}\mathbf{Q}_m + \mathbf{F}_m = \mathbf{Q}_{m+1}\underline{\mathbf{C}}_m$$

= $\mathbf{Q}_m\mathbf{C}_m + \mathbf{q}_{m+1}\mathbf{c}_{m+1,m}\mathbf{e}_m^\mathsf{T},$ (5)

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Equations like Eqn. (5) will be called perturbed Hessenberg decompositions.

To understand the perturbed case, we generalize and extend the polynomials based on the computed C_m (or \underline{C}_m) with their useful properties.

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The polynomials are named by their property. In (Z., 2007) we considered the following five types of polynomials:

• basis polynomials \mathcal{B}_m ,

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- residual polynomials \mathcal{R}_m and $\underline{\mathcal{R}}_m$.

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In this talk, we restrict ourselves to $\mathcal{L}_m[z^{-1}]$, $\mathcal{L}_m[1 - \delta_{z0}]$ and \mathcal{R}_m .

Adjugate polynomials

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This implies for all eigenvalues (Ritz values) θ_j of C_m (Z., 2006)

$$\mathcal{A}_m(\theta_j, \mathbf{C}_m)\mathbf{e}_1 = \mathbf{s}_j, \quad \mathbf{C}_m\mathbf{s}_j = \mathbf{s}_j\theta_j.$$

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Generalization:

$$\mathcal{A}_{\ell+1:m}(heta,z):=rac{\chi_{\ell+1:m}(heta)-\chi_{\ell+1:m}(z)}{ heta-z},\quad \ell=0,1,\ldots,m.$$

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Generalization:

$$\mathcal{L}_{\ell+1:m}[z^{-1}](z) := \frac{\chi_{\ell+1:m}(0) - \chi_{\ell+1:m}(z)}{z\chi_{\ell+1:m}(0)} = -\frac{\mathcal{A}_{\ell+1:m}(0,z)}{\chi_{\ell+1:m}(0)}, \quad \ell = 0, 1, \dots, m.$$

Lagrange polynomials and QOR iterates

Theorem (The finite precision QOR iterates)

Suppose that all $C_{\ell+1:m}$ are regular. We define the *m*th QOR solution by

$$\mathbf{z}_m := \mathbf{C}_m^{-1} \mathbf{e}_1 \|\mathbf{r}_0\|_2$$

and the mth QOR iterate by

 $\mathbf{x}_m := \mathbf{Q}_m \mathbf{z}_m.$

Then

$$\mathbf{x}_m = \mathcal{L}_m[z^{-1}](\mathbf{A})\mathbf{r}_0 - \sum_{\ell=1}^m \mathbf{z}_{\ell m} \,\mathcal{L}_{\ell+1:m}[z^{-1}](\mathbf{A})\mathbf{f}_\ell.$$

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Really sloppily speaking, in case of convergence,

$$\mathbf{x}_{\infty} = \mathbf{A}^{-1}\mathbf{r}_0 + \mathbf{A}^{-1}\mathbf{F}_{\infty}\mathbf{z}_{\infty} = \mathbf{A}^{-1}(\mathbf{r}_0 + \mathbf{F}_{\infty}\mathbf{z}_{\infty})$$

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Theorem (The finite precision QOR iterates)

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$$\mathbf{z}_m := \mathbf{C}_m^{-1} \mathbf{e}_1 \|\mathbf{r}_0\|_2$$

and the mth QOR iterate by

$$\mathbf{x}_m := \mathbf{Q}_m \mathbf{z}_m.$$

Then

$$\mathbf{x}_m = \mathcal{L}_m[z^{-1}](\mathbf{A})\mathbf{r}_0 - \sum_{\ell=1}^m \mathbf{z}_{\ell m} \,\mathcal{L}_{\ell+1:m}[z^{-1}](\mathbf{A})\mathbf{f}_\ell.$$

Really sloppily speaking, in case of convergence,

$$\mathbf{x}_{\infty} = \mathbf{A}^{-1}\mathbf{r}_0 + \mathbf{A}^{-1}\mathbf{F}_{\infty}\mathbf{z}_{\infty} = \mathbf{A}^{-1}(\mathbf{r}_0 + \mathbf{F}_{\infty}\mathbf{z}_{\infty})$$

Proving convergence is the hard task.

(6)

We consider Lagrange interpolation polynomials interpolating the inverse and a singularly perturbed identity.

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Properties:
\$\mathcal{L}_m^0[1-\delta_{z0}](\mathbf{C}_m) = \mathbf{I}_m, \quad \mathcal{L}_m^0[1-\delta_{z0}](0) = 0.\$
Definition:
\$\mathcal{L}_m^0[1-\delta_{z0}](z) := \frac{\chi_m(0) - \chi_m(z)}{\chi_m(0)} = \mathcal{L}_m[z^{-1}](z)z.\$

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$$\mathcal{L}^{0}_{\ell+1:m}[1-\delta_{z0}](z) := \frac{\chi_{\ell+1:m}(0) - \chi_{\ell+1:m}(z)}{\chi_{\ell+1:m}(0)}$$
$$= \mathcal{L}_{\ell+1:m}[z^{-1}](z)z, \quad \ell = 0, 1, \dots, m.$$

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Two types of polynomials \Rightarrow two expressions for the QOR residuals.

Residual polynomials and QOR residuals

Theorem (The finite precision QOR residuals)

Suppose that $\mathbf{q}_1 = \mathbf{r}_0 / \|\mathbf{r}_0\|_2$ and that all $C_{\ell+1:m}$ are regular. Let \mathbf{x}_m denote the *m*th QOR iterate and $\mathbf{r}_m := \mathbf{r}_0 - A\mathbf{x}_m$ the corresponding residual.

Then

$$\mathbf{r}_{m} = \mathcal{R}_{m}(\mathbf{A})\mathbf{r}_{0} + \sum_{\ell=1}^{m} \mathbf{z}_{\ell m} \mathcal{L}_{\ell+1:m}^{0} [1 - \delta_{z0}](\mathbf{A})\mathbf{f}_{\ell}$$
$$= \mathcal{R}_{m}(\mathbf{A})\mathbf{r}_{0} - \sum_{\ell=1}^{m} \mathbf{z}_{\ell m} \mathcal{R}_{\ell+1:m}(\mathbf{A})\mathbf{f}_{\ell} + \mathbf{F}_{m}\mathbf{z}_{m}.$$

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The first equation is related to the perturbation amplification. The second equation is related to the attainable accuracy. (7)

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Thus, we need to understand how the Ritz values behave in finite precision.

Outline

IDR and IDR(s) 1976-1980: IDR

Numerical experiments

Many pictures - less mathematics

Origin

In 1976 Sonneveld experimentally observed that for $\mathbf{B} \in \mathbb{C}^{n \times n}$ and a given starting vector $\mathbf{f}_0 \in \mathbb{C}^n$ and $\mathbf{f}_1 := \mathbf{B}\mathbf{f}_0$ the three-term recurrence

$$\mathbf{f}_{k+1} := \mathbf{B}(\mathbf{f}_k - \gamma_k(\mathbf{f}_k - \mathbf{f}_{k-1})), \quad \mathbf{\gamma}_k := rac{\mathbf{p}^{\mathsf{H}} \, \mathbf{f}_k}{\mathbf{p}^{\mathsf{H}}(\mathbf{f}_k - \mathbf{f}_{k-1})}$$

almost always stops after 2*n* steps with the zero vector $\mathbf{f}_{2n} = \mathbf{o}_n$ (Sonneveld, 2006; Sonneveld, 2008).

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He thus called this property "Induced Dimension Reduction" (IDR), and algorithms like the given three-term recurrence "IDR Algorithms".

IDR Theorem

Sonneveld first made experiments and then gave a rigorous proof. It is easy to see that apart from the first two (arbitrarily chosen) residuals the constructed residuals are in the B image of the space $\mathcal{S} := \mathbf{p}^{\perp}$.
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The same argument proves that in general (observe that the first two residuals f_0, f_1 are usually not in S) for $k \ge 1$

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

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Sonneveld proved that the dimensions of the spaces constructed are shrinking. This is the essence of the first IDR Theorem. He did not use the description as an orthogonal complement of a Krylov subspace as it is done here. We remark that generically $\dim(\mathcal{K}_n(\mathbf{B}^{-H}, \mathbf{B}^{-H}\mathbf{p})) = n$.

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

IDR Algorithms

The three-term recurrence

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

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

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

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

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The classical Richardson iteration with a starting guess x_0 is then given by

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

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

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

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

$$\mathbf{r}_{k+1} = (\mathbf{I} - \mathbf{A})(\mathbf{r}_k + \gamma_k(\mathbf{r}_k - \mathbf{r}_{k-1})), \quad \gamma_k = \frac{\mathbf{p}^{11}\mathbf{r}_k}{\mathbf{p}^{H}(\mathbf{r}_{k-1} - \mathbf{r}_k)}.$$

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The update of the iterates has to be modified accordingly,

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

= $(\mathbf{I} - \mathbf{A})(\mathbf{r}_k - \gamma_k \mathbf{A}(\mathbf{x}_k - \mathbf{x}_{k-1}) - \mathbf{r}_k$
= $-\mathbf{A}(\mathbf{r}_k + \gamma_k(\mathbf{I} - \mathbf{A})(\mathbf{x}_k - \mathbf{x}_{k-1}))$
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Sonneveld terms the outcome the Primitive IDR Algorithm (Sonneveld, 2006):

$$\mathbf{r}_{0} = \mathbf{b} - \mathbf{A}\mathbf{x}_{0}$$
$$\mathbf{x}_{1} = \mathbf{x}_{0} + \mathbf{r}_{0}$$
$$\mathbf{r}_{1} = \mathbf{r}_{0} - \mathbf{A}\mathbf{r}_{0}$$
For $k = 1, 2, \dots$ do
$$\gamma_{k} = \mathbf{p}^{\mathsf{T}}\mathbf{r}_{k}/\mathbf{p}^{\mathsf{T}}(\mathbf{r}_{k-1} - \mathbf{r}_{k})$$
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While "not converged" do

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 \mathbf{S}_k

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

 \mathbf{S}_k

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



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

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

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

 $\gamma_0 = 0$, $\mathbf{f}_0 = \mathbf{A}\mathbf{x}_0 - \mathbf{b}$, $\Delta \mathbf{g}_0 = \mathbf{o}_n$, $\Delta \mathbf{y}_0 = \mathbf{o}_n$ For k = 1, ... 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 $\Delta \mathbf{x}_k = \gamma_{k-1} \Delta \mathbf{y}_{k-1} - \omega_k \mathbf{s}_k$ $\Delta \mathbf{f}_k = \gamma_{k-1} \Delta \mathbf{g}_{k-1} - \omega_k \mathbf{t}_k$ $\mathbf{x}_k = \mathbf{x}_{k-1} + \Delta \mathbf{x}_k$ $\mathbf{f}_k = \mathbf{f}_{k-1} + \Delta \mathbf{f}_k$ if k is even $\Delta \mathbf{y}_k = \Delta \mathbf{y}_{k-1}$ $\Delta \mathbf{g}_k = \Delta \mathbf{g}_{k-1}$ else $\Delta \mathbf{y}_k = \Delta \mathbf{x}_k$ $\Delta \mathbf{g}_k = \Delta \mathbf{f}_k$ end $\gamma_k = -(\mathbf{p}^{\mathsf{H}}\mathbf{f}_k)/(\mathbf{p}^{\mathsf{H}}\Delta\mathbf{g}_k)$ done

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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 $\mathbf{I} - \omega_i \mathbf{A}$.

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



IDR and IDR(s) 1976–1980: IDR

Brothers of classical and primitive IDR

In 1976 Sonneveld considered the acceleration of Gauß-Seidel (AGS). Similarly, the IDR philisophy can be used as an accelerator for the other classical splitting methods like Jacobi, SOR, SSOR, or Chebyshev, or even more general semi-iterative methods.

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The numerical behavior is not very promising. But this picture changes, when we use more shadow vectors

Outline

Krylov methods in finite precision ...an introduction IDR and IDR(s) 1976–1980: IDR 2006–2010: IDR(s) IDR: tworelose relatives

IDR and Lanczos

Numerical experiments

Many pictures - less mathematics

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To analyze IDR and IDR(*s*), we have to consider generalized Hessenberg decompositions (also referred to as rational Hessenberg decompositions) and to generalize QOR, QMR and Ritz-Galërkin.

We have to prove that the expressions for the iterates and residuals based on polynomials are still valid. But: All these approaches extend easily to generalized Hessenberg decompositions.

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IDR(s)ORes is based on oblique projections and s + 1 consecutive multiplications with the same linear factor

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Understanding IDR: Hessenberg decompositions

We already noted that essential features of Krylov subspace methods can be described by a Hessenberg decomposition

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

Here, H_n denotes an unreduced Hessenberg matrix.

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

(8)

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IDR: Generalized Hessenberg decompositions

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

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Generalized Hessenberg decompositions correspond to an oblique 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,

$$\widehat{\mathbf{Q}}_{n}^{\mathsf{H}}(\mathbf{A},\mathbf{I})\mathbf{Q}_{n}\mathbf{U}_{n} = \widehat{\mathbf{Q}}_{n}^{\mathsf{H}}(\mathbf{A}\mathbf{Q}_{n}\mathbf{U}_{n},\mathbf{Q}_{n}\mathbf{U}_{n}) = \widehat{\mathbf{Q}}_{n}^{\mathsf{H}}(\mathbf{Q}_{n+1}\underline{\mathbf{H}}_{n},\mathbf{Q}_{n}\mathbf{U}_{n}) = (\underline{\mathbf{I}}_{n}^{\mathsf{T}}\underline{\mathbf{H}}_{n},\mathbf{U}_{n}) = (\mathbf{H}_{n},\mathbf{U}_{n}),$$
(12)

where $\widehat{\mathbf{Q}}_{n}^{\mathsf{H}} := \underline{\mathbf{I}}_{n}^{\mathsf{T}} \mathbf{Q}_{n+1}^{\dagger}$.

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IDR and IDR(s) 2006–2010: IDR(s)

IDR: The underlying Hessenberg decomposition

The IDR recurrences of IDR(s)ORes can be summarized by

$$\mathbf{v}_{n-1} := \mathbf{r}_{n-1} - \nabla \mathbf{R}_{n-s:n-1} \mathbf{c}_n = \mathbf{R}_{n-s-1:n-1} \mathbf{y}_n$$

= $(1 - \gamma_s^{(n)}) \mathbf{r}_{n-1} + \sum_{\ell=1}^{s-1} (\gamma_{s-\ell+1}^{(n)} - \gamma_{s-\ell}^{(n)}) \mathbf{r}_{n-\ell-1} + \gamma_1^{(n)} \mathbf{r}_{n-s-1},$
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IDR and IDR(s) 2006–2010: IDR(s)

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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

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

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/XXXX0000000\	(XXX0000000)
+ * * * * 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 X X 0 0 0 0 0 0 0 0 0 0
$\circ + \times \times \times \circ \circ \circ \circ \circ \circ \circ$	00X00000000
00+XXXX00000	000000000000
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000000+XXXX0	0000000000000
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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.


Understanding IDR: Deflation

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

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

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



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

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The extended matrix version \mathbf{L}_n satisfies

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

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

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The reduced residuals are defined by

$$\Omega_j(\mathbf{A})\mathbf{q}_{js+k} = \mathbf{r}_{j(s+1)+k} = (\mathbf{I} - \omega_j \mathbf{A})\mathbf{v}_{j(s+1)+k-k}$$

and every $\mathbf{v}_{j(s+1)+k-1}$ is orthogonal to **P**.

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Using induction (Sleijpen et al., 2008) one can prove that $\mathbf{q}_{js+k} \perp \mathcal{K}_j(\mathbf{A}^H, \mathbf{P})$; thus, this is a two-sided Lanczos process with *s* left and one right starting vectors.

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

$$\begin{split} \mathcal{G}_{0} &= \mathcal{K}(\mathbf{A}, \mathbf{r}_{0}), \quad \text{where } \mathcal{K}(\mathbf{A}, \mathbf{r}_{0}) \text{ denotes the } \textit{full Krylov subspace}, \\ \mathcal{G}_{j} &= \bigcap_{k=0}^{j-1} \Omega_{k}(\mathbf{A})^{-1} \Omega_{j}(\mathbf{A})(\mathcal{S}) = \left(\stackrel{j-1}{+} \Omega_{j}(\mathbf{A}) \stackrel{-\mathsf{H}}{\to} \Omega_{k}(\mathbf{A}) \stackrel{\mathsf{H}}{\to} \{\mathbf{P}\} \right)^{\perp} \\ &= \left(\Omega_{j}(\mathbf{A}) \stackrel{-\mathsf{H}}{\to} \mathcal{K}_{j}(\mathbf{A}^{\mathsf{H}}, \mathbf{P}) \right)^{\perp} = \Omega_{j}(\mathbf{A}) \left(\mathcal{K}_{j}(\mathbf{A}^{\mathsf{H}}, \mathbf{P}) \right)^{\perp} \end{split}$$

of the Sonneveld spaces.

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 G₁) are in the I − ω₁A image of S = P[⊥],
- the last s + 1 residuals are in the $\mathbf{I} \omega_j \mathbf{A}$ image of $S = \mathbf{P}^{\perp}$,
- ► 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 $S = \mathbf{P}^{\perp}$.

The second equality

j-1 $\bigcap^{j-1} \Omega_k(\mathbf{A})^{-1} \Omega_j(\mathbf{A})(\mathcal{S}) = \left(\begin{smallmatrix} j-1 \\ + \\ - \\ 0 \end{smallmatrix} \right) \Omega_j(\mathbf{A})^{-\mathsf{H}} \Omega_k(\mathbf{A})^{\mathsf{H}} \{ \mathbf{P} \} \right)^{\perp}$ k=0

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

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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 B,

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

The third and fourth equality

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

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

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In their new implementation IDR(*s*)BiO (van Gijzen and Sonneveld, 2008) of the IDR Theorem, they use basis vectors $\mathbf{g}_{-1}, \ldots, \mathbf{g}_{-s} \in \mathcal{G}_j$, which are not simply residual differences but linear combinations.

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

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

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

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- In (Sleijpen and Abe, 2010) the ideas behind BiCGStab2 (Gutknecht, 1993) and GPBiCG (Zhang, 1997) are considered.

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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}^{-H} , thus Simoncini and Szyld suggest to use a few steps of the Arnoldi method to compute some Ritz values, which are then used in some ordering as $1/\omega_j$ values.

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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}^{-H} , thus Simoncini and Szyld suggest to use a few steps of the Arnoldi method to compute some Ritz values, which are then used in some ordering as $1/\omega_j$ values.

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

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.

Outline

Krylov methods in finite presis ...an introduction IOR and IDR(s) 1976–1980: IDR 2006–2010: IDR(s)

IDR: two close relatives

IDR and Lanczos

IDR and Lanczos-type product methods

Numerical experiments

Many pictures - less mathematics

Similarities between Lanczos and IDR(1)

We have seen that IDR(*s*) is a Lanczos-type product method (LTPM), where the underlying Lanczos process uses *s* left and one right starting vectors.

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The only difference between the Lanczos process underlying IDR(1) and the finite precision Lanczos method is the perturbation term. Yet we will see that the structural constraints result in totally different deviations from the theoretical behavior of the Lanczos method.

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Thus far, this is maybe the only successful error analysis ever carried out for a perturbed short-term Krylov subspace method.

Lanczos' method in finite precision

We used the diagonal matrix

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A = diag([linspace(0, 1, 50), 3])
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and the starting vector

e = ones(51, 1)

in an implementation of Lanczos' method in MATLAB on a PC conforming to ANSI/IEEE 754 with machine precision eps (1) = $2^{-52} \approx 2.2204 \cdot 10^{-16}$.

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At step 10 the first Ritz value has converged (up to machine precision) to the eigenvalue 3, at step 27 the second one has converged. Detoriation reaches a maximum at step $19 = \lceil (10 + 27)/2 \rceil$.

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Lanczos' method in finite precision



IDR: two close relatives

R and Lanczos

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We note that we can observe multiple copies, but this time the approximation quality is reduced after a couple of steps, all Ritz values computed after certain steps show worse behavior than before.

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We show numerically that the Lanczos-part of finite precision BiCGStab behaves by no means similar to the Lanczos method in finite precision.

The eigenvalue approximations corresponding to BiCGStab are easier to analyze than those corresponding to IDR or IDR(1), since in BiCGStab the coefficients of the tridiagonal matrix of the underlying Lanczos method are explicitly computed.





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Since for real data all minimizers are real, we have run two sets of experiments with the same matrix and starting residual: The first experiment is based on an orthonormal random real matrix $\mathbf{P} \in \mathbb{R}^{n \times 2}$, the second experiment is based on an orthonormal random complex matrix $\mathbf{P} \in \mathbb{C}^{n \times 2}$.

Understanding IDR: Convergence for s = 2; **P** real



Understanding IDR: 20 steps for s = 2; **P** real



Understanding IDR: 50 steps for s = 2; **P** real



Understanding IDR: 100 steps for s = 2; **P** real



Understanding IDR: 150 steps for s = 2; **P** real



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Understanding IDR: 500 steps for s = 2; **P** real


Understanding IDR: 1000 steps for s = 2; **P** real



Understanding IDR: Convergence for s = 2; **P** complex



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Conclusions and Outlook

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- We still have to carefully look at the perturbation terms of the underlying perturbed Lanczos process.

Thank you very much for your attention!

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