Inference of thermo-physical properties

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MEASUREMENT & STANDARDS
Keys to COMPETITIVENESS and A SAFER WORLD

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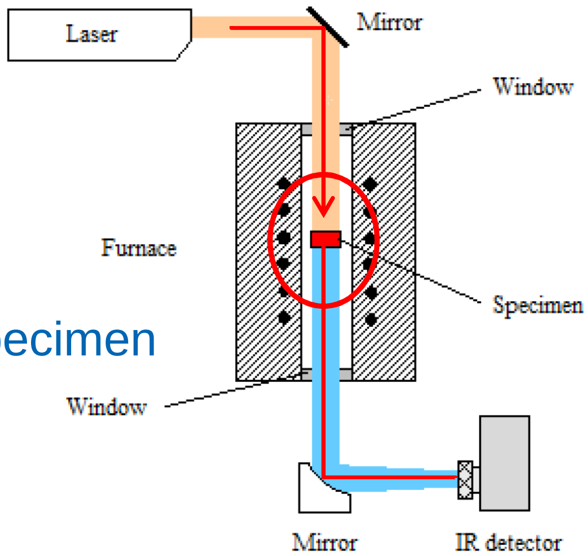
Inverse Problem : determination of thermal diffusivity

- Thermal diffusivity
  - Characteristic of a material that measures its ability to diffusing instead of absorbing thermal energy,
  - Important property in many fields (energy production, insulation of buildings, …)
- Measurement principle
  - FLASH method
  - Specimen in a furnace [20°C; 1400°C]
  - Short Laser flash on the front face
  - Transmission of thermal energy through the specimen
  - Measurement of the temperature rise on the back face using an IR detector



- Inverse problem
  - Thermal diffusivity is not observable, but is responsible for the observed temperature variations

GUM and inverse problems

GUM + supplements 1 et 2 : **direct measurement model**

$$Y = f\left(X_1, \ldots, X_N\right)$$

GUM + Supplements

Inverse problem (observation equation) :

$$\mathrm{Z} = \mathrm{g}(\mathrm{Y})$$

Beyond the GUM

Y : non-observable measurand

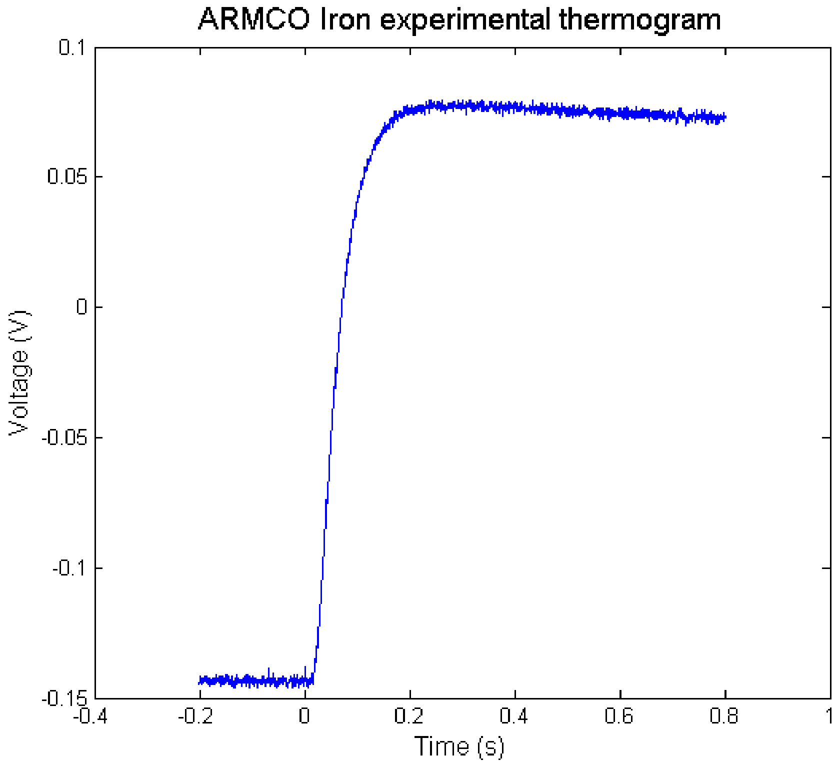
In an inverse problem, the measurand *Y* **determines** an observed indication *Z*.

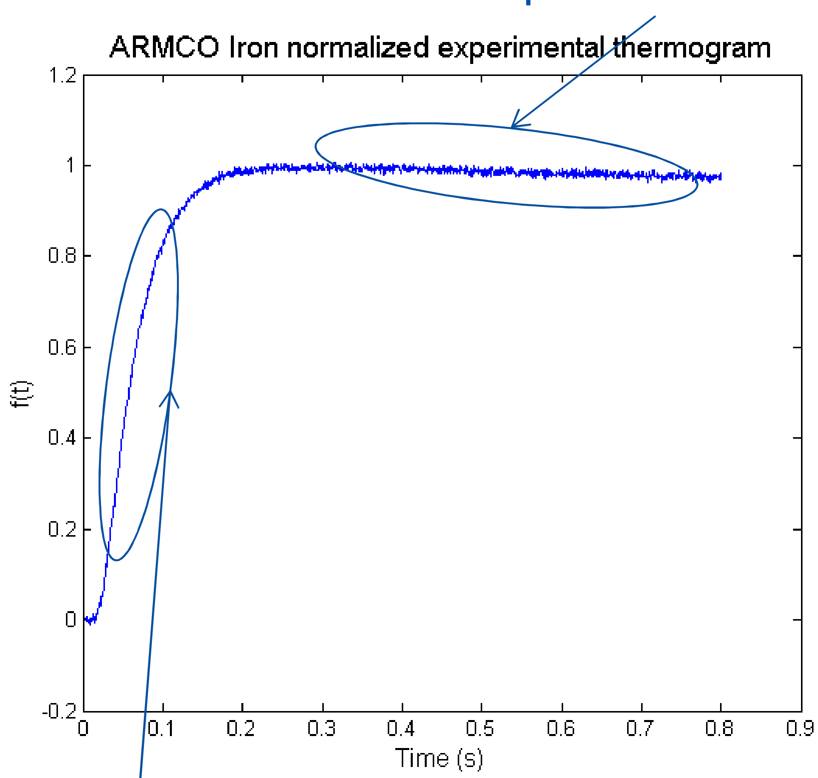
Laser flash : experimental thermogram

$$f(t) = \frac{U(t) - U_0}{U_{max} - U_0} = \frac{T(t) - T_0}{T_{max} - T_0}$$

$$Bi = \frac{he}{\lambda}$$

Decrease sensitive to parameter *Biot*





Increase sensitive to parameter τ
(characteristic time response in s)

$$\tau = \frac{e^2}{a}$$

Theoretical thermogram – heat equation

1-D cylindrical model

$$\lambda \frac{\partial^2 T(z,t)}{\partial z^2} + Q = \rho c_p \frac{\partial T(z,t)}{\partial t}$$

λ	Thermal conductivity ($W.m^{-1}.K^{-1}$)
ρ	Density ($kg.m^{-3}$)
c_p	Heat capacity ($J.kg^{-1}.K^{-1}$)
Q	Source term representing the laser heating ($J.m^{-3}.s^{-1}$)
e	Thickness of the specimen (m)
h	Heat exchange coefficient ($W.m^{-2}.K^{-1}$)

Boundary conditions :

at z = 0 : $\lambda \left.\frac{\partial T}{\partial z}\right|_{z=0} = h\left(T|_{z=0} - T_0\right)$

at z = e : $\lambda \left.\frac{\partial T}{\partial z}\right|_{z=e} = -h\left(T|_{z=e} - T_0\right)$

at t = 0 : $T(z,0) = T_0$

→ Solved in terms of τ and *Bi*

Step 1 - Statistical modeling

n = 1600 points between 0 et 0.8 s

Experimental thermogram = Theoretical thermogram + error

$$\boldsymbol{Y} = \boldsymbol{G}\left(\tau, Bi\right) + \boldsymbol{\epsilon}$$

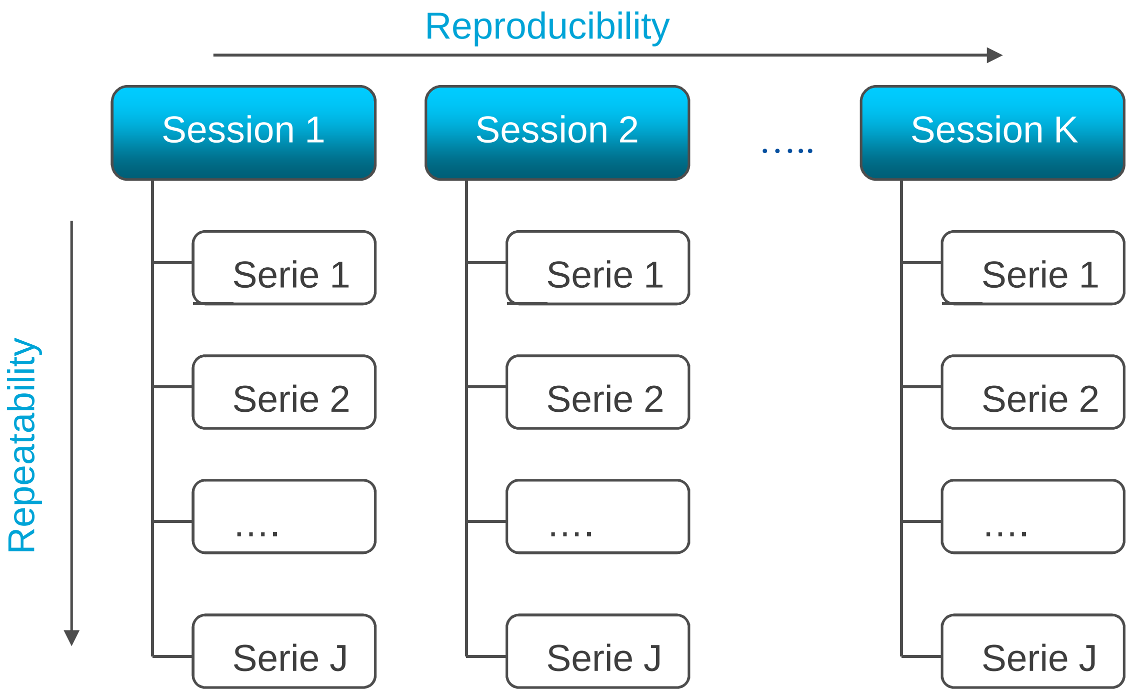
$$\boldsymbol{Y} = \begin{pmatrix} Y_1 \\ \vdots \\ Y_i \\ \vdots \\ Y_n \end{pmatrix} \in \mathbb{R}^n \qquad \boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_i \\ \vdots \\ \epsilon_n \end{pmatrix} \propto N_n\left(0, \sigma^2 Id_n\right) \qquad \tau > 0 \qquad Bi > 0$$

Unknown parameters $\boldsymbol{\theta} = \left(\tau, Bi, \sigma^2\right)$

Thermal diffusivity : $a = \dfrac{e^2}{\tau}$

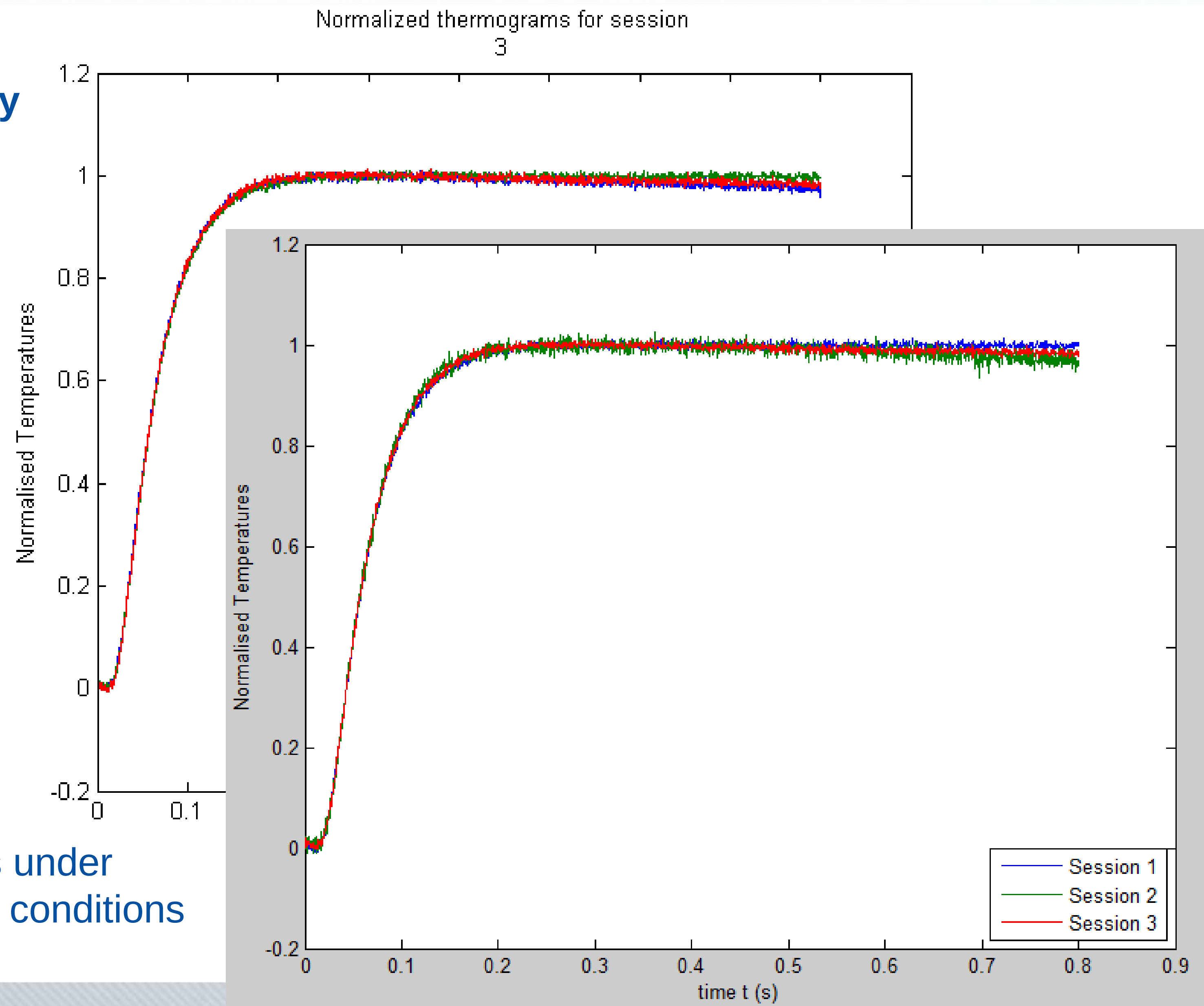
Use of a hierarchical model: motivations

- ✓ Neglected uncertainty sources
  - ✓ Power of the laser flash (sensitivity of the thermal diffusivity to the temperature)
  - ✓ Duration of the laser flash
  - ✓ Temperature in the furnace
  - ✓ Position of the sample in the furnace
  - ✓ …



Use of a hierarchical model : motivations

3 Thermograms under **repeatability** conditions



3 Thermograms under **reproducibility** conditions

Bayesian hierarchical model

$$\boldsymbol{Y}_{k,j} = \boldsymbol{G}\left(\tau_k, Bi_k\right) + \boldsymbol{\epsilon_{k,j}}$$

Sessions k
Series j

$$\begin{cases} 1 \leq k \leq K \\ 1 \leq j \leq J \end{cases}$$

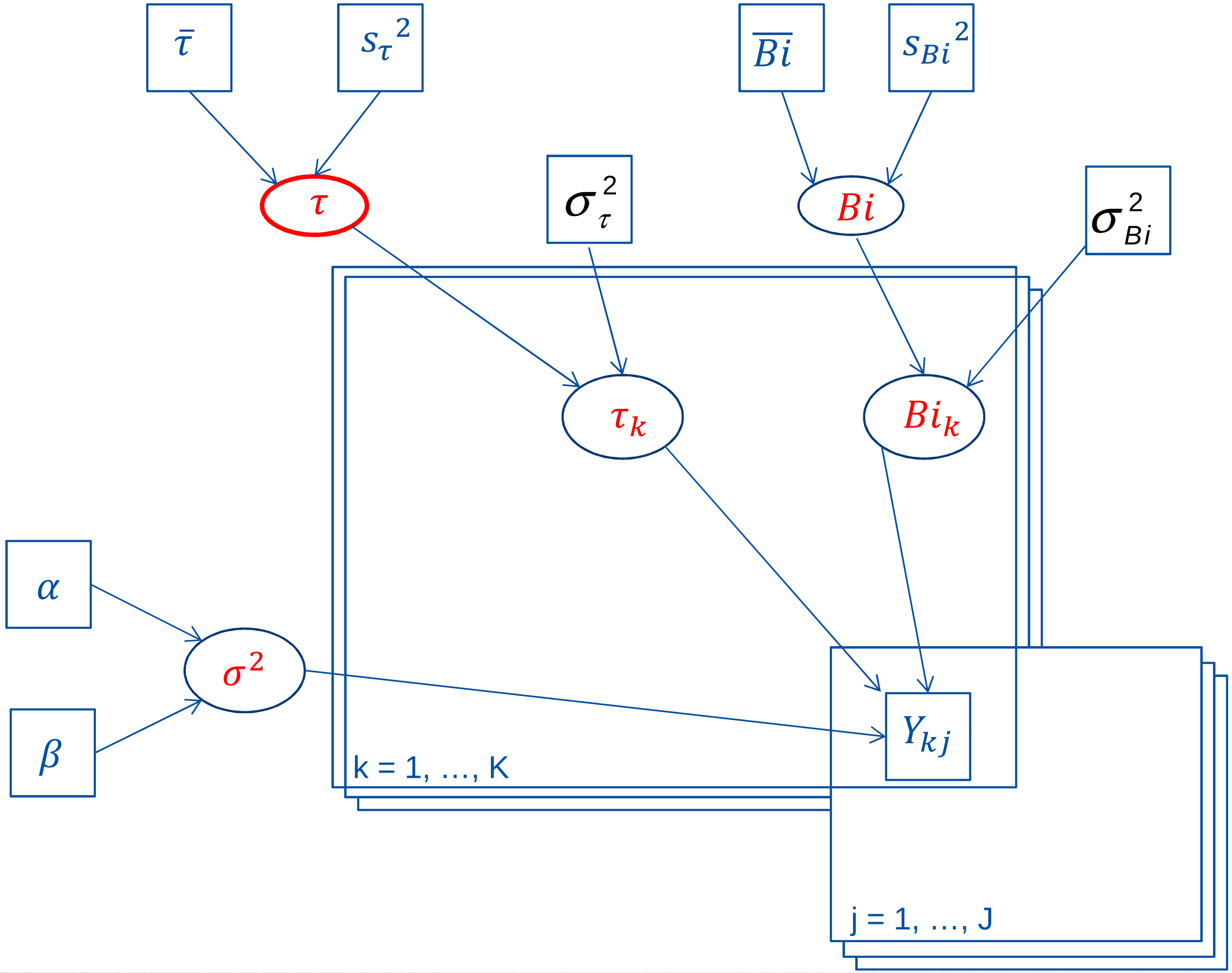
$$\boldsymbol{Y}_{k,j} \in \mathbb{R}^n \qquad \boldsymbol{\epsilon} \sim N_n\left(0, \sigma^2 Id_n\right)$$

$$\begin{cases} \tau_k \sim N\left(\tau, \sigma_\tau^2\right) \\ Bi_k \sim N\left(Bi, \sigma_{Bi}^2\right) \end{cases} \qquad \begin{cases} \tau > 0 \\ Bi > 0 \end{cases}$$

Parameter vector : $\boldsymbol{\theta} = \left(\tau, Bi, \tau_k, Bi_k, \sigma^2\right)$

More complex model : Directed Acyclic Graph (DAG) for a better visualization of the treatment of the parameters

Directed Acyclic Graph (DAG)



Step 2 : Choice of prior distributions

- ✓ Different prior distributions for different kinds of prior knowledge

Prior knowledge	Prior distributions
None	Wide rectangular
	Jeffreys
Interval endpoints	Rectangular
Best estimate with an associated uncertainty information	Gaussian

- ✓ Noise Variance σ^2
  - ✓ Known
  - ✓ Unknown : *Inverse gamma distribution IG(α;β)*

Step 3 : Numerical methods

- Determination of a sample from the posterior distribution for τ.
  - Metropolis-Hastings algorithm
- Propagation of distributions to determine the thermal diffusivity *a*
  - Monte Carlo simulation

Thickness e (m)	Characteristic time τ (s)
e_1	τ_1
⋮	⋮
e_i	τ_i
⋮	⋮
e_M	τ_M

$$a = \frac{e^2}{\tau}$$

Thermal diffusivity a ($m^2.s^{-1}$)
a_1
⋮
a_i
⋮
a_M

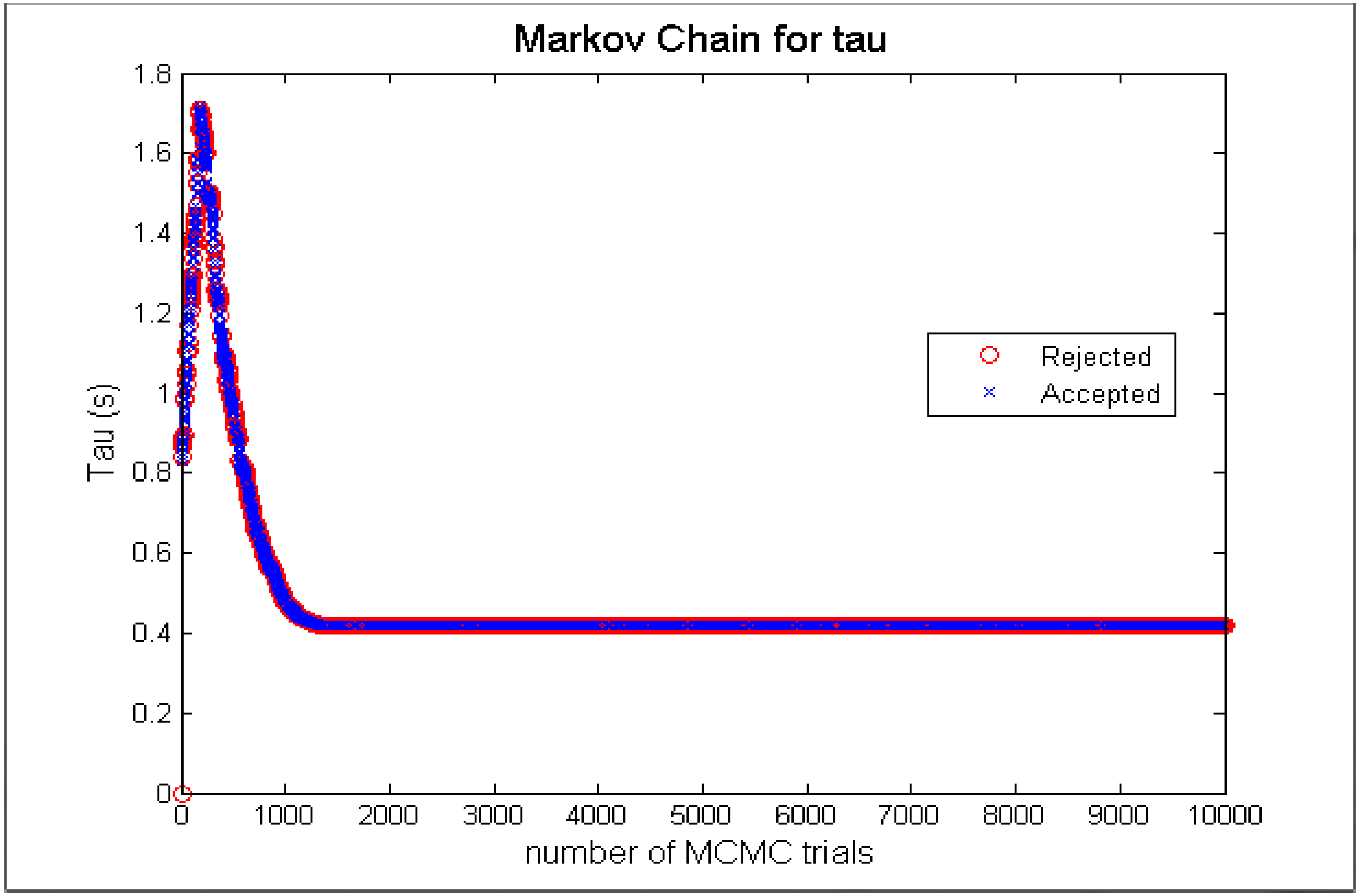
Simulation from a Gaussian distribution

Sample from the posterior distribution

Step 3 : Numerical methods – MH algorithm

Markov chain for τ

10000 trials



Brooks-Gelman [1] convergence criteria

[1] Gelman A., Brooks S. P., "General methods for monitoring convergence of iterative simulations",Journal of Computational and Graphical Statistics, 7, 4, 434-455, 1998.

Use of a hierarchical model : influence of the hyper parameters

σ_{τ}^{2} and σ_{Bi}^{2} characterize the dispersion of the parameters τ_k and Bi_k due to the influential quantities that are varied from one session of measurements to another

$\sigma_{\tau}^{2}=\sigma_{\mathrm{Bi}}^{2}$	$\mathrm{a}/10^{-6}.\mathrm{m}^{2}.\mathrm{s}^{-1}$	$\mathrm{u}(\mathrm{a})/10^{-6}.\mathrm{m}^{2}.\mathrm{s}^{-1}$	$\frac{\mathrm{u}(\mathrm{a})}{\mathrm{a}}/\%$
1×10^{-5}	20.439	0.082	0.40
5×10^{-5}	20.455	0.176	0.86
1×10^{-4}	20.443	0.247	1.21

The hyper parameters are used to take into account uncertainty sources that wouldn't be taken into account otherwise

Conclusion

- ✓ Bayesian framework adapted to inverse problems
  - ✓ When the measurand is the cause of another observed quantity
  - ✓ It provides a posterior probability dsitribution which combines information both from experimental data and from prior knowledge
- ✓ Use of a hierarchical model
  - ✓ Enables to deal with other uncertainty sources
  - ✓ Requires either additional knowledge or additional experimental data
- ✓ Best Practice Guide [Elster & all 2015]: « A guide to Bayesian inference for regression problems »

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