# Linear regression models and stopping criteria for Krylov methods 

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## Overview of talk

- Motivations and Modelling
- Perturbation Theory
- Statistical tests
- Least-squares and deterministic approach
- Stopping criteria
- Numerical examples


## Linear regression problem

Let $A \in \mathrm{R}^{m \times n}, \quad m \geq n$, with $\operatorname{Rank}(A)=n$. We consider the linear regression model

$$
\begin{equation*}
\mathbf{y}=A \mathfrak{X}+\mathbf{e}, \tag{1}
\end{equation*}
$$

where $E[\mathbf{e}]=0$ and $V[\mathbf{e}]=\sigma^{2} I_{m}$. We point out that $A$ defines a given model and $\mathfrak{X}$ is an unknown deterministic value. The minimum-variance unbiased (MVU) estimator of $\mathfrak{X}$ is related to $\mathbf{y}$ by the Gauss-Markov theorem.

## Gauss-Markov Theorem

For the linear model (1) the minimum-variance unbiased estimator of $\mathfrak{X}$ is given by

$$
\mathbf{x}^{*}=\left(A^{T} A\right)^{-1} A^{T} \mathbf{y}
$$

The variance $V\left[\mathbf{x}^{*}\right]=\sigma^{2}\left(A^{T} A\right)^{-1}$. If $\mathbf{e} \sim \mathcal{N}\left(0, \sigma^{2} I_{m}\right)$, and if we set

$$
\mathbf{s}^{2}=\frac{1}{m-n}\|\mathbf{r}\|_{2}^{2}, \quad \mathbf{r}=\mathbf{y}-A \mathbf{x}^{*}
$$

we have for our estimator of $\mathfrak{X}$ and for $\mathbf{s}^{\mathbf{2}}$, our estimator for $\sigma^{2}$,

$$
\mathbf{x}^{*} \sim \mathcal{N}\left(\mathfrak{x}, \sigma^{2}\left(A^{T} A\right)^{-1}\right), \quad \mathbf{s}^{2} \sim \frac{\sigma^{2}}{m-n} \chi^{2}(m-n)
$$

Moreover, the predicted value $\hat{\mathbf{y}}=A \mathbf{x}^{*}$ and the residual $\mathbf{r}$ are

$$
\hat{\mathbf{y}} \sim \mathcal{N}\left(A \mathfrak{x}, \sigma^{2} A\left(A^{T} A\right)^{-1} A^{T}\right) \text { and } \mathbf{r} \sim \mathcal{N}\left(0, \sigma^{2}\left(I-A\left(A^{T} A\right)^{-1} A^{T}\right)\right)
$$

## Perturbation theory

What we mean with PERTURBATION ?

## Perturbation theory

What we mean with PERTURBATION ?
Let $\delta \hat{\mathbf{y}}$ be a stochastic variable such that

$$
\delta \hat{\mathbf{y}} \sim \mathcal{N}\left(0, \tau^{2} A\left(A^{T} A\right)^{-1} A^{T}\right)
$$

Under the Hypotheses of Gauss-Markov, and assuming that $\hat{\mathbf{y}}$ and $\delta \hat{\mathbf{y}}$ are independently distributed, we have

$$
\hat{\mathbf{y}}+\delta \hat{\mathbf{y}} \sim \mathcal{N}\left(A \mathfrak{x},\left(\tau^{2}+\sigma^{2}\right) A\left(A^{T} A\right)^{-1} A^{T}\right)
$$

Moreover, we have that

$$
\|\delta \hat{\mathbf{y}}\|_{2}^{2} \sim \tau^{2} \chi^{2}(n)
$$

## Perturbation theory

Let $\delta \hat{\mathbf{y}} \sim \mathcal{N}\left(0, \tau^{2} A\left(A^{T} A\right)^{-1} A^{T}\right)$.
Under the hypotheses of Gauss-Markov and assuming that $\hat{\mathbf{y}}$ and $\delta \hat{\mathbf{y}}$ be uncorrelated, there exists

$$
\delta \mathbf{x}^{*} \sim \mathcal{N}\left(0, \tau^{2}\left(A^{T} A\right)^{-1}\right), \quad \delta \mathbf{y} \sim \mathcal{N}\left(0, \tau^{2} I_{m}\right)
$$

such that

1. $\hat{\mathbf{y}}+\delta \hat{\mathbf{y}}=A\left(\mathbf{x}^{*}+\delta \mathbf{x}^{*}\right)$,
2. $\mathbf{x}^{*}+\delta \mathbf{x}^{*}$ is the minimum-variance unbiased estimator of $\mathfrak{X}$ for the linear regression problem:

$$
\mathbf{y}+\delta \mathbf{y}=A \mathfrak{x}+\overline{\mathbf{e}}, \quad \overline{\mathbf{e}} \sim \mathcal{N}\left(0,\left(\sigma^{2}+\tau^{2}\right) I_{m}\right),
$$

3. and $\overline{\mathbf{s}}^{2}=\frac{1}{m-n}\left\|\mathbf{y}+\delta \mathbf{y}-A\left(\mathbf{x}^{*}+\delta \mathbf{x}^{*}\right)\right\|_{2}^{2}$, is the estimator for $\rho^{2}=\sigma^{2}+\tau^{2}$ with $\overline{\mathbf{s}}^{2} \sim \frac{\sigma^{2}+\tau^{2}}{m-n} \chi^{2}(m-n)$.

## Least-squares problem

The minimum-variance unbiased (MVU) estimators of $\mathfrak{X}$ and $\sigma^{2}$ are closely related to the solution of the least-squares problem (LSP),

$$
\begin{equation*}
\min _{x}\|y-A x\|_{2}^{2} \tag{2}
\end{equation*}
$$

where $y$ is a realization of $\mathbf{y}$. The least-squares problem (LSP) has the unique solution

$$
x^{*}=\left(A^{T} A\right)^{-1} A^{T} y
$$

and the corresponding minimum value is achieved by the $\|r\|_{2}$

$$
r=y-A x^{*}=(I-P) y, \quad\left(I-P=I-A\left(A^{T} A\right)^{-1} A^{T}\right)
$$

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$$

We remark here that the solution of LSP is deterministic and, therefore, supplies only a realization of the MVU $x^{*}$ and of $s^{2}$ the corresponding estimator of $\sigma^{2}$.

## Least-squares problem

The vector $x^{*}$ is also the solution of the normal equations, i.e. it is the unique stationary point of $\|y-A x\|_{2}^{2}$ :

$$
\begin{equation*}
A^{T} A x^{*}=A^{T} y \tag{3}
\end{equation*}
$$

We will denote in the following by

$$
R(x)=A^{T}(y-A x)
$$

the residual of (3).

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$$

the residual of (3). Moreover, we have

$$
\|y\|_{2}^{2}-\left\|x^{*}\right\|_{A^{T} A}^{2}=\|(I-P) y\|_{2}^{2}=\left\|y-A x^{*}\right\|_{2}^{2}
$$

## Least-squares problem

Given $\tilde{x}$ as an approximation of $x^{*}$,

$$
\delta y=-A\left(A^{T} A\right)^{-1} R(\tilde{x})
$$

is the minimum norm solution of

$$
\min _{w}\|w\|_{2}^{2} \quad \text { such that } \quad A^{T} A \tilde{x}=A^{T}(y+w) .
$$

Moreover, using $R(\tilde{x})=A^{T}(y-A \tilde{x})=A^{T} A\left(x^{*}-\tilde{x}\right)$, we have

$$
\|\delta y\|_{2}^{2}=\|R(\tilde{x})\|_{\left(A^{T} A\right)^{-1}}^{2}=\left\|x^{*}-\tilde{x}\right\|_{A^{T} A}^{2} .
$$

## A statistical point of view

How, we can link the deterministic theory for the least-squares perturbation to the Stochastic Perturbation theory?

## A statistical point of view

If $\delta y$ is a realization of a stochastic variable $\delta \mathbf{y}$ then $\|\delta y\|_{2}^{2}$ is a realization of $\|\delta \hat{\mathbf{y}}\|_{2}^{2} \sim \tau^{2} \chi^{2}(n)$.
Therefore, we consider that $\delta y$ is a sample of the stochastic variable $\delta \hat{\mathbf{y}}$ if for some small enough $\eta$,

$$
\text { Probability }\left(\|\delta \hat{\mathbf{y}}\|_{2}^{2} \geq\|\delta y\|_{2}^{2}\right) \geq 1-\eta
$$

where we assume that the random variable $\frac{\|\delta \hat{\mathbf{y}}\|_{2}^{2}}{\tau^{2}}$ follows a centered $\chi^{2}$ distribution with $n$ degrees of freedom. Thus, we can formulate our criterion as

$$
p_{\chi}\left(\frac{\|\delta y\|_{2}^{2}}{\tau^{2}}, n\right) \equiv \operatorname{Probability}\left(\frac{\|\delta \hat{\mathbf{y}}\|_{2}^{2}}{\tau^{2}} \leq \frac{\|\delta y\|_{2}^{2}}{\tau^{2}}\right) \leq \eta
$$

where, $p_{\chi}(., n)$ is the cumulative distribution function of the $\chi^{2}$ distribution.

## Preconditioned Conjugate Gradient for Normal equations 1

At each step $k$ the conjugate gradient method minimizes the energy norm of the error $\delta x^{(k)}=x^{*}-x^{(k)}$ on a Krylov space $x^{(0)}+\mathcal{K}_{k}$ :

$$
\min _{x^{(k)} \in x^{(0)}+\mathcal{K}_{k}} \delta x^{(k) T} A^{T} A \delta x^{(k)}
$$

where $\mathcal{K}_{k}=\operatorname{Span}\left(A^{T} y,\left(A^{T} A\right) A^{T} y, \ldots,\left(A^{T} A\right)^{k-1} A^{T} y\right)$. Let $R^{(k)}=A^{T}\left(y-A x^{(k)}\right)$ denote the normal equations residual at step $k$. Moreover, using $A^{T} A \delta x^{(k)}=A^{T}\left(y-A x^{(k)}\right)=R^{(k)}$, the value $\left\|\delta x^{(k)}\right\|_{A^{T} A}$ is equal to the dual norm of the residual $\left\|R^{(k)}\right\|_{\left(A^{\top} A\right)^{-1}}$.

## Preconditioned Conjugate Gradient for Normal equations 2

$$
\begin{aligned}
x^{(k)} & =x^{(k-1)}+\alpha_{k-1} q^{(k-1)}, \quad \alpha_{k-1}=\frac{R^{(k-1) T} R^{(k-1)}}{q^{(k-1) T} A^{T} A q^{(k-1)}}, \\
R^{(k)} & =R^{(k-1)}-\alpha_{k-1} A^{T} A q^{(k-1)}, \\
q^{(k)} & =R^{(k)}+\beta_{k-1} q^{(k-1)}, \quad \beta_{k-1}=\frac{R^{(k) T} R^{(k)}}{R^{(k-1) T} R^{(k-1)}} .
\end{aligned}
$$

The quantity $\alpha_{k-1}$ gives the step-size on the direction $q^{(k-1)}$ during the conjugate gradient algorithm.

## Preconditioned Conjugate Gradient for Normal equations 3

In exact arithmetic, we have that the energy norm of the error $\delta x^{(k)}=x^{*}-x^{(k)}$ is

$$
\left\|\delta x^{(k)}\right\|_{A^{T} A}^{2}=e_{A^{T} A}^{(k)}=\sum_{j=k}^{n-1} \alpha_{j} R^{(j) T} R^{(j)}
$$

and the energy norm of $x^{*}-x^{(0)}$ is

$$
\left\|x^{*}-x^{(0)}\right\|_{A^{T} A}^{2}=\sum_{j=0}^{n-1} \alpha_{j} R^{(j) T} R^{(j)}
$$

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$$
\left\|x^{*}-x^{(0)}\right\|_{A^{T} A}^{2}=\sum_{j=0}^{n-1} \alpha_{j} R^{(j) T} R^{(j)}
$$

Under the assumption that $e_{A^{\top} A}^{(k+d)} \ll e_{A^{\top} A^{\prime}}^{(k)}$, where the integer $d$ denotes a suitable delay, the Hestenes and Stiefel estimate $\xi_{k}$ of the energy-norm of the error will then be computed by the formula

$$
\xi_{k}=\sum_{j=k}^{k+d-1} \alpha_{j} R^{(j) T} R^{(j)} .
$$

## Preconditioned Conjugate Gradient for Normal equations 4

Finally,

$$
\left\|x^{*}-x^{(0)}\right\|_{A^{T} A}^{2} \geq \sum_{j=0}^{k-1} \alpha_{j} R^{(j) T} R^{(j)}=\nu_{k}
$$

Therefore,

$$
\left\|y-A x^{*}\right\|_{2}^{2}=\| y-A x^{(0)}-A\left(x^{*}-x^{(0)}\left\|_{2}^{2} \leq\right\| y-A x^{(0)} \|_{2}^{2}-\nu_{k} .\right.
$$

Introducing a preconditioner, we want to speed up the convergence rate of the conjugate gradient method but this will change the matrix and, therefore, the energy norm. However, we still want to estimate $e_{A^{T} A}^{(k)}$. It is proved that the energy norm of the preconditioned problem is equal to $e_{A^{T} A}^{(k)}$ (Arioli, Meurant). Moreover, when finite precision arithmetic is used, the Hestenes and Stiefel method for computing the error norm is numerically reliable (Strakos Tichy).

## Preconditioned Conjugate Gradient for Normal equations 5

```
PCGLS algorithm Given an initial guess x (0), compute r(0)}=(y-Ax(0) ), R(0)=\mp@subsup{A}{}{(0)}\mp@subsup{r}{}{(0)}\mathrm{ , and
solve Mz(0)}=\mp@subsup{R}{}{(0)}\mathrm{ . Set }\mp@subsup{q}{}{(0)}=\mp@subsup{z}{}{(0)},\mp@subsup{\beta}{0}{}=0,\mp@subsup{\nu}{0}{}=0,\mp@subsup{\chi}{1}{}=\mp@subsup{R}{}{(0)T}\mp@subsup{z}{}{(0)}\mathrm{ , and }\mp@subsup{\xi}{-d}{}=\infty\mathrm{ . Set }k=
while }\textrm{z}(\mp@subsup{\xi}{k-d}{},|\mp@subsup{r}{}{(0)}\mp@subsup{|}{2}{},\mp@subsup{\nu}{k}{},\mp@subsup{\tau}{}{2},\mp@subsup{\sigma}{}{2}))>\eta\mathrm{ do
    k=k+1;
    p=Aq(k-1);
    \alpha}k-1=\mp@subsup{\chi}{k}{}/|p|\mp@subsup{|}{2}{2}
```



```
    x}\mp@subsup{}{(k)}{(k)}\mp@subsup{x}{}{(k-1)}+\mp@subsup{\alpha}{k-1}{}\mp@subsup{q}{}{(k-1)}
    R
    Solve Mz }\mp@subsup{}{}{(k)}=\mp@subsup{R}{}{(k)}\mathrm{ ;
    \chi}\mp@subsup{k}{k+1}{}=\mp@subsup{R}{}{(k)T}\mp@subsup{z}{z}{(k)}
    \beta
    q}\mp@subsup{q}{}{(k)}=\mp@subsup{z}{}{(k)}+\mp@subsup{\beta}{k}{}\mp@subsup{q}{}{(k-1);
    if k>d}\mathrm{ then
        \mp@subsup{\xi}{k-d}{}=\mp@subsup{\sum}{j=k-d+1}{k}\mp@subsup{\psi}{j}{};
    else
        \xik-d}=\infty
    endif
end while.
```


## Stopping criteria $\eta$ and $\tau^{2}$

We stop when $\left.\mathbf{z}\left(\xi_{k-d},\left\|r^{(0)}\right\|_{2}, \nu_{k}, \tau^{2}, \sigma^{2}\right)\right) \leq \eta$

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1. $\eta$ is a probability (in our experiments $\eta=10^{-8}$ but $\eta=10^{-3}$ can realistic)

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1. $\eta$ is a probability (in our experiments $\eta=10^{-8}$ but $\eta=10^{-3}$ can realistic)
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1. $\eta$ is a probability (in our experiments $\eta=10^{-8}$ but $\eta=10^{-3}$ can realistic)
2. $\tau^{2}=\sigma^{2}$ can be fragile and it is better to impose $\tau^{2}=0.01 \sigma^{2}$
3. $\xi_{k}$ depend on $d$ the delay. When the preconditioned problem is still ill conditioned we must choose $d=20$ for reliability.
4. $p_{\chi}$ is cheap to compute (in our experiments we use the Matlab functions fcdf, and chis_cdf )

## Stopping criteria summary

1. $\mu_{1}=p_{F S}\left(\left(\frac{m-n}{n-k}\right) \frac{\xi_{k}}{\|y\|_{2}^{2}-\nu_{k}}, n-k, m-n\right)$ (F-test)
2. $\mu_{2}=p_{\chi}\left(\frac{\xi_{k}}{\tau^{2}}, n\right) \tau^{2}=0.1^{p} \sigma^{2}, p=0,2$,
3. $\mu_{3}=p_{\chi}\left(\frac{(m-n) \xi_{k}}{\tau_{k}^{2}}, n\right), \tau_{k}^{2}=0.1^{p}\left(\|y\|_{2}^{2}-\nu_{k}\right), p=0,2$.

## Test problems (Paige-Saunders)

| id | m | n | nnz | $\kappa(A)$ |
| :---: | :---: | :---: | :---: | :---: |
| well1033 | 1033 | 320 | 4732 | $1.610^{2}$ |
| illc1033 | 10033 | 320 | 4719 | $1.810^{4}$ |
| well1850 | 1850 | 712 | 8755 | $1.110^{2}$ |
| illc1850 | 1850 | 712 | 8636 | $1.410^{4}$ |

Dimensions, number of non zeros and $\kappa(A)=\left\|A^{+}\right\|_{2}\|A\|_{2}$ for Paige-Saunders tests.

In all the problems the standard deviation has been normalized

## Numerical tests $\left(\tau^{2}=\sigma^{2}\right)$

| id | $d$ | $\mathrm{IC}(1 \mathrm{e}-2)$ |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  | $\mu_{1}$ | $\mu_{2}$ | $\mu_{3}$ |
| Well1033 | 10 | $28(1.1 \mathrm{e}-03,1.061)$ | $28(1.1 \mathrm{e}-03,1.061)$ | $28(1.1 \mathrm{e}-03,1.061)$ |
|  | 20 | $28(1.1 \mathrm{e}-03,1.061)$ | $28(1.1 \mathrm{e}-03,1.061)$ | $28(1.1 \mathrm{e}-03,1.061)$ |
|  | 30 | $28(1.1 \mathrm{e}-03,1.061)$ | $28(1.1 \mathrm{e}-03,1.061)$ | $28(1.1 \mathrm{e}-03,1.061)$ |
| Well1850 | 10 | $22(2.0 \mathrm{e}-03,1.048)$ | $22(2.0 \mathrm{e}-03,1.048)$ | $22(2.0 \mathrm{e}-03,1.048)$ |
|  | 20 | $22(2.0 \mathrm{e}-03,1.048)$ | $22(2.0 \mathrm{e}-03,1.048)$ | $22(2.0 \mathrm{e}-03,1.048)$ |
|  | 30 | $22(2.0 \mathrm{e}-03,1.048)$ | $22(2.0 \mathrm{e}-03,1.048)$ | $22(2.0 \mathrm{e}-03,1.048)$ |
| illc 1033 | 10 | $124(4.9 \mathrm{e}-03,1.886)$ | $124(4.9 \mathrm{e}-03,1.886)$ | $59(2.0 \mathrm{e}-02,6.742)$ |
|  | 20 | $157(6.3 \mathrm{e}-04,1.021)$ | $156(1.3 \mathrm{e}-03,1.089)$ | $153(1.8 \mathrm{e}-03,1.160)$ |
|  | 30 | $157(6.3 \mathrm{e}-04,1.021)$ | $156(1.3 \mathrm{e}-03,1.089)$ | $153(1.8 \mathrm{e}-03,1.160)$ |
|  | 10 | $62(3.1 \mathrm{e}-02,5.010)$ | $120(7.9 \mathrm{e}-03,1.591)$ | $59(3.6 \mathrm{e}-02,5.770)$ |
|  | 20 | $140(4.2 \mathrm{e}-03,1.198)$ | $143(3.5 \mathrm{e}-03,1.144)$ | $93(1.3 \mathrm{e}-02,2.283)$ |
|  | 30 | $143(3.5 \mathrm{e}-03,1.144)$ | $145(3.0 \mathrm{e}-03,1.106)$ | $132(5.7 \mathrm{e}-03,1.343)$ |

Number of iterations for each stopping criterion $\eta=10^{-8}$ and $\tau^{2}=\sigma^{2}$. In bracket, the value of $\left\|x^{*}-\tilde{x}\right\|_{A^{T} A^{\prime}} /\left\|x^{*}\right\|_{A^{T}}^{A}$ and of the standard deviation of $r=b-A \tilde{x}$ at the corresponding iteration.

## Numerical tests $\left(\tau^{2}=\sigma^{2}\right)$

|  |  | IC $(1 \mathrm{e}-3)$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Well1033 | 10 | $9(7.8 \mathrm{e}-04,1.032)$ | $9(7.8 \mathrm{e}-04,1.032)$ | $9(7.8 \mathrm{e}-04,1.032)$ |  |
|  | 20 | $9(7.8 \mathrm{e}-04,1.032)$ | $9(7.8 \mathrm{e}-04,1.032)$ | $9(7.8 \mathrm{e}-04,1.032)$ |  |
|  | 30 | $9(7.8 \mathrm{e}-04,1.032)$ | $9(7.8 \mathrm{e}-04,1.032)$ | $9(7.8 \mathrm{e}-04,1.032)$ |  |
| Well1850 | 10 | $7(1.2 \mathrm{e}-03,1.017)$ | $7(1.2 \mathrm{e}-03,1.017)$ | $7(1.2 \mathrm{e}-03,1.017)$ |  |
|  | 20 | $7(1.2 \mathrm{e}-03,1.017)$ | $7(1.2 \mathrm{e}-03,1.017)$ | $7(1.2 \mathrm{e}-03,1.017)$ |  |
|  | 30 | $7(1.2 \mathrm{e}-03,1.017)$ | $7(1.2 \mathrm{e}-03,1.017)$ | $7(1.2 \mathrm{e}-03,1.017)$ |  |
| illc1033 | 10 | $59(1.4 \mathrm{e}-03,1.106)$ | $59(1.4 \mathrm{e}-03,1.106)$ | $57(1.8 \mathrm{e}-03,1.166)$ |  |
|  | 20 | $63(1.3 \mathrm{e}-03,1.082)$ | $63(1.3 \mathrm{e}-03,1.082)$ | $58(1.5 \mathrm{e}-03,1.122)$ |  |
|  | 30 | $63(1.3 \mathrm{e}-03,1.082)$ | $63(1.3 \mathrm{e}-03,1.082)$ | $58(1.5 \mathrm{e}-03,1.122)$ |  |
| illc1850 | 10 | $36(4.1 \mathrm{e}-03,1.186)$ | $37(2.7 \mathrm{e}-03,1.085)$ | $36(4.1 \mathrm{e}-03,1.186)$ |  |
|  | 20 | $37(2.7 \mathrm{e}-03,1.085)$ | $37(2.7 \mathrm{e}-03,1.085)$ | $36(4.1 \mathrm{e}-03,1.186)$ |  |
|  | 30 | $37(2.7 \mathrm{e}-03,1.085)$ | $37(2.7 \mathrm{e}-03,1.085)$ | $36(4.1 \mathrm{e}-03,1.186)$ |  |

Number of iterations for each stopping criterion $\eta=10^{-8}$ and $\tau^{2}=\sigma^{2}$. In bracket, the value of $\left\|x^{*}-\tilde{x}\right\|_{A}{ }^{T}{ }_{A} /\left\|x^{*}\right\|_{A^{T}}{ }_{A}$ and of the standard deviation of $r=b-A \tilde{x}$ at the corresponding iteration.

## Numerical tests $\left(\tau^{2}=\sigma^{2} / 100\right)$

| id | $d$ | $\mathrm{IC}(1 \mathrm{e}-2)$ |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  | $\mu_{1}$ | $\mu_{2}$ | $\mu_{3}$ |
| Well1033 | 10 | $28(1.1 \mathrm{e}-03,1.061)$ | $33(5.0 \mathrm{e}-05,1.000)$ | $33(5.0 \mathrm{e}-05,1.000)$ |
|  | 20 | $28(1.1 \mathrm{e}-03,1.061)$ | $33(5.0 \mathrm{e}-05,1.000)$ | $33(5.0 \mathrm{e}-05,1.000)$ |
|  | 30 | $28(1.1 \mathrm{e}-03,1.061)$ | $33(5.0 \mathrm{e}-05,1.000)$ | $33(5.0 \mathrm{e}-05,1.000)$ |
| Well1850 | 10 | $22(2.0 \mathrm{e}-03,1.048)$ | $25(1.7 \mathrm{e}-04,1.000)$ | $24(3.8 \mathrm{e}-04,1.002)$ |
|  | 20 | $22(2.0 \mathrm{e}-03,1.048)$ | $25(1.7 \mathrm{e}-04,1.000)$ | $24(3.8 \mathrm{e}-04,1.002)$ |
|  | 30 | $22(2.0 \mathrm{e}-03,1.048)$ | $25(1.7 \mathrm{e}-04,1.000)$ | $24(3.8 \mathrm{e}-04,1.002)$ |
| illc1033 | 10 | $124(4.9 \mathrm{e}-03,1.886)$ | $164(6.6 \mathrm{e}-05,1.000)$ | $138(2.1 \mathrm{e}-03,1.209)$ |
|  | 20 | $157(6.3 \mathrm{e}-04,1.021)$ | $164(6.6 \mathrm{e}-05,1.000)$ | $163(1.5 \mathrm{e}-04,1.001)$ |
|  | 30 | $157(6.3 \mathrm{e}-04,1.021)$ | $164(6.6 \mathrm{e}-05,1.000)$ | $163(1.5 \mathrm{e}-04,1.001)$ |
|  | 10 | $62(3.1 \mathrm{e}-02,5.010)$ | $178(6.1 \mathrm{e}-04,1.005)$ | $178(6.1 \mathrm{e}-04,1.005)$ |
|  | 20 | $140(4.2 \mathrm{e}-03,1.198)$ | $196(2.6 \mathrm{e}-04,1.001)$ | $195(3.6 \mathrm{e}-04,1.002)$ |
|  | 30 | $143(3.5 \mathrm{e}-03,1.144)$ | $196(2.6 \mathrm{e}-04,1.001)$ | $195(3.6 \mathrm{e}-04,1.002)$ |

Number of iterations for each stopping criterion $\eta=10^{-8}$ and $\tau^{2}=\sigma^{2} / 100$. In bracket, the value of $\left\|x^{*}-\tilde{x}\right\|_{A^{T} A^{\prime}} /\left\|x^{*}\right\|_{A^{T}}^{A}$ and of the standard deviation of $r=b-A \tilde{x}$ at the corresponding iteration.

## Numerical tests $\left(\tau^{2}=\sigma^{2} / 100\right)$

|  |  | IC $(1 \mathrm{e}-3)$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Well1033 | 10 | $9(7.8 \mathrm{e}-04,1.032)$ | $13(6.3 \mathrm{e}-05,1.000)$ | $13(6.3 \mathrm{e}-05,1.000)$ |  |
|  | 20 | $9(7.8 \mathrm{e}-04,1.032)$ | $13(6.3 \mathrm{e}-05,1.000)$ | $13(6.3 \mathrm{e}-05,1.000)$ |  |
|  | 30 | $9(7.8 \mathrm{e}-04,1.032)$ | $13(6.3 \mathrm{e}-05,1.000)$ | $13(6.3 \mathrm{e}-05,1.000)$ |  |
| Well1850 | 10 | $7(1.2 \mathrm{e}-03,1.017)$ | $8(2.2 \mathrm{e}-04,1.001)$ | $8(2.2 \mathrm{e}-04,1.001)$ |  |
|  | 20 | $7(1.2 \mathrm{e}-03,1.017)$ | $8(2.2 \mathrm{e}-04,1.001)$ | $8(2.2 \mathrm{e}-04,1.001)$ |  |
|  | 30 | $7(1.2 \mathrm{e}-03,1.017)$ | $8(2.2 \mathrm{e}-04,1.001)$ | $8(2.2 \mathrm{e}-04,1.001)$ |  |
| illc1033 | 10 | $59(1.4 \mathrm{e}-03,1.106)$ | $83(8.3 \mathrm{e}-05,1.000)$ | $83(8.3 \mathrm{e}-05,1.000)$ |  |
|  | 20 | $63(1.3 \mathrm{e}-03,1.082)$ | $83(8.3 \mathrm{e}-05,1.000)$ | $83(8.3 \mathrm{e}-05,1.000)$ |  |
|  | 30 | $63(1.3 \mathrm{e}-03,1.082)$ | $83(8.3 \mathrm{e}-05,1.000)$ | $83(8.3 \mathrm{e}-05,1.000)$ |  |
|  | 10 | $36(4.1 \mathrm{e}-03,1.186)$ | $55(3.2 \mathrm{e}-04,1.001)$ | $51(4.1 \mathrm{e}-04,1.002)$ |  |
|  | 20 | $37(2.7 \mathrm{e}-03,1.085)$ | $55(3.2 \mathrm{e}-04,1.001)$ | $51(4.1 \mathrm{e}-04,1.002)$ |  |
|  | 30 | $37(2.7 \mathrm{e}-03,1.085)$ | $55(3.2 \mathrm{e}-04,1.001)$ | $51(4.1 \mathrm{e}-04,1.002)$ |  |

Number of iterations for each stopping criterion $\eta=10^{-8}$ and $\tau^{2}=\sigma^{2} / 100$. In bracket, the value of $\left\|x^{*}-\tilde{x}\right\|_{A^{T}}{ }_{A} /\left\|x^{*}\right\|_{A^{T}}{ }_{A}$ and of the standard deviation of $r=b-A \tilde{x}$ at the corresponding iteration.

## Data Assimilation

Data assimilation purpose is to reconstruct the initial conditions at $t=0$ of a dynamical system based on knowledge of the system's evolution laws and on observations of the state at times $t_{i}$.

$$
\dot{u}=f(t, u) \quad u(t)=M(t) u_{0}
$$

Assume that the system state is observed (possibly only in parts) at times $\left\{t_{i}\right\}_{i=0}^{N}$, yielding observation vectors $\left\{y_{i}\right\}_{i=0}^{N}$, whose model is given by

$$
y_{i}=H u\left(t_{i}\right)+\epsilon, \quad \epsilon \sim \mathcal{N}\left(0, R_{i}=\sigma^{2} I\right)
$$

Find $u_{0}$ which minimizes

$$
\frac{1}{2} \sum_{i=0}^{N}\left\|H M\left(t_{i}\right) u_{0}-y_{i}\right\|_{R_{i}^{-1}}^{2}
$$

## Data Assimilation

Heat Equation model

$$
\begin{aligned}
& \frac{\partial u}{\partial t}=-\Delta u \quad \text { in } \quad S_{2}=[0,1] \times[0,1] \\
& u=0 \quad \text { on } \quad \partial S_{2}, \quad u(., 0)=u_{0} \quad \text { in } \quad S_{2}
\end{aligned}
$$

## Data Assimilation

The system is integrated with time-step $d t$, using an implicit Euler scheme. In the physical domain, a regular finite difference scheme is taken for the Laplace operator, with same spacing $h$ in the two spatial dimensions. The data of our problem is computed by imposing a solution $u_{0}(x, y, 0)$ computing the exact system trajectory and observing $H u$ at every point in the spatial domain and at every time step. In our application, $m=8100$, $n=900=30^{2}, d t=1, h=1 / 31, N=8$ and $H=\operatorname{diag}\left(1^{1.5}, 2^{1.5}, \ldots, n^{1.5}\right)$. The observation vector $y$ is obtained by imposing $u_{0}(x, y, 0)=\frac{1}{4} \sin \left(\frac{1}{4} x\right)(x-1) \sin (5 y)(y-1)$, and by adding a random measurement error with Gaussian distribution with zero mean and covariance matrix $R_{i}=\sigma^{2} I_{n}$, where $\sigma=10^{-3}$. In our numerical experiments, we use PCGLS without preconditioner.

## Data Assimilation: results $(\mathrm{d}=5)$


(a)

(b)


(d)
(a) Stopping criteria, (b) Energy norm of the error, (c)

$$
\zeta_{k}=\frac{\|y\|_{2}^{2}-\nu_{k}}{m-n} \text {, (d) Residual histogram. }
$$

## Conclusion

- F-test stopping rule for PCGLS


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- F-test stopping rule for PCGLS
- LSQR has similar behaviour
- Orthodir (or re-orthogonalization) can be a valuable alternative for LSP where $A$ is implicit
- How to generalize to other non linear regression problems or to NON-NORMAL distribution?

