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Fast iterative solvers

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Review. To simplify, take $\mathbf{x}_0 = \mathbf{0}$, assume $\|\mathbf{b}\|_2 = 1$.

Solving $\mathbf{Ax} = \mathbf{b}$ for a **general** square matrix $\mathbf{A}$.

Arnoldi decomposition: $\mathbf{AV}_k = \mathbf{V}_{k+1}\,\underline{H}_k$ with
$\mathbf{V}_k$ orthonormal, $\underline{H}_k$ Hessenberg. $\underline{H}_k = \underline{L}_k U_k = \underline{Q}_k R_k$.

$\mathbf{v}_1 = \mathbf{r}_0 = \mathbf{b}$, $\mathbf{x}_k = \mathbf{V}_k\,\vec{y}_k$, $\mathbf{r}_k = \mathbf{b} - \mathbf{Ax}_k$.

FOM:

$$\mathbf{r}_k \perp \mathbf{V}_k \quad \Leftrightarrow \quad H_k\,\vec{y}_k = e_1 \quad \Rightarrow \quad \mathbf{x}_k = \mathbf{V}_k(U_k^{-1}(L_k^{-1}e_1))$$

GMRES:

$$\vec{y}_k = \text{argmin}_{\vec{y}}\,\|\mathbf{b} - \mathbf{AV}_k\,\vec{y}\|_2 = \text{argmin}_{\vec{y}}\,\|e_1 - \underline{H}_k\,\vec{y}\|_2$$

$$\Rightarrow \quad \mathbf{x}_k = \mathbf{V}_k(R_k^{-1}(\underline{Q}_k^{*}e_1))$$

The columns of $\mathbf{V}_k$ span $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) \equiv \{p(\mathbf{A})\mathbf{r}_0 \mid p \in \mathcal{P}_{k-1}\}$.

$$\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) = \text{span}(\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_{k-1}).$$

Review. To simplify, take $\mathbf{x}_0 = \mathbf{0}$, assume $\|\mathbf{b}\|_2 = 1$.

Solving $\mathbf{A}\mathbf{x} = \mathbf{b}$ for a **Hermitian** matrix $\mathbf{A}$, $\|\mathbf{b}\|_2 = 1$

Lanczos decomposition: $\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{T}_k$ with
$\mathbf{V}_k$ orthonormal, $\underline{T}_k$ tri-diagonal. $\underline{T}_k = \underline{L}_k U_k = \underline{Q}_k R_k$.

$\mathbf{v}_1 = \mathbf{r}_0 = \mathbf{b}$, $\mathbf{x}_k = \mathbf{V}_k\,\vec{y}_k$, $\mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k$.

CG:

$$\mathbf{r}_k \perp \mathbf{V}_k \quad \Leftrightarrow \quad T_k\,\vec{y}_k = e_1 \quad \Rightarrow \quad \mathbf{x}_k = (\mathbf{V}_k\,U_k^{-1})(L_k^{-1}e_1)$$

MINRES:

$$\vec{y}_k = \text{argmin}_{\vec{y}}\,\|\mathbf{b} - \mathbf{A}\mathbf{V}_k\,\vec{y}\|_2 = \text{argmin}_{\vec{y}}\,\|e_1 - \underline{T}_k\,y\|_2$$

$$\Rightarrow \quad \mathbf{x}_k = (\mathbf{V}_k\,R_k^{-1})(\underline{Q}_k^{*}e_1)$$

Note. **Short recurrences** (eff. comp.) because of

- $\underline{T}_k$ tri-diagonal, and
- $\mathbf{U}_k\,U_k = \mathbf{V}_k$ (**CG**) and $\mathbf{W}_k\,R_k = \mathbf{V}_k$ (**MINRES**)

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$$\mathbf{r}_k \perp \mathbf{V}_k \quad \Leftrightarrow \quad T_k \vec{y}_k = e_1 \quad \Rightarrow \quad \mathbf{x}_k = (\mathbf{V}_k U_k^{-1})(L_k^{-1} e_1)$$

MINRES:

$$\vec{y}_k = \text{argmin}_{\vec{y}} \|\mathbf{b} - \mathbf{A}\mathbf{V}_k \vec{y}\|_2 = \text{argmin}_{\vec{y}} \|e_1 - \underline{T}_k y\|_2$$

$$\Rightarrow \quad \mathbf{x}_k = (\mathbf{V}_k R_k^{-1})(\underline{Q}_k^* e_1)$$

Details. For **MINRES**, see Exercise 7.8

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Note. **Less stable** because

- we rely on math. for orth. of $\mathbf{V}_k$ (**CG** & **MINRES**)
- $\mathbf{W}_k\,R_k = \mathbf{V}_k$ (**MINRES**) is a
  three term vector recurrence for the $\mathbf{w}_k$'s.

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$$\Rightarrow \quad \mathbf{x}_k = (\mathbf{V}_k\,R_k^{-1})(\underline{Q}_k^{*}e_1)$$

Note. If $\mathbf{A}$ is positive definite, then **CG** minimizes as well:

$$\vec{y}_k = \text{argmin}_{\vec{y}}\,\|\mathbf{x} - \mathbf{V}_k\,\vec{y}\|_A = \text{argmin}_{\vec{y}}\,\|\mathbf{b} - \mathbf{AV}_k\,\vec{y}\|_{A^{-1}}$$

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$$\Rightarrow \quad \mathbf{x}_k = (\mathbf{V}_k\,R_k^{-1})(\underline{Q}_k{}^* e_1)$$

SYMMLQ. Take $\mathbf{x}_k = \mathbf{A}\mathbf{V}_k\,\vec{y}_k$ with

$$\vec{y}_k \equiv \text{argmin}_{\vec{y}}\,\|\mathbf{x} - \mathbf{A}\mathbf{V}_k\,\vec{y}\|_2 \quad \Leftrightarrow \quad e_1 - \underline{T}_k{}^*\underline{T}_k\,\vec{y}_k = 0$$

$$\Rightarrow \mathbf{x}_k = \mathbf{V}_{k+1}\,\underline{T}_k(\underline{T}_k{}^*\underline{T}_k)^{-1}e_1 = (\mathbf{V}_{k+1}\underline{Q}_k)((R_k^*)^{-1}e_1)$$

Review. To simplify, take $\mathbf{x}_0 = \mathbf{0}$, assume $\|\mathbf{b}\|_2 = 1$.

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$$\Rightarrow \quad \mathbf{x}_k = (\mathbf{V}_k\, R_k^{-1})(\underline{Q}_k^{*} e_1)$$

Details. For **SYMMLQ**, see Exercise 7.9.

FOM residual polynomials and Ritz values

Property. $\mathbf{r}_k^{\mathsf{CG}} = \mathbf{r}_k^{\mathsf{FOM}} = p_k(\mathbf{A})\mathbf{r}_0 \perp \mathbf{V}_k$,

for some residual polynomial p_k of degree k, i.e., $p_k(0) = 1$.

$p_k^{\mathsf{FOM}} = p_k$ is the kth (CG or) **FOM residual polynomial**.

Theorem. $p^{\mathsf{FOM}}(\vartheta) = 0 \quad \Leftrightarrow \quad H_k\,\vec{y} = \vartheta\vec{y}$ for some $\vec{y} \neq \vec{0}$:

the zeros of p_k^{FOM} are precisely the kth order Ritz values.

In particular, $$p_k^{\mathsf{FOM}}(\lambda) = \prod_{j=1}^{k}\left(1 - \frac{\lambda}{\vartheta_j}\right) \qquad (\lambda \in \mathbb{C}).$$

Moreover, for a polynomial p of degree at most k with $p(0) = 1$, we have that that

$$p = p_k^{\mathsf{FOM}} \quad \Leftrightarrow \quad p(H_k) = 0.$$

Proof. Exercise 6.6.

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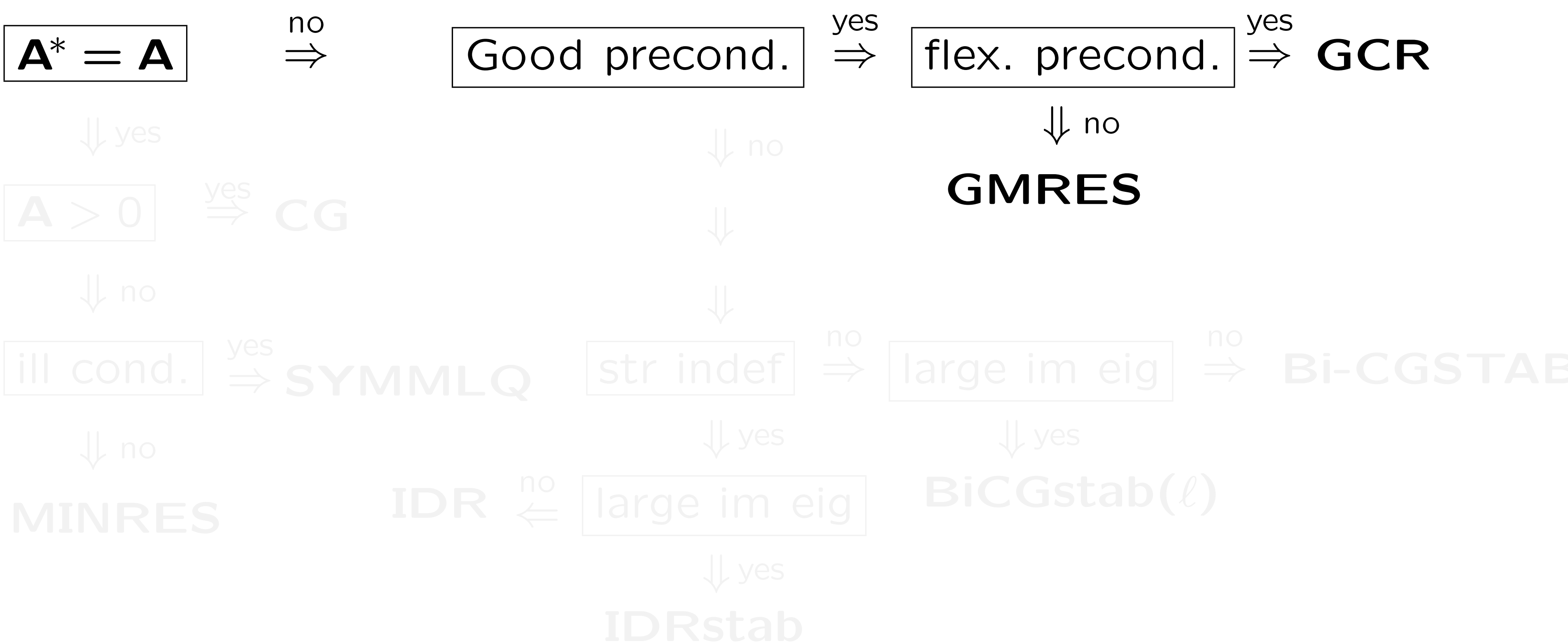
Theorem. Similarly relate zeros of p_k^{GMRES} to harmonic Ritz values of $\underline{H}_k$.

Solving $\mathbf{Ax} = \mathbf{b}$, an overview



a good preconditioner is available
the preconditioner is flexible
$\mathbf{A} + \mathbf{A}^*$ is strongly indefinite
$\mathbf{A}$ has large imaginary eigenvalues

Solving $\mathbf{Ax} = \mathbf{b}$, an overview

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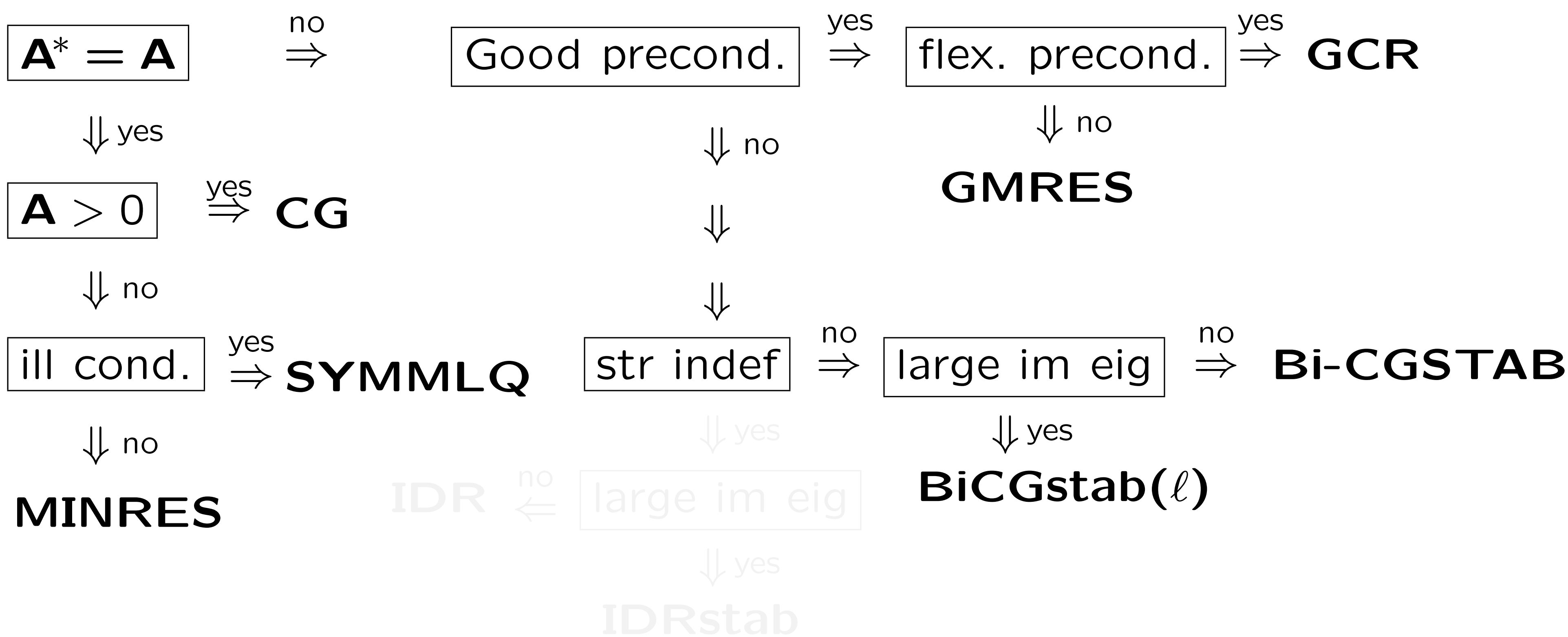
Solving $Ax = b$, an overview



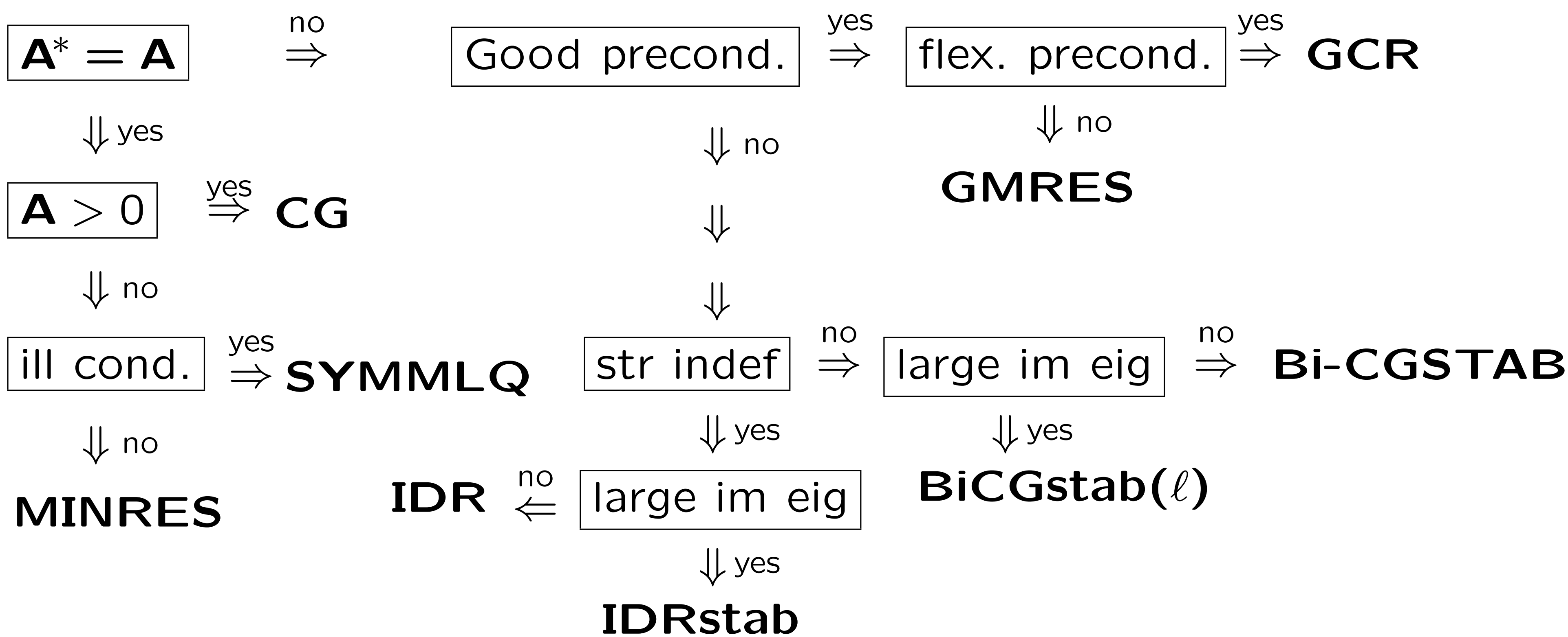
a good preconditioner is available

the preconditioner is flexible

$A + A^*$ is strongly indefinite

A has large imaginary eigenvalues

Solving $\mathbf{Ax} = \mathbf{b}$, an overview



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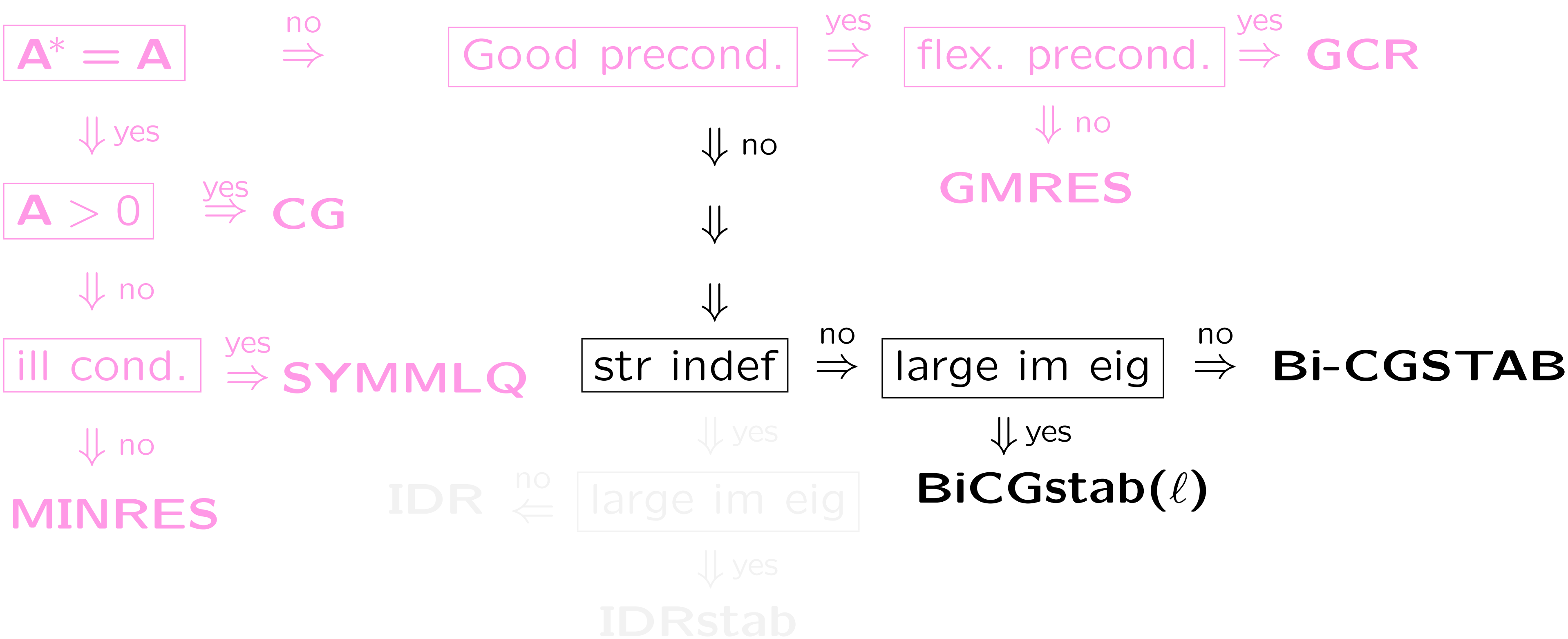
Solving $Ax = b$, an overview



a good preconditioner is available
the preconditioner is flexible
$\mathbf{A} + \mathbf{A}^*$ is strongly indefinite
$\mathbf{A}$ has large imaginary eigenvalues

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

with $\mathbf{A}$ $n \times n$ non-singular.

Today's topic. Iterative methods for general systems using short recurrences

Program Lecture 8

- **CG**
- **Bi-CG**
- Bi-Lanczos
- Hybrid **Bi-CG**
- **Bi-CGSTAB**, **BiCGstab**(ℓ)
- **IDR**

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[Hestenes Stiefel '52]

$\mathbf{A}^* = \mathbf{A} > 0$, Conjugate Gradient

$\mathbf{x} = \mathbf{0},\ \mathbf{r} = \mathbf{b},\ \mathbf{u} = \mathbf{0},\ \rho = 1$

While $\|\mathbf{r}\| > tol$ do

$\sigma = -\rho,\quad \rho = \mathbf{r}^*\mathbf{r},\quad \beta = \rho/\sigma$

$\mathbf{u} \leftarrow \mathbf{r} - \beta\,\mathbf{u},\quad \mathbf{c} = \mathbf{A}\mathbf{u}$

$\sigma = \mathbf{u}^*\mathbf{c},\quad \alpha = \rho/\sigma$

$\mathbf{r} \leftarrow \mathbf{r} - \alpha\,\mathbf{c}$

$\mathbf{x} \leftarrow \mathbf{x} + \alpha\,\mathbf{u}$

end while

Construction CG.

There are four alternative derivations of **CG**.

- **GCR** $\rightsquigarrow$ (use $\mathbf{A}^* = \mathbf{A}$) $\rightsquigarrow$ **CR** $\rightsquigarrow$
  use $\mathbf{A}^{-1}$ inner product $\quad + \quad$ efficient implementation.
- Lanczos $\quad + \quad T = LU \quad + \quad$ efficient implementation.
- **Orthogonalize residuals.** [Exercise 7.3]
- Nonlinear CG to solve $\mathbf{x} = \mathrm{argmin}_{\widetilde{\mathbf{x}}} \frac{1}{2}\|\mathbf{b} - \mathbf{A}\widetilde{\mathbf{x}}\|^2_{A^{-1}}$
- ...

Conjugate Gradients, $\mathbf{A}^* = \mathbf{A}$, $\mathbf{K}^* = \mathbf{K}$

$$\mathbf{u}_k = \mathbf{K}^{-1}\mathbf{r}_k - \beta_k\,\mathbf{u}_{k-1}$$

$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k\,\mathbf{A}\,\mathbf{u}_k$$

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Theorem. • $\mathbf{r}_k$, $\mathsf{K}\mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A}\mathsf{K}^{-1}, \mathbf{r}_0)$

• $\mathbf{r}_0, \ldots, \mathbf{r}_{k-1}$ is a **Krylov basis** of $\mathcal{K}_k(\mathbf{A}\mathsf{K}^{-1}, \mathbf{r}_0)$

• If $\mathbf{r}_k$, $\mathbf{A}\mathbf{u}_k \perp \mathsf{K}^{-1}\mathbf{r}_{k-1}$, then $\mathbf{r}_k$, $\mathbf{A}\mathbf{u}_k \perp \mathsf{K}^{-1}\mathcal{K}_k(\mathbf{A}\mathsf{K}^{-1}, \mathbf{r}_0)$

Conjugate Gradients, $\mathbf{A}^* = \mathbf{A}$, $\mathbf{K}^* = \mathbf{K}$

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Proof.

$\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1}\,\mathbf{A}\,\mathbf{u}_{k-1} \perp \mathbf{K}^{-1}\mathbf{r}_{k-1}$ — by construction α_{k-1}

$\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1}\,\mathbf{A}\,\mathbf{u}_{k-1} \perp \mathbf{K}^{-1}\mathcal{K}_{k-1}(\mathbf{A}\mathbf{K}^{-1}, \mathbf{r}_0)$ — by induction

Conjugate Gradients, $\mathbf{A}^* = \mathbf{A}$, $\mathbf{K}^* = \mathbf{K}$

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Proof.

$\mathbf{A}\,\mathbf{u}_k = \mathbf{A}\mathbf{K}^{-1}\mathbf{r}_k - \beta_k\,\mathbf{A}\,\mathbf{u}_{k-1} \perp \mathbf{K}^{-1}\mathbf{r}_{k-1}$ by construction β_k

$\mathbf{A}\,\mathbf{u}_k = \mathbf{A}\mathbf{K}^{-1}\mathbf{r}_k - \beta_k\,\mathbf{A}\,\mathbf{u}_{k-1} \perp \mathbf{K}^{-1}\mathcal{K}_{k-1}(\mathbf{A}\mathbf{K}^{-1}, \mathbf{r}_0)$ by induction:

$$\mathbf{A}\mathbf{K}^{-1}\mathbf{r}_k \perp \mathbf{K}^{-1}\mathcal{K}_{k-1}(\mathbf{A}\mathbf{K}^{-1}, \mathbf{r}_0) \quad\Leftrightarrow\quad \mathbf{r}_k \perp \mathbf{K}^{-1}\mathbf{A}\mathbf{K}^{-1}\mathcal{K}_{k-1}(\mathbf{A}\mathbf{K}^{-1}, \mathbf{r}_0)$$
$$\Leftarrow\quad \mathbf{r}_k \perp \mathbf{K}^{-1}\mathcal{K}_k(\mathbf{A}\mathbf{K}^{-1}, \mathbf{r}_0)$$

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$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k\,\mathbf{A}\,\mathbf{u}_k$$

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$$\Leftarrow \quad \mathbf{r}_k \perp \mathbf{K}^{-1}\mathcal{K}_k(\mathbf{A}\mathbf{K}^{-1}, \mathbf{r}_0)$$

$\mathbf{A}^* = \mathbf{A}$ & $\mathbf{K}^* = \mathbf{K}$: Preconditioned CG

$\mathbf{x} = \mathbf{0},\ \mathbf{r} = \mathbf{b},\ \mathbf{u} = \mathbf{0},\ \ \rho = 1$

```
While ‖r‖ > tol do
```

$\quad$ Solve $\mathbf{K}\mathbf{c} = \mathbf{r}$ for $\mathbf{c}$

$\quad \sigma = -\rho, \quad \rho = \mathbf{c}^*\mathbf{r}, \quad \beta = \rho/\sigma$

$\quad \mathbf{u} \leftarrow \mathbf{c} - \beta\,\mathbf{u}, \quad \mathbf{c} = \mathbf{A}\mathbf{u}$

$\quad \sigma \leftarrow \mathbf{u}^*\mathbf{c}, \quad \alpha = \rho/\sigma$

$\quad \mathbf{r} \leftarrow \mathbf{r} - \alpha\,\mathbf{c}$

$\quad \mathbf{x} \leftarrow \mathbf{x} + \alpha\,\mathbf{u}$

end while

Properties CG

Pros

- **Low costs per step**: 1 MV, 2 DOT, 3 AXPY
  to increase dimension Krylov subspace by one.
- **Low storage**: 5 large vectors (incl. $\mathbf{b}$).
- **Minimal res.** method **if A, K pos. def.**: $\|\mathbf{r}_k\|_{\mathbf{A}^{-1}}$ is min.
- **Orthogonal residual** method if $\mathbf{A}^* = \mathbf{A}$, $\mathbf{K}^* = \mathbf{K}$:
  $$\mathbf{r}_k \perp \mathbf{K}^{-1}\mathcal{K}_k(\mathbf{A}\mathbf{K}^{-1}; \mathbf{r}_0).$$
- No additional knowledge on properties of $\mathbf{A}$ is needed.
- **Robust**: **CG** always converges **if A, K pos. def.**.

Cons

- May **break down** if $\mathbf{A}^* = \mathbf{A} \not> 0$.
- Does **not** work if $\mathbf{A} \neq \mathbf{A}^*$.
- ◦ **CG** is sensitive to evaluation errors if $\mathbf{A}^* = \mathbf{A} \not> 0$.
  Often loss of a) super-linear conv., and b) accuracy.
  For two reasons:
  1) Loss of orthogonality in the Lanczos recursion
  2) As in FOM, bumps and peaks in CG conv. hist.

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For general square non-singular $\mathbf{A}$

- Apply **CG** to normal equations ($\mathbf{A}^*\mathbf{A}\mathbf{x} = \mathbf{A}^*\mathbf{b}$) $\rightsquigarrow$ **CGNE**
- Apply **CG** to $\mathbf{A}\mathbf{A}^*\mathbf{y} = \mathbf{b}$ (then $\mathbf{x} = \mathbf{A}^*\mathbf{y}$)
  $\rightsquigarrow$ **Graig's method**

Disadvantage. Search in $\mathcal{K}_k(\mathbf{A}^*\mathbf{A}, \ldots)$:

- If $\mathbf{A} = \mathbf{A}^*$ then convergence is determined by $\mathbf{A}^2$: condition number squared, ...
- Expansion $\mathcal{K}_k$ requires 2 MVs (i.e., many costly steps).

For a discussion on Graig's method, see Exercise 8.1.
For a Graig versus GCR, see Exercise 8.6.

For general square non-singular A

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[Faber Manteufel 90]

Theorem. For general square non-singular **A**, there is no Krylov solver that finds the best solution in de Krylov subspace $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$ using short recurrences.

For general square non-singular A

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[Faber Manteufel 90]

Theorem. For general square non-singular **A**, there is no Krylov solver that finds the best solution in de Krylov subspace $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$ using short recurrences.

Alternative. Construct residuals in a sequence of shrinking spaces (orthogonal to a sequence of growing spaces): adapt the construction of **CG**.

Conjugate Gradients, $\mathbf{A}^* = \mathbf{A}$. $\mathbf{K} = \mathbf{I}$

$$\mathbf{u}_k = \mathbf{r}_k - \beta_k \mathbf{u}_{k-1}$$
$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k \mathbf{A}\,\mathbf{u}_k$$

Theorem. • $\mathbf{r}_k,\ \mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A}, \mathbf{r}_0)$

• $\mathbf{r}_0, \ldots, \mathbf{r}_{k-1}$ is a **Krylov basis** of $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$

• If $\mathbf{r}_k,\ \mathbf{A}\mathbf{u}_k \perp \mathbf{r}_{k-1}$, then $\mathbf{r}_k,\ \mathbf{A}\mathbf{u}_k \perp \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$

Proof.

$\mathbf{A}\,\mathbf{u}_k = \mathbf{A}\,\mathbf{r}_k - \beta_k \mathbf{A}\,\mathbf{u}_{k-1} \perp \mathbf{r}_{k-1}$ — by construction β_{k-1}

$\mathbf{A}\,\mathbf{u}_k = \mathbf{A}\,\mathbf{r}_k - \beta_k \mathbf{A}\,\mathbf{u}_{k-1} \perp \mathcal{K}_{k-1}(\mathbf{A}, \mathbf{r}_0)$ — by induction:

$\mathbf{A}\mathbf{r}_k \perp \mathcal{K}_{k-1}(\mathbf{A}, \mathbf{r}_0) \quad \Leftrightarrow \quad \mathbf{r}_k \perp \mathbf{A}\mathcal{K}_{k-1}(\mathbf{A}, \mathbf{r}_0)$

$\Leftarrow \quad \mathbf{r}_k \perp \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$

Bi-Conjugate Gradients

$$\mathbf{u}_k = \mathbf{r}_k - \beta_k\,\mathbf{u}_{k-1}$$
$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k\,\mathbf{A}\,\mathbf{u}_k$$

Theorem. We have $\mathbf{r}_k,\ \mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A},\mathbf{r}_0)$.

Suppose $\widetilde{\mathbf{r}}_0,\ldots,\widetilde{\mathbf{r}}_{k-1}$ is a **Krylov basis** of $\mathcal{K}_k(\mathbf{A}^*,\widetilde{\mathbf{r}}_0)$.

If $\mathbf{r}_k,\ \mathbf{A}\mathbf{u}_k \perp \widetilde{\mathbf{r}}_{k-1}$, then $\mathbf{r}_k,\ \mathbf{A}\mathbf{u}_k \perp \mathcal{K}_k(\mathbf{A}^*,\widetilde{\mathbf{r}}_0)$.

Proof.

$\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1}\,\mathbf{A}\,\mathbf{u}_{k-1} \perp \widetilde{\mathbf{r}}_{k-1}$ by construction α_{k-1}

$\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1}\,\mathbf{A}\,\mathbf{u}_{k-1} \perp \mathcal{K}_{k-1}(\mathbf{A}^*,\widetilde{\mathbf{r}}_0)$ by induction

$\mathbf{A}\,\mathbf{u}_k = \mathbf{A}\,\mathbf{r}_k - \beta_k\,\mathbf{A}\,\mathbf{u}_{k-1} \perp \widetilde{\mathbf{r}}_{k-1}$ by construction β_{k-1}

$\mathbf{A}\,\mathbf{u}_k = \mathbf{A}\,\mathbf{r}_k - \beta_k\,\mathbf{A}\,\mathbf{u}_{k-1} \perp \mathcal{K}_{k-1}(\mathbf{A}^*,\widetilde{\mathbf{r}}_0)$ by induction:

$\mathbf{A}\mathbf{r}_k \perp \mathcal{K}_{k-1}(\mathbf{A}^*,\widetilde{\mathbf{r}}_0) \quad \Leftarrow \quad \mathbf{r}_k \perp \mathcal{K}_k(\mathbf{A}^*,\widetilde{\mathbf{r}}_0) \supset \mathbf{A}^*\mathcal{K}_{k-1}(\mathbf{A}^*,\widetilde{\mathbf{r}}_0)$

Bi-Conjugate Gradients

$$\mathbf{u}_k = \mathbf{r}_k - \beta_k \, \mathbf{u}_{k-1}$$
$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k \, \mathbf{A} \, \mathbf{u}_k$$

$\mathbf{r}_k,\ \mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A}, \mathbf{r}_0), \qquad \mathbf{r}_k,\ \mathbf{A}\mathbf{u}_k \perp \widetilde{\mathbf{r}}_{k-1}$

With $\qquad \rho_k \equiv (\mathbf{r}_k, \widetilde{\mathbf{r}}_k) \quad \& \quad \sigma_k \equiv (\mathbf{A}\mathbf{u}_k, \widetilde{\mathbf{r}}_k)$

and, since $\qquad \widetilde{\mathbf{r}}_k + \bar{\vartheta}_k \, \mathbf{A}^* \, \widetilde{\mathbf{r}}_{k-1} \in \mathcal{K}_k(\mathbf{A}^*, \widetilde{\mathbf{r}}_0) \qquad$ for some ϑ_k,

$\bar{\cdot}$ is the complex conjugate

we have that
$$\alpha_k = \frac{(\mathbf{r}_k, \widetilde{\mathbf{r}}_k)}{(\mathbf{A}\mathbf{u}_k, \widetilde{\mathbf{r}}_k)} = \frac{\rho_k}{\sigma_k}$$

and
$$\beta_k = \frac{(\mathbf{A}\mathbf{r}_k, \widetilde{\mathbf{r}}_{k-1})}{(\mathbf{A}\mathbf{u}_{k-1}, \widetilde{\mathbf{r}}_{k-1})} = \frac{(\mathbf{r}_k, \mathbf{A}^*\widetilde{\mathbf{r}}_{k-1})}{\sigma_{k-1}} = \frac{-\rho_k}{\vartheta_k \, \sigma_{k-1}}$$

Bi-Conjugate Gradients

$$\mathbf{u}_k = \mathbf{r}_k - \beta_k\,\mathbf{u}_{k-1}$$
$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k\,\mathbf{A}\,\mathbf{u}_k$$

$$\mathbf{r}_k,\ \mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A},\mathbf{r}_0), \qquad \mathbf{r}_k,\ \mathbf{A}\mathbf{u}_k \perp \widetilde{\mathbf{r}}_{k-1}$$

With $\rho_k \equiv (\mathbf{r}_k, \bar{q}_k(\mathbf{A}^*)\widetilde{\mathbf{r}}_0)$ & $\sigma_k \equiv (\mathbf{A}\mathbf{u}_k, \bar{q}_k(\mathbf{A}^*)\widetilde{\mathbf{r}}_0)$

and, since $q_k(\zeta) + \vartheta_k\,\zeta\,q_{k-1}(\zeta) \in \mathcal{P}_{k-1}$ for some ϑ_k,

we have that $\alpha_k = \dfrac{\rho_k}{\sigma_k}$ & $\beta_k = \dfrac{-\rho_k}{\vartheta_k\,\sigma_{k-1}}$

Bi-Conjugate Gradients

Classical **Bi-CG** [Fletcher '76] generates the **shadow** residuals $\widetilde{\mathbf{r}}_k = \bar{q}_k(\mathbf{A}^*)\widetilde{\mathbf{r}}_0$ with the same polynomal as $\mathbf{r}_k$ $(q_k = p_k)$

$$\mathbf{r}_k = p_k(\mathbf{A})\mathbf{r}_0, \qquad \widetilde{\mathbf{r}}_k = \bar{p}_k(\mathbf{A}^*)\widetilde{\mathbf{r}}_0:$$

i.e., compute $\widetilde{\mathbf{r}}_{k+1}$ as

$$\widetilde{\mathbf{r}}_{k+1} = \widetilde{\mathbf{r}}_k - \bar{\alpha}_k\,\mathbf{A}^*\widetilde{\mathbf{u}}_k, \qquad \text{with} \qquad \widetilde{\mathbf{u}}_k = \widetilde{\mathbf{r}}_k - \bar{\beta}_k\,\widetilde{\mathbf{u}}_{k-1}.$$

In particular, $\vartheta_k = \alpha_{k-1}$.

However, other choices for q_k are possible as well.

Example. $q_k(\zeta) = (1 - \omega_{k-1}\zeta)\,q_{k-1}(\zeta) \quad (\zeta \in \mathbb{C})$.

Then, $\vartheta_k = \omega_{k-1}$ and $\widetilde{\mathbf{r}}_k = \widetilde{\mathbf{r}}_{k-1} - \bar{\omega}_{k-1}\,\mathbf{A}^*\widetilde{\mathbf{r}}_{k-1}$,

with, for instance, $\bar{\omega}_{k-1}$ to minimize $\|\widetilde{\mathbf{r}}_k\|_2$.

The next transparancy displays classical **Bi-CG**.

[Fletcher 76]

Bi-CG

$\mathbf{x} = \mathbf{0}, \quad \mathbf{r} = \mathbf{b}.$ Choose $\tilde{\mathbf{r}}$

$\mathbf{u} = \mathbf{0}, \quad \rho = 1$ $\tilde{\mathbf{u}} = \mathbf{0}$

While $\|\mathbf{r}\| > tol$ do

$\sigma = -\rho, \quad \rho = (\mathbf{r}, \tilde{\mathbf{r}}), \quad \beta = \rho/\sigma$

$\mathbf{u} \leftarrow \mathbf{r} - \beta\,\mathbf{u}, \quad \mathbf{c} = \mathbf{A}\mathbf{u},$ $\tilde{\mathbf{u}} \leftarrow \tilde{\mathbf{r}} - \bar{\beta}\,\tilde{\mathbf{u}}, \quad \tilde{\mathbf{c}} = \mathbf{A}^*\tilde{\mathbf{u}}$

$\sigma = (\mathbf{c}, \tilde{\mathbf{r}}), \quad \alpha = \rho/\sigma$

$\mathbf{r} \leftarrow \mathbf{r} - \alpha\,\mathbf{c},$ $\tilde{\mathbf{r}} \leftarrow \tilde{\mathbf{r}} - \bar{\alpha}\,\tilde{\mathbf{c}}$

$\mathbf{x} \leftarrow \mathbf{x} + \alpha\,\mathbf{u}$

end while

[Fletcher 76]

Bi-CG

$\mathbf{x} = \mathbf{0}, \quad \mathbf{r} = \mathbf{b}.$ Choose $\widetilde{\mathbf{r}}$

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$\mathbf{u} \leftarrow \mathbf{r} - \beta\,\mathbf{u}, \quad \mathbf{c} = \mathbf{A}\mathbf{u},$ $\widetilde{\mathbf{c}} \leftarrow \mathbf{A}^*\widetilde{\mathbf{r}} - \bar{\beta}\,\widetilde{\mathbf{c}}$

$\sigma = (\mathbf{c}, \widetilde{\mathbf{r}}), \quad \alpha = \rho/\sigma$

$\mathbf{r} \leftarrow \mathbf{r} - \alpha\,\mathbf{c},$ $\widetilde{\mathbf{r}} \leftarrow \widetilde{\mathbf{r}} - \bar{\alpha}\,\widetilde{\mathbf{c}}$

$\mathbf{x} \leftarrow \mathbf{x} + \alpha\,\mathbf{u}$

end while

Selecting the initial shadow residual $\widetilde{\mathbf{r}}_0$.

- Often recommended: $\widetilde{\mathbf{r}}_0 = \mathbf{r}_0$.
- Practical experience: select $\widetilde{\mathbf{r}}_0$ randomly (unless $\mathbf{A}^* = \mathbf{A}$).

Exercise. **Bi-CG** and **CG** coincide

if $\mathbf{A}$ is Hermitian and $\widetilde{\mathbf{r}}_0 = \mathbf{r}_0$.

Exercise. Derive a version of **Bi-CG** that includes a pre-conditioner $\mathbf{K}$.

Show that **Bi-CG** and **CG** coincide

if $\mathbf{A}$ and $\mathbf{K}$ are Hermitian and $\widetilde{\mathbf{r}}_0 = \mathbf{K}^{-1}\mathbf{r}_0$.

Exercise 8.9 gives an alternative derivation of **Bi-CG**.

Properties Bi-CG

Pros

- Usually selects good approximations from the search subspaces (Krylov subspaces).
- **Low costs per step**: 2 DOT, 5 AXPY.
- **Low storage**: 7 large vectors.
- No knowledge on properties of $\mathbf{A}$ is needed.

Cons

- ∘ Non-optimal Krylov subspace method.
- Not robust: **Bi-CG** may break down.
- **Bi-CG** is sensitive to evaluation errors (often loss of super-linear convergence).
- ∘ Convergence depends on **shadow** residual $\widetilde{\mathbf{r}}_0$.
- **2 MV needed to expand search subspace by 1 vector.**
- **1 MV is by $\mathbf{A}^*$.**

Properties Bi-CG

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- Usually selects good approximations from
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Program Lecture 8

- **CG**
- **Bi-CG**
- Bi-Lanczos
- Hybrid **Bi-CG**
- **Bi-CGSTAB, BiCGstab**(ℓ)
- **IDR**

Bi-Lanczos

Find coefficients α_k, β_k, $\widetilde{\alpha}_k$ and $\widetilde{\beta}_k$ such that (**bi-orthogonalize**)

$$\gamma_k \mathbf{v}_{k+1} = \mathbf{A}\mathbf{v}_k - \alpha_k \mathbf{v}_k - \beta_k \mathbf{v}_{k-1} - \ldots \perp \mathbf{w}_k, \mathbf{w}_{k-1}, \ldots$$

$$\widetilde{\gamma}_k \mathbf{w}_{k+1} = \mathbf{A}^* \mathbf{w}_k - \widetilde{\alpha}_k \mathbf{w}_k - \widetilde{\beta}_k \mathbf{w}_{k-1} - \ldots \perp \mathbf{v}_k, \mathbf{v}_{k-1}, \ldots$$

Select appropriate scaling coefficients γ_k and $\widetilde{\gamma}_k$.

Then

$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1} \underline{H}_k$ with $\underline{H}_k$ Hessenberg

$\mathbf{A}^*\mathbf{W}_k = \mathbf{W}_{k+1} \widetilde{\underline{H}_k}$ with $\widetilde{\underline{H}_k}$ Hessenberg

and $\mathbf{W}_{k+1}^* \mathbf{V}_{k+1} = D_{k+1}$ diagonal

Exercise. $T_k \equiv \mathbf{W}_k^* \mathbf{A} \mathbf{V}_k = D_k H_k = \widetilde{H_k}^* D_k$ is tridiagonal.

Exploit $\widetilde{H_k} = D_k H_k^* D_k^*$ and tridiagonal structure:

$\rightsquigarrow$ **Bi-Lanczos**.

Bi-Lanczos

Find coefficients α_k, β_k, $\widetilde{\alpha}_k$ and $\widetilde{\beta}_k$ such that (**bi-orthogonalize**)

$$\gamma_k \mathbf{v}_{k+1} = \mathbf{A}\mathbf{v}_k - \alpha_k \mathbf{v}_k - \beta_k \mathbf{v}_{k-1} - \ldots \perp \mathbf{w}_k, \mathbf{w}_{k-1}, \ldots$$

$$\widetilde{\gamma}_k \mathbf{w}_{k+1} = \mathbf{A}^* \mathbf{w}_k - \widetilde{\alpha}_k \mathbf{w}_k - \widetilde{\beta}_k \mathbf{w}_{k-1} - \ldots \perp \mathbf{v}_k, \mathbf{v}_{k-1}, \ldots$$

Select appropriate scaling coefficients γ_k and $\widetilde{\gamma}_k$.

Then

$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\underline{H}_k$ with $\underline{H}_k$ Hessenberg

$\mathbf{A}^*\mathbf{W}_k = \mathbf{W}_{k+1}\underline{\widetilde{H}_k}$ with $\underline{\widetilde{H}_k}$ Hessenberg

and $\mathbf{W}_{k+1}^*\mathbf{V}_{k+1} = D_{k+1}$ diagonal

Exercise. $T_k \equiv \mathbf{W}_k^*\mathbf{A}\mathbf{V}_k = D_k H_k = \widetilde{H_k}^* D_k$ is tridiagonal.

Exploit $\widetilde{H_k} = D_k H_k^* D_k^*$ and tridiagonal structure:

$\rightsquigarrow$ **Bi-Lanczos**. See Exercise 8.7 for details.

[Lanczos '50]

Lanczos

$$\rho = \|\mathbf{r}_0\|, \quad \mathbf{v}_1 = \mathbf{r}_0/\rho$$

$$\beta_0 = 0, \quad \mathbf{v}_0 = \mathbf{0}$$

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

$$\widetilde{\mathbf{v}} = \mathbf{A}\,\mathbf{v}_k - \beta_{k-1}\,\mathbf{v}_{k-1}$$

$$\alpha_k = \mathbf{v}_k^*\,\widetilde{\mathbf{v}}, \quad \widetilde{\mathbf{v}} \leftarrow \widetilde{\mathbf{v}} - \alpha_k\,\mathbf{v}_k$$

$$\beta_k = \|\widetilde{\mathbf{v}}\|, \quad \mathbf{v}_{k+1} = \widetilde{\mathbf{v}}/\beta_k$$

end while

[Lanczos '50]

Bi-Lanczos

Select a $\mathbf{r}_0$,	and a $\widetilde{\mathbf{r}}_0$
$\mathbf{v}_1 = \mathbf{r}_0/\|\mathbf{r}_0\|,\ \mathbf{v}_0 = \mathbf{0}$,	$\mathbf{w}_1 = \widetilde{\mathbf{r}}_0/\|\widetilde{\mathbf{r}}_0\|,\ \mathbf{w}_0 = \mathbf{0}$
$\gamma_0 = 0,\ \delta_0 = 1$,	$\widetilde{\gamma}_0 = 0,\ \widetilde{\delta}_0 = 1$
For $k = 1, 2, \ldots$ do	
$\quad \delta_k = \mathbf{w}_k^* \mathbf{v}_k$,	
$\quad \widetilde{\mathbf{v}} = \mathbf{A}\,\mathbf{v}_k$,	$\widetilde{\mathbf{w}} = \mathbf{A}^*\,\mathbf{w}_k$
$\quad \beta_k = \overline{\widetilde{\gamma}}_{k-1}\delta_k/\delta_{k-1}$,	$\widetilde{\beta}_k = \overline{\gamma}_{k-1}\overline{\delta}_k/\overline{\delta}_{k-1}$
$\quad \widetilde{\mathbf{v}} \leftarrow \widetilde{\mathbf{v}} - \beta_k \mathbf{v}_{k-1}$,	$\widetilde{\mathbf{w}} \leftarrow \widetilde{\mathbf{w}} - \widetilde{\beta}_k \mathbf{w}_{k-1}$
$\quad \alpha_k = \mathbf{w}_k^* \widetilde{\mathbf{v}}/\delta_k$,	$\widetilde{\alpha}_k = \overline{\alpha}_k$
$\quad \widetilde{\mathbf{v}} \leftarrow \widetilde{\mathbf{v}} - \alpha_k\,\mathbf{v}_k$,	$\widetilde{\mathbf{w}} \leftarrow \widetilde{\mathbf{w}} - \widetilde{\alpha}_k\,\mathbf{w}_k$
$\quad$ Select a $\gamma_k \neq 0$	and a $\widetilde{\gamma}_k \neq 0$
$\quad \mathbf{v}_{k+1} = \widetilde{\mathbf{v}}/\gamma_k$,	$\mathbf{w}_{k+1} = \widetilde{\mathbf{w}}/\widetilde{\gamma}_k$,
$\quad \mathbf{V}_k = [\,\mathbf{V}_{k-1}, \mathbf{v}_k\,]$,	$\mathbf{W}_k = [\,\mathbf{W}_{k-1}, \mathbf{w}_k\,]$
end while	

Arnoldi: $\mathbf{AV}_k = \mathbf{V}_{k+1}\underline{H}_k$.

If $\mathbf{A}^* = \mathbf{A}$, then $\underline{T}_k \equiv \underline{H}_k$ tridiagonal $\rightsquigarrow$ Lanczos

---

Lanczos $\quad + \quad T = LU \quad + \quad$ efficient implementation

$\rightsquigarrow$ **CG**

Bi-Lanczos $\quad + \quad T = LU \quad + \quad$ efficient implementation

$\rightsquigarrow$ **Bi-CG**

[Fletcher 76]

Bi-CG

$\mathbf{x} = \mathbf{0}, \quad \mathbf{r} = \mathbf{b}.$ Choose $\widetilde{\mathbf{r}}$

$\mathbf{u} = \mathbf{0}, \quad \rho = 1$ $\widetilde{\mathbf{c}} = \mathbf{0}$

While $\|\mathbf{r}\| > tol$ do

$\sigma = -\rho, \quad \rho = (\mathbf{r}, \widetilde{\mathbf{r}}), \quad \beta = \rho/\sigma$

$\mathbf{u} \leftarrow \mathbf{r} - \beta\,\mathbf{u}, \quad \mathbf{c} = \mathbf{A}\mathbf{u},$ $\widetilde{\mathbf{c}} \leftarrow \mathbf{A}^*\widetilde{\mathbf{r}} - \bar{\beta}\,\widetilde{\mathbf{c}}$

$\sigma = (\mathbf{c}, \widetilde{\mathbf{r}}), \quad \alpha = \rho/\sigma$

$\mathbf{r} \leftarrow \mathbf{r} - \alpha\,\mathbf{c},$ $\widetilde{\mathbf{r}} \leftarrow \widetilde{\mathbf{r}} - \bar{\alpha}\,\widetilde{\mathbf{c}}$

$\mathbf{x} \leftarrow \mathbf{x} + \alpha\,\mathbf{u}$

end while

Bi-CG may break down

0) **Lucky** breakdown if $\mathbf{r}_k = \mathbf{0}$.

1) **Pivot breakdown** or **LU-breakdown**,
i.e., LU-decomposition may not exist.

Corresponds to $\sigma = 0$ in **Bi-CG**

Remedy.

- Composite step **Bi-CG** (skip once forming $T_k = L_k U_k$)
- Form $T = QR$ as in **MINRES** (from the beginning): simple **Quasi Minimal Residuals**

2) **Bi-Lanczos** may **break down**,
i.e., a diagonal element of D_k may be zero.

Corresponds to $\rho = 0$ in **Bi-CG**

Remedy. ∘ Look ahead

General remedy. ∘ Restart ∘ Look ahead in **QMR**

Note. **CG** may suffer from pivot breakdown
when applied to a Hermitian, non definite matrix
($\mathbf{A}^* = \mathbf{A}$ with positive as well as negative eigenvalues):

MINRES and **SYMMLQ** cure this breakdown.

Note. Exact breakdowns are rare.
However, near breakdowns lead to irregular convergence and instabilities. This leads to

- loss of speed of convergence
- loss of accuracy

Properties Bi-CG

Advantages

- Usually selects good approximations from the search subspaces (Krylov subspaces).
- 2 DOT, 5 AXPY per step.
- Storage: 8 large vectors.
- No knowledge on properties of $\mathbb{A}$ is needed.

Drawbacks

- ◦ Non-optimal Krylov subspace method.
- Not robust: **Bi-CG** may break down.
- **Bi-CG** is sensitive to evaluation errors (often loss of super-linear convergence).
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Program Lecture 8

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- **Bi-CG**
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- Hybrid **Bi-CG**
- **Bi-CGSTAB, BiCGstab**(ℓ)
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Bi-Conjugate Gradients, K=I

$$\mathbf{u}_k = \mathbf{r}_k - \beta_k\,\mathbf{u}_{k-1}$$
$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k\,\mathbf{A}\,\mathbf{u}_k$$

$\mathbf{r}_k,\ \mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A},\mathbf{r}_0),\qquad \mathbf{r}_k,\ \mathbf{A}\mathbf{u}_k \perp \widetilde{\mathbf{r}}_{k-1}$

With $\quad \rho_k \equiv (\mathbf{r}_k, \bar{q}_k(\mathbf{A}^*)\widetilde{\mathbf{r}}_0) \quad \& \quad \sigma_k \equiv (\mathbf{A}\mathbf{u}_k, \bar{q}_k(\mathbf{A}^*)\widetilde{\mathbf{r}}_0)$

and, since $\quad q_k(\zeta) + \vartheta_k\,\zeta\,q_{k-1}(\zeta) \in \mathcal{P}_{k-1} \quad$ for some ϑ_k,

we have that $\quad \alpha_k = \dfrac{\rho_k}{\sigma_k} \quad \& \quad \beta_k = \dfrac{-\rho_k}{\vartheta_k\,\sigma_{k-1}}$

[Sonneveld '89]

Transpose-free Bi-CG

$$\rho_k = (\mathbf{r}_k, \bar{q}_k(\mathbf{A}^*)\,\widetilde{\mathbf{r}}_0) = (q_k(\mathbf{A})\mathbf{r}_k, \widetilde{\mathbf{r}}_0),$$
$$\sigma_k = (\mathbf{A}\mathbf{u}_k, \bar{q}_k(\mathbf{A}^*)\,\widetilde{\mathbf{r}}_0) = (\mathbf{A}q_k(\mathbf{A})\mathbf{u}_k, \widetilde{\mathbf{r}}_0)$$

$$\mathbf{Q}_k \equiv q_k(\mathbf{A})$$

$$\text{(Bi-CG)}\quad \begin{cases} \rho_k, & \mathbf{Q}_k\mathbf{u}_k = \mathbf{Q}_k\mathbf{r}_k - \beta_k\,\mathbf{Q}_k\mathbf{u}_{k-1}, \\ \sigma_k, & \mathbf{Q}_k\mathbf{r}_{k+1} = \mathbf{Q}_k\mathbf{r}_k - \alpha_k\,\mathbf{A}\mathbf{Q}_k\mathbf{u}_k, \end{cases}$$

(Pol) Compute q_{k+1} of degree $k+1$ **s.t.** $q_{k+1}(0) = 1$.

Compute $\mathbf{Q}_{k+1}\mathbf{u}_k$, $\mathbf{Q}_{k+1}\mathbf{r}_{k+1}$

(from $\mathbf{Q}_k\mathbf{u}_k, \mathbf{Q}_k\mathbf{r}_{k+1}, \ldots$

[Sonneveld '89]

Transpose-free Bi-CG

$\rho_k = (\mathbf{r}_k, \bar{q}_k(\mathbf{A}^*)\,\widetilde{\mathbf{r}}_0) = (q_k(\mathbf{A})\mathbf{r}_k, \widetilde{\mathbf{r}}_0),$

$\sigma_k = (\mathbf{A}\mathbf{u}_k, \bar{q}_k(\mathbf{A}^*)\,\widetilde{\mathbf{r}}_0) = (\mathbf{A}q_k(\mathbf{A})\mathbf{u}_k, \widetilde{\mathbf{r}}_0)$

$\mathbf{Q}_k \equiv q_k(\mathbf{A})$

$$\text{(Bi-CG)} \quad \begin{cases} \rho_k, & \mathbf{Q}_k\mathbf{u}_k = \mathbf{Q}_k\mathbf{r}_k - \beta_k\,\mathbf{Q}_k\mathbf{u}_{k-1}, \\ \sigma_k, & \mathbf{Q}_k\mathbf{r}_{k+1} = \mathbf{Q}_k\mathbf{r}_k - \alpha_k\,\mathbf{A}\mathbf{Q}_k\mathbf{u}_k, \end{cases}$$

(Pol) Compute q_{k+1} of degree $k+1$ **s.t.** $q_{k+1}(0) = 1$.

Compute $\mathbf{Q}_{k+1}\mathbf{u}_k$, $\mathbf{Q}_{k+1}\mathbf{r}_{k+1}$

Example. $q_{k+1}(\zeta) = (1 - \omega_k\zeta)q_k(\zeta)$

[Sonneveld '89]

Transpose-free Bi-CG

$$\rho_k = (\mathbf{r}_k, \bar{q}_k(\mathbf{A}^*)\,\widetilde{\mathbf{r}}_0) = (q_k(\mathbf{A})\mathbf{r}_k, \widetilde{\mathbf{r}}_0),$$
$$\sigma_k = (\mathbf{A}\mathbf{u}_k, \bar{q}_k(\mathbf{A}^*)\,\widetilde{\mathbf{r}}_0) = (\mathbf{A}q_k(\mathbf{A})\mathbf{u}_k, \widetilde{\mathbf{r}}_0)$$

$$\mathbf{Q}_k \equiv q_k(\mathbf{A})$$

$$\text{(Bi-CG)} \quad \begin{cases} \rho_k, & \mathbf{Q}_k\mathbf{u}_k = \mathbf{Q}_k\mathbf{r}_k - \beta_k\,\mathbf{Q}_k\mathbf{u}_{k-1}, \\ \sigma_k, & \mathbf{Q}_k\mathbf{r}_{k+1} = \mathbf{Q}_k\mathbf{r}_k - \alpha_k\,\mathbf{A}\mathbf{Q}_k\mathbf{u}_k, \end{cases}$$

(Pol) Compute q_{k+1} of degree $k+1$ **s.t.** $q_{k+1}(0) = 1$.

Compute $\mathbf{Q}_{k+1}\mathbf{u}_k$, $\mathbf{Q}_{k+1}\mathbf{r}_{k+1}$

Example. $q_{k+1}(\zeta) = (1 - \omega_k\zeta)q_k(\zeta) \quad (\zeta \in \mathbb{C})$.

$$\begin{cases} \omega_k, & \mathbf{Q}_{k+1}\mathbf{u}_k = \mathbf{Q}_k\mathbf{u}_k - \omega_k\,\mathbf{A}\mathbf{Q}_k\mathbf{u}_k, \\ & \mathbf{Q}_{k+1}\mathbf{r}_{k+1} = \mathbf{Q}_k\mathbf{r}_{k+1} - \omega_k\,\mathbf{A}\mathbf{Q}_k\mathbf{r}_{k+1}, \end{cases}$$

Transpose-free Bi-CG; Practice

Work with $\mathbf{u}'_k \equiv \mathbf{Q}_k \mathbf{u}_k^{\text{BiCG}}$ and $\mathbf{r}'_k \equiv \mathbf{Q}_k \mathbf{r}_{k+1}^{\text{BiCG}}$

Write $\mathbf{u}_{k-1}$ and $\mathbf{r}_k$, instead of $\mathbf{Q}_k \mathbf{u}_{k-1}^{\text{BiCG}}$ and $\mathbf{Q}_k \mathbf{r}_k^{\text{BiCG}}$, resp.

$$\rho_k = (\mathbf{r}_k, \widetilde{\mathbf{r}}_0), \qquad \sigma_k = (\mathbf{A}\mathbf{u}'_k, \widetilde{\mathbf{r}}_0)$$

$$\text{(Bi-CG)} \quad \begin{cases} \rho_k = (\mathbf{r}_k, \widetilde{\mathbf{r}}_0), & \mathbf{u}'_k = \mathbf{r}_k - \beta_k \mathbf{u}_{k-1}, \\ \sigma_k = (\mathbf{A}\mathbf{u}'_k, \widetilde{\mathbf{r}}_0), & \mathbf{r}'_k = \mathbf{r}_k - \alpha_k \mathbf{A}\mathbf{u}'_k, \qquad \mathbf{x}'_k = \mathbf{x}_k + \alpha_k \mathbf{u}'_k \end{cases}$$

(Pol) Compute updating coefficients for q_{k+1}.

Compute $\mathbf{u}_k$, $\mathbf{r}_{k+1}$, $\mathbf{x}_{k+1}$

Example.

$$\begin{cases} \omega_k, & \mathbf{u}_{k+1} = \mathbf{u}'_k - \omega_k \mathbf{A}\mathbf{u}'_k, \\ & \mathbf{r}_{k+1} = \mathbf{r}'_k - \omega_k \mathbf{A}\mathbf{r}'_k, \qquad \mathbf{x}_{k+1} = \mathbf{x}'_k + \omega_k \mathbf{r}'_k \end{cases}$$

Example. $q_{k+1}(\zeta) = (1 - \omega_k \zeta) q_k(\zeta) \qquad (\zeta \in \mathbb{C})$.

How to choose ω_k?

Bi-CGSTABilized. With $\mathbf{s}_k \equiv \mathbf{A}\mathbf{r}'_k$,

$$\omega_k \equiv \mathrm{argmin}_\omega \|\mathbf{r}'_k - \omega\, \mathbf{A}\mathbf{r}'_k\|_2 = \frac{\mathbf{s}_k^* \mathbf{r}'_k}{\mathbf{s}_k^* \mathbf{s}_k}$$

as in Local Minimal Residual method,

or, equivalently, as in GCR(1).

[van der Vorst 92]

BiCGSTAB

$\mathbf{x} = \mathbf{0}, \quad \mathbf{r} = \mathbf{b}.$ Choose $\tilde{\mathbf{r}}$

$\mathbf{u} = 0, \quad \omega = \sigma = 1.$

While $\|\mathbf{r}\| > tol$ do

$\sigma \leftarrow -\omega\sigma, \quad \rho = (\mathbf{r}, \tilde{\mathbf{r}}), \quad \beta = \rho/\sigma$

$\mathbf{u} \leftarrow \mathbf{r} - \beta\,\mathbf{u}, \qquad \mathbf{c} = \mathbf{A}\mathbf{u}$

$\sigma = (\mathbf{c}, \tilde{\mathbf{r}}), \qquad \alpha = \rho/\sigma$

$\mathbf{r} \leftarrow \mathbf{r} - \alpha\,\mathbf{c},$

$\mathbf{x} \leftarrow \mathbf{x} + \alpha\,\mathbf{u}$

$\mathbf{s} = \mathbf{A}\mathbf{r}, \qquad \omega = (\mathbf{r}, \mathbf{s})/(\mathbf{s}, \mathbf{s})$

$\mathbf{u} \leftarrow \mathbf{u} - \omega\,\mathbf{c}$

$\mathbf{x} \leftarrow \mathbf{x} + \omega\,\mathbf{r}$

$\mathbf{r} \leftarrow \mathbf{r} - \omega\,\mathbf{s}$

end while

Hybrid Bi-CG or product type Bi-CG

$$\mathbf{r}_k \equiv q_k(\mathbf{A})\mathbf{r}_k^{\text{Bi-CG}} = q_k(\mathbf{A})\, p_k^{\text{BiCG}}(\mathbf{A})\,\mathbf{r}_0$$

p_k^{BiCG} is the kth "**Bi-CG** residual polynomial"

How to select q_k**??**

q_k for **efficient steps** & **fast convergence**.

Fast convergence by

- reducing the residual
- stabilizing the **Bi-CG** part
- other   when used as linear solver for the Jacobian system in a Newton scheme for non-linear equations, by reducing the number of Newton steps

Hybrid Bi-CG

Examples.

CGS	**Bi-CG** $\times$ **Bi-CG**	Sonneveld [1989]
Bi-CGSTAB	**GCR**(1) $\times$ **Bi-CG**	van der Vorst [1992]
GPBi-CG	2-truncated **GCR** $\times$ **Bi-CG**	Zhang [1997]
BiCGstab(ℓ)	**GCR**(ℓ) $\times$ **Bi-CG**	Sl. Fokkema [1993]

For more details on hybrid Bi-CG,
see Exercise 8.11 and Exercise 8.12.
For a derivation of GPBi-CG, see Exercise 8.13.

Properties hybrid Bi-CG

Pros

- Converges often twice as fast as **Bi-CG** w.r.t. # MVs:
  each MV expands the search subspace
  Bi-CG: $\mathbf{x}_k - \mathbf{x}_0 \in \mathcal{K}_k(\mathbf{A}; \mathbf{r}_0)$ à 2k MV.
  Hybrid **Bi-CG**: $\mathbf{x}_k - \mathbf{x}_0 \in \mathcal{K}_{2k}(\mathbf{A}; \mathbf{r}_0)$ à 2k MV.
- Work/MV and storage similar to **Bi-CG**.
- Transpose free.
- ○ Explicit computation of **Bi-CG** scalars.

Cons

- Non-optimal Krylov subspace method.
- Peaks in the convergence history.
- Large intermediate residuals.
- ○ Breakdown possibilities.

[Sonneveld '89]

Conjugate Gradients Squared

$$\mathbf{r}_k = p_k^{\mathsf{BiCG}}(\mathbf{A})\, p_k^{\mathsf{BiCG}}(\mathbf{A})\, \mathbf{r}_0$$

CGS exploits recurrence relations for the **Bi-CG** polynomials to design a very efficient algorithm.

Properties

\+ Hybrid **Bi-CG**.

\+ A very efficient algorithm:
 1 DOT/MV, 3.25 AXPY/MV;
 storage: 7 large vectors.

− Often high peaks in its convergence history

− Often large intermediate residuals

\+ Seems to do well as linear solver in a Newton scheme

[Sonneveld 89]

Conjugate Gradients Squared

$\mathbf{x} = \mathbf{0}$, $\mathbf{r} = \mathbf{b}$. Choose $\tilde{\mathbf{r}}$.

$\mathbf{u} = \mathbf{w} = \mathbf{0}$, $\rho = 1$.

While $\|\mathbf{r}\| > tol$ do

$\sigma = -\rho, \quad \rho = (\mathbf{r}, \tilde{\mathbf{r}}), \quad \beta = \rho/\sigma$

$\mathbf{w} \leftarrow \mathbf{u} - \beta\,\mathbf{w}$

$\mathbf{v} = \mathbf{r} - \beta\,\mathbf{u}$

$\mathbf{w} \leftarrow \mathbf{v} - \beta\,\mathbf{w}, \quad \mathbf{c} = \mathbf{A}\mathbf{w}$

$\sigma = (\mathbf{c}, \tilde{\mathbf{r}}), \quad \alpha = \rho/\sigma$

$\mathbf{u} = \mathbf{v} - \alpha\,\mathbf{c}$

$\mathbf{r} \leftarrow \mathbf{r} - \alpha\,\mathbf{A}(\mathbf{v} + \mathbf{u})$

$\mathbf{x} \leftarrow \mathbf{x} + \alpha\,(\mathbf{v} + \mathbf{u})$

end while

Program Lecture 8

- **CG**
- **Bi-CG**
- Bi-Lanczos
- Hybrid **Bi-CG**
- **Bi-CGSTAB, BiCGstab**(ℓ)
- **IDR**

Properties Bi-CGSTAB

Pros

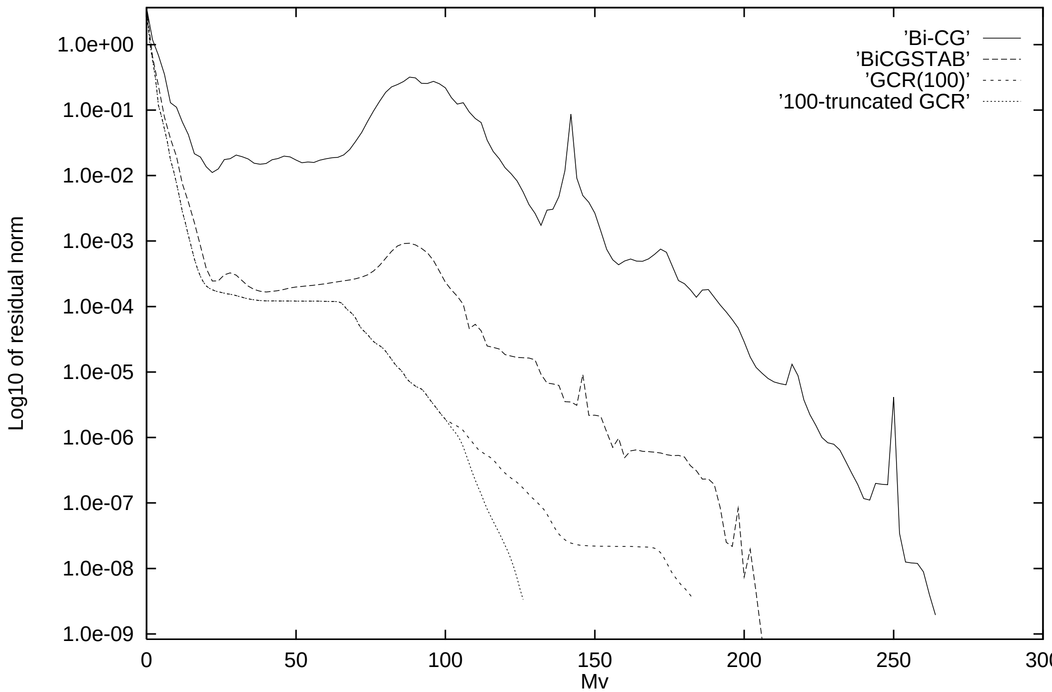
- Hybrid **Bi-CG**.
- Converges faster (& smoother) than **CGS**.
- More accurate than **CGS**.
- 2 DOT/MV, 3 AXPY/MV.
- Storage: 6 large vectors.

Cons Danger of

(A) Lanczos breakdown ($\rho_k = 0$),

(B) pivot breakdown ($\sigma_k = 0$),

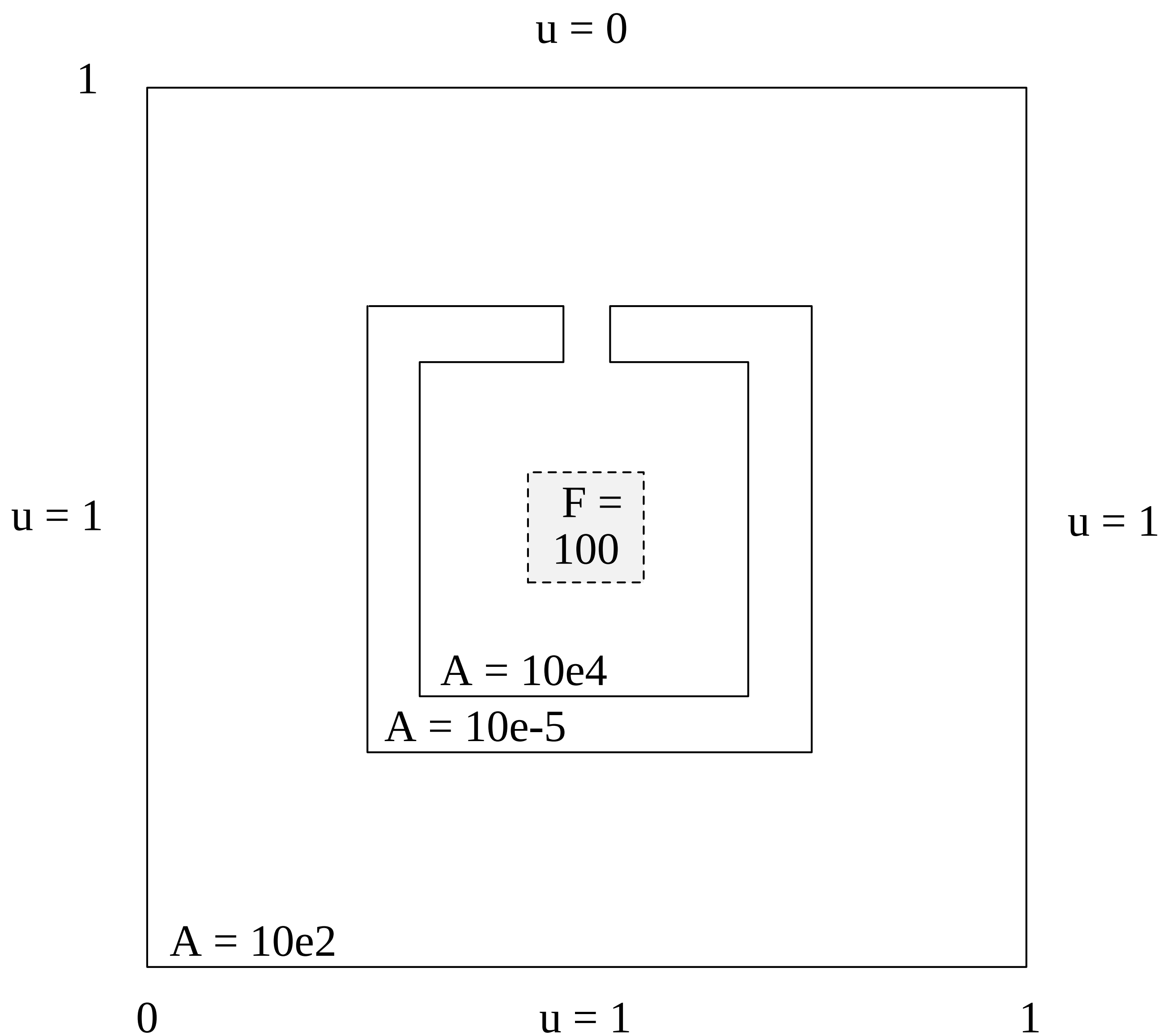
(C) breakdown minimization ($\omega_k = 0$).



$$-(a\,u_x)_x - (a\,u_y)_y = 1 \text{ on } [0,1] \times [0,1].$$

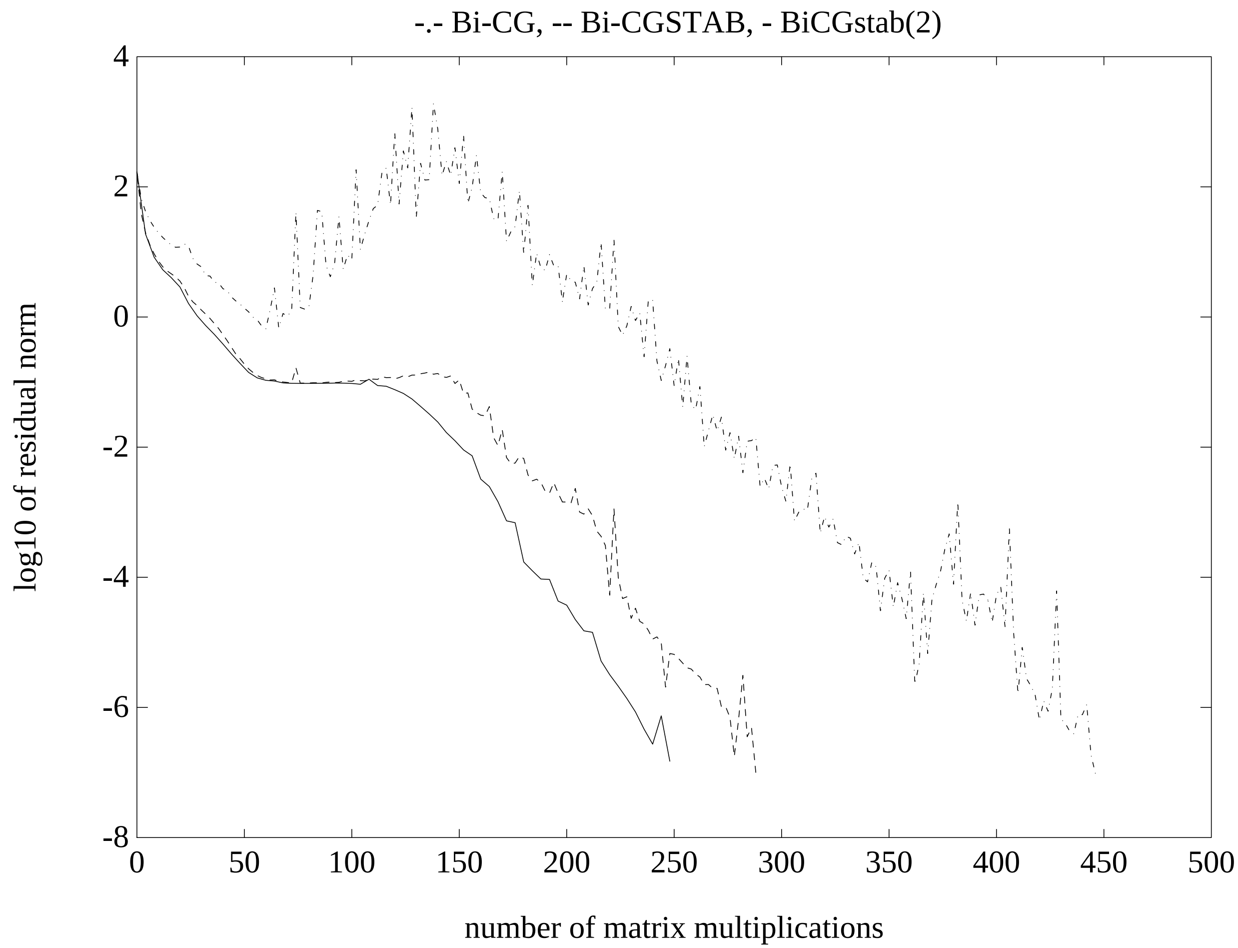
$a = 1000$ for $0.1 \leq x, y \leq 0.9$ and $a = 1$ elsewhere.

Dirichlet BC on $y = 0$, Neumann BC on other parts of Boundary.
82×82 volumes. ILU Decomp.



$-(a\,u_x)_x - (a\,u_y)_y + b\,u_x = f$ on $[0,1] \times [0,1]$.

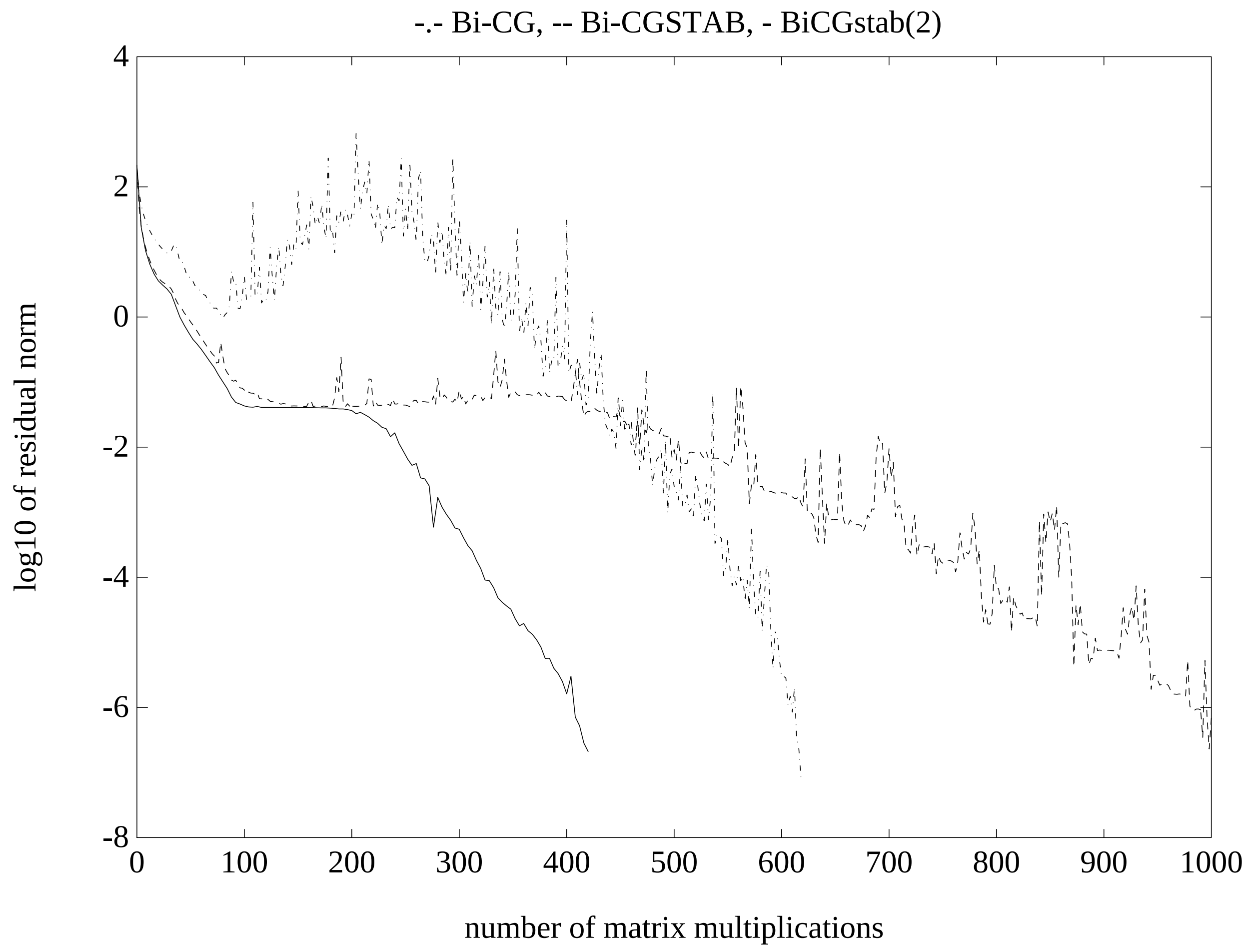
definition of $a = A$ and of $f = F$; $F = 0$ except . . .



$$-(a\,u_x)_x - (a\,u_y)_y + bu_x = f \text{ on } [0,1] \times [0,1].$$

$b(x,y) = 2\exp(2(x^2 + y^2))$, a changes strongly

Dirichlet BC. 129×129 volumes. ILU Decomp.



$-(a\, u_x)_x - (a\, u_y)_y + b u_x = f$ on $[0,1] \times [0,1]$.

$b(x,y) = 2\exp(2(x^2 + y^2))$, a changes strongly

Dirichlet BC. 201×201 volumes. ILU Decomp.

Breakdown of the minimization

Exact arithmetic, $\omega_k = 0$:

— No reduction of residual by

$$\mathbf{Q}_{k+1}\, r_{k+1} = (\mathbf{I} - \omega_k \mathbf{A}\,)\, \mathbf{Q}_k\, \mathbf{r}_{k+1}^{\mathrm{BiCG}}. \qquad (\star)$$

— q_{k+1} is of degree k: **Bi-CG** scalars can not be computed;
breakdown of incorporated **Bi-CG**.

Finite precision arithmetic, $\omega_k \approx 0$:

— Poor reduction of residual by $(\star)$

— **Bi-CG** scalars are seriously affected by evaluation errors:
drop of speed of convergence.

$\omega_k \approx 0$ to be expected if **A** is real and

A has eigenvalues with rel. large imaginary part: ω_k is real!

Example. $q_{k+1}(\zeta) = (1 - \omega_k \zeta) q_k(\zeta) \quad (\zeta \in \mathbb{C})$.

How to choose ω_k?

Bi-CGSTABilized. With $\mathbf{s}_k \equiv \mathbf{A}\mathbf{r}'_k$,

$$\omega_k \equiv \text{argmin}_\omega \|\mathbf{r}'_k - \omega\, \mathbf{A}\mathbf{r}'_k\|_2 = \frac{\mathbf{s}_k^* \mathbf{r}'_k}{\mathbf{s}_k^* \mathbf{s}_k}$$

as in Local Minimal Residual method,

or, equivalently, as in GCR(1).

BiCGstab(ℓ). Cycle ℓ times through the **Bi-CG** part

to compute $\mathbf{A}^j \mathbf{u}'$, $\mathbf{A}^j \mathbf{r}'$ for $j = 0, \ldots, \ell$,

where now $\mathbf{u}' \equiv \mathbf{Q}_k \mathbf{u}_{k+\ell-1}^{\text{BiCG}}$ and $\mathbf{r}' \equiv \mathbf{Q}_k \mathbf{r}_{k+\ell}^{\text{BiCG}}$ for $k = m\ell$.

$$\vec{\gamma}_m \equiv \text{argmin}_{\vec{\gamma}} \|\mathbf{r}' - [\mathbf{A}\mathbf{r}', \ldots, \mathbf{A}^\ell \mathbf{r}']\vec{\gamma}\|_2$$

$$\mathbf{r}_{k+\ell} = \mathbf{r}' - [\mathbf{A}\mathbf{r}', \ldots, \mathbf{A}^{\ell}\mathbf{r}']\vec{\gamma}_m$$

$$q_{k+\ell}(\zeta) = (1 - [\zeta, \ldots, \zeta^{\ell}]\vec{\gamma}_m)q_k(\zeta) \quad (\zeta \in \mathbb{C})$$

BiCGstab(ℓ) for $\ell \geq 2$ [Sl Fokkema 93, Sl vdV Fokkema 94]

$$\begin{cases} q_{k+1}(\mathbf{A}) = \mathbf{A}\, q_k(\mathbf{A}) & k \neq m\ell \\ q_{m\ell+\ell}(\mathbf{A}) = \phi_m(\mathbf{A})\, q_{m\ell}(\mathbf{A}) & k = m\ell \end{cases}$$

where ϕ_m of exact degree ℓ, $\phi_m(0) = 1$ and

$$\phi_m \quad \text{minimizes} \quad \|\phi_m(\mathbf{A})\, \underbrace{q_{m\ell}(\mathbf{A})\, \mathbf{r}^{\text{BiCG}}_{m\ell+\ell}}_{\mathbf{r}'}\|_2.$$

ϕ_m is a **GCR** residual polynomial of degree ℓ.

Note that real polynomials of degree ≥ 2 can have complex zeros.

BiCGstab(ℓ) for $\ell \geq 2$ [Sl Fokkema 93, Sl vdV Fokkema 94]

$$\begin{cases} q_{k+1}(\mathbf{A}) = \mathbf{A}\, q_k(\mathbf{A}) & k \neq m\ell \\ q_{m\ell+\ell}(\mathbf{A}) = \phi_m(\mathbf{A})\, q_{m\ell}(\mathbf{A}) & k = m\ell \end{cases}$$

where ϕ_m of exact degree ℓ, $\phi_m(0) = 1$ and

$$\phi_m \quad \text{minimizes} \quad \|\phi_m(\mathbf{A}) \underbrace{q_{m\ell}(\mathbf{A})\, \mathbf{r}^{\text{BiCG}}_{m\ell+\ell}}_{\mathbf{r}'}\|_2.$$

Minimization in practice: $p_m(\zeta) = 1 - \sum_{j=1}^{\ell} \gamma_j^{(m)}\, \zeta^j$

$$(\gamma_j^{(m)}) \equiv \text{argmin}_{(\gamma_j)} \|\mathbf{r}' - \sum_{j=1}^{\ell} \gamma_j\, \mathbf{A}^j\, \mathbf{r}'\|_2,$$

Compute $\mathbf{A}\mathbf{r}'$, $\mathbf{A}^2\,\mathbf{r}'$, . . . , $\mathbf{A}^\ell\,\mathbf{r}'$ explicitly.

With $\mathbf{R} \equiv \left[\mathbf{A}\mathbf{r}', \ldots, \mathbf{A}^\ell\,\mathbf{r}'\right]$, $\vec{\gamma}_m \equiv (\gamma_1^{(m)}, \ldots, \gamma_\ell^{(m)})^{\mathsf{T}}$ we have

[Normal Equations, use Choleski] $(\mathbf{R}^*\mathbf{R})\vec{\gamma}_m = \mathbf{R}^*\mathbf{r}'$

BiCGstab(ℓ)

$\mathbf{x} = \mathbf{0}$, $\mathbf{r} = [\,\mathbf{b}\,]$. Choose $\widetilde{\mathbf{r}}$.
$\mathbf{u} = [\,\mathbf{0}\,]$, $\gamma_\ell = \sigma = 1$.

While $\|\,\mathbf{r}\,\| > tol$ do

$\quad \sigma \leftarrow -\gamma_\ell\,\sigma$

$\quad$ For $j = 1$ to ℓ do

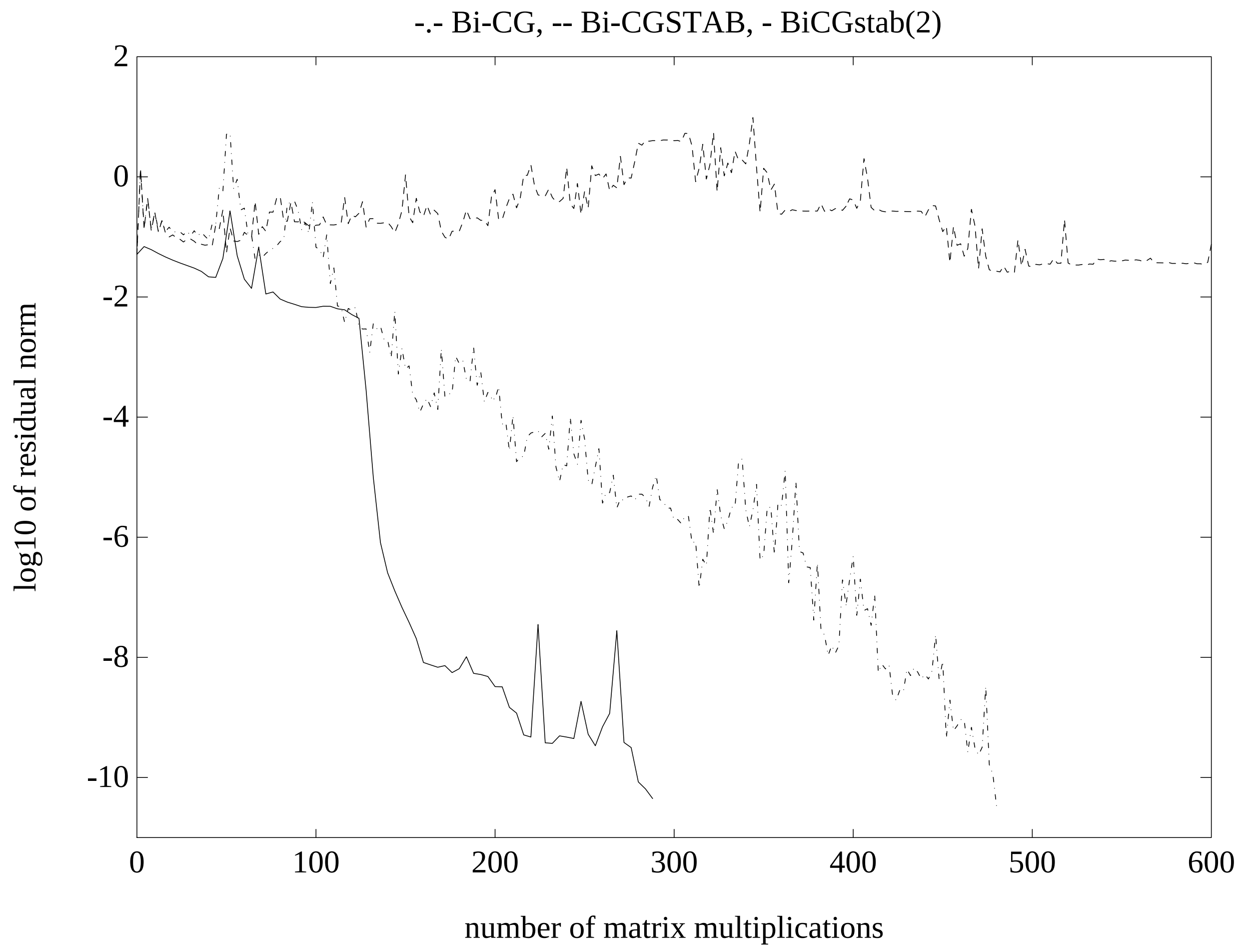
$\quad\quad \rho = (\mathbf{r}_j, \widetilde{\mathbf{r}})$, $\quad \beta = \rho/\sigma$
$\quad\quad \mathbf{u} \leftarrow \mathbf{r} - \beta\,\mathbf{u}$, $\quad \mathbf{u} \leftarrow [\,\mathbf{u}, \mathbf{A}\mathbf{u}_j\,]$
$\quad\quad \sigma = (\mathbf{u}_{j+1}, \widetilde{\mathbf{r}})$, $\quad \alpha = \rho/\sigma$
$\quad\quad \mathbf{r} \leftarrow \mathbf{r} - \alpha\,\mathbf{u}_{2:j+1}$, $\quad \mathbf{r} \leftarrow [\,\mathbf{r}, \mathbf{A}\mathbf{r}_j\,]$
$\quad\quad \mathbf{x} \leftarrow \mathbf{x} + \alpha\,\mathbf{u}_1$

$\quad$ end for

$\quad \mathbf{R} \equiv \mathbf{r}_{2:\ell+1}$. Solve $(\mathbf{R}^*\mathbf{R})\vec{\gamma} = \mathbf{R}^*\mathbf{r}_1$ for $\vec{\gamma}$
$\quad \mathbf{u} \leftarrow [\,\mathbf{u}_1 - (\gamma_1\mathbf{u}_2 + \ldots + \gamma_\ell\mathbf{u}_{\ell+1})\,]$
$\quad \mathbf{r} \leftarrow [\,\mathbf{r}_1 - (\gamma_1\mathbf{r}_2 + \ldots + \gamma_\ell\mathbf{r}_{\ell+1})\,]$
$\quad \mathbf{x} \leftarrow \mathbf{x} + (\gamma_1\mathbf{r}_1 + \ldots + \gamma_\ell\mathbf{r}_\ell)$

end while

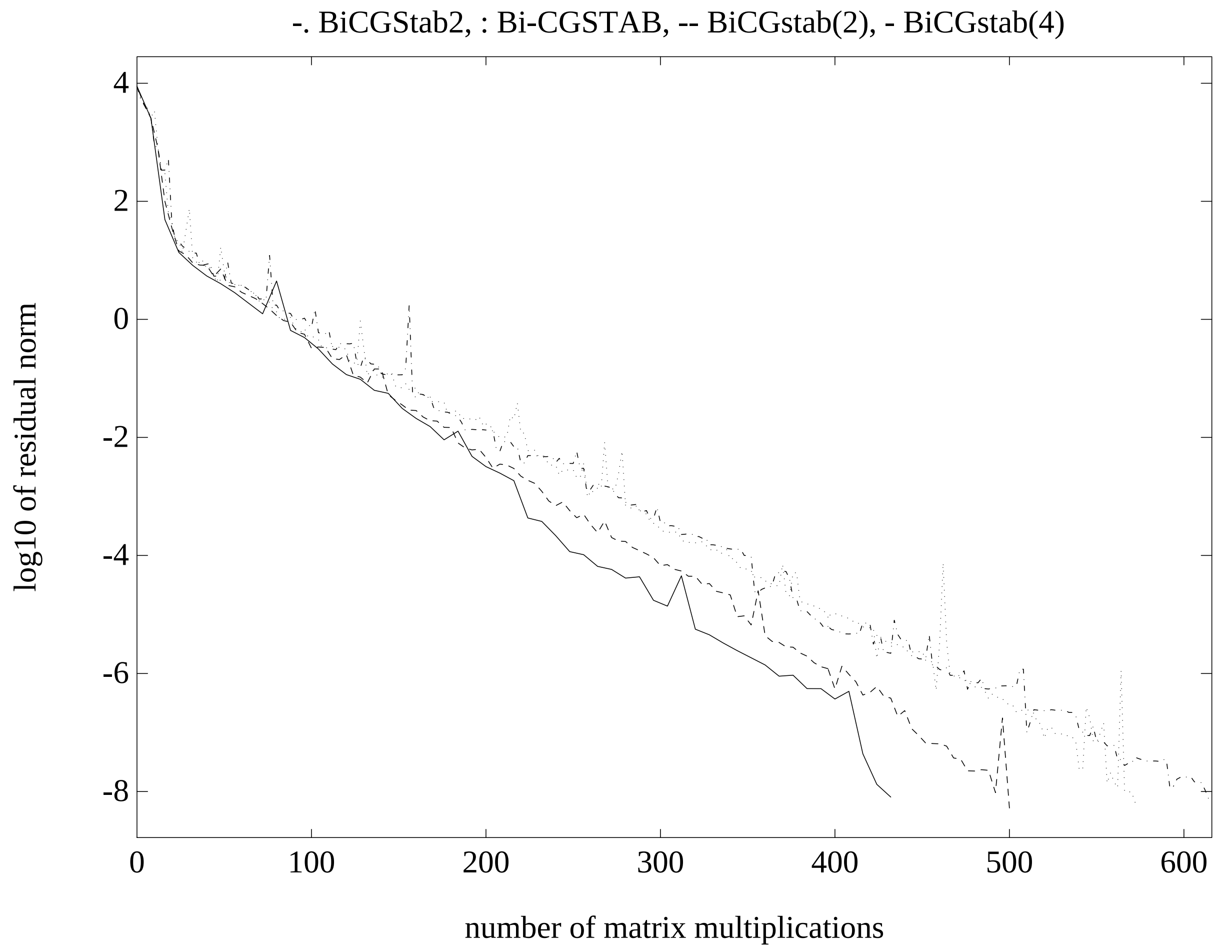
```
epsilon = 10^(-16);  ell = 4;
x = zeros(b);   rt = rand(b);
sigma = 1;   omega = 1;   u = zeros(b);

y = MV(x);  r = b-y;

norm = r'*r;   nepsilon = norm*epsilon^2;   L = 2:ell+1;
while norm > nepsilon
   sigma = -omega*sigma;  y = r;
   for j = 1:ell
        rho = rt'*y;         beta = rho/sigma;
        u = r-beta*u;
        y = MV(u(:,j));   u(:,j+1) = y;
        sigma = rt'*y;    alpha = rho/sigma;
        r = r-alpha*u(:,2:j+1);
        x = x+alpha*u(:,1);
        y = MV(r(:,j));   r(:,j+1) = y;
   end

   G = r'*r;   gamma = G(L,L)\G(L,1);   omega = gamma(ell);
   u = u*[1;-gamma];  r = r*[1;-gamma];  x = x+r*[gamma;0];
   norm = r'*r;
end
```



$$u_{xx} + u_{yy} + u_{zz} + 1000u_x = f.$$

f s.t. $u(x,y,z) = \exp(xyz)\sin(\pi x)\sin(\pi y)\sin(\pi z)$.

$(52 \times 52 \times 52)$ volumes. No preconditioning.

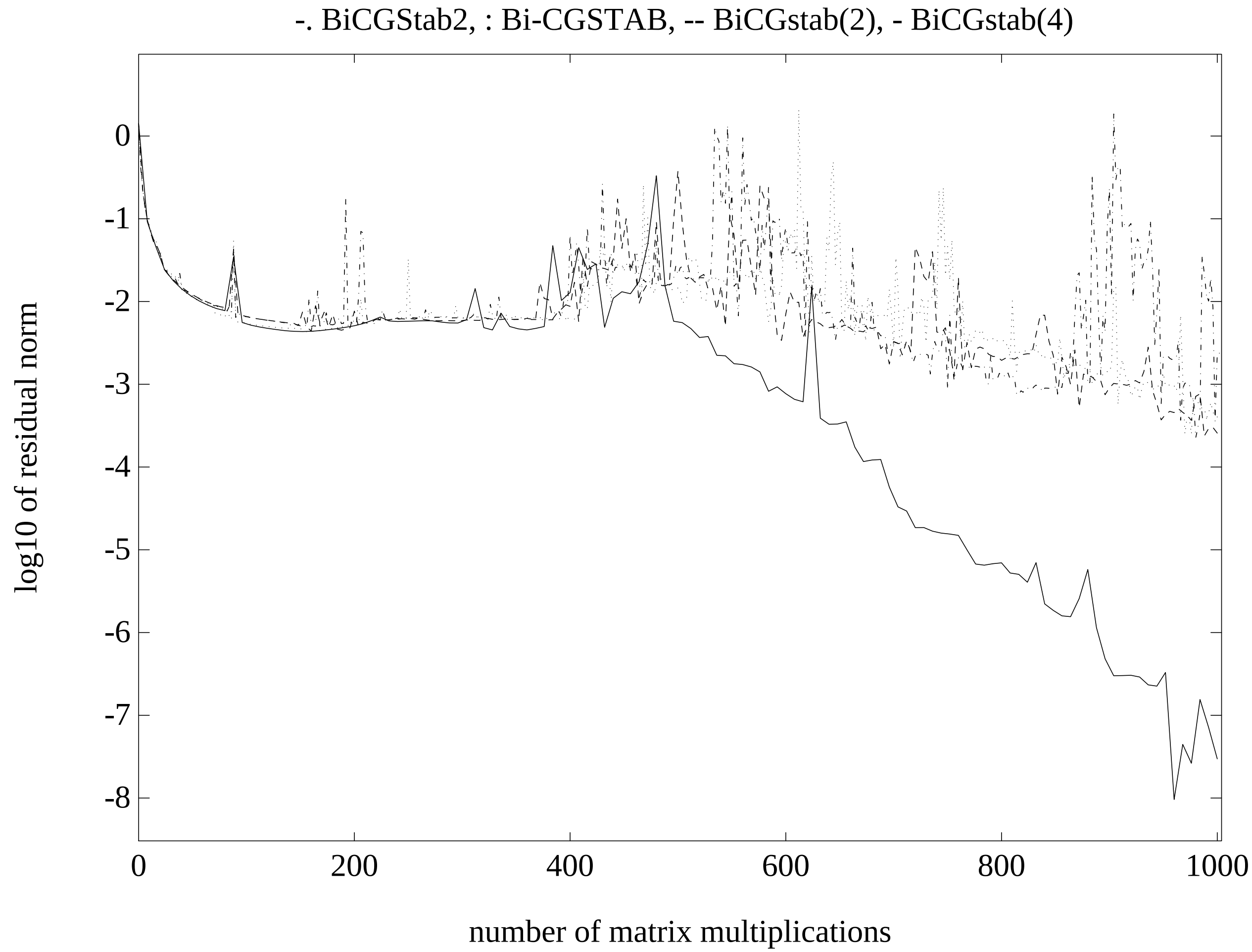


$$-(a\,u_x)_x - (a\,u_y)_y = 1 \text{ on } [0,1]\times[0,1].$$

$a = 1000$ for $0.1 \le x, y \le 0.9$ and $a = 1$ elsewhere.

Dirichlet BC on $y = 0$, Neumann BC on other parts of Boundary.

200×200 volumes. ILU Decomp.

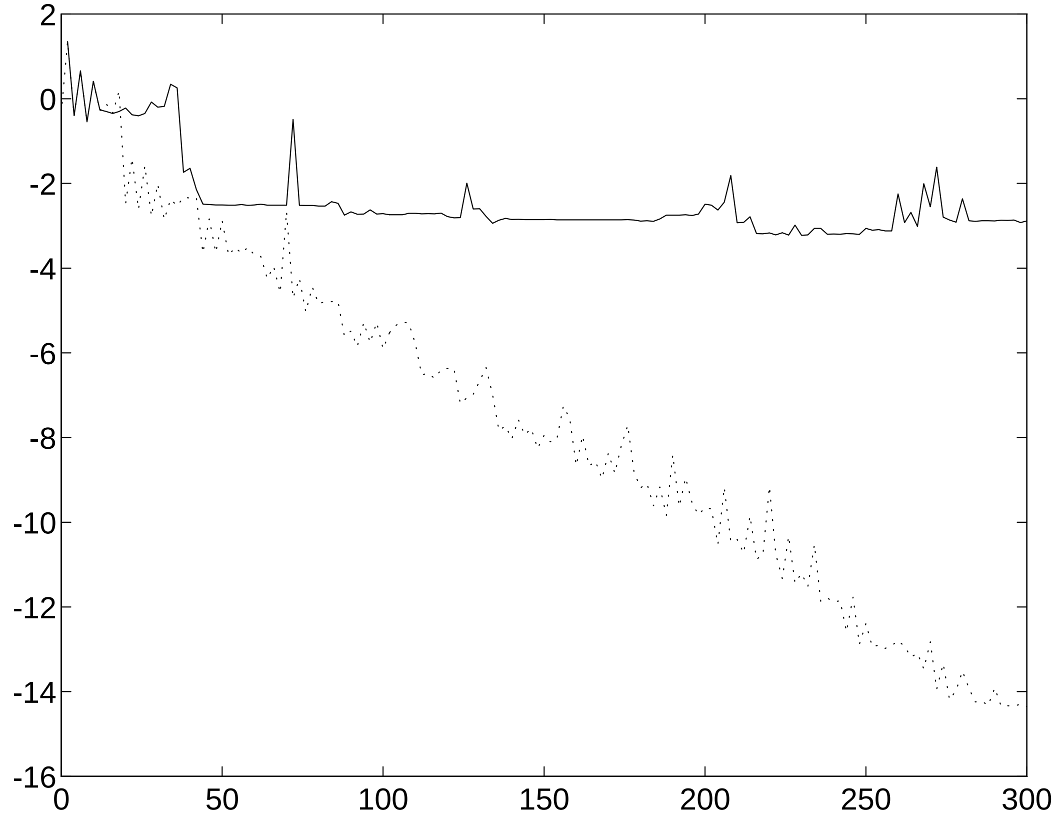


$$-\epsilon(u_{xx}+u_{yy})+a(x,y)u_x+b(x,y)u_y=0 \text{ on } [0,1]\times[0,1], \text{ Dirichlet BC}$$

$$\epsilon=10^{-1}, \quad a(x,y)=4x(x-1)(1-2y), \quad b(x,y)=4y(1-y)(1-2x),$$

$$u(x,y)=\sin(\pi x)+\sin(13\pi x)+\sin(\pi y)+\sin(13\pi y)$$

(201×201) volumes, no preconditioning.



$$u_{xx} + u_{yy} + u_{zz} + 1000\, u_x = f.$$

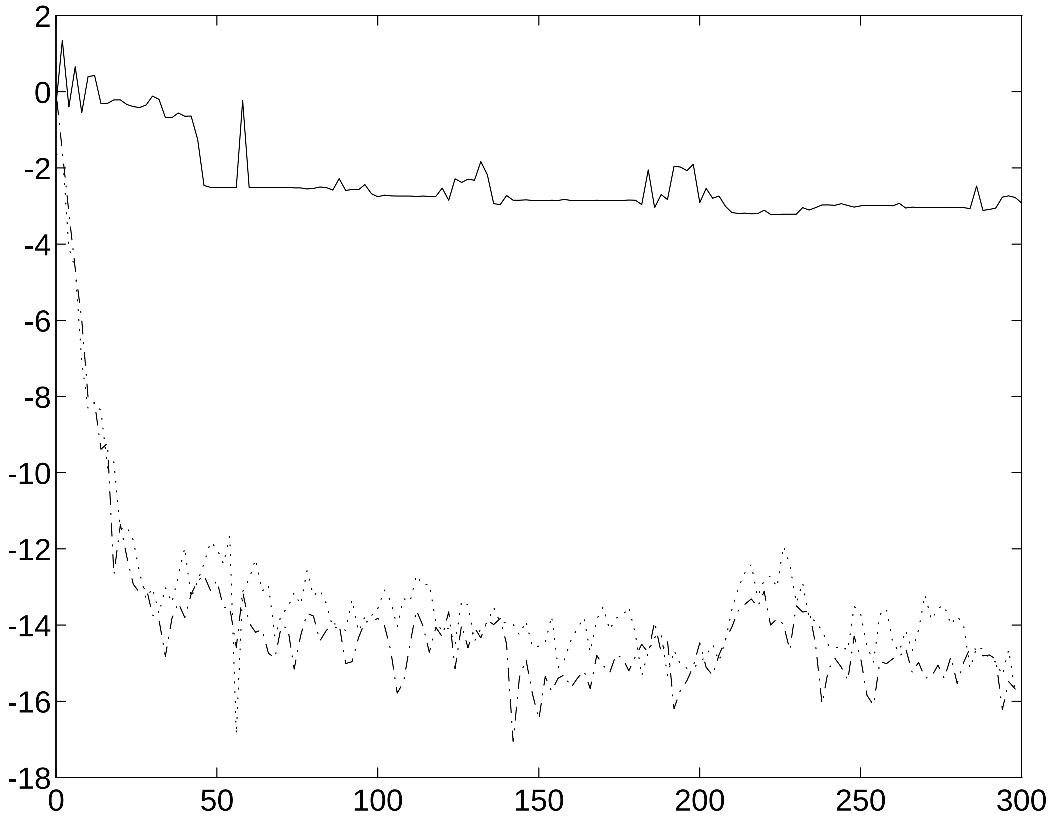
f is defined by the solution

$$u(x, y, z) = \exp(xyz)\sin(\pi x)\sin(\pi y)\sin(\pi z).$$

($10 \times 10 \times 10$) volumes. No preconditioning .

Accurate Bi-CG coefficients

$$|\epsilon| \leq n\,\overline{\xi}\,\frac{\|\,\mathbf{r}_k\,\|_2\,\|\,\widetilde{\mathbf{r}}_0\|_2}{|(\mathbf{r}_k, \widetilde{\mathbf{r}}_0)|} \quad = \frac{n\,\overline{\xi}}{\widehat{\rho}_k} \quad \text{where} \quad \widehat{\rho}_k \equiv \frac{|(\mathbf{r}_k, \widetilde{\mathbf{r}}_0)|}{\|\,\mathbf{r}_k\|_2\,\|\,\widetilde{\mathbf{r}}_0\|_2}$$



Why using pol. factors of degree ≥ 2?

Hybrid **Bi-CG**, that is faster than **Bi-CGSTAB**

1 sweep **BiCGstab**(ℓ) versus ℓ steps **Bi-CGSTAB**:

- Reduction with MR-polynomial of degree ℓ is better than $\ell\times$ MR-pol. of degr. 1.
- MR-polynomial of degree ℓ contributes only once to an increase of $\widehat{\rho}_k$

Why not?

- Efficiency:
  $1.75 + 0.25 \cdot \ell$ DOT/MV, $\quad 2.5 + 0.5 \cdot \ell$ AXPY/MV
  Storage: $\quad 2\ell + 5$ large vector.

- Loss of accuracy:

$$\Big|\|\mathbf{r}_k\| - \|\mathbf{b} - \mathbf{A}\mathbf{x}_k\|\Big| \leq \ldots + c\,\bar{\xi}\,\max\Big(|\gamma_i|\,\Big\|\,|\mathbf{A}|\,|\mathbf{A}^{i-1}\widehat{\mathbf{r}}|\,\Big\|\Big)$$

- break-downs are possible

Properties Bi-CG

Advantages

- Usually selects good approximations from the search subspaces (Krylov subspaces).
- 2 DOT, 5 AXPY per step.
- Storage: 8 large vectors.
- No knowledge on properties of $\mathbb{A}$ is needed.

Drawbacks

- ◦ Non-optimal Krylov subspace method.
- Not robust: **Bi-CG** may break down.
- **Bi-CG** is sensitive to evaluation errors (often loss of super-linear convergence).
- ◦ Convergence depends on **shadow** residual $\widetilde{\mathbf{r}}_0$.
- 2 MV needed to expand search subspace.
- 1 MV is by $\mathbf{A}^*$.

Program Lecture 8

- **CG**
- **Bi-CG**
- Bi-Lanczos
- Hybrid **Bi-CG**
- **Bi-CGSTAB**, **BiCGstab**(ℓ)
- **IDR**

Hybrid Bi-CG

Notation. If p_k is a polynomial of exact degree k,

$\widetilde{\mathbf{r}}_0$ n-vector, let

$$\mathcal{S}(p_k, \mathbf{A}, \widetilde{\mathbf{r}}_0) \equiv \{p_k(\mathbf{A})\mathbf{v} \mid \mathbf{v} \perp \mathcal{K}_k(\mathbf{A}^*, \widetilde{\mathbf{r}}_0)\}$$

Theorem. Hybrid **Bi-CG** find residuals $\mathbf{r}_k \in \mathcal{S}(p_k, \mathbf{A}, \widetilde{\mathbf{r}}_0)$.

Example.

Bi-CGSTAB: $\quad p_k(\lambda) = (1 - \omega_k \lambda)\, p_{k-1}(\lambda)$

where, in every step,

$\omega_k = \text{minarg}_\omega \|\mathbf{r} - \omega \mathbf{A}\mathbf{r}\|_2$, where $\mathbf{r} = p_{k-1}(\mathbf{A})\mathbf{v}$, $\mathbf{v} = \mathbf{r}_k^{\text{Bi-CG}}$

Hybrid Bi-CG

Notation. If p_k is a polynomial of exact degree k,

$\widetilde{\mathbf{r}}_0$ n-vector, let

$$\mathcal{S}(p_k, \mathbf{A}, \widetilde{\mathbf{r}}_0) \equiv \{p_k(\mathbf{A})\mathbf{v} \mid \mathbf{v} \perp \mathcal{K}_k(\mathbf{A}^*, \widetilde{\mathbf{r}}_0)\}$$

Theorem. Hybrid **Bi-CG** find residuals $\mathbf{r}_k \in \mathcal{S}(p_k, \mathbf{A}, \widetilde{\mathbf{r}}_0)$.

Example.

BiCGstab(ℓ): $\quad p_k(\lambda) = (1 - \omega_k\lambda)\, p_{k-1}(\lambda)$

where, every ℓth step

$\vec{\gamma} = \text{minarg}_{\vec{\gamma}} \|\mathbf{r} - [\mathbf{Ar}, \ldots, \mathbf{A}^\ell\mathbf{r}]\vec{\gamma}\|_2$, where $\mathbf{r} = p_{k-\ell}(\mathbf{A})\mathbf{r}_k^{\text{Bi-CG}}$.

$(1 - \gamma_1\lambda - \ldots - \gamma_\ell\lambda^\ell) = (1 - \omega_k\lambda) \cdot \ldots \cdot (1 - \omega_{k-\ell}\lambda)$

Induced Dimension Reduction

Definition. If p_k is a polynomial of exact degree k, $\widetilde{\mathbf{R}} \equiv \widetilde{\mathbf{R}}_0 = [\,\tilde{\mathbf{r}}_1, \ldots, \tilde{\mathbf{r}}_s\,]$ an $n \times s$ matrix, then

$$\mathcal{S}(p_k, \mathbf{A}, \widetilde{\mathbf{R}}) \equiv \left\{ p_k(\mathbf{A})\mathbf{v} \mid \mathbf{v} \perp \mathcal{K}_k(\mathbf{A}^*, \widetilde{\mathbf{R}}) \right\},$$

is the p_k-**Sonneveld** subspace. Here

$$\mathcal{K}_k(\mathbf{A}^*, \widetilde{\mathbf{R}}) \equiv \left\{ \sum_{j=0}^{k-1} (\mathbf{A}^*)^j \, \widetilde{\mathbf{R}} \, \vec{\gamma}_j \mid \vec{\gamma}_j \in \mathbb{C}^s \right\}.$$

Theorem. **IDR** find residuals $\mathbf{r}_k \in \mathcal{S}(p_k, \mathbf{A}, \widetilde{\mathbf{R}})$.

Example.

Bi-CGSTAB: $\quad p_k(\lambda) = (1 - \omega_k \lambda)\, p_{k-1}(\lambda)$

where, in every step,

$\omega_k = \text{minarg}_\omega \|\mathbf{r} - \omega \mathbf{A}\mathbf{r}\|_2$, where $\mathbf{r} = p_{k-1}(\mathbf{A})\mathbf{v}$, $\mathbf{v} = \mathbf{r}_k^{\text{Bi-CG}}$

[van Gijzen Sonneveld 07]

IDR

Select an $\mathbf{x}_0$.

Select $n \times s$ matrices $\mathbf{U}$ and $\widetilde{\mathbf{R}}$.

Compute $\mathbf{C} \equiv \mathbf{A}\mathbf{U}$.

$\mathbf{x} = \mathbf{x}_0$, $\mathbf{r} - \mathbf{b} - \mathbf{A}\mathbf{x}$, $j = s$, $i = 1$

while $\|\mathbf{r}\| > \mathit{tol}$ do

  Solve $\widetilde{\mathbf{R}}^* \mathbf{C}\vec{\gamma} = \widetilde{\mathbf{R}}^* \mathbf{r}$ for $\vec{\gamma}$

  $\mathbf{v} = \mathbf{r} - \mathbf{C}\vec{\gamma}$, $\mathbf{s} = \mathbf{A}\mathbf{v}$

  $j{+}{+}$, if $j > s$, $\omega = \mathbf{s}^*\mathbf{v}/\mathbf{s}^*\mathbf{s}$, $j = 0$

  $\mathbf{U}e_i \leftarrow \mathbf{U}\vec{\gamma} + \omega\mathbf{v}$, $\mathbf{x} = \mathbf{x} + \mathbf{U}e_i$

  $\mathbf{r}_0 = \mathbf{r}$, $\mathbf{r} = \mathbf{v} - \omega\mathbf{s}$, $\mathbf{C}e_i = \mathbf{r}_0 - \mathbf{r}$

  $i{+}{+}$, if $i > s$, $i = 1$

end while

Select $n \times \ell$ matricex $\mathbf{U}$ and $\widetilde{\mathbf{R}}$

Experiments suggest $\widetilde{\mathbf{R}} = \mathtt{qr}(\text{rand}(n, \ell), 0)$

$\mathbf{U}$ and $\mathbf{C}$ can be constructed from ℓ steps of **GCR**.

We will discuss IDR in more detail in Lecture 11.

See also Exercise 11.1–Exercise 11.5.