

# Bayesian Modelling Numerical Inference

satRday

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- ▶ your dataset is cleaned
- ▶ data stored in a secure database, copied in 3 (or more) places

you are now in front of your computer screen

you open R

you import your dataset

you check it

and you are happy with that

- ▶ now you are remembering the hypotheses you want to test
- ▶ and you are beginning to realize how complex can be your hypotheses and how complex may be science
- ▶ so that you start drawing some convoluted relationships between variables, twisted processes and wawering distorted curves

but..

• •

after a while, you type on the keyboard  $lm()$  or perhaps  $glm()$ ...

..

already resigned to think *linearly*

# work program

- 1 bayesian vs frequentist inference
  - elements of theory
  - application to DBH distribution
- 2 MCMC numerical methods
  - principles
  - the algorithm
  - Application
- 3 some comments
- 4 why bayesian modeling in R

# probabilist roots of bayesian statistics

## Bayes Theorem

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

$$P(A|B)P(B) = P(A \cap B) = P(B|A)P(A)$$

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$



Rev. Thomas Bayes  
1702-1761

## in terms of density

let  $X$  and  $Y$  be 2 random variables with densities  $\pi_X$  et  $\pi_Y$

$$\pi_{X|Y}(x|y) = \frac{\pi_{Y|X}(y|x)\pi_X(x)}{\pi_Y(y)}$$

## formalisation for model inference

- ▶ your dataset  $y_1, \dots, y_n$
- ▶ your dataset are observations from a parametric model

$$Y_1, \dots, Y_n \sim \pi_{Y|\theta} \quad i.i.d.$$

- ▶ the likelihood of this model is  $L(y_1, \dots, y_n; \theta) = \prod_{i=1}^n \pi_{Y|\theta}(y_i|\theta)$

### frequentist estimation of $\theta$

$\hat{\theta}$  maximize  $L(y_1, \dots, y_n; \theta)$

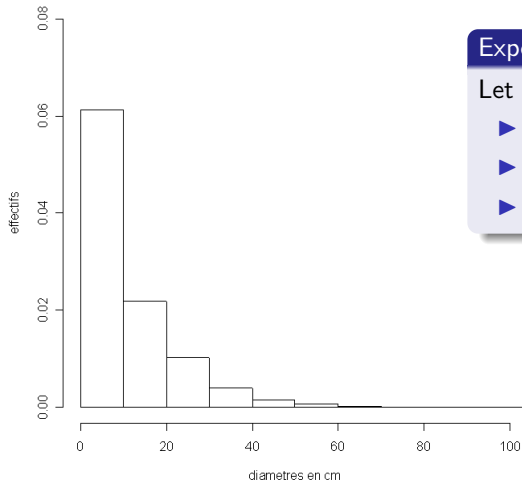
### bayesian estimation of $\theta$

- ▶ *a priori* law on  $\theta$  with density  $\pi_\theta$
- ▶ calculate the *a posteriori* law

$$\pi_{\theta|Y}(\theta|y_1, \dots, y_n) = \frac{L(y_1, \dots, y_n; \theta)\pi_\theta(\theta)}{\int L(y_1, \dots, y_n; \theta)\pi_\theta(\theta)d\theta}$$

# Diameter distribution in natural forests

Histogramme des diametres des arbres



## Exponential model

Let  $Y$  be the DBH of a tree

- ▶ law :  $Y \sim \exp(\theta)$
- ▶ density :  $\pi_{Y|\theta}(y|\theta) = \theta \exp(-\theta y)$
- ▶ data :  $\mathbf{y} = (y_1, \dots, y_n)$

# Diameter distribution in natural forests

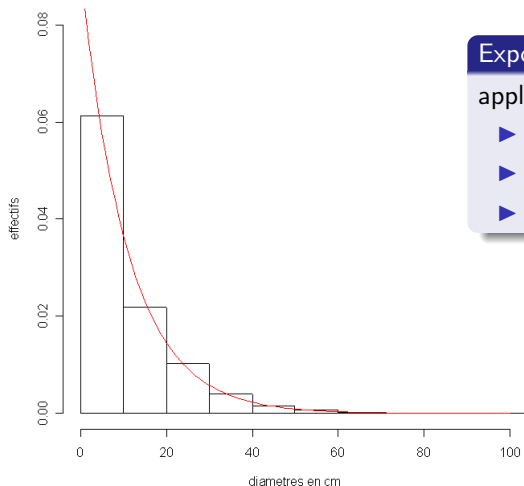
## frequentist inference

- ▶ the likelihood is  $L(\mathbf{y}; \theta) = \prod_{i=1}^n \theta \exp(-\theta y_i) = \theta^n \exp(-\theta \sum_{i=1}^n y_i)$
- ▶ the log-likelihood is  $\ell(\theta) = n \log \theta - \theta \sum_{i=1}^n y_i$
- ▶  $\theta$  estimate at maximum likelihood is given by

$$\frac{\partial \ell(\hat{\theta})}{\partial \theta} = 0 \iff \frac{n}{\theta} - \sum_{i=1}^n y_i = 0 \implies \hat{\theta} = \frac{n}{\sum_{i=1}^n y_i}$$

# Diameter distribution in natural forests

Histogramme des diametres des arbres



## Exponential model

application to real data

- ▶  $n = 39858$
- ▶  $\sum y_i = 434131.1$
- ▶  $\hat{\theta} = 0.0918$



# Diameter distribution in natural forests

## bayesian inference

- ▶ the likelihood does not change  $L(\mathbf{y}; \theta) = \theta^n \exp(-\theta \sum_{i=1}^n y_i)$
- ▶ we choose an *a priori* law on  $\theta$  :  $\pi(\theta)$
- ▶  $\theta$  estimate is given by the *a posteriori* law

$$\pi_{\theta|\mathbf{y}}(\theta|y_1, \dots, y_n) = \frac{L(\mathbf{y}; \theta)\pi(\theta)}{\int L(\mathbf{y}; \theta)\pi(\theta)d\theta} \propto L(\mathbf{y}; \theta)\pi(\theta)$$

- ▶ the choice of the *a priori* law is fundamental

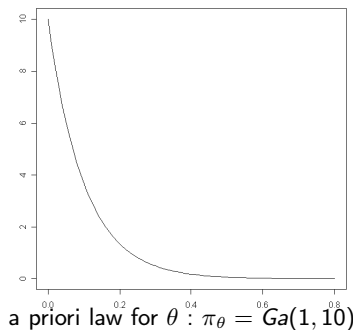
# Diameter distribution in natural forests

you have to **choose** an *a priori* law for  $\theta$  :

- ▶ common laws on  $\mathbb{R}^+$  → no explicit *a posteriori* law
- ▶ conjugated law → known *a posteriori* law
- ▶ the **Gamma law is conjugated to the exponential law**

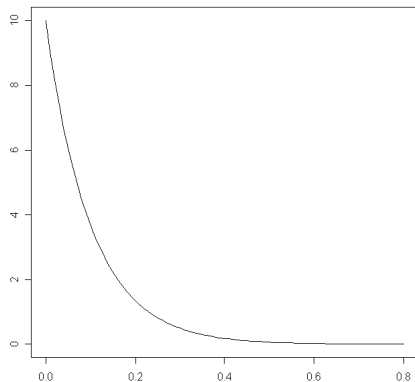
## Exponential model

- ▶ prior of  $\theta$  :  $\pi_{\theta}(\theta) = Ga(\theta|\alpha, \beta)$
- ▶ posterior of  $\theta$  :  
 $\pi_{\theta|y} = Ga(\alpha + n, \beta + \sum y_i)$
- ▶ posterior of  $Y$  :  
 $\pi_{Y|y} = Gg(\alpha + n, \beta + \sum y_i, 1)$



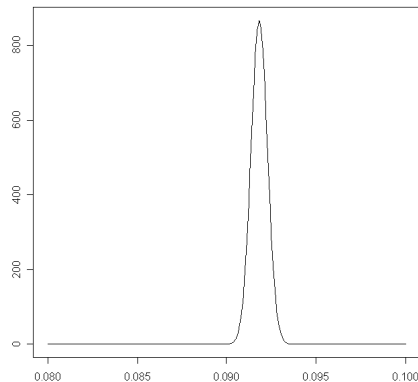
# Diameter distribution in natural forests

with real data :  $n = 39858$  et  $\sum y_i = 434131.1$



prior law for  $\theta$  :

$$\pi_{\theta} = \text{Ga}(1, 10)$$



posterior law for  $\theta$  :

$$\pi_{\theta|y} = \text{Ga}(1 + 39858, 10 + 434131.1)$$

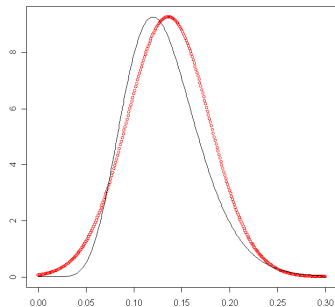
A histogram showing the frequency distribution of tree diameters. The x-axis is labeled 'diametres en cm' and ranges from 0 to 100. The y-axis is labeled 'effectifs' and ranges from 0.00 to 0.08. The histogram bars are white with black outlines. A smooth, dark curve is overlaid on the histogram, representing a fitted probability density or a smoothed frequency curve. The distribution is right-skewed, with a peak at the first bin (0-10 cm) and a long tail extending towards 100 cm.

A set of small navigation icons typically found in Beamer presentations, including symbols for back, forward, search, and other slide controls.

# Diameter distribution : bayesian $\leftrightarrow$ frequentist

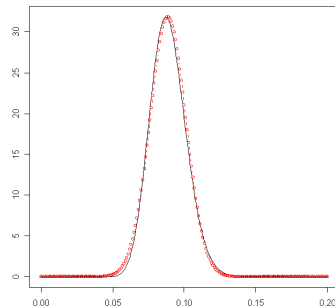
## Impact of the sample size $n$

Sample size  $n = 10$



$$\pi_{\theta|y}(\theta|y) \text{ (-)} \quad \leftrightarrow \quad \mathcal{N}(\hat{\theta}, \frac{\hat{\sigma}^2}{n}) \text{ (}\circ\circ\text{)}$$

Sample size  $n = 50$



$$\pi_{\theta|y}(\theta|y) \text{ (-)} \quad \leftrightarrow \quad \mathcal{N}(\hat{\theta}, \frac{\hat{\sigma}^2}{n}) \text{ (}\circ\circ\text{)}$$

# Comments

- ▶ the added values of bayesian inference is greater when the sample size is low
  - supplementary information from the *a priori* law
  - the *a priori* greatly helps inference but **may also biased**
  - the choice of the *a priori* law is crucial

- ▶ practical scheme

$$\left. \begin{array}{c} a \text{ priori law } \pi_{\theta}(\theta) \\ + \\ \text{data } \mathbf{y} \end{array} \right\} \longrightarrow a \text{ posteriori law } \pi_{\theta|\mathbf{y}}(\theta|\mathbf{y})$$

- ▶ moving from «a priori» → «a posteriori» is nearly impossible analytically (excepted for conjugated laws)

⇒ numerical methods **MCMC** to infer *a posteriori* laws

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# Markov Chain Monte Carlo methods

## Monte Carlo methods

- ▶ inference technique based on the simulation of a high number of random variables

## advantages

- ▶ may be applied to a wide range of problems
- ▶ a few underlying hypotheses
- ▶ easy to implement

## constraints

- ▶ a good random generator
- ▶ computational power
- ▶ likelihood-explicit



# Markov Chain Monte Carlo methods

## ► objective

- sample a target law of density  $\pi(z)$  where  $Z$  is a real variable with  $n$ -dimensions

## ► principle

- we build a Markov  $(Z^{(k)})_{k \geq 0}$  chain on  $\mathbb{R}^n$  for which the asymptotic law is  $\pi$
- when the chain is stationary, we extract a random sample from the chain  $(Z^{(k_1)}, \dots, Z^{(k_N)})$  in order to estimate the parameter a *posteriori* distribution

# Metropolis-Hastings (MH) sampler

- ▶ objective : build a Markov with  $\pi$  invariant
- ▶ ingredients :
  - ① a proposal law/kernel  $\pi^{prop}$
  - ② a measurable function  $\alpha \mapsto [0, 1]$ .
- ▶ principle :
  - ① starting from  $z \in E$ ,  $\pi^{prop}$  give a new candidate  $\tilde{z} \in E$ .
  - ② this new candidate is accepted with probability  $\alpha(z, \tilde{z})$ , if not we conserve  $z$ .
- ▶ in practice
  - the proposal law/kernel  $\pi^{prop}$  is chosen by you
  - the MH algorithm determine  $\alpha$

# the algorithm

Given  $\pi$  the density of the target law,  $\pi^{prop}$  the density of the proposal law/kernel

► initialisation : set  $z^{(0)}$

► iteration  $t$

① Given  $z^{(t-1)}$ , sample  $\tilde{z} \sim \pi^{prop}(z^{(t-1)})$

②  $\alpha(z^{(t-1)}, \tilde{z}) = \min \left( \frac{\pi(\tilde{z})/\pi^{prop}(z^{(t-1)}, \tilde{z})}{\pi(z^{(t-1)})/\pi^{prop}(\tilde{z}, z^{(t-1)})}, 1 \right)$

③  $z^{(t)} = \begin{cases} \tilde{z} & \text{with probability } \alpha \\ z^{(t-1)} & \text{with probability } 1 - \alpha \end{cases}$

# Application to DBH distribution

## the exponential model

model law	$\pi_{Y \theta}(y) = \exp(\theta)$
likelihood	$L(\mathbf{y}; \theta) = \theta^n \exp(-\theta \sum_{i=1}^n y_i)$
<i>a priori</i> law	$\pi_{\theta}(\theta) = \text{Ga}(\theta, 1, 10) = 10 \exp(-10 \theta)$
<i>a posteriori</i> law	$\pi_{\theta \mathbf{y}} = \text{Ga}(1 + n, 10 + \sum y_i)$

imagine we do not know that  $\pi_{\theta|\mathbf{y}} = \text{Ga}(1 + n, 10 + \sum y_i)$

$$\begin{aligned} \pi_{\theta|\mathbf{y}}(\theta|y_1, \dots, y_n) &= \frac{L(y_1, \dots, y_n; \theta) \pi_{\theta}(\theta)}{\int L(y_1, \dots, y_n; \theta) \pi_{\theta}(\theta) d\theta} = \frac{\theta^n \exp(-\theta \sum_{i=1}^n y_i) \times 10 \exp(-10 \theta)}{\int \theta^n \exp(-\theta \sum_{i=1}^n y_i) \times 10 \exp(-10 \theta) d\theta} \\ &\propto \theta^n \exp(-\theta(10 + \sum_{i=1}^n y_i)) \end{aligned}$$

however you know that

$$\pi_{\theta|\mathbf{y}}(\theta|y_1, \dots, y_n) \propto \theta^n \exp(-\theta(10 + \sum_{i=1}^n y_i))$$

## here we are : inferring the model with MCMC

building the Markov chain  $\theta^{(1)}, \dots, \theta^{(t)}, \dots$  with asymptotic law  $\pi_{\theta|y}$

- ▶ the target law :  $\pi_{\theta|y}(\theta|y_1, \dots, y_n) \propto \theta^n \exp\{-\theta(10 + \sum_{i=1}^n y_i)\}$
- ▶ the proposal law : gaussian random walk  $\tilde{\theta} \sim \mathcal{N}(\theta^{(t-1)}, \sigma^2)$

$$\pi^{prop}(\theta^{(t-1)}, \tilde{\theta}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}(\theta^{(t-1)} - \tilde{\theta})^2\right\}$$

- ▶ the Metropolis-Hastings ratio is

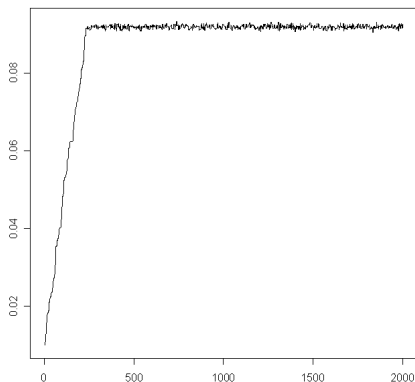
$$r = \frac{\tilde{\theta}^n \exp\{-\tilde{\theta}(10 + \sum_{i=1}^n y_i)\}}{(\theta^{(t-1)})^n \exp\{-\theta^{(t-1)}(10 + \sum_{i=1}^n y_i)\}}$$

- ▶ updating the chain

- $u \sim \mathcal{U}[0, 1]$
- $\theta^{(t)} = \begin{cases} \tilde{\theta} & \text{if } u \leq r \\ \theta^{(t-1)} & \text{if not} \end{cases}$

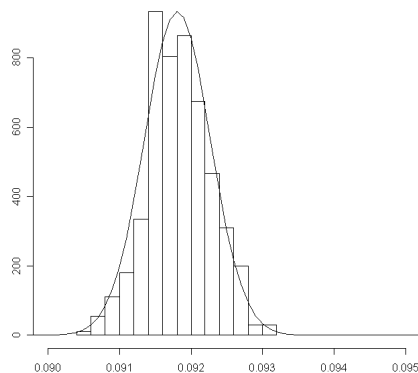
# Application to DBH distribution

Markov chain for  $\theta^{(t)}$



$\sigma = 0.001$  et  $\theta^{(0)} = 0.01$

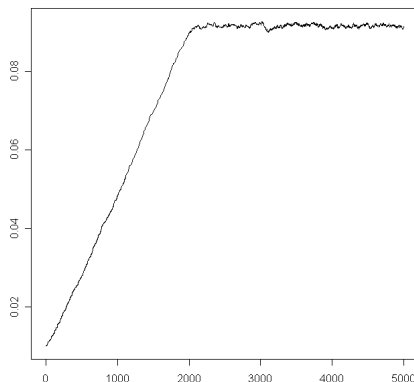
Estimate of  $\pi_{\theta|y}$



# Impact of the proposal law

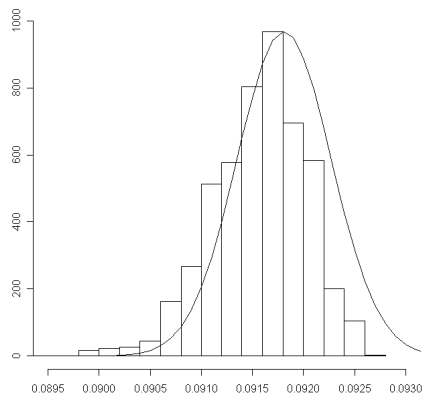
results with  $\sigma = 0.0001$ , *i.e.* a smaller step

Markov chain of  $\theta^{(t)}$



$\sigma = 0.0001$  et  $\theta^{(0)} = 0.01$

Estimate of  $\pi_{\theta|y}$

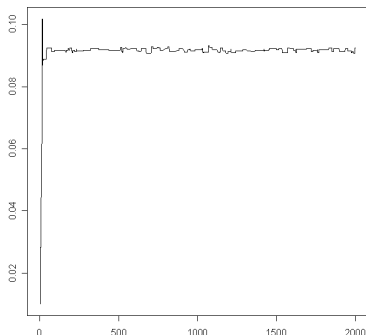


# Application to DBH distribution

impact of the proposal law

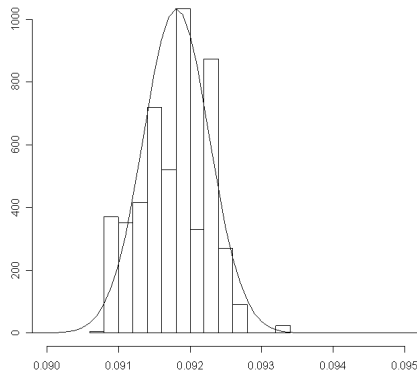
results for  $\sigma = 0.01$ , *i.e.* a bigger step

Markov chain of  $\theta^{(t)}$



$\sigma = 0.01$  et  $\theta^{(0)} = 0.01$

Estimation de  $\pi_{\theta|y}$





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in practice some critical points

- ▶ initial values may be critical
- ▶ uneasy to optimize the proposal law / to diagnose convergence
- ▶ burning time maybe **too** long

## other MC algorithms

- ▶ Gibbs : sequential updates of model parameters  
iteration  $Z^{(k)} \rightarrow Z^{(k+1)}$  is  $\begin{cases} Z_\ell^{(k+1)} \sim \pi_{\ell|\neg\ell} \\ \text{for } \ell \in \{1, \dots, n\} \end{cases}$   
with  $\pi_{\ell|\neg\ell}$  the marginal law of  $Z_\ell$  given  $Z_1, \dots, Z_{\ell-1}, Z_{\ell+1}, \dots, Z_n$
- ▶ Metropolis within Gibbs : mixing MH and Gibbs
- ▶ Hamiltonian MC : oriented walk  
Implied in Rstan <http://mc-stan.org/>

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# the bayesian future

## ECOLOGY LETTERS

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### Why environmental scientists are becoming Bayesians

[James S. Clark](#)

First published: 15 December 2004 [Full publication history](#)

DOI: 10.1111/j.1461-0248.2004.00702.x [View/save citation](#)

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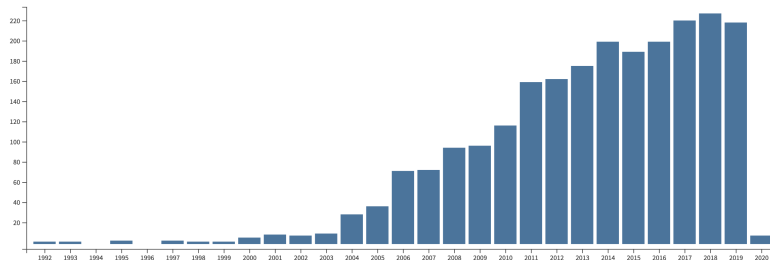


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Volume 8, Issue 1  
January 2005  
Pages 2-14

# the bayesian future

Total Publications

**2305** Analyze



Keywords : Bayes + Africa

# the bayesian way of thinking

DID THE SUN JUST EXPLODE?  
(IT'S NIGHT, SO WE'RE NOT SURE)



FREQUENTIST STATISTICIAN:

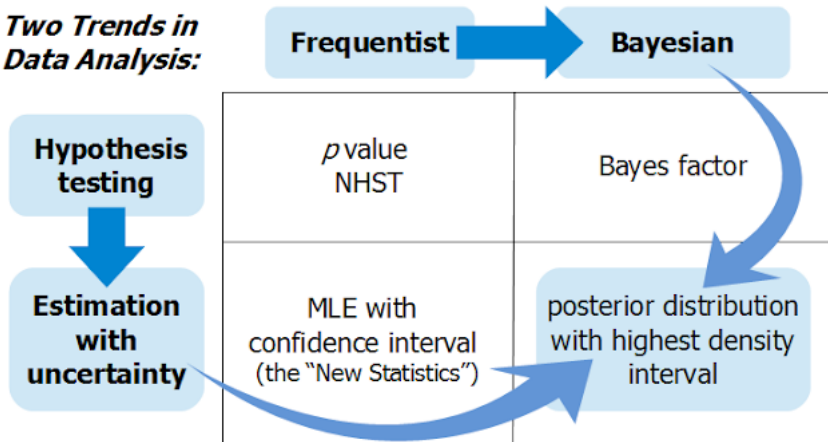


BAYESIAN STATISTICIAN:



# the bayesian way of thinking

*Two Trends in Data Analysis:*



# the bayesian advantages

You can

- ▶ incorporate prior knowledge
- ▶ design your own model
- ▶ inspect your posterior distribution
- ▶ easily propagate uncertainties, even for complex models
- ▶ update your models as soon as you want



## the bayesian advantages

You will

- ▶ separate creativity from inference
- ▶ build very complex models
- ▶ not forget your prior results each time you start modeling
- ▶ be useful for decision making
- ▶ have fun in modeling

# the bayesian niche

