CG versus MINRES on Positive Definite Systems

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SOL and ICME, Stanford University
Joint work with David Fong

Recent Advances on Optimization
In honor of Philippe Toint
Toulouse, France, July 24–26, 2013

Meeting for Philippe

First thought:

The trust-region subproblem

$\|x_k\| \nearrow$ for CG

The trust-region subproblem

$$\min\ g^T p + \frac{1}{2} p^T H p \ \text{ st } \ \|p\|_M \leq \Delta$$

Apply PCG to $Hp = -g$
Exit if $d^T H d < 0$
or $\|p\|_M > \Delta$

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Focus on $Ax = b$, $A \succ 0$, $M = I$
Backward errors
Stopping early

Part I: CG and MINRES

Iterative algorithms for $Ax = b$, $A = A^T$
based on the Lanczos process

Krylov-subspace methods: $x_k = V_k y_k$

Lanczos process (summary)

$$\beta_1 v_1 = b \qquad AV_k = V_{k+1} H_k$$

$$V_k = \begin{pmatrix} v_1 & v_2 & \dots & v_k \end{pmatrix}$$

$$T_k = \begin{pmatrix} \alpha_1 & \beta_2 & & \\ \beta_2 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_k \\ & & \beta_k & \alpha_k \end{pmatrix}$$

$$H_k = \begin{pmatrix} & T_k & \\ 0 \; \dots \; 0 & & x \end{pmatrix}$$

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$$\begin{aligned} r_k &= b - Ax_k \\ &= \beta_1 v_1 - AV_k y_k \\ &= V_{k+1}(\beta_1 e_1 - H_k y_k), \end{aligned}$$

Aim: $\beta_1 e_1 \approx H_k y_k$

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Two subproblems

CG	$T_k y_k = \beta_1 e_1$	$x_k = V_k y_k$
MINRES	$\min \lVert H_k y_k - \beta_1 e_1 \rVert$	$x_k = V_k y_k$

Common practice

$$Ax = b, \quad A = A^T$$

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A indefinite	$\Rightarrow$	Use MINRES

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Experiment: CG vs MINRES on $A \succ 0$

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A positive definite	$\Rightarrow$	Use CG
A indefinite	$\Rightarrow$	Use MINRES

Experiment: CG vs MINRES on $A \succ 0$

- Hestenes and Stiefel (1952) proposed both CG and CR for $A \succ 0$ and proved many properties
- CR $\equiv$ MINRES when $A \succ 0$
  They both minimize $\|r_k\| = \|b - Ax_k\|$ in the Krylov subspace

Theoretical properties for $Ax = b$, $A \succ 0$

		CG	CR (MINRES)
$\|x^* - x_k\|$	$\searrow$	HS 1952	HS 1952
$\|x^* - x_k\|_A$	$\searrow$	HS 1952	HS 1952
$\|x_k\|$	$\nearrow$	Steihaug 1983	Fong 2011

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		CR (MINRES)
$\|r_k\|$	$\searrow$	HS 1952
$\|r_k\| / \|x_k\|$	$\searrow$	Fong 2011

Backward error for square systems $Ax = b$

Stopping tolerances α, β

x_k is an acceptable solution iff there exist E, f st

$$(A+E)x_k = b+f \qquad \frac{\|E\|}{\|A\|} \le \alpha \qquad \frac{\|f\|}{\|b\|} \le \beta$$

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Smallest perturbations E, f: (Titley-Peloquin 2010)

$$E = \frac{\alpha\|A\|}{\psi\|x_k\|} r_k x_k^T \qquad \frac{\|E\|}{\|A\|} = \alpha\frac{\|r_k\|}{\psi}$$

$$f = -\frac{\beta\|b\|}{\psi} r_k \qquad \frac{\|f\|}{\|b\|} = \beta\frac{\|r_k\|}{\psi}$$

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$$f = -\frac{\beta\|b\|}{\psi} r_k \qquad \frac{\|f\|}{\|b\|} = \beta\frac{\|r_k\|}{\psi}$$

Backward error: $\|r_k\|/\psi$

Stopping rule: $\|r_k\| \le \psi \equiv \alpha\|A\|\|x_k\| + \beta\|b\|$

Backward error for square systems, $\beta = 0$

$$(A + E_k)x_k = b$$

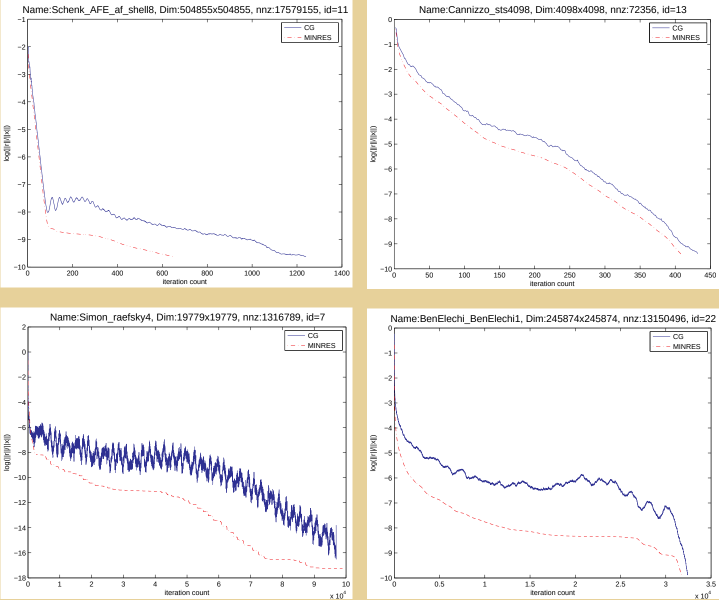
$$E_k = \frac{r_k x_k^T}{\|x_k\|^2} \qquad \|E_k\| = \frac{\|r_k\|}{\|x_k\|}$$

Data: Tim Davis's sparse matrix collection

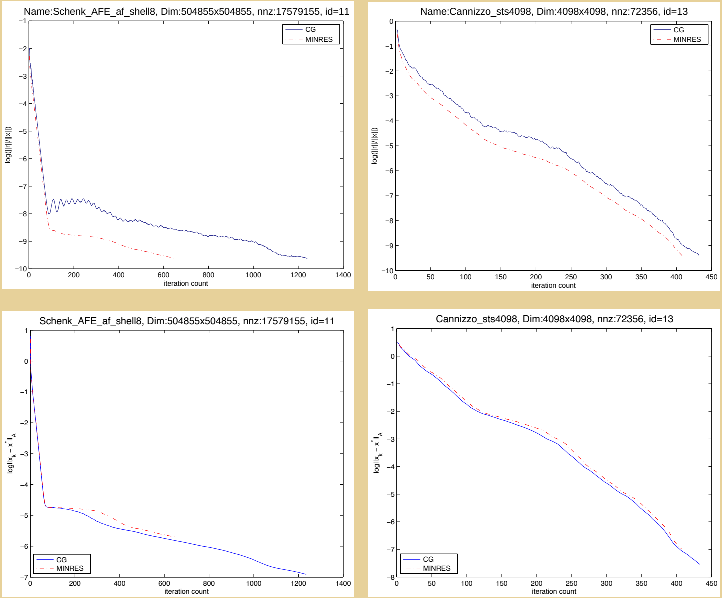
Real, symmetric posdef examples that include b

Plot $\log_{10}\|E_k\|$ for CG and MINRES

$\|r_k\|/\|x_k\|$ for $A \succ 0$ MINRES can stop sooner



$\|r_k\|/\|x_k\|$ and $\log_{10}\|x - x_k\|_A$



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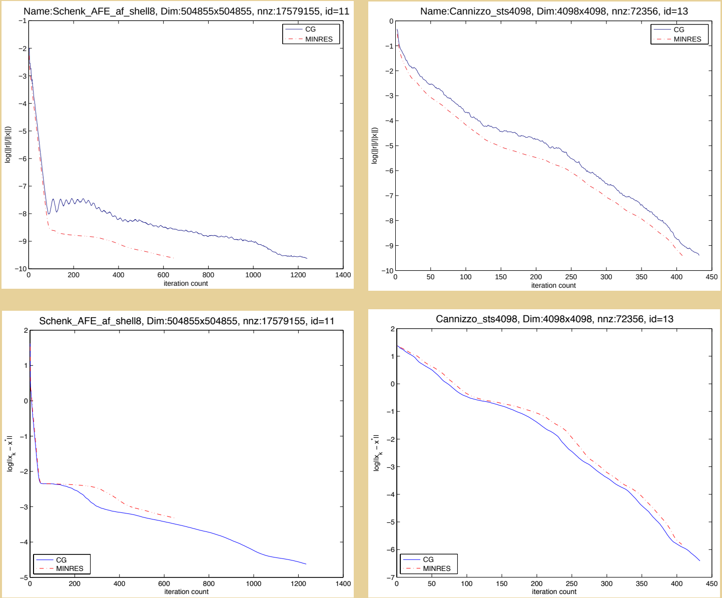
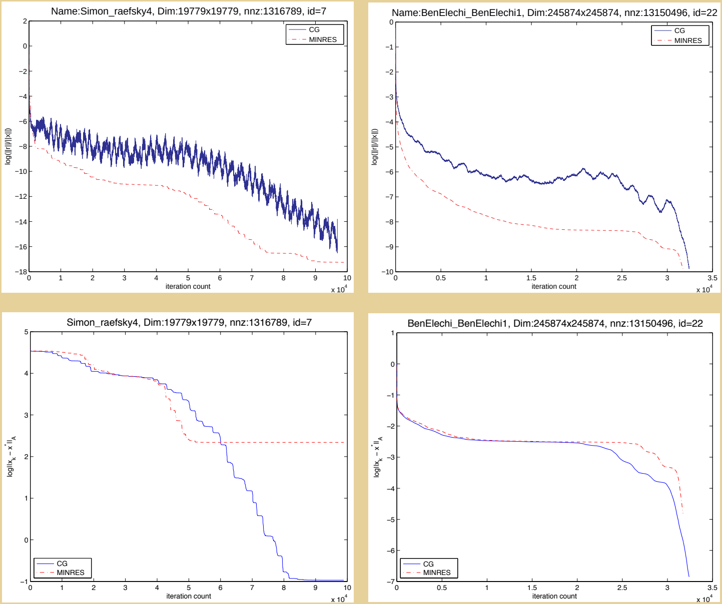


$\|r_k\| / \|x_k\|$ and $\log_{10} \|x - x_k\|_A$



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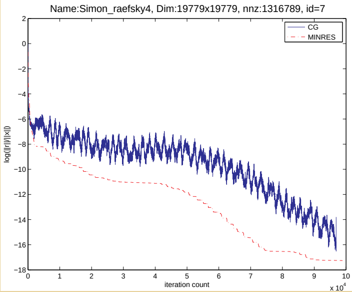
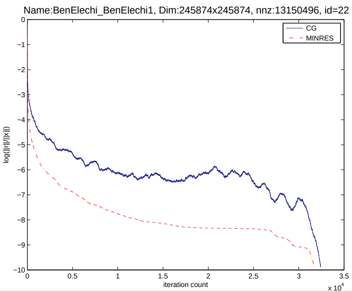
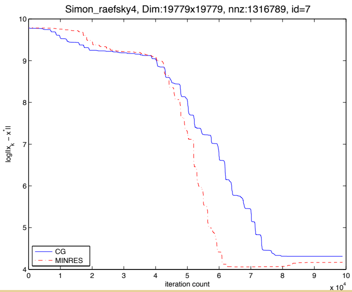
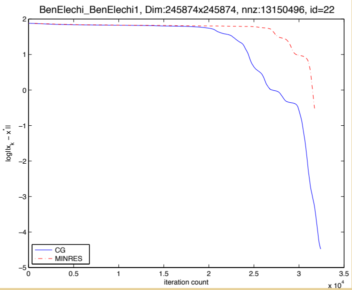
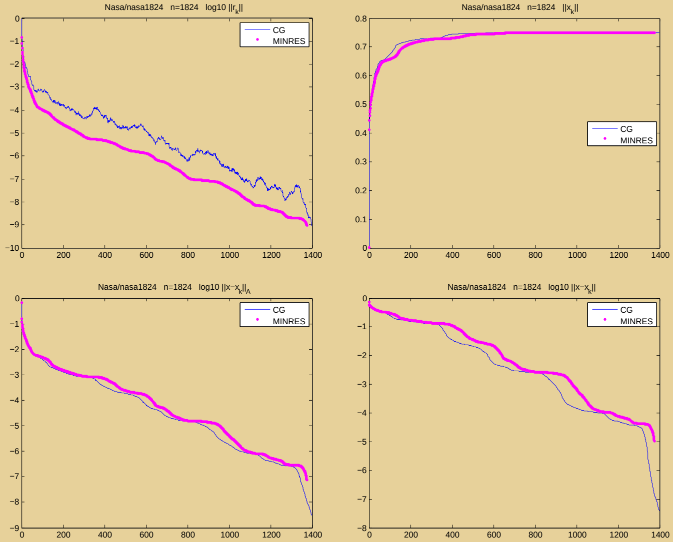




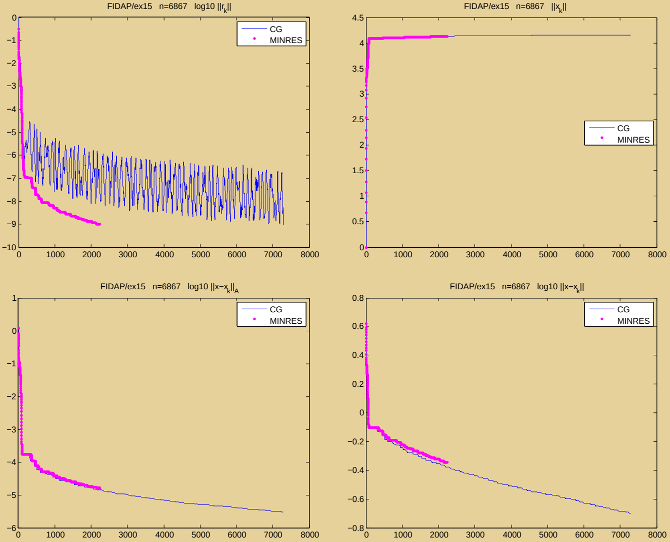




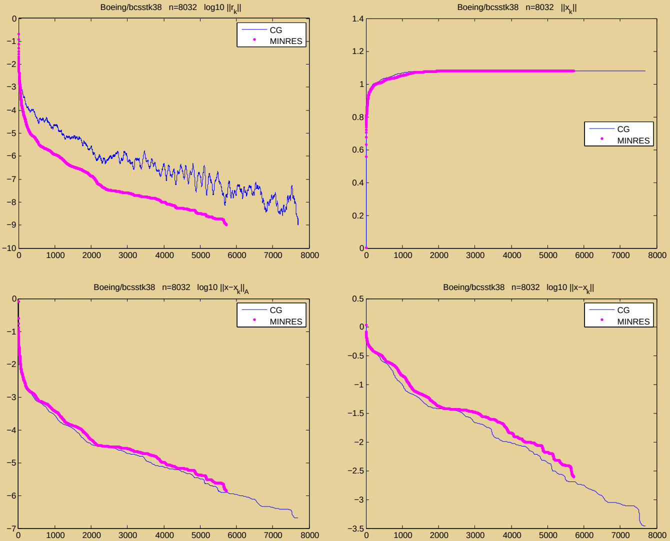
$\|r_k\| \quad \|x_k\| \quad \|x - x_k\|_A \quad \|x - x_k\| \quad \kappa(A) = 10^6$



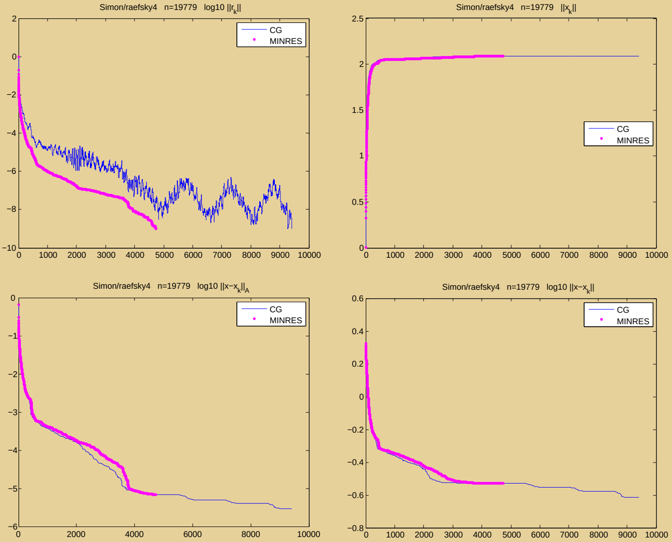
$\|r_k\| \quad \|x_k\| \quad \|x - x_k\|_A \quad \|x - x_k\| \quad \kappa(A) = 10^{11}$



$\|r_k\|$ $\|x_k\|$ $\|x - x_k\|_A$ $\|x - x_k\|$ $\kappa(A) = 10^7$



$\|r_k\| \quad \|x_k\| \quad \|x - x_k\|_A \quad \|x - x_k\| \quad \kappa(A) = 10^{12}$



Why does $\|r_k\|$ for CG lag behind MINRES?

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Greenbaum 1997: (Thanks David Titley-Peloquin)

$$\|r_k^C\| = \frac{\|r_k^M\|}{\sqrt{1 - \|r_k^M\|^2 / \|r_{k-1}^M\|^2}}$$

$\Rightarrow \|r_k^C\| \gg \|r_k^M\|$ if MINRES is almost stalling

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Fong 2011: If $\alpha = 0$ in stopping rule, stop when $\|r_l\| \le \beta \|b\|$

$$\prod_{k=1}^{l} \frac{\|r_k\|}{\|r_{k-1}\|} = \frac{\|r_l\|}{\|b\|} \approx \beta$$

$\Rightarrow \|r_k^M\| / \|r_{k-1}^M\|$ closer to 1 on average if l is large
$\Rightarrow$ bigger gap on average between $\|r_k^C\|$ and $\|r_k^M\|$

Posdef systems and least squares

LS $\equiv$ PSD system

$$\min \|Ax - b\| \qquad \Rightarrow \qquad A^T Ax = A^T b$$

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$$\min \|Ax - b\| \quad \Rightarrow \quad A^T A x = A^T b$$

Conversely, let $A = U^T U$ (Cholesky) and solve $U^T c = b$

PSD system $\equiv$ LS

$$Ax = b \quad \Rightarrow \quad U^T U x = U^T c \quad \Rightarrow \quad \min \|Ux - c\|$$

Part II: LSQR and LSMR

LSQR $\equiv$ CG on $A^TAx = A^Tb$

LSMR $\equiv$ MINRES on $A^TAx = A^Tb$

Based on Golub-Kahan bidiagonalization

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solve $Ax = b$	$\min \|x\|$ st $Ax = b$
$\min \|Ax - b\|$	$\min \left\| \begin{pmatrix} A \\ \lambda I \end{pmatrix} x - \begin{pmatrix} b \\ 0 \end{pmatrix} \right\|$

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- A can be an operator ($\Rightarrow$ allows preconditioning)
- Av, $A^T u$ plus $O(m+n)$ operations per iteration

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- June 2013: F90 complex implementations
  Austin Benson and Victor Minden, ICME

LSQR on $Ax = b$

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  Backward errors are monotonic for LSQR on $Ax = b$
  (like CG and MINRES when $A \succ 0$):

$$\|r_k\|/(\alpha\|A\|\|x_k\| + \beta\|b\|) \quad \searrow$$

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What about GMRES?

LSQR and LSMR on $\min \|Ax - b\|$

Stewart backward error

$$r_k = b - Ax_k$$

$$\frac{\|A^T r_k\|}{\|A\|\|r_k\|} \le \alpha$$

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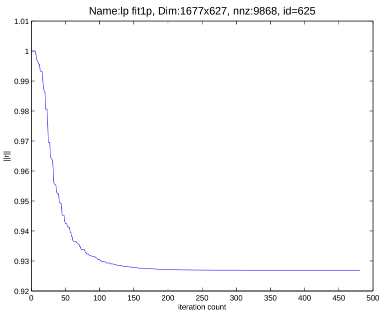
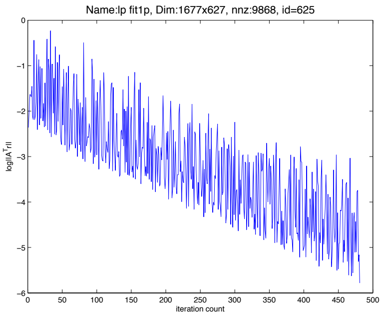
LSQR $\|r_k\|$



LSQR $\log \|A^T r_k\|$



LSQR and LSMR on $\min \|Ax - b\|$

Stewart backward error

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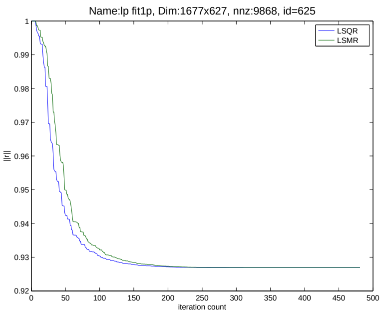
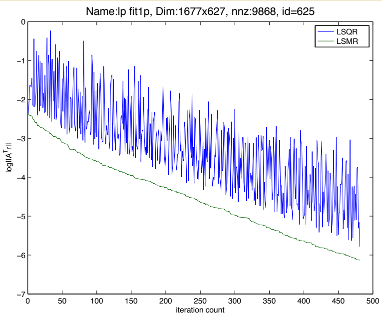
$\|r_k\|$



$\log \|A^T r_k\|$



Overdetermined systems

Test Data

- Tim Davis, University of Florida Sparse Matrix Collection
- $\mathrm{LPnetlib}$: Linear Programming Problems
- $\mathrm{A} = (\mathrm{Problem.A})'$ $\quad \mathrm{b} = \mathrm{Problem.c}$ $\quad$ (127 problems)

Overdetermined systems

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- Tim Davis, University of Florida Sparse Matrix Collection
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- A = (Problem.A)' b = Problem.c (127 problems)

$$\text{Solve } \min \|Ax - b\|_2$$

with LSQR and LSMR

Backward error – estimates

$A^T A\hat{x} = A^T b$	$\hat{r} = b - A\hat{x}$	exact
$(A+E_i)^T(A+E_i)x = (A+E_i)^T b$	$r = b - Ax$	any x

Backward error – estimates

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$$(A+E_i)^T(A+E_i)x = (A+E_i)^T b \qquad r = b - Ax \qquad \text{any } x$$

Two estimates given by Stewart (1975 and 1977)

$$E_1 = \frac{ex^T}{\|x\|^2} \qquad \|E_1\| = \frac{\|e\|}{\|x\|} \qquad e = \hat{r} - r$$

$$E_2 = -\frac{rr^TA}{\|r\|^2} \qquad \|E_2\| = \frac{\|A^Tr\|}{\|r\|} \qquad \text{computable}$$

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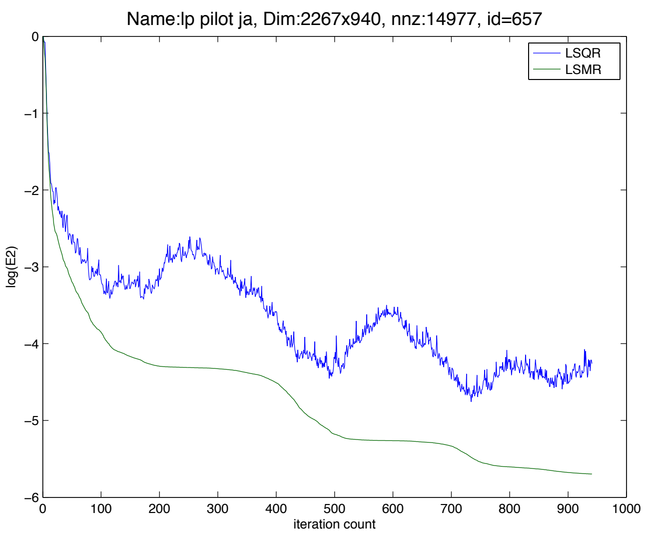
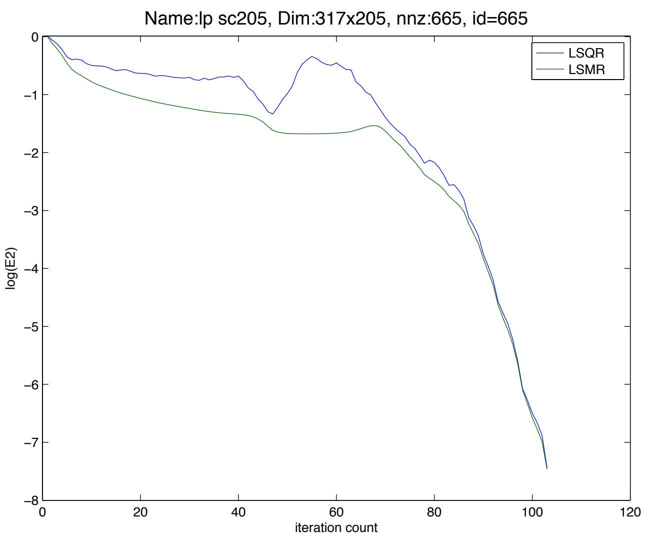
Theorem

$$\|E_2^{\text{LSMR}}\| \le \|E_2^{\text{LSQR}}\|$$

$\log_{10} \|E_2\|$ for LSQR and LSMR – typical



$\log_{10} \|E_2\|$ for LSQR and LSMR – rare



Backward error - optimal

$$\mu(x) \equiv \min_E \|E\| \quad \text{st} \quad (A+E)^T(A+E)x = (A+E)^T b$$

Exact $\mu(x)$ (Waldén, Karlson, & Sun 1995, Higham 2002)

$$C \equiv \left[A \quad \frac{\|r\|}{\|x\|}\left(I - \frac{rr^T}{\|r\|^2}\right)\right] \qquad \mu(x) = \sigma_{\min}(C)$$

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Cheaper estimate $\tilde{\mu}(x)$ (Grcar, Saunders, & Su 2007)

$$K = \begin{pmatrix} A \\ \frac{\|r\|}{\|x\|} I \end{pmatrix} \qquad v = \begin{pmatrix} r \\ 0 \end{pmatrix}$$

$$\min_y \|Ky - v\| \qquad \tilde{\mu}(x) = \frac{\|Ky\|}{\|x\|}$$

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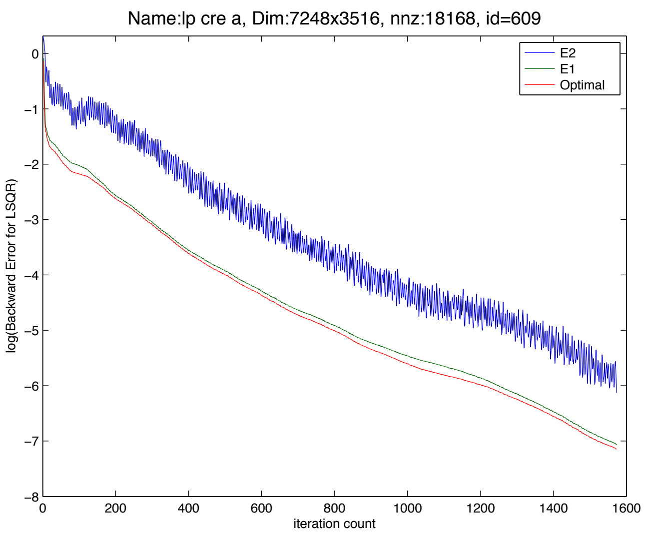
```
r       = b - A*x;
p       = colamd(A);
eta     = norm(r)/norm(x);
K       = [A(:,p); eta*speye(n)];
v       = [r; zeros(n,1)];
[c,R]   = qr(K,v,0);
mutilde = norm(c)/norm(x);
```

Backward errors for LSQR – typical



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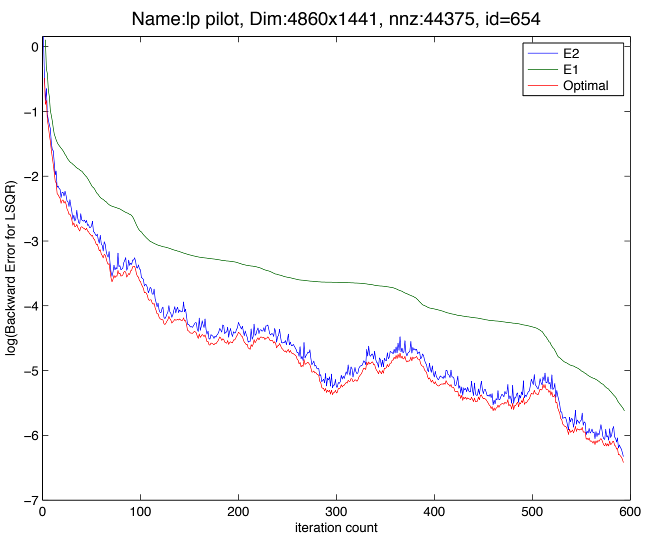
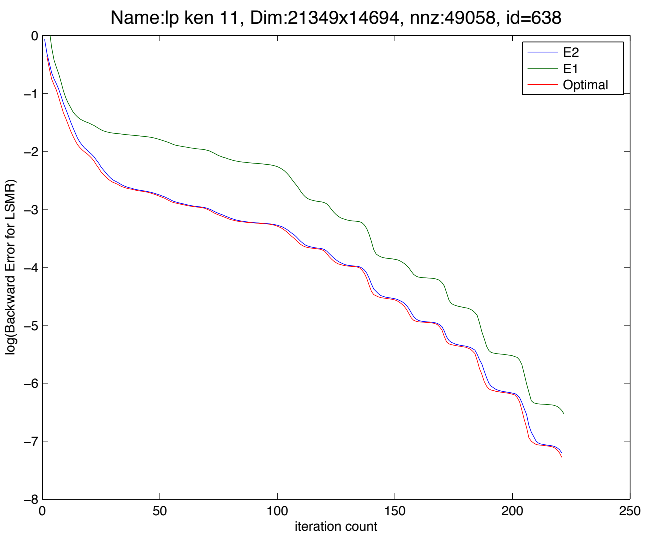
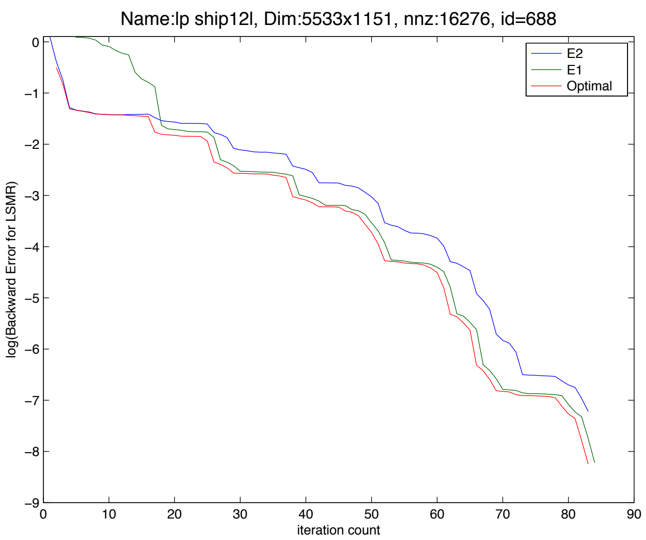


Backward errors for LSMR – typical



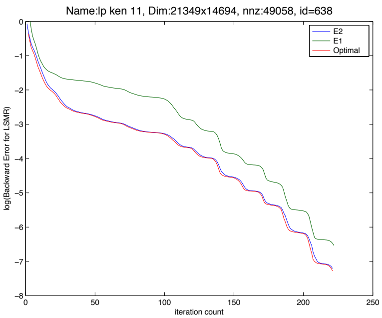
Backward errors for LSMR – rare



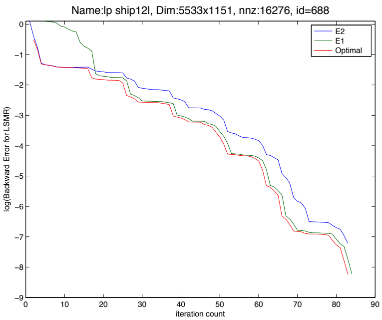
For LSMR

$\|E_2\| \approx$ optimal BE almost always

Typical: $\|E_2\| \approx \tilde{\mu}(x)$



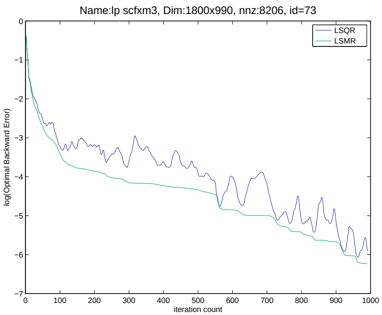
Rare: $\|E_1\| \approx \tilde{\mu}(x)$



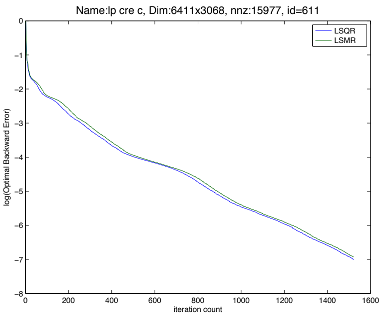
Optimal backward errors $\tilde{\mu}(x)$

Seem monotonic for LSMR Usually not for LSQR

Typical for LSQR and LSMR



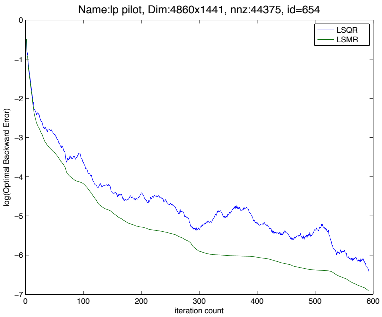
Rare LSQR, typical LSMR



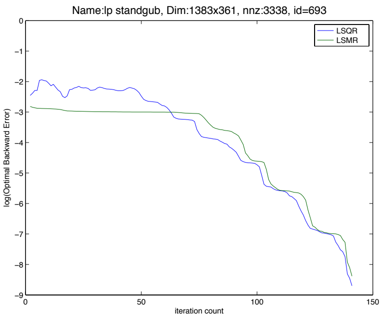
Optimal backward errors

$\tilde{\mu}(x^{\mathrm{LSMR}}) \leq \tilde{\mu}(x^{\mathrm{LSQR}})$ almost always

Typical



Rare



Summary

Theoretical properties for $Ax = b$

CG and MINRES, $A \succ 0$

$$\|x^* - x_k\|,\ \|x^* - x_k\|_A \quad \searrow$$

$$\|x_k\| \quad \nearrow$$

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CG and MINRES, $A \succ 0$

$$\|x^* - x_k\|,\ \|x^* - x_k\|_A \quad \searrow$$

$$\|x_k\| \quad \nearrow$$

MINRES, $A \succ 0$

$$\|r_k\| \quad \searrow$$

$$\|r_k\|/(\alpha\|A\|\|x_k\| + \beta\|b\|) \quad \searrow$$

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LSQR and LSMR, any A

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LSQR and LSMR, any A

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$$\|r_k\|/(\alpha\|A\|\|x_k\| + \beta\|b\|) \quad \searrow$$

Monotonic backward errors
$\Rightarrow$ safe to stop early

Theoretical properties for $\min \|Ax - b\|$

LSQR and LSMR

$$\begin{array}{rl} \|x^* - x_k\|,\ \|r^* - r_k\| & \searrow \\ \|r_k\| & \searrow \\ \|x_k\| & \nearrow \\ x_k \to \text{min-length } x^* & \text{if } \operatorname{rank}(A) < n \end{array}$$

Theoretical properties for $\min \|Ax - b\|$

LSQR and LSMR

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LSMR

$$\begin{array}{rl} \|A^T r_k\| & \searrow \\ \|A^T r_k\| / \|r_k\| & \searrow \text{ almost always} \\ & \approx \text{ optimal BE almost always} \\ & \leq \ (\|A^T r_k\| / \|r_k\|)^{\text{LSQR}} \end{array}$$

Theoretical properties for $\min \|Ax - b\|$

LSQR and LSMR

$$\begin{array}{rl} \|x^* - x_k\|,\ \|r^* - r_k\| & \searrow \\ \|r_k\| & \searrow \\ \|x_k\| & \nearrow \\ x_k \rightarrow \text{min-length } x^* & \text{if } \operatorname{rank}(A) < n \end{array}$$

LSMR

$$\begin{array}{rl} \|A^T r_k\| & \searrow \\ \|A^T r_k\| / \|r_k\| & \searrow \ \text{almost always} \\ & \approx \ \text{optimal BE almost always} \\ & \leq \ (\|A^T r_k\| / \|r_k\|)^{\text{LSQR}} \end{array}$$

For LSMR, optimal backward errors **seem** monotonic

$\Rightarrow$ safe to stop early

Final thoughts

We learn from history

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that we don't learn from history
– G. W. F. Hegel

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If you're not fired with enthusiasm,

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If you’re not fired with enthusiasm,
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