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The main effects of rounding errors in Krylov solvers for symmetric linear systems

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Program

$$\mathbf{A}\mathbf{x}=\mathbf{b} \quad \text{with} \quad \mathbf{A}=\mathbf{A}^{\mathsf{T}}$$

- Introduction & numerical examples
- MINRES versus GMRES
- CG
- SYMMLQ
- Conclusions

Notation: $\|\cdot\| = \|\cdot\|_2$, $\quad \kappa_2(\mathbf{A}) = \|\mathbf{A}\|\,\|\mathbf{A}^{-1}\|$

Assumptions (for the purpose of this talk):

$\mathbf{x}_0 = 0$, $\quad \mathbf{r}_0 = \mathbf{b}$, $\quad \|\mathbf{r}_0\| = 1$

$\mathbf{A}\mathbf{y} = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ $\quad\quad \mathbf{A}\mathbf{y} = \mathbf{b}/\|\mathbf{b}\|$

$\mathbf{x} = \mathbf{x}_0 + \mathbf{y}$ $\quad\quad \mathbf{x} = \|\mathbf{b}\|\,\mathbf{y}$

$$\mathbf{A}\mathbf{x}=\mathbf{b}, \quad \mathbf{A}^{\mathsf{T}}=\mathbf{A}$$

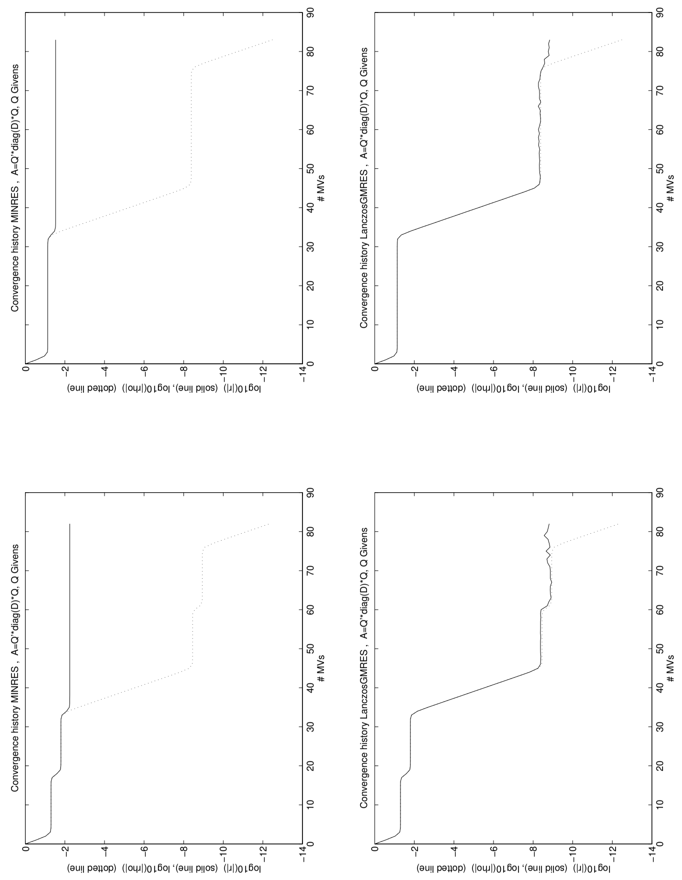
Numerical examples

I. $\mathbf{A} = \mathbf{G}\,\mathrm{diag}(10^{-8}, 2\,10^{-8}, 2:h:3)\,\mathbf{G}^{\mathsf{T}}$
with $h = 1/789$ and $\mathbf{G}$ Givens rotation (45°) in $(1,30)$-plane.

II. $\mathbf{A} = \mathbf{G}\,\mathrm{diag}(-10^{-8}, 10^{-8}, 2:h:3)\,\mathbf{G}^{\mathsf{T}}$
with $h = 1/389$ and $\mathbf{G}$ Givens rotation (45°) in $(1,30)$-plane.

$\mathbf{A}$ ill-conditioned, $\kappa_2(\mathbf{A}) = 3\,10^8$, non-diag., sparse.
In I: $\mathbf{A}$ is pos. def. In II: $\mathbf{A}$ is non-def.

$\mathbf{b} = (1,1,\dots,1)^{\mathsf{T}}$, $\quad \mathbf{x}_0 = (0,0,\dots,0)^{\mathsf{T}}$



Problems

Why is MINRES unstable?

Least square system is solved?

Modified Gram-Schmidt is unstable?

Lanczos is unstable?

What about other methods?

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

What is stable?

Suppose $\mathbf{x}$ is exact known. Then,

in rounded arithmetic, $\mathbf{u}$ rel.mach. precision,

$$\Delta\mathbf{r} = \mathbf{b} - \widehat{\mathbf{A}\mathbf{x}}$$

$$|\Delta\mathbf{r}| \leq n_A\,\mathbf{u}\,|\mathbf{A}|\,|\mathbf{x}|, \qquad n_A = \max_i \#\{j | a_{ij} \neq 0\}$$

$$\|\Delta\mathbf{r}\| \leq n_A^{3/2}\,\mathbf{u}\,\kappa_2(\mathbf{A})\,\|\mathbf{b}\|$$

$\|\Delta\mathbf{r}\|$ of order

- $\mathbf{u}\,\kappa_2(\mathbf{A})\,\|\mathbf{b}\|$ is acceptable
- say, $\mathbf{u}\,\kappa_2(\mathbf{A})^2\,\|\mathbf{b}\|$ is not acceptable

[Lanczos '50]

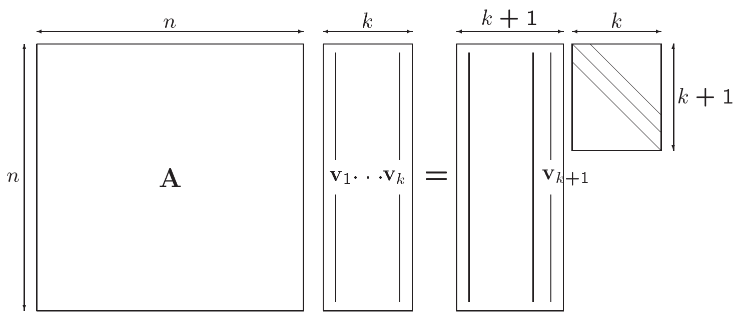
Lanczos

$\mathbf{r}_0 = \mathbf{b}, \qquad \mathbf{v}_1 = \mathbf{r}_0$

$\tilde{\mathbf{v}} = \mathbf{A}\mathbf{v}_k - \alpha_k\mathbf{v}_k \qquad \alpha_k$ s.t. $\tilde{\mathbf{v}} \perp \mathbf{v}_k$

$\tilde{\mathbf{v}} = \tilde{\mathbf{v}} - \beta_{k-1}\mathbf{v}_{k-1} \qquad \beta_{k-1}$ s.t. $\tilde{\mathbf{v}} \perp \mathbf{v}_{k-1}$

$\beta_k = \|\tilde{\mathbf{v}}\|, \qquad \mathbf{v}_{k+1} = \tilde{\mathbf{v}}/\beta_k$

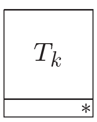


$\mathbf{A} \qquad \mathbf{V}_k \quad = \quad \mathbf{V}_{k+1} \qquad \underline{T}_k$

$\mathbf{V}_k \qquad n \times k$ orthonormal (in exact arithm.),

$\underline{T}_k \qquad$ tri-diagonal $(k+1) \times k$,

$T_k \qquad k \times k$ upper block of $\underline{T}_k$. $\qquad \underline{T}_k =$



$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{T}_k$

MINRES & GMRES

$$\mathbf{x}_k = \mathbf{V}_k y_k$$

Minimize $\quad \|\mathbf{r}_0 - \mathbf{A}\mathbf{V}_k\,y_k\|$

$$= \left\|\,\mathbf{V}_{k+1}e_1 - \mathbf{V}_{k+1}\,\underline{T}_k\,y_k\right\|$$

$$= \|\,e_1 - \underline{T}_k\,y_k\|$$

Solve $\quad \underline{T}_k\,y_k = e_1 \quad$ in least square sense.

$$\underline{T}_k = \underline{Q}_k\,R_k$$

$\underline{Q}_k \quad (k+1) \times k$ orth. (product Givens rot.)

$R_k \quad k \times k$ upper Δ, tri-diagonal.

GMRES: $\quad \mathbf{x}_k = \mathbf{V}_k(R_k^{-1}z_k)$

with $z_k = \underline{Q}_k^T e_1$

MINRES: $\quad \mathbf{x}_k = (\mathbf{V}_k\,R_k^{-1})z_k$

GMRES: $\mathbf{x}_k = \mathbf{V}_k(R_k^{-1} z_k)$
MINRES: $\mathbf{x}_k = (\mathbf{V}_k\, R_k^{-1}) z_k$

$\|\mathbf{r}_k\| = \rho_k$ where $\rho_k = |\sin_1 \cdot \ldots \cdot \sin_k|$

MINRES: Use $\mathbf{W}_k = [\mathbf{w}_1, \ldots, \mathbf{w}_k] = \mathbf{V}_k R_k^{-1}$.

Solve $\mathbf{W}_k R_k = \mathbf{V}_k$: R_k upper Δ., tri-diag.

$\mathbf{w}_k$ solution inhom. 3-term recurrence

& $\mathbf{x}_k = \mathbf{x}_{k-1} + \rho_{k-1} \cos_k \mathbf{w}_k$

MINRES:

+: efficient use of memory

-: instable for ill-conditioned $\mathbf{A}$ $\Leftarrow$

GMRES:

-: memory requirements prop. k

+: stable also for ill-conditioned $\mathbf{A}$ $\Leftarrow$

GMRES: $\mathbf{x}_k = \mathbf{V}_k(R_k^{-1} z_k) = \mathbf{V}_k y_k$
MINRES: $\mathbf{x}_k = (\mathbf{V}_k\, R_k^{-1}) z_k = \mathbf{W}_k z_k$

In rounded arithmetic: $\mathbf{u}$ rel. mach. prec.

$$\widehat{\alpha\beta} = (\alpha + \xi\alpha)\beta = \alpha(\beta + \xi\beta), \qquad |\xi| \leq \mathbf{u}$$

$$\begin{aligned} \widehat{\alpha\mathbf{w}} &= \alpha(\mathbf{w} + \Delta\mathbf{w}), \qquad |\Delta\mathbf{w}| \leq \mathbf{u}\,|\mathbf{w}| \\ &\neq (\alpha + \xi\alpha)\mathbf{w} \end{aligned}$$

Scalar recurrence:

$$(R_k + \Delta_R)\widehat{y}_k = z_k$$

with $|\Delta_R| \leq 3\,\mathbf{u}\,|R_k| + \mathcal{O}(\mathbf{u}^2)$

Vector recurrence:

$$\widehat{\mathbf{W}}_k R_k = \mathbf{V}_k + \Delta_V$$

with
$$\begin{aligned} |\Delta_V| &\leq 3\,\mathbf{u}\,|\widehat{\mathbf{W}}_k|\,|R_k| + \mathcal{O}(\mathbf{u}^2) \\ &\leq 3\,\mathbf{u}\,|\mathbf{V}_k R_k^{-1}|\,|R_k| + \mathcal{O}(\mathbf{u}^2) \end{aligned}$$

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{T}_k, \qquad \underline{T}_k = \underline{Q}_k\, R_k$$

$\boxed{\text{GMRES:} \quad \mathbf{x}_k = \mathbf{V}_k(R_k^{-1} z_k) = \mathbf{V}_k y_k}$

MINRES: $\mathbf{x}_k = (\mathbf{V}_k\, R_k^{-1}) z_k$

In rounded arithmetic: $\mathbf{u}$ rel. mach. prec.

$$(R_k + \Delta_R)\widehat{y}_k = z_k$$

with $|\Delta_R| \leq 3\,\mathbf{u}\,|R_k| + \mathcal{O}(\mathbf{u}^2)$

$$\Delta y_k = -R_k^{-1}\Delta_R R_k^{-1} z_k$$

$$\Delta \mathbf{x}_k = -\mathbf{V}_k R_k^{-1}\Delta_R R_k^{-1} z_k$$

$$\Delta \mathbf{r}_k = \mathbf{A}\mathbf{V}_k R_k^{-1}\Delta_R R_k^{-1} z_k = \mathbf{V}_{k+1}\,\underline{Q}_k\,\Delta_R R_k^{-1} z_k$$

$$\boxed{\|\Delta\mathbf{r}_k\| \leq 3\sqrt{k+1}\,\mathbf{u}\,\kappa_2(\mathbf{A})}$$

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{T}_k, \qquad \underline{T}_k = \underline{Q}_k\, R_k$$

Theorem. $\|\,|R_k|\,\|\,\|R_k^{-1}\| \leq \sqrt{3}\,\kappa_2(\mathbf{A})$

$\|\,|R_k|\,\| \leq \sqrt{3}\,\|R_k\|$ [van der Sluis '69]

$$\begin{aligned} \sigma_j(R_k)^2 &= \lambda_j(R_k^{\mathsf{T}} R_k) = \lambda_j(R_k^{\mathsf{T}}\,\underline{Q}_k^{\mathsf{T}}\,\underline{Q}_k\,R_k) \\ &= \lambda_j(\underline{T}_k^{\mathsf{T}}\,\underline{T}_k) = \lambda_j(\underline{T}_k^{\mathsf{T}}\,\mathbf{V}_{k+1}^{\mathsf{T}}\mathbf{V}_{k+1}\,\underline{T}_k) \\ &= \lambda_j(\mathbf{V}_k^{\mathsf{T}}\mathbf{A}^{\mathsf{T}}\mathbf{A}\mathbf{V}_k) \end{aligned}$$

Use Cauchy's interlace theorem:

$$\sigma_{\min}(\mathbf{A}) \leq \sigma_j(R_k) \leq \sigma_{\max}(\mathbf{A})$$

Remark. $\sigma_{\min}(\mathbf{A}) \not\leq \sigma_j(T_k) \leq \sigma_{\max}(\mathbf{A})$

Ritz values (eigenv. T_k) can be 0

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{T}_k\,, \quad \underline{T}_k = \underline{Q}_k\,R_k$$

In rounded arithmetic:

Theorem. [Paige '71, Parlett '80]

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{T}_k + \Delta, \quad \|\Delta\| \leq \mathbf{u}\,\|\mathbf{A}\|$$

$\underline{T}_k$ tri-diag, $\quad \|\mathbf{V}_{k+1}\| \leq \sqrt{k+1}$

$$\|\mathbf{V}_{k+1}\| \leq \sqrt{m}$$

with m max. # "duplicated Ritz values"

(usually: $m \leq 3$)

QR-decomposition using Givens rotation:

errors small as compared to other sources of errors

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{T}_k\,, \quad \underline{T}_k = \underline{Q}_k\,R_k$$

GMRES: $\mathbf{x}_k = \mathbf{V}_k(R_k^{-1}z_k)$

$\boxed{\text{MINRES: } \mathbf{x}_k = (\mathbf{V}_k\,R_k^{-1})z_k = \mathbf{W}_k z_k}$

In rounded arithmetic: $\quad$ $\mathbf{u}$ rel. mach. prec.

$$\widehat{\mathbf{W}}_k R_k = \mathbf{V}_k + \Delta_V$$

with $\quad |\Delta_V| \leq 3\,\mathbf{u}\,|\mathbf{V}_k R_k^{-1}|\,|R_k| + \mathcal{O}(\mathbf{u}^2)$

$$\Delta\mathbf{x}_k = -\Delta_W z_k = -\Delta_V R_k^{-1} z_k$$

$$\Delta\mathbf{r}_k = \mathbf{A}\Delta_V R_k^{-1} z_k$$

$$|\Delta\mathbf{r}_k| \leq 3\,\mathbf{u}\,|\mathbf{A}|\,|\mathbf{V}_k R_k^{-1}|\,|R_k|\,|R_k^{-1}|\,|\mathbf{r}_0|$$

$$\boxed{\|\Delta\mathbf{r}_k\| \leq 3\sqrt{3k}\,\mathbf{u}\,\kappa_2(\mathbf{A})^2}$$

[Paige & Saunders '75]

MINRES

```
Choose x0
x = x0,  r = b − Ax,  ρ = ‖r‖,  v = r/ρ
β = 0,  β̃ = 0,  c = −1,  s = 0
v_old = 0,  w = 0,  w̃̃ = v,  κ = ρ
while  |ρ| > tol  do
    ṽ ← A v − β v_old
    α ← v* ṽ,  ṽ ← ṽ − α v
    β ← ‖ṽ‖,  v_old ← v,  v ← ṽ/β

    l1 ← s α − c β̃,  l2 ← s β
    α̃ ← −s β̃ − c α,  β̃ ← c β
    l0 ← sqrt(α̃² + β²),  c ← α̃/l0,  s ← β/l0
    w̃ ← w̃̃ − l1 w,  w̃̃ ← v − l2 w,  w ← w̃/l0
    x ← x + (ρ c) w,  ρ ← s ρ
end while
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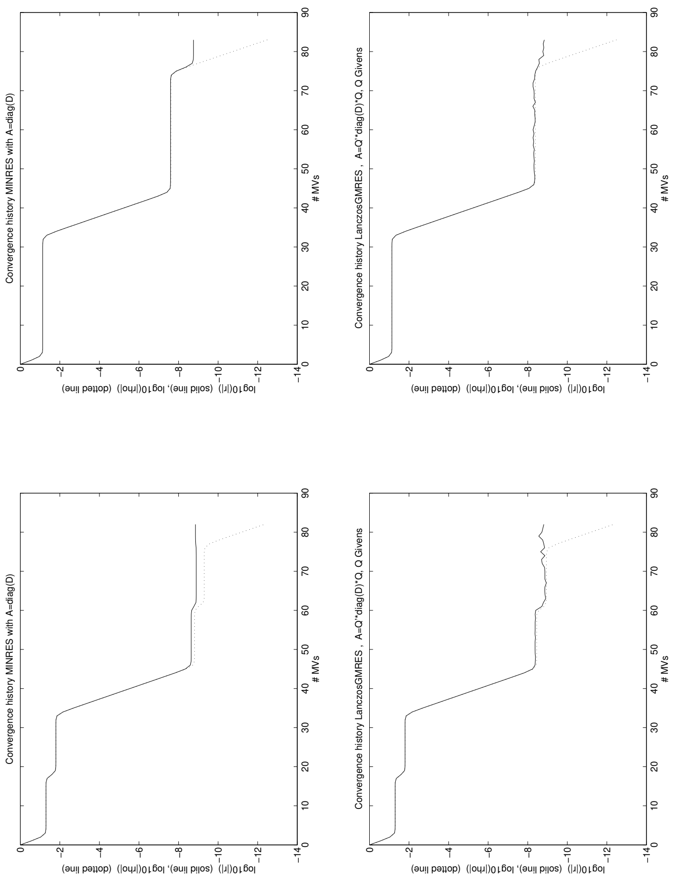


GMRES: $\mathbf{x}_k = \mathbf{V}_k(R_k^{-1} z_k) = \mathbf{V}_k y_k$

MINRES: $\mathbf{x}_k = (\mathbf{V}_k\, R_k^{-1}) z_k = \mathbf{W}_k z_k$

In rounded arithmetic: $\quad$ $\mathbf{u}$ rel. mach. prec.

$$\widehat{\alpha\beta} = (\alpha + \xi\alpha)\beta = \alpha(\beta + \xi\beta), \qquad |\xi| \le \mathbf{u}$$

$$\begin{aligned} \widehat{\alpha\mathbf{w}} &= \alpha(\mathbf{w} + \Delta\mathbf{w}), \qquad |\Delta\mathbf{w}| \le \mathbf{u}\,|\mathbf{w}| \\ &\neq (\alpha + \xi\alpha)\mathbf{w} \end{aligned}$$

Scalar recurrence:

$$(R_k + \Delta_R)\widehat{y}_k = z_k$$

with $\quad |\Delta_R| \le 3\,\mathbf{u}\,|R_k| + \mathcal{O}(\mathbf{u}^2)$

Vector recurrence: for the jth row vector

$$(\widehat{\mathbf{W}}_k)_j (R_k + \Delta_R^{(j)}) = (\mathbf{V}_k)_j = e_j^{\mathsf{T}} \mathbf{V}_k$$

with $\quad |\Delta_R^{(j)}| \le 3\,\mathbf{u}\,|R_k| + \mathcal{O}(\mathbf{u}^2)$

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\, \underline{T}_k\,, \qquad \underline{T}_k = \underline{Q}_k\, R_k$$

GMRES: $\mathbf{x}_k = \mathbf{V}_k(R_k^{-1} z_k)$

$\boxed{\text{MINRES: } \mathbf{x}_k = (\mathbf{V}_k\, R_k^{-1}) z_k = \mathbf{W}_k z_k}$

In rounded arithmetic: $\quad$ $\mathbf{u}$ rel. mach. prec.

$$(e_j^{\mathsf{T}} \widehat{\mathbf{W}}_k)(R_k + \Delta_R^{(j)}) = e_j^{\mathsf{T}} \mathbf{V}_k$$

with $\quad |\Delta_R^{(j)}| \le 3\,\mathbf{u}\,|R_k| + \mathcal{O}(\mathbf{u}^2)$

For the jth coordinate:

$$\Delta\mathbf{x}_{jk} = e_j^{\mathsf{T}} \mathbf{V}_k R_k^{-1} \Delta_R^{(j)} R_k^{-1} z_k$$

If $\mathbf{A}$ diagonal:

$$\begin{aligned} \Delta\mathbf{r}_{jk} &= -e_j^{\mathsf{T}} \mathbf{A}\mathbf{V}_k R_k^{-1} \Delta_R^{(j)} R_k^{-1} z_k \\ &= e_j^{\mathsf{T}} \mathbf{V}_{k+1}\, \underline{Q}_k\, \Delta_R^{(j)} R_k^{-1} z_k \end{aligned}$$

$$\boxed{\|\Delta\mathbf{r}_k\| \le 3\,\sqrt{k+1}\,\mathbf{u}\,\kappa_2(\mathbf{A})}$$

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\, \underline{T}_k\,, \qquad \underline{T}_k = \underline{Q}_k\, R_k$$

SYMMLQ

$$\mathbf{x}_k = \mathbf{A}\mathbf{V}_k y_k$$

Minimize $\quad \|\mathbf{x} - \mathbf{x}_0 - \mathbf{A}\mathbf{V}_k\, y_k\|$

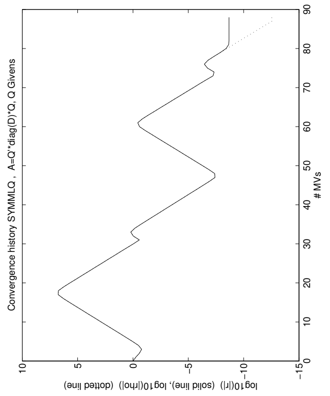
$$\begin{aligned} &\Leftrightarrow\ \mathbf{x} - \mathbf{x}_0 - \mathbf{A}\mathbf{V}_k y_k \perp \mathbf{A}\mathbf{V}_k \\ &\Leftrightarrow\ \mathbf{V}_k^{\mathsf{T}}(\mathbf{r}_0 - \mathbf{A}^{\mathsf{T}}\mathbf{A}\mathbf{V}_k y_k) = 0 \\ &\Leftrightarrow\ (\mathbf{A}\mathbf{V}_k)^{\mathsf{T}}(\mathbf{A}\mathbf{V}_k) y_k = \underline{T}_k^{\mathsf{T}}\, \underline{T}_k\, y_k \\ &\qquad = R_k^{\mathsf{T}} R_k y_k = e_1 \end{aligned}$$

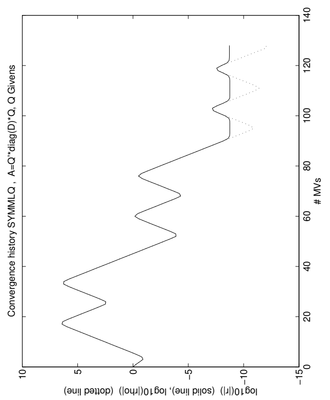
SYMMLQ:

$$\begin{aligned} \mathbf{x}_k &= \mathbf{A}\mathbf{V}_k R_k^{-1} R_k^{-\mathsf{T}} e_1 \\ &= \left(\mathbf{V}_{k+1}\, \underline{Q}_k\right)\left(R_k^{-\mathsf{T}} e_1\right) \end{aligned}$$

+: efficient use of memory

+: stable also for ill-conditioned $\mathbf{A}$ $\Leftarrow$





$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\,\underline{T}_k, \qquad \underline{T}_k = \underline{Q}_k\,R_k$$

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

$$R_k^{\mathsf{T}} g = e_1, \qquad \Delta g = -R_k^{-\mathsf{T}}\Delta_L R_k^{-\mathsf{T}} e_1$$

with $\quad |\Delta_L| \le 3\,\mathbf{u}\,|R_k^{\mathsf{T}}| + \mathcal{O}(\mathbf{u})^2$

Problem: $\quad \mathbf{A}\mathbf{V}_{k+1}\,\underline{Q}_k\,\Delta g = \mathbf{V}_{k+2}\,\underline{T}_{k+1}\,\underline{Q}_k\,\Delta g$

$$= \mathbf{V}_k R_k^{\mathsf{T}}\Delta g + [\mathbf{v}_{k+1}, \mathbf{v}_{k+2}]\begin{bmatrix} * \\ * \end{bmatrix}$$

$$\Delta\mathbf{r}_k = \mathbf{V}_k R_k^{\mathsf{T}}\Delta g + [\mathbf{v}_{k+1}, \mathbf{v}_{k+2}]\left(\widehat{t}_k - t_k\right)$$

with $t_k = M_k \begin{bmatrix} g_{k-1} \\ g_k \end{bmatrix}$, M_k a 2×2 subbl. R_{k+2}^{T}

$$\boxed{\|\Delta\mathbf{r}_k\| \le 3\sqrt{3k}\,\mathbf{u}\,\kappa_2(\mathbf{A}) + \|\widehat{t}_k - t_k\|}$$

$$R_k^{\mathsf{T}} g = e_1$$

$\Delta g = -R_k^{-\mathsf{T}}\Delta_L R_k^{-\mathsf{T}} e_1$ with $|\Delta_L| \le 3\,\mathbf{u}\,|R_k^{\mathsf{T}}| + \mathcal{O}(\mathbf{u})^2$

$t_k = M_k \begin{bmatrix} g_{k-1} \\ g_k \end{bmatrix}$, with M_k a 2×2 subbl. R_{k+2}^{T}

Straight-forward estimate:

$$\|\widehat{t}_k - t_k\| \le 3\,\mathbf{u}\,\kappa_2(R_k^{\mathsf{T}})^2$$

In exact arithmetic: $\|t_k\| = \|\mathbf{r}_k\|$.

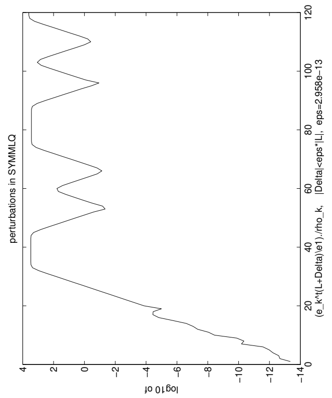
Problem: $\|\mathbf{r}_k\| \to 0$?

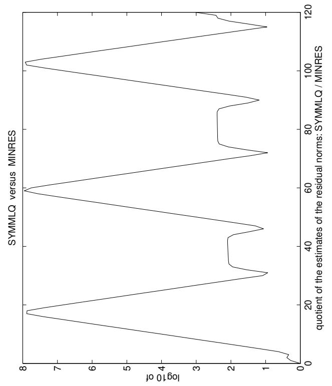
Theorem.

$$\|t_k\| \lesssim k\ \overbrace{|s_1\cdots s_k|}^{\|\mathbf{r}_k^{\mathsf{MR}}\|}\ \kappa_2(\mathbf{A})$$

Theorem.

$$\|\widehat{t}_k - t_k\| \le k^3\,\mathbf{u}\,|s_1\cdots s_k|\,\kappa_2(\mathbf{A})^2$$





In exact arithmetic.

Residual relation MINRES & SYMMLQ

Theorem. $\|\mathbf{r}_{k+1}^{\mathsf{MINRES}}\| \le \|\mathbf{r}_k^{\mathsf{SYMMLQ}}\|$

$$\|\mathbf{r}_k^{\mathsf{SYMMLQ}}\| \le \nu_{k+1}\,\kappa_2(\mathbf{A})\,\|\mathbf{r}_k^{\mathsf{MINRES}}\|$$

with $\qquad \nu_k := k + \frac{1}{2}\ln k$

MINRES selects $\mathbf{x}_k^{\mathsf{MINRES}}$ from $\mathcal{K}_k(\mathbf{A};\mathbf{r}_0)$

SYMMLQ slects $\mathbf{x}_k^{\mathsf{SYMMLQ}}$ from $\mathbf{A}\mathcal{K}_k(\mathbf{A};\mathbf{r}_0)$

$$\mathbf{A}\mathcal{K}_k(\mathbf{A};\mathbf{r}_0) \subset \mathcal{K}_{k+1}(\mathbf{A};\mathbf{r}_0)$$

Problem: $\quad \mathcal{K}_k(\mathbf{A};\mathbf{r}_0) \not\subset \mathbf{A}\mathcal{K}_{k+i}(\mathbf{A};\mathbf{r}_0)$

Corollary. $\|t_k\| \le \nu_{k+1}\,|s_1\cdots s_k|\,\kappa_2(\mathbf{A})$

[Paige & Saunders '75]

SYMMLQ

Choose $\mathbf{x}_0$

$\mathbf{x}=\mathbf{x}_0,\quad \mathbf{r}=\mathbf{b}-\mathbf{A}\mathbf{x},\quad \rho=\|\mathbf{r}\|,\quad \mathbf{v}=\mathbf{r}/\rho$

$\beta=0,\quad \widetilde{\beta}=0,\quad c=-1,\quad s=0,\quad \kappa=\rho$

$\mathbf{v}_{\mathrm{old}}=\mathbf{0},\quad \mathbf{w}=\mathbf{v},\quad g=0,\quad \widetilde{\widetilde{g}}=\rho$

while $\kappa > \mathtt{tol}$ do

- $\widetilde{\mathbf{v}} \leftarrow \mathbf{A}\,\mathbf{v}-\beta\,\mathbf{v}_{\mathrm{old}}$
- $\alpha \leftarrow \mathbf{v}^*\,\widetilde{\mathbf{v}},\quad \widetilde{\mathbf{v}} \leftarrow \widetilde{\mathbf{v}}-\alpha\,\mathbf{v}$
- $\beta \leftarrow \|\widetilde{\mathbf{v}}\|,\quad \mathbf{v}_{\mathrm{old}} \leftarrow \mathbf{v},\quad \mathbf{v} \leftarrow \widetilde{\mathbf{v}}/\beta$
- $l_1 \leftarrow s\,\alpha - c\,\widetilde{\beta},\quad l_2 \leftarrow s\,\beta$
- $\widetilde{\alpha} \leftarrow -s\,\widetilde{\beta}-c\,\alpha,\quad \widetilde{\beta} \leftarrow c\,\beta$
- $l_0 \leftarrow \sqrt{\widetilde{\alpha}^2+\beta^2},\quad c \leftarrow \widetilde{\alpha}/l_0,\quad s \leftarrow \beta/l_0$
- $\widetilde{g} \leftarrow \widetilde{\widetilde{g}}-l_1\,g,\quad \widetilde{\widetilde{g}} \leftarrow -l_2\,g,\quad g \leftarrow \widetilde{g}/l_0$
- $\mathbf{x} \leftarrow \mathbf{x}+(g\,c)\,\mathbf{w}+(g\,s)\,\mathbf{v}$
- $\mathbf{w} \leftarrow s\,\mathbf{w}-c\,\mathbf{v},\quad \kappa \leftarrow \sqrt{\widetilde{g}^2+\widetilde{\widetilde{g}}^2}$

end while

$$\mathbf{A}\mathbf{V}_k=\mathbf{V}_{k+1}\underline{T}_k,\qquad \mathbf{V}_k^{\mathsf{T}}\mathbf{A}\mathbf{V}_k=T_k=L_kL_k^{\mathsf{T}}$$

L_k lower Δ, bi-diagonal (Choleski)

Variant of Conjugate Gradients

$$\mathbf{x}_k=\mathbf{V}_k y_k$$

such that $\quad \mathbf{r}_0-\mathbf{A}\mathbf{V}_k y_k \perp \mathbf{V}_k$

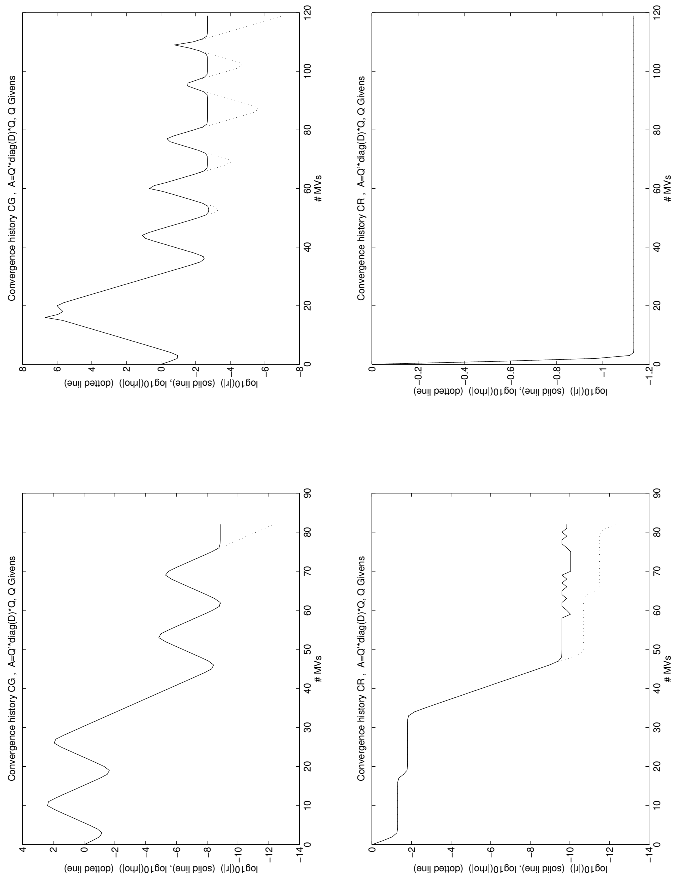
Var. of CG: $\mathbf{x}_k=\left(\mathbf{V}_k L_k^{-\mathsf{T}}\right)\left(L_k^{-1}e_1\right)$

+: efficient (comp. work per step & memory)

+: stable if $\mathbf{A}>0$ $\left(\kappa_2(T_k)=\kappa_2(L_k)^2\leq\kappa_2(\mathbf{A})\right)$ $\Leftarrow$

-: unstable if $\mathbf{A}$ not definite

also for well-cond. $\mathbf{A}$ (T_k can be singular)!



GMRES: $\mathbf{x}_k=\mathbf{V}_k(R_k^{-1}z_k)=\mathbf{V}_k y_k$

MINRES: $\mathbf{x}_k=(\mathbf{V}_k\,R_k^{-1})z_k=\mathbf{W}_k z_k$

CG: $\mathbf{x}_k=\left(\mathbf{V}_k L_k^{-\mathsf{T}}\right)\left(L_k^{-1}e_1\right)$

In rounded arithmetic: $\mathbf{u}$

Scalar recurrence: $\quad R_k y_k = z_k$

$$(R_k+\Delta_R)\widehat{y}_k=z_k$$

with $\quad |\Delta_R|\leq 3\,\mathbf{u}\,|R_k|+\mathcal{O}(\mathbf{u}^2)$

$$\Delta y_k \sim 3\,\mathbf{u}\,R_k^{-1}\,|R_k^{-1}|\,R_k^{-1}\,z_k$$

3-term vector recurrence: $\quad \mathbf{W}_k R_k=\mathbf{V}_k$

$$\widehat{\mathbf{W}}_k R_k=\mathbf{V}_k+\Delta_V$$

with $\quad |\Delta_V|\leq 3\,\mathbf{u}\,|\mathbf{V}_k R_k^{-1}|\,|R_k|+\mathcal{O}(\mathbf{u}^2)$

$$\Delta_W=-\Delta_V R_k^{-1}\sim 3\,\mathbf{u}\,|\mathbf{V}_k R_k^{-1}|\,|R_k|\,|R_k^{-1}|$$

2-term vector recurrence: $\quad \mathbf{U}_k L_k^{\mathsf{T}}=\mathbf{V}_k$

$$(\widehat{\mathbf{U}}_k+\Delta_U)L_k^{\mathsf{T}}=\mathbf{V}_k+\Delta_V$$

with $\quad |\Delta_U|\leq 3\,\mathbf{u}\,|\mathbf{U}_k|=3\,\mathbf{u}\,|\mathbf{V}_k L_k^{-\mathsf{T}}|,$

$\quad |\Delta_V|\leq \mathbf{u}\,|\mathbf{V}_k|$

$\mathbf{U}_k L_k^{\mathsf{T}} = \mathbf{V}_k$ (CG), $\mathbf{W}_k R_k = \mathbf{V}_k$ (MINRES)

In rounded arithmetic: $|\xi| \leq \mathbf{u}$ rel. mach. prec.

2-term vector recurrence: ith row

$$\widehat{\mathbf{u}}_{ik} = \frac{(\mathbf{v}_{ik} - \ell_{k\,k-1}\widehat{\mathbf{u}}_{i\,k-1}(1+\xi))\,(1+2\xi')}{\ell_{kk}}$$

$$= \frac{\mathbf{v}_{ik}(1+\xi'') - \ell_{k\,k-1}\widehat{\mathbf{u}}_{i\,k-1}}{\ell_{kk}(1+3\xi''')}$$

New errors can be cast on new columns.

3-term vector recurrence: ith row

$$\widehat{\mathbf{w}}_{ik} = \frac{\mathbf{v}_{ik}(1+2\xi) - r_{k\,k-1}\widehat{\mathbf{w}}_{i\,k-1}(1+3\xi') - r_{k\,k-2}\widehat{\mathbf{w}}_{i\,k-2}(1+3\xi'')}{r_{kk}}$$

New errors can<u>not</u> be cast to new columns only!

[S., van der Vorst, Fokkema '94, Greenbaum '96]

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

In rounded arithmetic:

$$\widehat{\mathbf{x}}_{k+1} = \widehat{\mathbf{x}}_k + \alpha_k \widehat{\mathbf{u}}_k + \delta$$
$$\widehat{\mathbf{r}}_{k+1} = \widehat{\mathbf{r}}_k - \alpha_k \mathbf{A}\widehat{\mathbf{u}}_k + \mathbf{f}_k$$

with $\|\mathbf{f}_k\| \lesssim \mathbf{u}\, n_A\, \|\mathbf{A}\|\, \|\widehat{\mathbf{x}}_{k+1} - \widehat{\mathbf{x}}_k\|$

Theorem. For CG and CR:

$$\|(\mathbf{b} - \mathbf{A}\widehat{\mathbf{x}}_k) - \widehat{\mathbf{r}}_k\| \leq 2k\, n_A^{3/2}\, \kappa_2(\mathbf{A})$$

Proof.

$$\|\mathbf{x} - \mathbf{x}_k\| \leq \|\mathbf{A}^{-\gamma}\|\, \|\mathbf{x} - \mathbf{x}_k\|_{\mathbf{A}^{2\gamma}}$$
$$= \|\mathbf{A}^{-\gamma}\|\, \|\mathbf{r}_k\|_{\mathbf{A}^{2\gamma-2}} \leq \|\mathbf{A}^{-\gamma}\|_{\mathbf{A}^{2\gamma-2}}$$
$$\leq \|\mathbf{A}^{-\gamma}\|\, \|\mathbf{A}^{\gamma-1}\|_2 = \|\mathbf{A}^{-1}\|$$

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\underline{T}_k, \quad T_k = L_k L_k^{\mathsf{T}}$$
$$\mathbf{x}_k = \left(\mathbf{V}_k L_k^{-\mathsf{T}}\right)\left(L_k^{-1} e_1\right)$$

Additional problems CG: CG uses

- other scaling LU-decomposition T_k
  $|L_k^{-\mathsf{T}}|\,|L_k^{-1}| = |U_k^{-1}|\,|\widetilde{L}_k^{-1}|$
- other scaling on Lanczos: $\mathbf{A}\mathbf{R}_k = \mathbf{R}_{k+1}\underline{\widetilde{T}}_k$
- coupled 2-term: $\mathbf{U}_k L_k^{\mathsf{T}} = \mathbf{V}_k$, $\mathbf{A}\mathbf{U}_k = \mathbf{V}_{k+1}\underline{L}_k$
- $\mathbf{r}_k$ is obtained recursively ($\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k \mathbf{A}\mathbf{u}_k$) rather than as $\mathbf{b} - \mathbf{A}\mathbf{x}_k$

$$\boxed{\left|\|\mathbf{b} - \mathbf{A}\widehat{\mathbf{x}}_k\| - \|\mathbf{r}_k\|\right| \leq \mathbf{u}\,\gamma_k\,\kappa_2(\mathbf{A})}$$

$\gamma_k \sim k$

Conclusions

Lanczos errors: delay in convergence

GMRES, SYMMLQ and CG (if $\mathbf{A} > 0$):
perturb. errors of order $\mathbf{u}\,\kappa_2(\mathbf{A})$: acceptable

MINRES perturb. errors of order $\mathbf{u}\,\kappa_2(\mathbf{A})^2$

SYMMLQ slower than GMRES
GMRES requires more memory

$\mathbf{A} > 0$: CG the best choice

$\mathbf{A}^{\mathsf{T}} = \mathbf{A}$ non-def.: CG & CR may break-down

$\mathbf{A}^{\mathsf{T}} = \mathbf{A}$ non-def. & $\mathbf{A}$ ill-conditioned:
SYMMLQ or Lanczos b. GMRES best choice