The extended normal equations: conditioning and iterative solution

# E. Riccietti (ENS Lyon) http://perso.ens-lyon.fr/elisa.riccietti/

Joint work with: H. Calandra (TOTAL) S. Gratton (IRIT-INP, Toulouse) X. Vasseur (ISAE-SUPAERO, Toulouse)

Communications in NLA 28th September, 2020

## Context

Given  $A \in \mathbb{R}^{m \times n}$ ,  $m \ge n$  with rank(A) = n,  $b \in \mathbb{R}^m$  and  $x, c \in \mathbb{R}^n$ , we consider the *extended least squares problem* 

$$\min_{\mathbf{x}\in\mathbb{R}^n} \frac{1}{2} \|A\mathbf{x} - b\|^2 - \mathbf{c}^T \mathbf{x},$$
(ELS)

whose solution satisfies the extended normal equations

$$A^T A x = A^T b + c. \tag{ENE}$$

 $\rightarrow$  This is a generalization of the least squares problem (case c = 0)

# Motivating applications

#### • Multilevel Levenberg-Marquardt method



Calandra, H., Gratton, S., Riccietti, E., Vasseur, X., On the approximation of the solution of partial differential equations by artificial neural networks trained by a multilevel Levenberg-Marquardt method, OMS, 2020

$$\min_{x\in\mathbb{R}^n}f(x)=\frac{1}{2}\|F(x)\|^2.$$

#### • Penalty function method



Fletcher, R., A class of methods for nonlinear programming: III. Rates of convergence, Numerical Methods for Nonlinear Optimization, 1973



Estrin, R. and Orban, D. and Saunders, M. A., LNLQ: An iterative method for least-norm problems with an error minimization property, SIMAX, 2019

 $\min_{x} f(x)$ <br/>s.t. g(x) = 0.

## Our questions

### Practical aspects:

• How to numerically solve (ENE) by a stable iterative method?

#### O Theoretical aspects:

- How to build a good bound for the forward error on the computed solution by such method?
  - What is the conditioning of (ENE)?
  - What is the backward error of (ENE)?

## NUMERICAL SOLUTION OF THE SYSTEM

# Exploit the structure of the problem

## Case c = 0

- Forming matrix  $A^T A$  leads to a loss of accuracy
- Practical solution methods do not form this product:

$$A^{T}Ax - A^{T}b = A^{T}(Ax - b)$$

- Direct methods: employ a factorization of A rather than of  $A^T A$
- Iterative methods: perform matrix-vector multiplications Ax and  $A^Ty$ .

## **2** Case $c \neq 0$ ?

# CG vs CGLS for normal equations

Same method in exact arithmetic, different performance in finite precision for some problems:

• in CGLS  $d_k = b - Ax_k$  is recurred and  $r_k = A^T d_k$ .

|  | - Algorithm 2 CGLS for $A^T A x = A^T b$  |
|--|---|
| <b>Algorithm 1</b> CG for $A^T A x = A^T b$  |   |
| Input: A, b, x <sub>0</sub> .  | Input: A, b, $x_0$ .<br>Define $d_0 = b - Ax_0$ , $r_0 = A^T d_0$ , $p_1 = r_0$ . |
| Define $r_0 = A^T (b - Ax_0), p_1 = r_0.$  | for $k = 1, 2,$ do  |
| for $k = 1, 2,$ do   | $t_k = A p_k$ ,   |
| $\alpha_k = \frac{r_{k-1}^T r_{k-1}}{\ Ap_k\ ^2},$   | $\alpha_k = \frac{r_{k-1}^{\tau} r_{k-1}}{\ t_k\ ^2},$                            |
| $\begin{aligned} x_k &= x_{k-1}^{-1} + \alpha_k p_k, \\ r_k &= r_{k-1} - \alpha_k A^T (Ap_k), \end{aligned}$ | $x_k = x_{k-1} + \alpha_k p_k,$   |
|  | $d_k = d_{k-1} - \alpha_k t_k,$<br>$r_k = A^T d_k,$                               |
| $\rho r_k^T r_k$   |   |
| $\beta_k = \frac{r_k^T r_k}{r_{k-1}^T r_{k-1}},$   | $\beta_k = \frac{r_k^T r_k}{r_{k-1}^T r_{k-1}},$                                  |
| $p_{k+1} = r_k + \beta_k p_k.$   |   |
| end for  | $p_{k+1} = r_k + \beta_k p_k.$  |
|  | end for   |



Paige, C. C. and Saunders, M. A., *LSQR: An Algorithm for Sparse Linear Equations and Sparse Least Squares*, ACM Trans. Math. Softw., 1982

Björck, A. and Elfving, T. and Strakos, Z. , *Stability of conjugate gradient and Lanczos methods for linear least squares problems*, SIMAX, 1998

# Stable method for solving (ENE): CGLSc

• Extend the successful algorithmic procedures to the case  $c \neq 0$ 

|  | - Algorithm 4 CGLSc for $A^T A x = A^T b + c$                        |  |  |
|--|--|--|--|
| <b>Algorithm 3</b> CG for $A^T A x = A^T b + c$  | Algorithm 4 CGLSc for $A^{T}Ax = A^{T}D + c$                         |  |  |
|  | - Input: $A, b, x_0$   |  |  |
| Input: A. b. c. $x_0$ .  | Define $r_0 = b - Ax_0$ , $s_0 = A^T r_0 + c$ , $p_1 = s_0$ .        |  |  |
| Input: A, b, c, $x_0$ .<br>Define $r_0 = A^T (b - Ax_0) + c$ , $p_1 = r_0$ .                 | for $k = 1, 2,$ do   |  |  |
| for $k = 1, 2,$ do   | $t_k = A \rho_k$   |  |  |
| $\alpha_k = \ r_{k-1}\ ^2 / \ Ap_k\ ^2,$   | $\alpha_k = \ s_{k-1}\ ^2 / \ t_k\ ^2$                               |  |  |
| $x_k = x_{k-1} + \alpha_k p_k,$  | $x_k = x_{k-1} + \alpha_k p_k$                                       |  |  |
| $\mathbf{r}_{k} = \mathbf{r}_{k-1} - \alpha_{k} \mathbf{A}^{T} (\mathbf{A} \mathbf{p}_{k}),$ | $r_k = r_{k=1} - \alpha_k t_k$                                       |  |  |
| $\beta_k = \ r_k\ ^2 / \ r_{k-1}\ ^2,$   | $s_k = A^T r_k + c$  |  |  |
| $p_{k+1} = r_k + \beta_k p_k$  | $\beta_k = \ \mathbf{s}_k\ ^2 / \ \mathbf{s}_{k-1}\ ^2$              |  |  |
| end for  | $\boldsymbol{p}_{k+1} = \boldsymbol{r}_k + \beta_k \boldsymbol{p}_k$ |  |  |
|  | - end for  |  |  |

## Numerical tests: setting

- All the numerical methods have been implemented in Matlab
- Matrix of dimensions m = 100, n = 50 with known singular values distribution
- Performance profiles: 55 matrices, with condition number between 1 and 10<sup>10</sup>. The optimality measure is <sup>||x x̂||</sup>/<sub>||x||</sub>, with x the exact solution (x = (n − 1 : −1 : 0)). A simulation is considered unsuccessful if the relative solution accuracy is larger than 10<sup>-2</sup>.

## Remark

(ENE) is equivalent to the augmented system

$$\begin{bmatrix} \xi I_m & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} b \\ -c/\xi \end{bmatrix}, \quad r = \xi y = b - Ax,$$
(AUG)

## Comparison with iterative methods

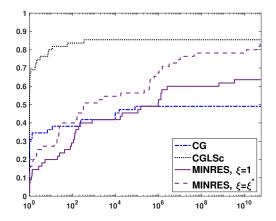
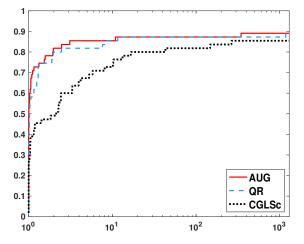


Figure: Performance profile in logarithmic scale. The optimality measure considered is the relative solution accuracy  $||x - \hat{x}|| / ||x||$ .

## Comparison with direct methods



- QR: solves (AUG) with ξ = 1, employing the QR factorization of [A, b].
- AUG: solves (AUG) with  $\xi = \xi^*$  using an  $LBL^T$ factorization (Matlab ldl).

 $\rightarrow$  CGLSc can compare with direct methods in terms of solution accuracy

## THEORETICAL RESULTS: Error bounds

Why can't we use existing theory?

# Can we use standard linear systems theory?

This gives underwhelming results already for normal equations.

Let x and  $\hat{x}$  be an exact and a perturbed solution of (LS),  $\delta x = x - \hat{x}$ , u the machine precision, r = b - Ax the residual.

Forward error bound

Linear systems' theory:

Least squares theory:

$$\frac{\|\delta x\|}{\|x\|} \le \kappa(A)^2 u \qquad \qquad \frac{\|\delta x\|}{\|x\|} \le \frac{m}{1-mu} \kappa(A) \left(1 + \frac{\|A^{\dagger}\| \|r\|}{\|x\|}\right) u$$

## Underwhelming result!

The conditioning of the problem depends on  $\kappa(A)^2$  only if ||r|| is large! The bound from linear systems' theory is pessimistic.

# Why such underwhelming results?

Standard linear systems theory:

- Based on the assumption that the matrix  $A^T A$  is formed explicitly.
- Practical solution methods do not form this product:

$$A^T A x - A^T b = A^T (A x - b)$$

- Direct methods: employ a factorization of A rather than of  $A^T A$
- Iterative methods: perform matrix-vector multiplications Ax and  $A^Ty$ .
- We should consider perturbations on matrix A rather than on matrix  $A^T A$ : we need a structured analysis to obtain condition number and backward error
- Better error bounds:

$$FE \coloneqq \frac{\|x - \hat{x}\|}{\|x\|} \sim \text{relative condition number} \times \text{backward error}$$

# Condition number

### Definition

If F is a continuously differentiable function

 $F: \mathcal{X} \to \mathcal{Y}$  $x \longmapsto F(x),$ 

the absolute condition number of F at x is the scalar

$$\|F'(x)\|_{\mathrm{op}} \coloneqq \sup_{\|v\|_{\mathcal{X}}=1} \|F'(x)v\|_{\mathcal{Y}},$$

where F'(x) is the Fréchet derivative of F at x. The relative condition number of F at x is

$$\frac{\|F'(x)\|_{\mathrm{op}}\,\|x\|_{\mathcal{X}}}{\|F(x)\|_{\mathcal{Y}}}.$$

# Conditioning, normal equations (c = 0)

## Definition of F

We consider F as the function that maps A, b to the solution x of a least squares problem:

$$F: \mathbb{R}^{m \times n} \times \mathbb{R}^m \to \mathbb{R}^n$$
$$(A, b) \longmapsto F(A, b) = A^{\dagger}b.$$

## Explicit formula for the conditioning

The absolute condition number of the normal equations, with Euclidean norm on the solution and Frobenius norm on the data<sup>a</sup>, is given by

$$\kappa_{NE} = \|A^{\dagger}\|\sqrt{1+\|x\|^2+\|A^{\dagger}\|^2\|r\|^2}$$

Gratton, S., On the condition number of linear least squares problems in a weighted Frobenius norm, BIT Numerical Mathematics, 1996

 $^{a}\|[A,b]\|_{F}^{2}\coloneqq \|A\|_{F}^{2}+\|b\|^{2}$ 

## Backward error

Let  $A \in \mathbb{R}^{m \times n}$ ,  $b \in \mathbb{R}^m$  and  $\tilde{x}$  a perturbed solution of the normal equations. Find the smallest perturbation (E, f) of (A, b) such that the vector  $\tilde{x}$  exactly solves

$$(A+E)^{T}(A+E)x = (A+E)^{T}(b+f),$$

i.e. given

$$\mathcal{G} \coloneqq \{ (E, f) \in \mathbb{R}^{m \times n+1} \colon (A+E)^T (A+E) \tilde{x} = (A+E)^T (b+f) \},\$$

we want to compute the quantity:

$$\eta(\tilde{x}) = \min_{(E,f)\in\mathcal{G}} \|[E,f]\|_{F}.$$

Well studied problem  $\rightarrow$  explicit formula for  $\eta(\tilde{x})$ 

# Why can't we use standard least squares theory?

Presence of *c*:

- Conditioning: different mapping from data to solution.
- Backward error: different set of admissible perturbations.

# Conditioning for (ENE)

We consider F as the function that maps A, b, c to the solution x of ENE

$$F: \mathbb{R}^{m \times n} \times \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}^n$$
$$(A, b, c) \longmapsto F(A, b, c) = A^{\dagger}b + A^{\dagger}(A^{\dagger})^{T}c.$$

#### Lemma

The absolute condition number of the problem ENE is given by

$$\|F'(A,b,c)\|_{\mathrm{op}} = \|[(r^{\mathsf{T}} \otimes (A^{\mathsf{T}}A)^{-1})L_{\mathsf{T}} + x^{\mathsf{T}} \otimes A^{\dagger}, A^{\dagger}, (A^{\mathsf{T}}A)^{-1}]\|,$$

where  $L_T$  is the linear operator such that  $vec(A^T) = L_T vec(A)$  and r = b - Ax.

Case c = 0

$$\|F'(A,b,c)\|_{\mathrm{op}} = \|[(r^{\mathsf{T}}\otimes (A^{\mathsf{T}}A)^{-1})L_{\mathsf{T}} + x^{\mathsf{T}}\otimes A^{\dagger},A^{\dagger}]\|.$$

# An explicit formula for the condition number, $c \neq 0$

## Theorem

The absolute condition number of problem (ENE), with Euclidean norm on the solution and Frobenius norm on the data<sup>a</sup>, is  $\sqrt{\|\bar{M}\|}$ , with  $\bar{M} \in \mathbb{R}^{n \times n}$  given by

$$\bar{M} = (1 + \|r\|^2)(A^T A)^{-2} + (1 + \|x\|^2)(A^T A)^{-1} - 2 \operatorname{sym}(B)$$

with  $B = A^{\dagger} r x^{T} (A^{T} A)^{-1}$ , sym $(B) = \frac{1}{2} (B + B^{T})$  and x the exact solution of (ENE).

 ${}^{a} \| (A, b, c) \|_{F}^{2} \coloneqq \| A \|_{F}^{2} + \| b \|^{2} + \| c \|^{2}$ 

### Remark

The structured relative condition number is

$$\kappa_{S} = \frac{\sqrt{\|\bar{M}\|} \|A, b, c\|_{F}}{\|x\|}$$

There are problems in which  $\kappa_S$  can be as large as a quantity of order  $\kappa(A)^2$ , while in others it can be as low as  $\kappa(A)$ .

# Backward error for (ENE)

Let  $A \in \mathbb{R}^{m \times n}$ ,  $b \in \mathbb{R}^m$ ,  $c \in \mathbb{R}^n$  and  $\tilde{x}$  a perturbed solution to (ENE). Find the smallest perturbation (E, f, g) of (A, b, c) such that the vector  $\tilde{x}$  exactly solves

$$(A+E)^{T}(A+E)x = (A+E)^{T}(b+f) + (c+g),$$

i.e. given

 $\mathcal{G} \coloneqq \{ E \in \mathbb{R}^{m \times n}, f \in \mathbb{R}^m, g \in \mathbb{R}^n \colon (A + E)^T (A + E) \tilde{x} = (A + E)^T (b + f) + (c + g) \},\$ 

we want to compute the quantity:

$$\eta(\tilde{x}) = \min_{(E,f,g)\in\mathcal{G}} \|(E,f,g)\|_F := \sqrt{\|E\|_F^2 + \|f\|^2 + \|g\|^2}$$

Difficult to solve  $\rightarrow$  we use a linearized estimate  $\bar{\eta}$ 

# First order approximation for the forward error

• Classical analysis:

$$\Delta_{\mathcal{C}} = \kappa(\mathcal{A})^2 \frac{\|\mathcal{A}^T \mathcal{A} \hat{x} - \mathcal{A}^T b - c\|}{\|\mathcal{A}\|^2 \|\hat{x}\|}$$

• Structured analysis:

$$\Delta_{S} = \frac{\sqrt{\|\overline{M}\|} \|(A, b, c)\|_{F}}{\|\hat{x}\|} \overline{\eta}_{r}(\hat{x}).$$

This is valid only if matrix  $A^T A$  is not explicitly formed.

# Validation of the structured error bound

Table:  $\kappa(A)$ : condition number,  $\kappa_S$ : structured condition number, FE:  $||x - \hat{x}|| / ||x||$  forward error,  $\Delta_C$ : standard bound,  $\Delta_S$ : structured estimate.

| Pb. | $\kappa(A)$      | ĸs               | FE                 | $\Delta_{C}$       | $\Delta_S$         |
|-----|------------------|------------------|--------------------|--------------------|--------------------|
| 1   | $9 \cdot 10^2$   | $1 \cdot 10^6$   | $5 \cdot 10^{-13}$ | $2 \cdot 10^{-10}$ | $1 \cdot 10^{-11}$ |
| 2   | $2 \cdot 10^{3}$ | $4 \cdot 10^3$   | $7 \cdot 10^{-15}$ | $3 \cdot 10^{-10}$ | $3 \cdot 10^{-13}$ |
| 3   | $5 \cdot 10^5$   | $6 \cdot 10^5$   | $1 \cdot 10^{-12}$ | $3 \cdot 10^{-5}$  | $5\cdot 10^{-11}$  |
| 4   | $4 \cdot 10^{7}$ | $4 \cdot 10^7$   | $4 \cdot 10^{-11}$ | $6 \cdot 10^{-2}$  | $4 \cdot 10^{-9}$  |
| 5   | $1 \cdot 10^9$   | $5 \cdot 10^8$   | $3 \cdot 10^{-8}$  | $7 \cdot 10^2$     | $3 \cdot 10^{-7}$  |
| 6   | $1 \cdot 10^{5}$ | $3\cdot 10^{10}$ | $2 \cdot 10^{-8}$  | $3 \cdot 10^{-6}$  | $1 \cdot 10^{-7}$  |
| 7   | $1 \cdot 10^4$   | $5 \cdot 10^5$   | $6 \cdot 10^{-13}$ | $2 \cdot 10^{-8}$  | $2 \cdot 10^{-12}$ |
| 8   | $1 \cdot 10^4$   | $8\cdot 10^9$    | $9 \cdot 10^{-10}$ | $8 \cdot 10^{-8}$  | $7 \cdot 10^{-8}$  |
| 9   | $1 \cdot 10^4$   | $3 \cdot 10^7$   | $5\cdot 10^{-11}$  | $2 \cdot 10^{-8}$  | $1\cdot 10^{-10}$  |
| 10  | $1 \cdot 10^7$   | $3\cdot 10^{10}$ | $3 \cdot 10^{-8}$  | $3\cdot 10^{-2}$   | $1\cdot 10^{-7}$   |

CGLS*c* 

## THANK YOU FOR YOUR ATTENTION



Calandra, H., Gratton, S., Riccietti, E., Vasseur, X., On iterative solution of the extended normal equations, SIMAX, 2020 http://perso.ens-lyon.fr/elisa.riccietti/doc/linear.pdf

## QR method

• Solves the augmented system:

$$\begin{bmatrix} \xi I_m & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} b \\ -c/\xi \end{bmatrix}, \quad r = \xi y = b - Ax,$$

with  $\xi = 1$ , employing the QR factorization of [A, b], as described in theorem below.

#### Theorem

Let  $A \in \mathbb{R}^{m \times n}$ ,  $m \ge n$ ,  $b \in \mathbb{R}^m$ ,  $c \in \mathbb{R}^n$ . Assume that rank(A) = n and let

$$\begin{bmatrix} A, b \end{bmatrix} = Q \begin{bmatrix} R & d_1 \\ 0 & d_2 \end{bmatrix}$$

For any  $\xi \neq 0$ , the solution to the augmented system can be computed from

$$R^T z = -c, \quad Rx = (d_1 - z), \quad r = Q \begin{bmatrix} z \\ d_2 \end{bmatrix}.$$

## Remark

• (ENE) and (AUG) also give the first-order optimality conditions for the problems

$$\min_{x,r} \frac{1}{2} \|r\|^2 - c^T x \text{ subject to } Ax + r = b, \qquad (\text{ELS-primal})$$

and

$$\min_{r} \frac{1}{2} \|r\|^2 - b^T r \quad \text{subject to} \quad A^T r = -c. \quad (\text{ELS-dual})$$

# Motivating applications (I)

• Multilevel Levenberg-Marquardt method



Calandra, H., Gratton, S., Riccietti, E., Vasseur, X., On the approximation of the solution of partial differential equations by artificial neural networks trained by a multilevel Levenberg-Marquardt method, OMS, 2020

$$\min_{x\in\mathbb{R}^n}f(x)=\frac{1}{2}\|F(x)\|^2.$$

We have at disposal an approximation to the objective function:

$$f^{H}(x^{H}) = \frac{1}{2} \|F^{H}(x^{H})\|^{2}, \quad x^{H} \in \mathbb{R}^{n_{H}}, \ n_{H} < n$$

Coarse model:

$$m_{k}^{H}(x_{k}^{H}, s^{H}) = \frac{1}{2} \|F^{H}(x_{k}^{H}) + J^{H}(x_{k}^{H})s^{H}\|^{2} + \frac{\lambda_{k}}{2} \|s^{H}\|^{2} + (R \nabla f(x_{k}) - \nabla f^{H}(x_{0}^{H}))^{T}s^{H},$$

with  $J^H(x_k^H)$  the Jacobian matrix of  $F^H$  at  $x_k^H$ , R a full-rank linear restriction operator and  $x_0^H = Rx_k$ .

# Motivating applications (II)

## • Penalty function method

- Fletcher, R., A class of methods for nonlinear programming: III. Rates of convergence, Numerical Methods for Nonlinear Optimization, 1973
- Estrin, R. and Orban, D. and Saunders, M. A., LNLQ: An iterative method for least-norm problems with an error minimization property, SIMAX, 2019

$$\min_{x} f(x)$$
  
s.t.  $g(x) = 0$ ,

Penalty function :

$$\Phi_{\sigma}(x) = f(x) - g(x)^{T} y_{\sigma}(x),$$

where  $y_{\sigma}(x) \in \mathbb{R}^m$  is the solution of

$$\min_{y} \|A(x)^{\mathsf{T}}y - \nabla f(x)\|^2 + \sigma g(x)^{\mathsf{T}}y,$$

with A(x) the Jacobian matrix of g(x) at x and  $\sigma > 0$ , a given real-valued penalty parameter.

#### Theorem

The absolute condition number of problem (ENE), with Euclidean norm on the solution and Frobenius norm (parameterized by  $\alpha, \beta, \gamma$ ) on the data, is  $\sqrt{\|\bar{M}\|}$ , with  $\bar{M} \in \mathbb{R}^{n \times n}$  given by

$$\bar{M} = \left(\frac{1}{\gamma^2} + \frac{\|r\|^2}{\alpha^2}\right) (A^T A)^{-2} + \left(\frac{1}{\beta^2} + \frac{\|x\|^2}{\alpha^2}\right) (A^T A)^{-1} - \frac{2}{\alpha^2} \operatorname{sym}(B), \quad (1)$$

with  $B = A^{\dagger} r x^{T} (A^{T} A)^{-1}$ , sym $(B) = \frac{1}{2} (B + B^{T})$  and x the exact solution of (ENE).

The structured conditioning of the normal equations is

$$|F'(A,b)|| = ||A^{\dagger}||\sqrt{\frac{1}{\beta^2} + \frac{||x||^2 + ||A^{\dagger}||^2 ||r||^2}{\alpha^2}}.$$

If c = 0 and  $\gamma \to \infty$ , the known result for least squares problems is recovered (note that in this case B = 0 as  $A^T r = 0$ ). Taking large values of  $\gamma$  allows us to perturb A and b only, and to include the case c = 0. This is because the condition  $\gamma \to \infty$  implies  $g \to 0$ , from the constraint  $\alpha^2 \|E\|_{c}^{2} + \beta^2 \|f\|^{2} + \gamma^2 \|g\|^{2} = 1$  in the definition of the condition number.

# Set of admissible perturbations on the matrix

#### Theorem

Let  $A \in \mathbb{R}^{m \times n}$ ,  $b \in \mathbb{R}^m$ ,  $c, \tilde{x} \in \mathbb{R}^n$  and assume that  $\tilde{x} \neq 0$ . Let  $\tilde{r} = b - A\tilde{x}$  and define two sets  $\mathcal{E}, \mathcal{M}$  by

$$\mathcal{E} = \{ E \in \mathbb{R}^{m \times n} : (A + E)^T (b - (A + E)\tilde{x}) = -c \}, \\ \mathcal{M} = \{ v (\alpha c^T - v^{\dagger} A) + (I_m - vv^{\dagger}) (\tilde{r}\tilde{x}^{\dagger} + Z(I_n - \tilde{x}\tilde{x}^{\dagger})) : \\ v \in \mathbb{R}^m, Z \in \mathbb{R}^{m \times n}, \alpha \in \mathbb{R}, s.t. \ \alpha \|v\|^2 (v^{\dagger} b - \alpha c^T \tilde{x}) = -1 \}.$$

Then  $\mathcal{E} = \mathcal{M}$ .

Case c = 0

$$\mathcal{E} = \{ E \in \mathbb{R}^{m \times n} : (A + E)^T (b - (A + E)\tilde{x}) = 0 \},$$
  
$$\mathcal{M} = \{ -vv^{\dagger}A + (I_m - vv^{\dagger})(\tilde{r}\tilde{x}^{\dagger} + Z(I_n - \tilde{x}\tilde{x}^{\dagger})) : v \in \mathbb{R}^m, Z \in \mathbb{R}^{m \times n} \}.$$

## Lower bound on the backward error

#### Lemma

The set of admissible perturbations  ${\cal E}$  defined in Theorem is such that  ${\cal E}\subseteq {\cal M}_2,$  with

$$\mathcal{M}_{2} = \{ v \left( \alpha c^{T} - v^{\dagger} A \right) + (I_{m} - vv^{\dagger}) (\tilde{r} \tilde{x}^{\dagger} + Z(I_{n} - \tilde{x} \tilde{x}^{\dagger})) : v \in \mathbb{R}^{m}, Z \in \mathbb{R}^{m \times n}, \alpha \in \mathbb{R} \}.$$

Then,

$$\min_{\mathcal{E}} \|E\|_{F}^{2} \geq \min_{\mathcal{M}_{2}} \|E\|_{F}^{2} = \frac{\|\tilde{F}\|^{2}}{\|\tilde{x}\|^{2}} + \min\{\lambda_{*}, 0\},$$
  
for  $\lambda_{*} = \lambda_{\min} \left( A(I_{n} - cc^{T})A^{T} - \frac{\tilde{r}\tilde{r}^{T}}{\|\tilde{x}\|^{2}} \right)$ , with  $\lambda_{\min}(M)$  denoting the smallest eigenvalue of the matrix  $M$ .

Case c = 0

$$\min_{\mathcal{E}} \|E\|_{F}^{2} = \frac{\|\tilde{r}\|^{2}}{\|\tilde{x}\|^{2}} + \min\{\lambda_{*}, 0\}, \quad \lambda_{*} = \lambda_{\min}\left(AA^{T} - \frac{\tilde{r}\tilde{r}^{T}}{\|\tilde{x}\|^{2}}\right).$$

# Linearization estimate of $\eta(\tilde{x})$

Given  $h(A, b, c, x) = A^T(b - Ax) + c$ , find (E, f, g) such that

$$\bar{\eta}(\tilde{x}) = \min \|[E, f, g]\|_F \quad \text{s.t.} \quad h(A, b, c, \tilde{x}) + [J_A, J_b, J_c] \begin{bmatrix} \operatorname{vec}(E) \\ f \\ g \end{bmatrix} = 0,$$

where  $J_A$ ,  $J_b$  and  $J_c$  are the Jacobian matrices of h with respect to vec(A), b, c. Lemma

$$\bar{\eta}(\tilde{x}) = \left\| \begin{bmatrix} \operatorname{vec}(E) \\ f \\ g \end{bmatrix} \right\| = \|J^{\dagger}h(A, b, c, \tilde{x})\|, \quad J \coloneqq [I_n \otimes \tilde{r}^T - A^T(\tilde{x} \otimes I_m), A^T, I_n].$$

Moreover, assume that  $\tilde{r} \neq 0$ . If  $4\sqrt{2 + \|\tilde{x}\|^2} \|J^{\dagger}\| \eta(\tilde{x}) \leq 1$ , then

$$\frac{2}{1+\sqrt{2}} \ \bar{\eta}(\tilde{x}) \leq \eta(\tilde{x}) \leq 2 \ \bar{\eta}(\tilde{x}),$$

Backup slides

## Comparison with CG: solution accuracy

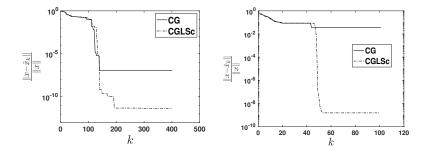


Figure: Left:  $\kappa(A) = 10^5$ . Right:  $\kappa(A) = 5 \times 10^7$ .