## On the iterative solution of systems of the form $A^{\top} A x=A^{\top} b+c$

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## Context

Given $A \in \mathbb{R}^{m \times n}, m \geq n$ with $\operatorname{rank}(A)=n, b \in \mathbb{R}^{m}$ and $x, c \in \mathbb{R}^{n}$, solve

$$
\begin{equation*}
A^{\top} A x=A^{\top} b+\mathbf{c} \tag{SYS}
\end{equation*}
$$

or

$$
\min _{x}\|A x-b\|^{2}-x^{\top} \mathbf{c}
$$

Remarks

- This is a generalization of the normal equations for least-squares problems (case $c=0$ )


## 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, arXiv e-print, 2019

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

We have at disposal an approximation to the objective function:

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

Coarse model:

$$
\begin{aligned}
m_{k}^{H}\left(x_{k}^{H}, s^{H}\right)= & \frac{1}{2}\left\|F^{H}\left(x_{k}^{H}\right)+J^{H}\left(x_{k}^{H}\right) s^{H}\right\|^{2}+\frac{\lambda_{k}}{2}\left\|s^{H}\right\|^{2}+ \\
& \left(R \nabla f\left(x_{k}\right)-\nabla f^{H}\left(x_{0}^{H}\right)\right)^{\top} s^{H},
\end{aligned}
$$

with $J^{H}\left(x_{k}^{H}\right)$ the Jacobian matrix of $F^{H}$ at $x_{k}^{H}, R$ a full-rank linear restriction operator and $x_{0}^{H}=R x_{k}$.

## Motivating applications (II)

- Penalty function method

显
Fletcher, R., A class of methods for nonlinear programming: III. Rates of convergence, Numerical Methods for Nonlinear Optimization, 1973
通
Estrin, R. and Orban, D. and Saunders, M. A., LNLQ: An iterative method for least-norm problems with an error minimization property, technical report, 2018

$$
\begin{aligned}
& \min _{x} f(x) \\
\text { s.t. } & g(x)=0,
\end{aligned}
$$

Penalty function :

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

where $y_{\sigma}(x) \in \mathbb{R}^{m}$ is defined as the solution of the following minimization problem:

$$
\min _{y}\left\|A(x)^{\top} y-\nabla f(x)\right\|^{2}+\sigma g(x)^{\top} y
$$

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

## Interesting questions

- What is the conditioning of $A^{\top} A x=A^{\top} b+c$ ?
- Standard theory for linear systems do no take into account structured perturbations and gives underwhelming results
- Structured conditioning analysis is necessary. Presence of $c$ results in a different mapping from data to solution
- What is the backward error?
- Different set of admissible perturbations on the matrix
- How to numerically solve it by an iterative method?
- Methods for normal equations such as CGLS cannot be used.

THEORETICAL RESULTS

## Conditioning, case $c=0$

Let $\delta x=x-\hat{x}, \hat{x}$ a perturbed solution.
Forward error bound
From standard theory on linear systems:

$$
\frac{\|\delta x\|}{\|x\|} \leq \kappa(A)^{2} u
$$

For least squares problems:

$$
\frac{\|\delta x\|}{\|x\|} \leq \gamma_{m} \kappa_{L S} u, \quad \kappa_{L S}=\kappa(A)\left(1+\frac{\left\|A^{\dagger}\right\|\|r\|}{\|x\|}\right), \quad r=b-A x
$$

Underwhelming result!
The conditioning of the problem depends on $\kappa(A)^{2}$ only if $\|r\|$ is large!

## Conditioning

Definition
If $F$ is a continuously differentiable function

$$
\begin{aligned}
F & : \mathcal{X} \\
& \rightarrow \mathcal{Y} \\
& \longmapsto F(x),
\end{aligned}
$$

the absolute condition number of $F$ at $x$ is the scalar $\left\|F^{\prime}(x)\right\|_{\text {op }}$. The relative condition number of $F$ at $x$ is

$$
\frac{\left\|F^{\prime}(x)\right\|_{\mathrm{op}}\|x\|_{\mathcal{X}}}{\|F(x)\|_{\mathcal{Y}}} .
$$

R J R . Rice, A theory of condition, SIAM J. Numer . Anal ., 1966

## Conditioning, case $c=0$

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

$$
\begin{gathered}
F: \mathbb{R}^{m \times n} \times \mathbb{R}^{m} \rightarrow \mathbb{R}^{n} \\
(A, b) \longmapsto F(A, b)=A^{\dagger} b
\end{gathered}
$$

Explicit formula for the conditioning
The absolute condition number of a least-squares problem, with Euclidean norm on the solution and Frobenius norm on the data ${ }^{a}$, is given by

$$
\kappa_{N E}=\left\|A^{\dagger}\right\| \sqrt{1+\|x\|^{2}+\left\|A^{\dagger}\right\|^{2}\|r\|^{2}}
$$



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

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

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

## Lemma

The absolute condition number of the problem SYS is given by

$$
\left\|F^{\prime}(A, b, c)\right\|_{\mathrm{op}}=\left\|\left[\left(r^{\top} \otimes\left(A^{T} A\right)^{-1}\right) L_{T}+x^{\top} \otimes A^{\dagger}, A^{\dagger},\left(A^{\top} A\right)^{-1}\right]\right\|,
$$

where $L_{T}$ is the linear operator such that $\operatorname{vec}\left(A^{\top}\right)=L_{T} \operatorname{vec}(A)$ and $r=b-A x$.

Case $c=0$

$$
\left\|F^{\prime}(A, b, c)\right\|_{\mathrm{op}}=\left\|\left[\left(r^{\top} \otimes\left(A^{T} A\right)^{-1}\right) L_{T}+x^{\top} \otimes A^{\dagger}, A^{\dagger}\right]\right\|
$$

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

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

$$
\begin{gathered}
F: \mathbb{R}^{m \times n} \times \mathbb{R}^{m} \times \mathbb{R}^{n} \rightarrow \mathbb{R}^{n} \\
(A, b, c) \longmapsto F(A, b, c)=A^{\dagger} b+A^{\dagger}\left(A^{\dagger}\right)^{\top} c .
\end{gathered}
$$

Theorem
The absolute condition number of problem SYS, with Euclidean norm on the solution and Frobenius norm on the data ${ }^{a}$, is $\sqrt{\|\bar{M}\|}$, with $\bar{M} \in \mathbb{R}^{n \times n}$ given by

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

with $B=A^{\dagger} r x^{\top}\left(A^{\top} A\right)^{-1}, \operatorname{sym}(B)=\frac{1}{2}\left(B+B^{\top}\right)$ and $x$ the exact solution of SYS.

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

Upper bound for the condition number

$$
\sqrt{\|\bar{M}\|} \leq(1+\|r\|+2 \sqrt{\|c\|\|x\|})\left\|A^{\dagger}\right\|^{2}+(1+\|x\|)\left\|A^{\dagger}\right\| .
$$

## Backward error analysis

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 SYS . Find the smallest perturbation $E$ of $A$ such that the vector $\tilde{x}$ exactly solves

$$
(A+E)^{\top}(A+E) x=(A+E)^{\top} b+c,
$$

i.e. given

$$
\mathcal{G}:=\left\{E \in \mathbb{R}^{m \times n}:(A+E)^{\top}(A+E) \tilde{x}=(A+E)^{\top} b+c\right\},
$$

we want to compute the quantity:

$$
\eta(\tilde{x})=\min _{E \in \mathcal{G}}\|E\|_{F}
$$

## 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

$$
\begin{aligned}
\mathcal{E}= & \left\{E \in \mathbb{R}^{m \times n}:(A+E)^{\top}(b-(A+E) \tilde{x})=-c\right\}, \\
\mathcal{M}= & \left\{v\left(\alpha c^{\top}-v^{\dagger} A\right)+\left(I_{m}-v v^{\dagger}\right)\left(\tilde{r} \tilde{x}^{\dagger}+Z\left(I_{n}-\tilde{x} \tilde{x}^{\dagger}\right)\right):\right. \\
& \left.v \in \mathbb{R}^{m}, Z \in \mathbb{R}^{m \times n}, \alpha \in \mathbb{R}, \text { s.t. } \alpha\|v\|^{2}\left(v^{\dagger} b-\alpha c^{\top} \tilde{x}\right)=-1\right\} .
\end{aligned}
$$

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

Case $c=0$

$$
\begin{aligned}
\mathcal{E} & =\left\{E \in \mathbb{R}^{m \times n}:(A+E)^{\top}(b-(A+E) \tilde{x})=0\right\}, \\
\mathcal{M} & =\left\{-v v^{\dagger} A+\left(I_{m}-v v^{\dagger}\right)\left(\tilde{r} \tilde{x}^{\dagger}+Z\left(I_{n}-\tilde{x} \tilde{x}^{\dagger}\right)\right): v \in \mathbb{R}^{m}, Z \in \mathbb{R}^{m \times n}\right\} .
\end{aligned}
$$

## Lower bound on the backward error

## Lemma

The set of admissible perturbations $\mathcal{E}$ defined in Theorem is such that $\mathcal{E} \subseteq \mathcal{M}_{2}$, with

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

Then,

$$
\min _{\mathcal{E}}\|E\|_{F}^{2} \geq \min _{\mathcal{M}_{2}}\|E\|_{F}^{2}=\frac{\|\tilde{r}\|^{2}}{\|\tilde{x}\|^{2}}+\min \left\{\lambda_{*}, 0\right\}
$$

for $\lambda_{*}=\lambda_{\text {min }}\left(A\left(I_{n}-c C^{\top}\right) A^{\top}-\frac{\tilde{r} \tilde{r}^{\top}}{\|\tilde{x}\|^{2}}\right)$, with $\lambda_{\text {min }}(M)$ denoting the smallest eigenvalue of the matrix $M$.

Case $c=0$

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

## NUMERICAL SOLUTION OF THE SYSTEM

## CG vs CGLS for normal equations

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

- in CGLS $d_{k}=b-A x_{k}$ is recurred and $r_{k}=A^{\top} d_{k}$.

Algorithm 1 CG for $A^{\top} A x=A^{\top} b$

```
Input: \(A, b, x_{0}\).
Define \(r_{0}=A^{\top}\left(b-A x_{0}\right), p_{1}=r_{0}\).
    for \(k=1,2, \ldots\) do
        \(\alpha_{k}=\frac{r_{k-1}^{\top} r_{k-1}}{\left\|A p_{k}\right\|^{2}}\),
        \(x_{k}=x_{k-1}+\alpha_{k} p_{k}\),
\(r_{k}=r_{k-1}-\alpha_{k} A^{\top}\left(A p_{k}\right)\),
        \(x_{k}=x_{k-1}+\alpha_{k} p_{k}\),
\(r_{k}=r_{k-1}-\alpha_{k} A^{\top}\left(A p_{k}\right)\),
        \(\beta_{k}=\frac{r_{k}^{\top} r_{k}}{r_{k-1}^{\top} r_{k-1}}\),
        \(p_{k+1}=r_{k}+\beta_{k} p_{k}\).
    end for
```

```
Algorithm 2 CGLS for \(A^{\top} A x=A^{\top} b\)
    Input: \(A, b, x_{0}\).
    Define \(d_{0}=b-A x_{0}, r_{0}=A^{\top} d_{0}, p_{1}=r_{0}\).
    for \(k=1,2, \ldots\) do
        \(t_{k}=A p_{k}\),
        \(\alpha_{k}=\frac{r_{k-1}^{\top} r_{k-1}}{\left\|t_{k}\right\|^{2}}\),
        \(x_{k}=x_{k-1}+\alpha_{k} p_{k}\),
        \(d_{k}=d_{k-1}-\alpha_{k} t_{k}\),
        \(r_{k}=A^{\top} d_{k}\),
        \(\beta_{k}=\frac{r_{k}^{\top} r_{k}}{r_{k-1}^{\top} r_{k-1}}\),
        \(p_{k+1}=r_{k}+\beta_{k} p_{k}\).
    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
$\square$ Björck, A. and Elfving, T. and Strakos, Z., Stability of conjugate gradient and Lanczos methods for linear least squares problems, SIMAX, 1998

## CG for $A^{\top} A x=A^{\top} b+c$

Initial rounding error due to the product $r_{0}=A^{T} b+c-A^{T} A x_{0}$ :

$$
\|\delta x\| \leq \kappa(A)^{2} u\left(\frac{\|b\|}{\|A\|}+\frac{\|c\|}{\|A\|^{2}}\right)
$$

This initial error cannot be canceled, and the best error bound we can hope for will include the term given above.
Optimal bound:

$$
\|\delta x\| \leq \sqrt{\|\bar{M}\|}\|[A, b, c]\|_{F u}
$$

If

$$
\|b\|\|A\|+\|c\| \gg\left[1+\|r\|+2 \sqrt{\|c\|\|x\|}+\frac{1+\|x\|}{\left\|A^{\dagger}\right\|}\right] \sqrt{\|A\|_{F}^{2}+\|b\|^{2}+\|c\|^{2}}
$$

CG can be expected to produce less than optimal accuracy.

## IDEA to design a stable method

- Extend the successful algorithmic procedures to the case $c \neq 0$
- Need to factorize matrix $A$ in both the left and right hand sides

$$
A^{T}\left(A^{T} x-b\right)
$$

Two solution methods
We propose two iterative methods based on two different reformulations of the problem

## Proposed methods (I) CGLS $\epsilon$

Given $\epsilon>0$, let us then define

$$
A_{\epsilon}=\left[\begin{array}{c}
A \\
\epsilon C^{\top}
\end{array}\right], \quad b_{\epsilon}=\left[\begin{array}{c}
b \\
1 / \epsilon
\end{array}\right] .
$$

We then consider the following linear least squares problem:

$$
\min _{x}\left\|A_{\epsilon} x-b_{\epsilon}\right\|^{2}
$$

with normal equations

$$
\left(A^{\top} A+\epsilon^{2} c c^{\top}\right) x=A^{\top} b+c .
$$

## CGLS $\epsilon$ solves $S Y S \epsilon$ with CGLS method

## Lemma

Let $x_{\epsilon}$ be the solution of SYS $\epsilon$ and $x$ be the solution of SYS. Then, $\lim _{\epsilon \rightarrow 0} x_{\epsilon}=x$ and the relative norm of the error satisfies

$$
\frac{\left\|x_{\epsilon}-x\right\|}{\|x\|} \leq \epsilon^{2} \frac{\|c\|\|w\|}{1+\epsilon^{2} c^{\top} w}, \quad w=\left(A^{\top} A\right)^{-1} c
$$

## Remarks (I)

- Will a really small $\epsilon$ may cause large errors in finite arithmetic?
- A perturbed solution $\tilde{x}_{\epsilon}=x_{\epsilon}+\delta x_{\epsilon}$ will be such that:

$$
\left(A_{\epsilon}^{\top} A_{\epsilon}\right)\left(\delta x_{\epsilon}\right)=\delta\left(A_{\epsilon}^{\top} b_{\epsilon}\right) . \quad\left|\delta\left(A_{\epsilon}^{\top} b_{\epsilon}\right)\right| \leq \gamma_{m+1}\left|A_{\epsilon}^{\top} \| b_{\epsilon}\right|
$$

This overestimates the error!

$$
\mathrm{fl}\left(A_{\epsilon}^{\top} b_{\epsilon}\right)=\mathrm{fl}\left(A^{\top} b\right)+\mathrm{fl}\left(\epsilon c \frac{1}{\epsilon}\right)+\delta_{s},
$$

with $\delta_{s}$ error due to the summation.

- If $\epsilon=2^{i}$ for $i \in \mathbb{Z}$, then $\mathrm{fl}\left(\epsilon \subset \frac{1}{\epsilon}\right)=c$. Then,

$$
\mathrm{fl}\left(A_{\epsilon}^{\top} b_{\epsilon}\right)=A^{\top} b+c+\delta_{p}+\delta_{s}, \quad \text { with } \quad\left|\delta_{s}\right| \leq u\left|\mathrm{fl}\left(A^{\top} b\right)+c\right|,\left|\delta_{p}\right| \leq \gamma_{m}|A||b|,
$$

and the bound does not depend on $\epsilon$.

## Remarks (II)

- What about the conditioning of the problem?
- Due to the presence of small $\epsilon$ in the right-hand side the residual will generally be really large.
- Standard conditioning analysis of least squares problems is not well-suited in this case
- We can show that the conditioning does not depend on $\left\|b_{\epsilon}-A_{\epsilon} x_{\epsilon}\right\|$, that will be really large, but rather on $\left\|r_{\epsilon}\right\|=\left\|b-A x_{\epsilon}\right\|$, that will be indeed much smaller


## Conditioning

- Let $F_{\epsilon}$ be the function that maps $A, b, c$ to the solution $x_{\epsilon}$ of SYS $\epsilon$

$$
\begin{gathered}
F_{\epsilon}: \mathbb{R}^{m \times n} \times \mathbb{R}^{m} \times \mathbb{R}^{n} \rightarrow \mathbb{R}^{n} \\
(A, b, c) \longmapsto F_{\epsilon}(A, b, c)=\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-1}\left(A^{\top} b+c\right),
\end{gathered}
$$

and let $r_{\epsilon}=b-A x_{\epsilon}$.

- The absolute condition number of problem $\mathrm{SYS} \epsilon$, with Euclidean norm on the solution and Frobenius norm on the data, is then given by:

$$
\begin{aligned}
\left\|F_{\epsilon}^{\prime}(A, b, c)\right\|_{\mathrm{op}}= & \|\left[\left(r_{\epsilon}^{\top} \otimes\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-1}\right) L_{T}+x_{\epsilon}^{\top} \otimes\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-1} A^{\top},\right. \\
& \left.\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-1} A^{\top},\left(1-2 \epsilon c^{\top} x_{\epsilon}\right)\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-1}\right] \| .
\end{aligned}
$$

- Computable formula: $\sqrt{\left\|\bar{M}_{\epsilon}\right\|}$, with

$$
\begin{aligned}
\bar{M}_{\epsilon}= & \left(\left(1-2 \epsilon c^{\top} x_{\epsilon}\right)^{2}+\left\|r_{\epsilon}\right\|^{2}\right)\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-2} \\
& +\left(1+\left\|x_{\epsilon}\right\|^{2}\right)\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-1} A^{\top} A\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-1}-2 \operatorname{sym}\left(B_{\epsilon}\right)
\end{aligned}
$$

with $B_{\epsilon}=\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-1} A^{\top} r_{\epsilon} \tau_{\epsilon}^{\top}\left(A_{\epsilon}^{\top} A_{\epsilon}\right)^{-1}$ and $\operatorname{sym}\left(B_{\epsilon}\right)=\frac{1}{2}\left(B_{\epsilon}+B_{\epsilon}^{\top}\right)$.

## Proposed method (II) CGLSI

Given $\hat{l} \in \mathbb{R}^{(m+1) \times(m+1)}$, we define $\hat{A} \in \mathbb{R}^{(m+1) \times n}$ and $\hat{b} \in \mathbb{R}^{m+1}$ as:

$$
\hat{A}=\left[\begin{array}{c}
A \\
C^{\top}
\end{array}\right], \quad \hat{I}=\left[\begin{array}{cc}
I_{m} & 0 \\
0 & 0
\end{array}\right], \quad \hat{b}=\left[\begin{array}{l}
b \\
1
\end{array}\right] .
$$

We then reformulate SYS as:

$$
\hat{A}^{\top} \hat{l} \hat{A} x=\hat{A}^{\top} \hat{b}
$$

- Possible to factorize $\hat{A}^{\top}$ in both the right and the left-hand sides:
- no need of recurring the residual $r=\hat{A}^{\top}(\hat{l} \hat{A} x-\hat{b})$ (simply update $\hat{d}=\hat{l} \hat{A} x-\hat{b}$ along the iterations and form $r$ by multiplication with $\hat{A}^{\top}$ )
- computation of $p_{k}^{\top} A^{\top} A p_{k}$ as $\left\|\hat{I} \hat{A} p_{k}\right\|^{2}$

We can therefore expect the same benefits of CGLS as compared to CG.

## Algorithm

Algorithm 3 CGLSI for $A^{\top} A x=A^{\top} b+c$
Input: $\hat{A}, \hat{b}, x_{0}$
Define $\hat{d}_{0}=\hat{b}-\hat{A} x_{0}, r_{0}=\hat{A}^{\top}\left(\hat{b}-\hat{A} x_{0}\right), p_{1}=r_{0}$.
for $k=1,2, \ldots$ do
$\hat{t}_{k}=\hat{I} \hat{A} p_{k}$,
$\alpha_{k}=\frac{r_{k-1}^{\top} r_{k-1}}{\hat{t}_{k}^{\top} \hat{k}_{k}}$,
$x_{k}=x_{k-1}+\alpha_{k} p_{k}$,
$\hat{d}_{k}=\hat{d}_{k-1}-\alpha_{k} \hat{t}_{k}$,
$r_{k}=\hat{A}^{\top} \hat{d}_{k}$,
$\beta_{k}=\frac{r_{k}^{\top} r_{k}}{r_{k-1}^{\top} r_{k-1}}$,
$p_{k+1}=r_{k}+\beta_{k} p_{k}$.
end for

## First order approximation for the forward error

First order approximation for the forward error can be obtained as

$$
\frac{\|x-\hat{x}\|}{\|x\|} \sim \frac{\kappa_{S Y S}\|[A, b, c]\| F}{\|x\|} u, \quad u \text { machine precision }
$$

We define the following error estimates:

$$
\begin{aligned}
& \hat{E}_{C G L S I}:=\frac{\sqrt{\|\bar{M}\|\|[A, b, c]\|_{F}}}{\|x\|} u, \\
& \hat{E}_{C G L S_{\epsilon}}:=\epsilon^{2} \frac{\|c\|\|w\|}{1+\epsilon^{2} c^{\top} w}+\frac{\sqrt{\left\|\bar{M}_{\epsilon}\right\|\|[A, b, c]\|_{F}}}{\|x\|} u I_{n}-\frac{\epsilon^{2} w c^{\top}}{1+\epsilon^{2} c^{\top} w} \|,
\end{aligned}
$$

$u$ being the machine precision.

- CGLS $\epsilon$ : the error on the computed solution $\hat{x}_{\epsilon}$ depends on two terms:

$$
\frac{\left\|x-\hat{x}_{\epsilon}\right\|}{\|x\|} \leq \frac{\left\|x-x_{\epsilon}\right\|}{\|x\|}+\frac{\left\|x_{\epsilon}-\hat{x}_{\epsilon}\right\|}{\|x\|}=\frac{\left\|x-x_{\epsilon}\right\|}{\|x\|}+\frac{\left\|x_{\epsilon}-\hat{x}_{\epsilon}\right\|}{\left\|x_{\epsilon}\right\|} \frac{\left\|x_{\epsilon}\right\|}{\|x\|} .
$$

## NUMERICAL TESTS

## Numerical tests: setting

- All the numerical methods have been implemented in Matlab
- $A \in \mathbb{R}^{m \times n}, A=U \Sigma V^{\top}$, where $U$ and $V$ from gallery('orthog', $m / n, j$ ), $j=1, \ldots, 6$.
- C1: $\Sigma_{i i}=a^{-i}$, for $a>0$,

C2 : $\Sigma_{i i}=u_{i}, u=\operatorname{linspace}(d w, u p, n)$, with dw, up $>0$, for $i=1, \ldots, n$.

- Matrix dimensions: $m=40$ and $n=20$ for the tests and $m=100, n=50$ for performance profiles
- Performance profiles: 40 matrices, with condition number between 1 and $10^{10}$. The optimality measure is $\frac{\|x-\hat{x}\|}{\|x\|}$, with $x$ the exact solution $(x=(n-1:-1: 0))$. A simulation is considered unsuccessful if the relative solution accuracy is larger than $10^{-2}$.


## How to choose $\epsilon$ ?




$$
\frac{\left\|x-\hat{x}_{\epsilon}\right\|}{\|x\|} \leq \frac{\left\|x-x_{\epsilon}\right\|}{\|x\|}+\frac{\left\|x_{\epsilon}-\hat{x}_{\epsilon}\right\|}{\|x\|}=\frac{\left\|x-x_{\epsilon}\right\|}{\|x\|}+\frac{\left\|x_{\epsilon}-\hat{x}_{\epsilon}\right\|}{\left\|x_{\epsilon}\right\|} \frac{\left\|x_{\epsilon}\right\|}{\|x\|} .
$$



Figure: Left: right hand side of small norm, Right: right hand side of large norm


## Comparison with CG



Figure: Left: $\kappa(A)=10^{5}, \kappa(\hat{A})=10^{5}$. Right: $\kappa(A)=10^{7}, \kappa(\hat{A})=10^{10}$.


Performance of CGLSI and CGLS $\epsilon$ is comparable but

- CGLSI is parameter free
- CGLS/ is less sensible to the right hand side

Much better performance than CG

## Validation of error bounds

| Problem | $\kappa(A)^{2} u$ | $E_{C G L S I}$ | $\hat{E}_{C G L S I}$ | $E_{C G L S \epsilon}$ | $\hat{E}_{C G L S \epsilon}$ |
| :---: | :---: | :--- | :--- | :--- | :--- |
| $a=2.0$ | $10^{-10}$ | $10^{-11}$ | $10^{-8}$ | $10^{-9}$ | $10^{-9}$ |
| $a=2.5$ | $10^{-2}$ | $10^{-9}$ | $10^{-6}$ | $10^{-9}$ | $10^{-6}$ |
| $a=1.5$ | $10^{-10}$ | $10^{-13}$ | $10^{-11}$ | $10^{-13}$ | $10^{-11}$ |
| $a=1.3$ | $10^{-12}$ | $10^{-13}$ | $10^{-13}$ | $10^{-14}$ | $10^{-13}$ |
| $a=1.1$ | $10^{-14}$ | $10^{-14}$ | $10^{-13}$ | $10^{-14}$ | $10^{-14}$ |
| $a=0.7$ | $10^{-10}$ | $10^{-12}$ | $10^{-12}$ | $10^{-12}$ | $10^{-12}$ |
| up $=1$ | $10^{-2}$ | $10^{-9}$ | $10^{-7}$ | $10^{-8}$ | $10^{-8}$ |
| up $=1$ | $10^{-2}$ | $10^{-8}$ | $10^{-4}$ | $10^{-4}$ | $10^{-6}$ |
| $a=1.5$ | $10^{-10}$ | $10^{-13}$ | $10^{-12}$ | $10^{-10}$ | $10^{-10}$ |

- Better performance that standard CG, both in terms of accuracy and of rate of convergence.
- The error bounds much better predict forward errors than classical bounds.


## Comparison with QR method



- Propose method can compare with direct methods in terms of solution accuracy


## THANK YOU FOR YOUR ATTENTION

Calandra, H., Gratton, S., Riccietti, E., Vasseur, X., On the solution of systems of the form $A^{T} A x=A^{T} b+c$, $\operatorname{In}$ preparation

## Effect of large right-hand sides

Let us assume to apply CG to SYS and CGLS to SYS $\epsilon$. We would respectively compute:

$$
\alpha_{1}=\frac{\left\|r_{0}\right\|^{2}}{p_{1}^{\top} A^{\top} A p_{1}}=\frac{\left\|A^{\top} b+c\right\|^{2}}{\left\|A\left(A^{\top} b+c\right)\right\|^{2}}, \quad x_{1}=\alpha_{1}\left(A^{\top} b+c\right)=\alpha_{1} p_{1}
$$

and

$$
\alpha_{1}(\epsilon)=\frac{\left\|A^{\top} b+c\right\|^{2}}{\left\|A\left(A^{\top} b+c\right)\right\|^{2}+\epsilon\left\|c^{\top}\left(A^{\top} b+c\right)\right\|}, \quad x_{1}(\epsilon)=\alpha_{1}(\epsilon) p_{1}(\epsilon)=\alpha_{1}(\epsilon) p_{1}
$$

Notice that if $\epsilon$ tends to zero, so does the term $\epsilon\left\|c^{\top}\left(A^{\top} b+c\right)\right\|$ in the denominator of $\alpha_{1}(\epsilon)$. Consequently $\alpha_{1}(\epsilon)$ tends toward $\alpha_{1}$ and $x_{1}(\epsilon)$ tends toward $x_{1}$. If $\epsilon$ has to be fixed, its value should be small enough to let $\epsilon\left\|c^{\top}\left(A^{\top} b+c\right)\right\|$ be small compared to $\left\|A\left(A^{\top} b+c\right)\right\|^{2}$, otherwise the found approximation will be close to a solution of $\mathrm{SYS} \epsilon$ rather than to one of SYS. This choice is then particularly difficult when $\left\|A^{\top} b+c\right\|$ is large.

