Backward Perturbation Analysis

for Scaled Total Least Squares Problems

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Computational Methods with Applications

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Outline

- **The scaled total least squares problem**
- **Backward perturbation analysis**
- **A pseudo-minimal backward error** μ
- **A lower bound for** μ
- **An asymptotic estimate for** μ
- **Numerical experiments and conclusion**

Notation

Matrices: A, ΔA, E, ...

Vectors: b, Δb, f, ...

Scalars: γ, β, ξ, ...

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Matrix norms: $\|A\|_2 \equiv \sigma_{\max}(A)$, $\quad \|A\|_F^2 \equiv \mathrm{trace}(A^T A)$

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$\sigma_{\min}(A)$**:** smallest singular value of A

$\lambda_{\min}(A)$**:** smallest eigenvalue of (real symmetric) A

$A^\dagger$**:** Moore-Penrose generalized inverse of A
(for a non-zero vector $v^\dagger = v^T/\|v\|_2^2$)

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The scaled total least squares problem

Given $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$, the least squares problem is

$$\min_{f,x} \left\{ \|f\|_2^2 \;:\; Ax = b + f \right\}$$

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The scaled total least squares (STLS) problem is

$$\min_{E,f,x} \left\{ \|[E, \gamma f]\|_F^2 \;:\; (A + E)x = b + f \right\}$$

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The STLS problem reduces to

- the least squares (LS) problem as $\gamma \to 0$
- the total least squares (TLS) problem if $\gamma = 1$
- the data least squares (DLS) problem as $\gamma \to \infty$

STLS optimality conditions

The STLS problem is equivalent to

$$\min_x \frac{\|b - Ax\|_2^2}{\gamma^{-2} + \|x\|_2^2}$$

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Lemma (Paige and Strakoš, 2002)

- *under mild conditions on A and b, a unique STLS solution exists*

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Lemma (Paige and Strakoš, 2002)

- *under mild conditions on A and b, a unique STLS solution exists*
- *assuming these conditions hold, $\hat{x}$ is optimal* **if and only if**

$$A^T(b - A\hat{x}) = -\frac{\|b - A\hat{x}\|_2^2}{\gamma^{-2} + \|\hat{x}\|_2^2}\hat{x} \qquad \textit{and} \qquad \frac{\|b - A\hat{x}\|_2^2}{\gamma^{-2} + \|\hat{x}\|_2^2} < \sigma_{min}^2(A)$$

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Backward perturbation analysis

Recent research:

- Consistent linear systems:
  Oettli & Prager (64), Rigal & Gaches (67), D. Higham & N. Higham (92), Varah (94), J.G. Sun & Z. Sun (97), Sun (99), etc.

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- DLS problems: Chang, Golub & Paige (06)

Backward perturbation analysis for STLS

Given an approximate STLS solution $0 \neq y \in \mathbb{R}^n$, we seek minimal perturbations ΔA and Δb such that y is the exact STLS solution of the perturbed problem:

$$y = \arg\min_x \frac{\|(b + \Delta b) - (A + \Delta A)x\|_2^2}{\gamma^{-2} + \|x\|_2^2}$$

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- this can be used to design stopping criteria for iterative methods for large sparse problems

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The minimal backward error problem

The minimal backward error problem:

$$\min_{[\Delta A, \Delta b] \in \mathcal{G}} \left\{ \, \|[\Delta A, \Delta b]\|_F \, \right\}$$

where

$$\mathcal{G} \equiv \left\{ \, [\Delta A, \Delta b] \; : \; y = \arg\min_x \frac{\|(b + \Delta b) - (A + \Delta A)x\|_2^2}{\gamma^{-2} + \|x\|_2^2} \, \right\}$$

The set $\mathcal{G}$

Recall the STLS optimality conditions:

$$\begin{cases} h(A, b, \hat{x}) & \equiv & A^T(b - A\hat{x}) + \frac{\|b-A\hat{x}\|_2^2}{\gamma^{-2}+\|\hat{x}\|_2^2}\hat{x} & = & 0, \\ \frac{\|b-A\hat{x}\|_2^2}{\gamma^{-2}+\|\hat{x}\|_2^2} & < & \sigma_{min}^2(A) \end{cases}$$

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Therefore

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Therefore

$$\mathcal{G} \equiv \left\{ [\Delta A, \Delta b] \;:\; y = \arg\min_x \frac{\|(b+\Delta b)-(A+\Delta A)x\|_2^2}{\gamma^{-2}+\|x\|_2^2} \right\}$$

$$= \left\{ \begin{array}{ll} [\Delta A, \Delta b] \;:\; h(A+\Delta A, b+\Delta b, y) = 0, \\ \qquad\qquad \frac{\|(b+\Delta b)-(A+\Delta A)y\|_2^2}{\gamma^{-2}+\|y\|_2^2} < \sigma_{min}^2(A+\Delta A) \end{array} \right\}$$

The superset $\mathcal{G}^+$

The inequality makes the problem difficult...

$$\mathcal{G} = \left\{ \begin{array}{lcl} [\Delta A, \Delta b] \;:\; h(A+\Delta A, b+\Delta b, y) & = & 0, \\ \frac{\|(b+\Delta b)-(A+\Delta A)y\|_2^2}{\gamma^{-2}+\|y\|_2^2} & < & \sigma_{min}^2(A+\Delta A) \end{array} \right\}$$

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We will consider the following pseudo-minimal backward error μ:

$$\mu \equiv \min_{[\Delta A, \Delta b] \in \mathcal{G}^+} \ \{ \ \|[\Delta A, \Delta b]\|_F \}$$

Can we really ignore the inequality?

We are ignoring the inequality in the set $\mathcal{G}$ and solving

$$\mu \equiv \min_{[\Delta A, \Delta b] \in \mathcal{G}^+} \{ \, \|[\Delta A, \Delta b]\|_F \}$$

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Theorem

Let $\hat{x}$ be the true STLS solution.
There exists an $\epsilon > 0$ such that when $\|y - \hat{x}\|_2 < \epsilon$,

$$\mu(y) \text{ is indeed the true minimal backward error.}$$

A pseudo-minimal backward error

We can find an explicit representation of $\mathcal{G}^+$ and minimize over this set.

Theorem

Define $r \equiv b - Ay$ *and*

$$M \equiv A(I - yy^\dagger)A^T - \frac{rr^T}{1 + \|y\|_2^2} + \frac{(Ay + \gamma^2\|y\|_2^2 b)(Ay + \gamma^2\|y\|_2^2 b)^T}{\|y\|_2^2 + \gamma^4\|y\|_2^4}$$

Then

$$\mu^2 = \frac{\|r\|_2^2}{1 + \|y\|_2^2} + \min\{\lambda_{\min}(M), 0\}$$

Limits $\gamma \to 0$ and $\gamma \to \infty$

When $\gamma \to 0$,

$$M \to AA^T - \frac{rr^T}{1 + \|y\|_2^2}$$

This is consistent with the result of Waldén, Karlson & Sun (95).

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When $\gamma \to \infty$,

$$M \to A(I - yy^\dagger)A^T - \frac{rr^T}{1 + \|y\|_2^2} + bb^T$$

This is consistent with the result of Chang, Golub & Paige (06).

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Rearranging terms and taking the 2-norm:

$$\|[\Delta A, \Delta b]\|_2^2 \; + \; \beta_1 \cdot \|[\Delta A, \Delta b]\|_2 \; - \; \beta_0 \geq 0$$

where $\beta_0, \beta_1 \geq 0$ are independent of ΔA and Δb.

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$$\mu \;\geq\; 2\beta_0 \left(\beta_1 + \sqrt{\beta_1^2 + 4\beta_0} \right)^{-1} \equiv \mu_{lb}$$

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This lower bound can be estimated in $\mathcal{O}(mn)$ flops.

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Theorem

$$\lim_{y \to \hat{x}} \tilde{\mu}/\mu = 1$$

Computing the asymptotic estimate

Theorem

Define $r \equiv b - Ay$,

$$\xi_0 \equiv \sqrt{1 + \|y\|_2^2}\,, \quad \xi_1 \equiv \sqrt{\gamma^{-2} + \|y\|_2^2}\,, \quad \xi_2 \equiv \frac{\|y\|_2^2 - \gamma^{-2} + 2}{\xi_0 \xi_1^2}\,,$$

and

$$B \equiv \begin{bmatrix} \xi_0 A + \xi_2 r y^T \\ \xi_0^{-1} \|r\|_2 I \\ \xi_0^{-1} \|r\|_2 \|y\|_2 (I - y y^\dagger) \end{bmatrix}, \quad c \equiv \begin{bmatrix} \xi_0^{-1} r \\ -\xi_1 \|r\|_2 y \\ 0 \end{bmatrix}$$

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Then

$$\tilde{\mu} = \|B B^\dagger c\|_2$$

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Sample numerical test

Tests:

- When is μ actually the minimal backward error?
  (How close does y have to be to the true STLS solution for

$$\frac{\|(b+\Delta b)-(A+\Delta A)y\|_2^2}{\gamma^{-2}+\|y\|_2^2} < \sigma_{min}^2(A+\Delta A)$$

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- Are μ_{lb} and $\tilde{\mu}$ good estimates of μ?

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Data:

- $\gamma = 1$
- 100×40 "random" A with $\|A\|_F = 1$ and $\kappa_2(A) = 10^5$
- E and f are "random" with $\|E\|_F, \|f\|_2 \leq 10^{-2}$
- $b = (A + E)x + f$ where $x = [1, 1, \ldots, 1]^T$

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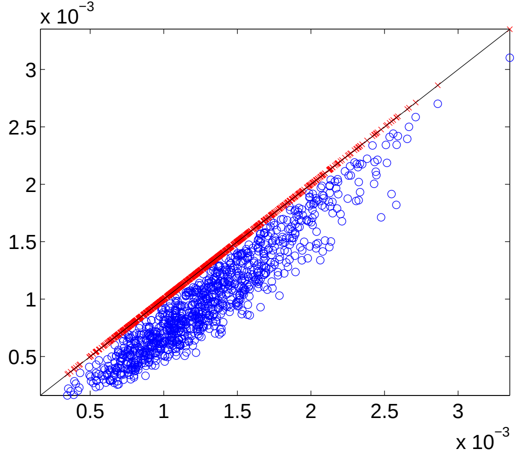
- E and f are "random" with $\|E\|_F, \|f\|_2 \leq 10^{-2}$
- $b = (A + E)x + f$ where $x = [1, 1, \ldots, 1]^T$
- Obtain the STLS solution $\hat{x}$
- Perturb $\hat{x}$ "randomly" to obtain y, with $\frac{\|y-\hat{x}\|_2}{\|\hat{x}\|_2} \leq \delta_x$
- Run 1000 tests with $\delta_x = 10^{-2}$ and $\delta_x = 10^{-1}$

Sample test result: $\delta_x = 10^{-2}$

μ_{lb} vs μ: blue dots; $\tilde{\mu}$ vs μ: red stars



Sample test result: $\delta_x = 10^{-1}$

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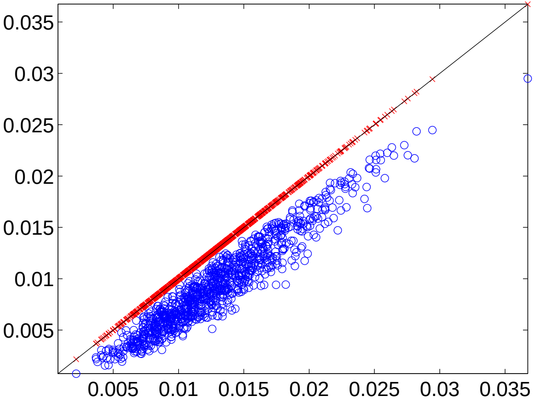

Summary and future work

Given an approximate STLS solution $0 \neq y \in \mathbb{R}^n$, we have found:

- a pseudo-minimal backward error μ
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Thank you for your attention!