Error norm estimation in CG-like methods for solving linear least-squares problems

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based on joint work with

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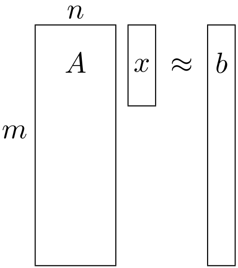


$$\min_{x \in \mathbb{R}^n} \| \, b - Ax \, \|$$

$$A^T A \, x \; = \; A^T b \, , \qquad A \, x \; = \; b_{|\mathcal{R}(A)}$$

A has full column rank (for simplicity)

Solving system of normal equations

using conjugate gradients (CG)

$$\min_{x \in \mathbb{R}^n} \| b - Ax \| \quad \Leftrightarrow \quad A^T A\, x = A^T b.$$

CG for normal equations ($x_0 = 0$ for simplicity) constructs

$$x_k \in \mathcal{K}_k(A^T A, A^T b)$$

which minimize

$$\| x - x_k \|_{A^T A}^2 = \| \underbrace{b - Ax_k}_{r_k} \|^2 - \| \underbrace{b - b_{|\mathcal{R}(A)}}_{r} \|^2.$$

algorithms ?

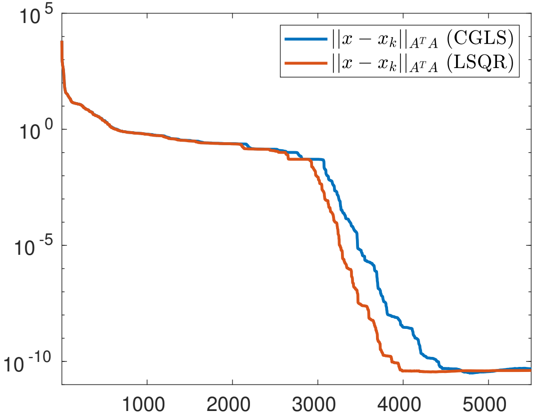
stopping ?

CG for normal equations

CGLS and LSQR algorithms

CGLS [Hestenes & Stiefel, 1952]

LSQR [Paige & Saunders, 1982]



Stopping criteria

Backward error and $A^T A$-norm of the error

1. **Backward error**: Given ε, stop if x_k solves

$$\min_{x \in \mathbb{R}^n} \| (b + f) - (A + E)x \| , \quad \frac{\|E\|}{\|A\|} \leq \varepsilon , \quad \frac{\|f\|}{\|b\|} \leq \varepsilon .$$

[Paige & Saunders, 1982]

2. **Error norms**: Recall

$$\| x - x_k \|_{A^T A}^2 = \| r_k \|^2 - \| r \|^2.$$

Stop if

$$\frac{\| r_k \|^2 - \| r \|^2}{\| r \|^2} \leq \varepsilon \quad \Leftrightarrow \quad \| x - x_k \|_{A^T A}^2 \leq \frac{\varepsilon}{1 + \varepsilon} \|r_k\|^2 .$$

[Papež & Tichý, 2024]

Normwise relative backward error criterion

and sufficient conditions

$$(A+E)^T(A+E)\,x_k \;=\; (A+E)^T(b+f) \qquad (1)$$

$$\min_{E,f,\xi}\left\{\xi : (1) \text{ holds with } \frac{\|E\|}{\|A\|}\le\xi,\ \frac{\|f\|}{\|b\|}\le\xi\right\} \;\le\; \varepsilon$$

- Sufficient conditions (too conservative)

$$\begin{aligned}\|r_k\| &\le \varepsilon\,(\,\|A\|\,\|x_k\| + \|b\|\,)\,,\\ \|A^T r_k\| &\le \varepsilon\,\|A\|\,\|r_k\|\,.\end{aligned}$$

[Paige & Saunders, 1982]

- Sufficient condition (asymptotically tight)

$$\frac{\|\,x - x_k\,\|_{A^T A}}{\|A\|\,\|x_k\| + \|b\|} \le \varepsilon\,.$$

[Chang & Paige & Titley-Peloquin, 2009]

How to estimate $\| x - x_k \|_{A^T A}$?

The conjugate gradient (CG) algorithm is almost always the iterative method of choice for solving linear systems with symmetric positive definite matrices. This book

- describes and analyzes techniques based on Gauss quadrature rules to cheaply compute bounds on norms of the error and that can be used to derive reliable stopping criteria;
- shows how to compute estimates of the smallest and largest eigenvalues during CG iterations; and
- illustrates algorithms using many numerical experiments; these algorithms also can be easily incorporated into existing CG codes.

Error Norm Estimation in the Conjugate Gradient Algorithm is intended for those in academia and industry who use the conjugate gradient algorithm, including the many branches of science and engineering in which symmetric linear systems have to be solved.

Gérard Meurant is retired from the French Atomic Energy Commission (CEA), where he worked in applied mathematics from 1970 to 2008. He was research director at the time of his retirement. He is the author of more than 60 papers on numerical linear algebra and six books, including two books co-authored with Gene H. Golub.

Petr Tichý is an associate professor at the Faculty of Mathematics and Physics at Charles University in Prague, Czech Republic. He is the author of more than 27 journal publications and one textbook. His research covers a variety of topics in numerical linear algebra, optimization, approximation of functions, and round-off error analysis of algorithms.

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Error Norm Estimation in the Conjugate Gradient Algorithm

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Petr Tichý

Error norm estimation in CG

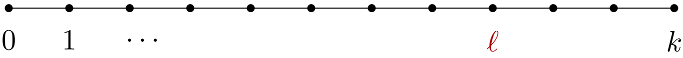
A is symmetric and positive definite, $Ax = b$

input A, b, x_0, τ
$r_0 = b - Ax_0$, $p_0 = r_0$
for $k = 0, \dots$ **do**
$\quad\vdots$
$\quad x_{k+1} = x_k + \gamma_k p_k$
$\quad r_{k+1} = r_k - \gamma_k A p_k$
$\quad\vdots$
$\quad \Delta_k = \gamma_k \|r_k\|^2$
$\quad (\ell, \mathtt{EST}) = \mathtt{adaptive}(\{\Delta_j\}_{j=0}^{k}, \tau)$
end for

Heuristically,

$$\frac{\|\, x - x_\ell \,\|_A^2 \; - \; \mathtt{EST}}{\|\, x - x_\ell \,\|_A^2} \;\leq\; \tau$$

$$\mathtt{EST} \;=\; \sum_{j=\ell}^{k} \Delta_j$$



[Meurant & Papež & Tichý, 2021], [Papež & Tichý, 2024]

Error norm estimation in CGLS

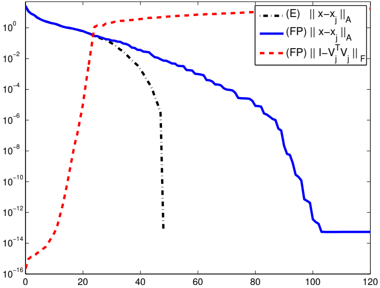
for solving least-squares problems

input A, b, x_0, τ
$r_0 = b - Ax_0$
$s_0 = p_0 = A^T r_0$
for $k = 0, 1, \ldots$ **do**
  $q_k = Ap_k$
  $\gamma_k = \|s_k\|^2 / \|q_k\|^2$
  $x_{k+1} = x_k + \gamma_k p_k$
  $r_{k+1} = r_k - \gamma_k q_k$
  $s_{k+1} = A^T r_{k+1}$
  $\delta_{k+1} = \|s_{k+1}\|^2 / \|s_k\|^2$
  $p_{k+1} = s_{k+1} + \delta_{k+1} p_k$
  $\Delta_k^{\mathrm{CGLS}} = \gamma_k \, \|s_k\|^2$
  $(\ell, \texttt{EST}) = \texttt{adaptive}(\{\Delta_j^{\mathrm{CGLS}}\}_{j=0}^{k}, \tau)$
end for

[Papež & Tichý, 2024]

Finite precision computations

and the estimates



Estimates are reliable, if **local orthogonality** is preserved

$$\frac{|s_k^T p_{k-1}|}{\|s_{k-1}\|^2} \ll 1,$$

where $s_k = A^T A x_k - A^T b$.

[Strakoš & Tichý, 2002], [Papež & Tichý, 2024]

Preconditioning

and the A^TA-norm of the error

- L nonsingular, modify the problem

$$\min_{z\in\mathbb{R}^n} \|b - \underbrace{AL^{-T}}_{\hat{A}}\underbrace{L^Tz}_{\hat{z}}\|\,.$$

- Solve the corresponding system of normal equations

$$\underbrace{L^{-1}A^T}_{\hat{A}^T}\underbrace{AL^{-T}}_{\hat{A}}\underbrace{L^Tx}_{\hat{x}} = \underbrace{L^{-1}A^T}_{\hat{A}^T}b.$$

$L \to$ a **split preconditioner** for A^TA.

- It holds that

$$\|\hat{x} - \hat{x}_k\|^2_{\hat{A}^T\hat{A}} = \|x - x_k\|^2_{A^TA}$$

and our techniques can be used in PCGLS and PLSQR.

Numerical experiments

Test problems

SuiteSparse Matrix collection

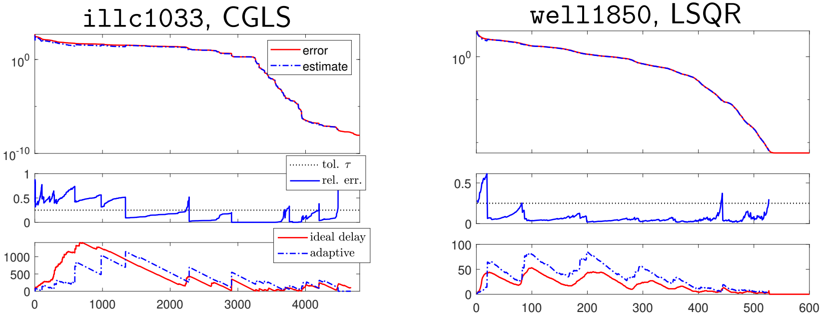
problem	m	n	b	precond
illc1033	1033	320	✓	no
well1850	1850	712	✓	no
illc1850	1850	712	✓	✓
sls	1 748 122	62 729	rand	✓

- b comes together with the matrix or randomly generated.
- L constructed using the incomplete Cholesky of $A^T A$ without explicitly forming it $\to$ MATLAB interface of HSL_MI35.

[HSL library], [Scott & Tůma, 2014]

Problems without preconditioning

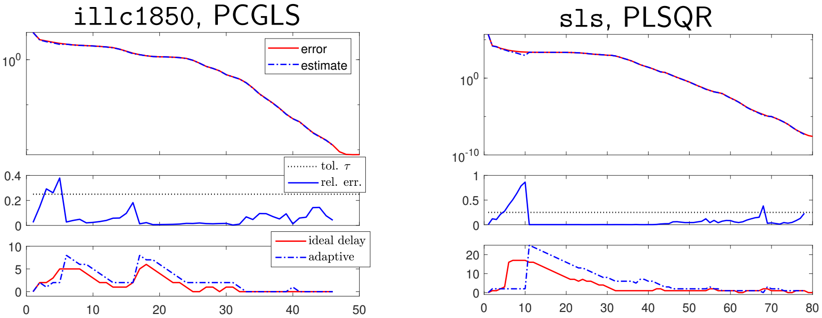
`illc1033` and `well1850`



$$\frac{\| x - x_\ell \|^2_{A^TA} - \mathtt{EST}}{\| x - x_\ell \|^2_{A^TA}} \leq \tau = 0.25$$

Problems with preconditioning

`illc1850` and `sls`



$$\frac{\| x - x_\ell \|^2_{A^TA} - \mathtt{EST}}{\| x - x_\ell \|^2_{A^TA}} \leq \tau = 0.25$$

Conclusions

- The techniques for **error estimation** developed for CG can also be used in **CGLS** and **LSQR**.
- The estimates are **cheap**, numerically reliable, and work with preconditioning.
- The **heuristic strategy** for estimating the quantity of interest with a tolerance τ has shown to be **robust** and **reliable**.
- In the final stage, the suggested ℓ is usually **almost optimal**. Important for stopping the iterations.

Related papers

J. Papež, P. Tichý,

[Estimating error norms in CG-like algorithms for least-squares and least-norm problems, Numer. Algorithms, 2024.]

- G. Meurant, P. Tichý, [Error Norm Estimation in the Conjugate Gradient Algorithm, SIAM Spotlights, Philadelphia, PA, 2024, x+127 p.]
- G. Meurant, J. Papež, P. Tichý, [Accurate error estimation in CG, Numer. Algorithms 88, 2021, pp. 1337-1359.]
- X.W. Chang, C.C. Paige, D. Titley-Peloquin, [Stopping criteria for the iterative solution of linear least squares problems. SIAM J. Matrix Anal. Appl. 31, 2009, pp. 831-852.]
- Z. Strakoš, P. Tichý, [On error estimation in CG and why it works in FP computations, Electron. Trans. Numer. Anal. 13, 2002, pp. 56–80.]

Thank you for your attention!