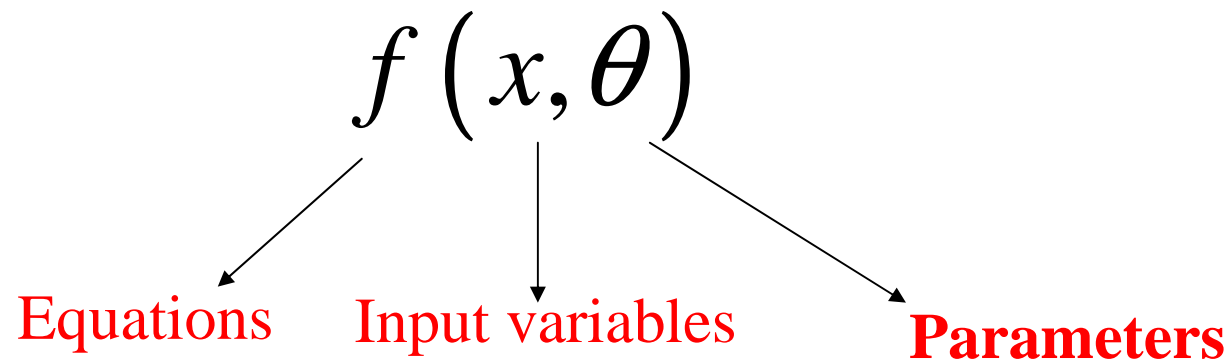


An introduction to modelling, Poznan, Nov. 2008

# Estimation of model parameters

**David Makowski**  
**INRA**

# Parameters



« **A parameter** is a numerical value which is not calculated by the model and is not measured »

# Parameter estimation

« aims at approximating the parameter values by using *experimental data* and/or *expert knowledge* »

## It is important because

« *Model performances* depend on the accuracy of the parameter estimates »

# The Bayesians and the Frequentists

**For Frequentists,**

- parameters are fixed
- parameters are estimated by points values for a given dataset
- estimation is performed by using data **only**

**For Bayesians,**

- parameters are defined as random variables
- parameters are estimated by distributions for a given dataset
- estimation is performed from **both** data and prior information
- computations more complex, but results more intuitive

## **Four steps for estimating parameters**

### **1. How many and which parameters should be estimated?**

- In simple models, all parameters
- In complex models, a subset of parameters is estimated

### **2. What kind of information is available?**

- Data
- Prior information (expert knowledge, literature)

### **3. Which estimation method?**

- Ordinary least squares
- Weighted/Generalized least squares, maximum likelihood
- Bayesian method

### **4. What is the accuracy of the parameter estimator?**

- Theoretical consideration, variances, residuals

# Four estimation problems

**Pb.A: One parameter**

**Pb.B: Linear with 2 parameters**

**Pb.C: Non linear with 18 parameters**

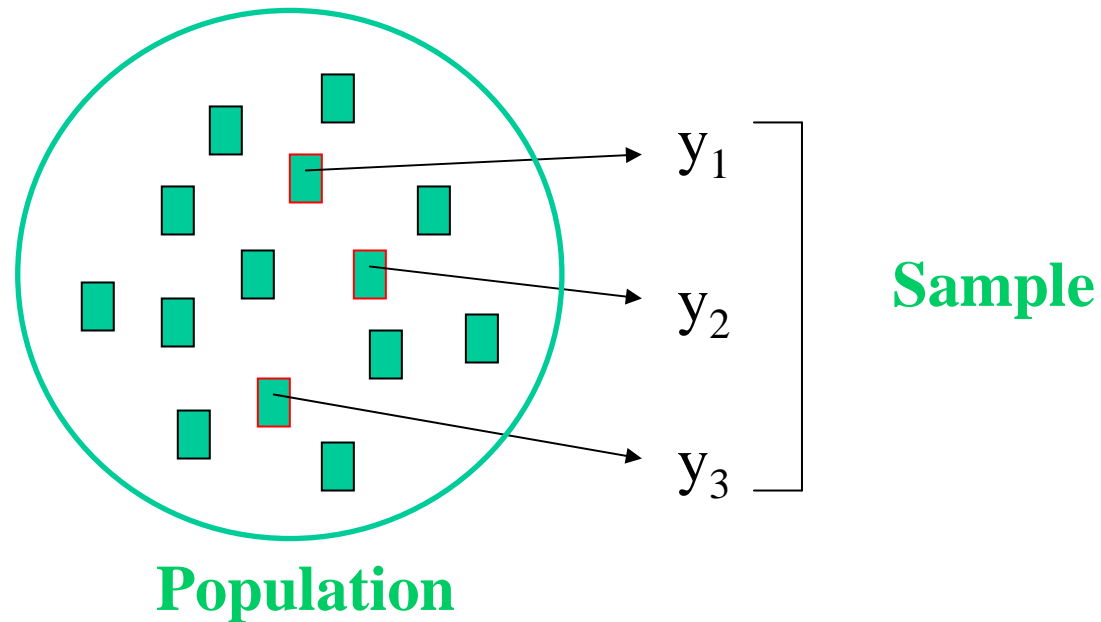
**Pb.D: Estimation from data and prior information**

**Estimation  
from data only**

# Problem A

**« Estimation of the average oilseed rape yield in 2004 in a small area**

**from 3 yield measurements collected in three different plots »**



## Step 1. Which parameters?

**A single parameter**, the average yield in the considered area, noted  $\theta$ .



## Step 2. What kind of information?

**Available information:** a *sample* of three measures collected in three plots from the *population of plots* of interest

## Step 3. Which method?

**An estimator** of the average yield is:

$$\hat{\theta} = \frac{y_1 + y_2 + y_3}{3}$$

Example :

- If  $y_1=30$ ,  $y_2=39$  et  $y_3=35$ , the estimated average yield is **34.7** q/ha.
- If  $y_1=32$ ,  $y_2=38$  et  $y_3=39$ , the estimated average yield is **36.3** q/ha.

*« An estimator is a function relating the parameter to the observations »*

Data set 1  $\longrightarrow$   $\hat{\theta}_1$

Data set 2  $\longrightarrow$   $\hat{\theta}_2$

Data set  $N$   $\longrightarrow$   $\hat{\theta}_N$

## Step 4. Is the estimator accurate?

$$E\left[\left(\hat{\theta} - \theta\right)^2\right] = \left[E\left(\hat{\theta}\right) - \theta\right]^2 + \text{var}\left(\hat{\theta}\right)$$

**Mean squared  
error**

**Bias<sup>2</sup>**

**Variance**

## Step 4. Is the estimator accurate?

### a. Theoretical consideration

« Under some assumptions, our estimator is *unbiased* and of *minimum variance* among the unbiased estimators »

## Step 4. Is the estimator accurate?

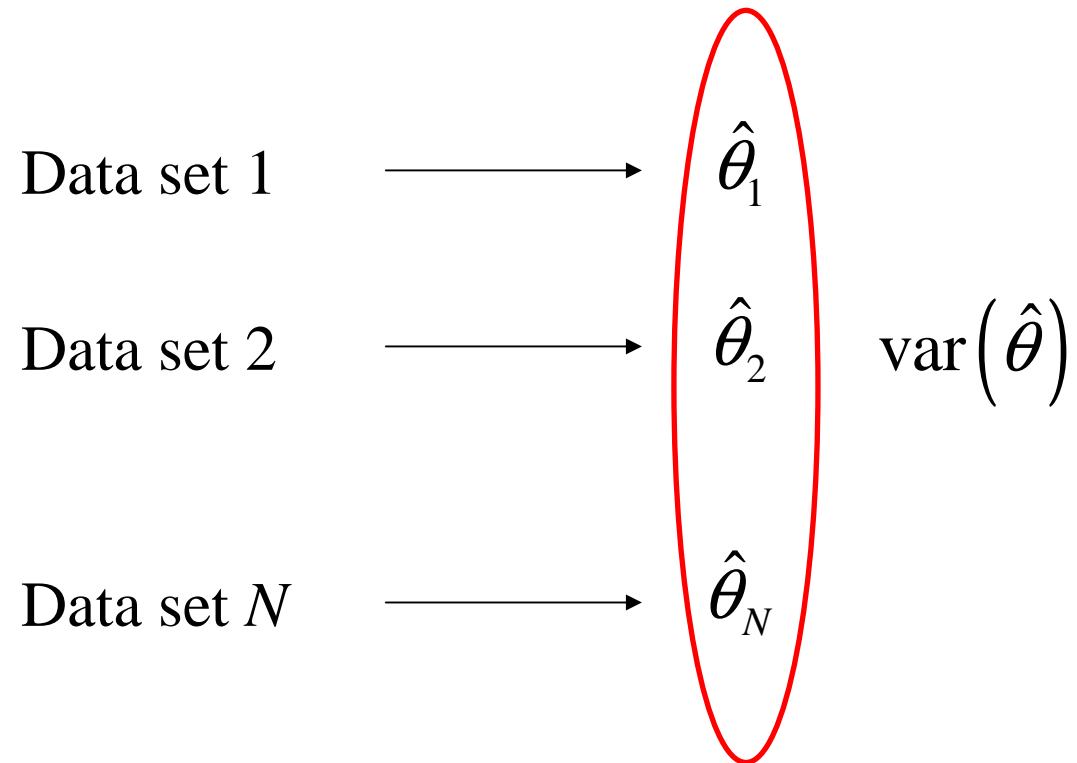
### b. Estimator variance

$\text{var}(\hat{\theta})$  can be estimated from data

Example :

- If  $y_1=30$ ,  $y_2=39$  and  $y_3=35$ , the estimated variance is **6.78** q<sup>2</sup>/ha<sup>2</sup>, standard deviation=**2.6** q/ha.
- If  $y_1=32$ ,  $y_2=38$  and  $y_3=39$ , the estimated variance is **4.78** q<sup>2</sup>/ha<sup>2</sup>, standard deviation=**2.19** q/ha.

**The variance of an estimator measures  
its variability across datasets**



## Problem B

« *Estimation of the parameters of the model*  
 *$f(x; \theta_1, \theta_2)$*  »

$$f(x; \theta_1, \theta_2) = \theta_1 + \theta_2 x$$

Nitrogen uptake in oilseed  
rape crop

Nitrogen fertilizer dose

***This model computes nitrogen uptake in  
function of fertilizer dose***

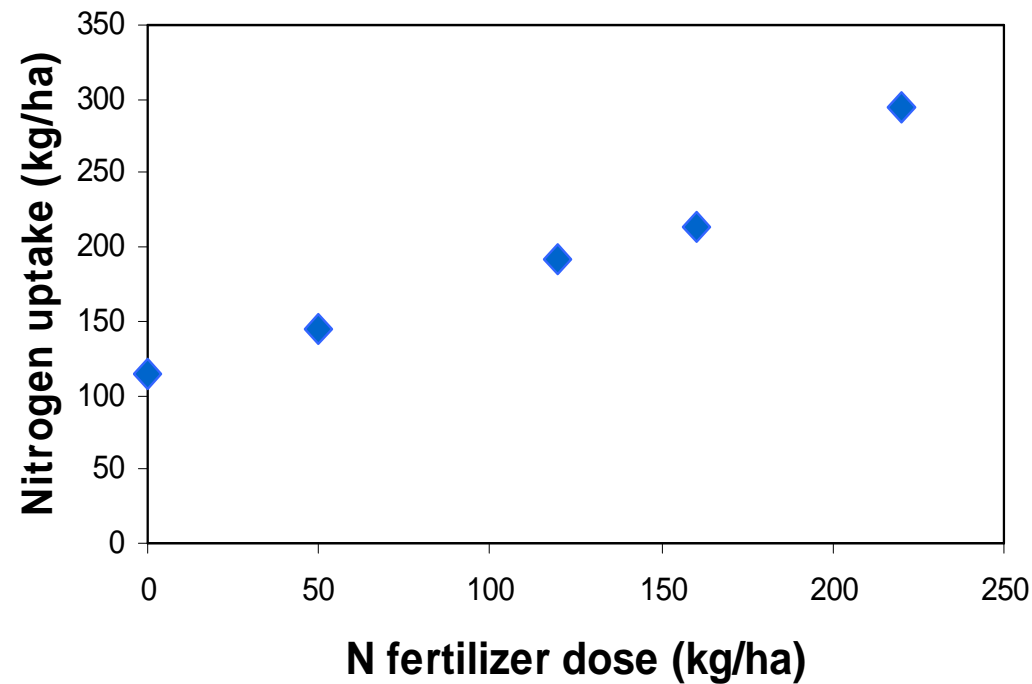


## Step 1. Which parameters?

Two model parameters:  $\theta_1$  and  $\theta_2$

## Step 2. What kind of information?

A **sample** of 5 nitrogen uptake measurements obtained in 5 plots in the **population of interest** (an area in France)



## Step 3. Which method?

### Ordinary least squares

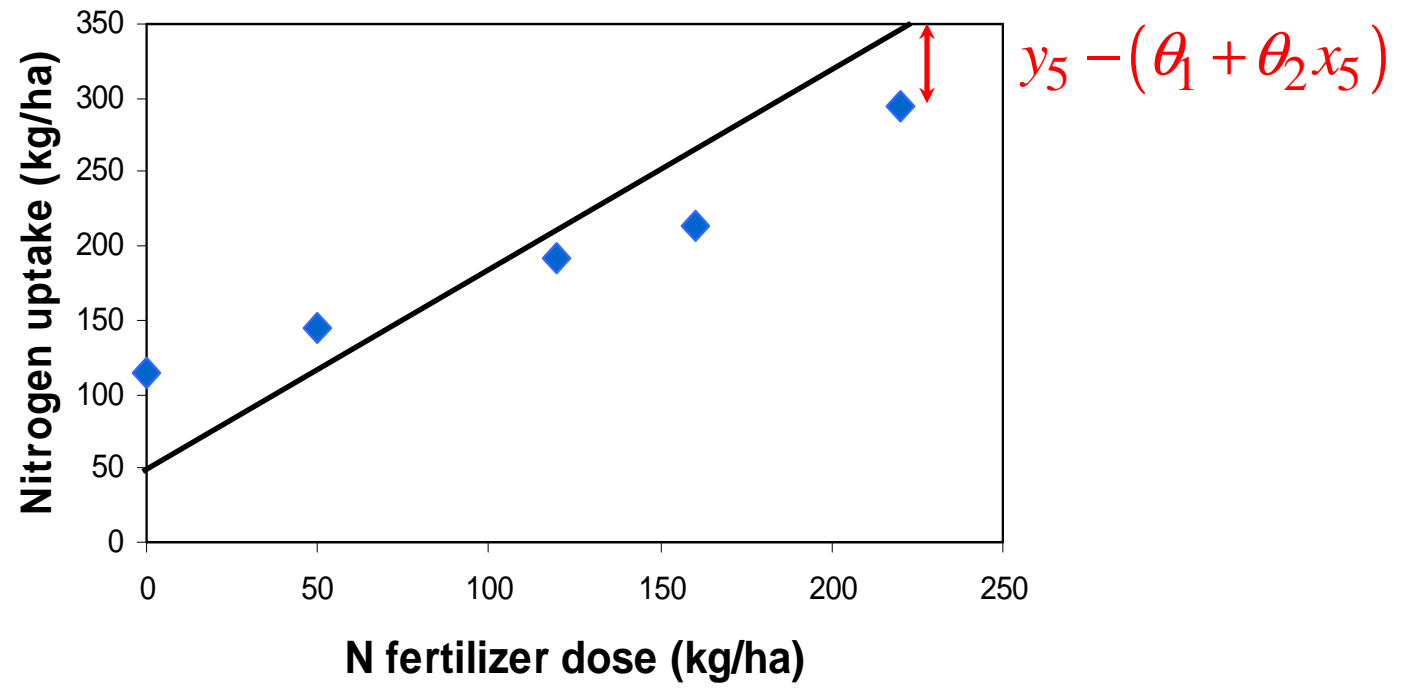
The parameter estimators are the values of  $\theta_1$  and  $\theta_2$  minimizing

$$\sum_{i=1}^N (y_i - \theta_1 - \theta_2 x_i)^2$$

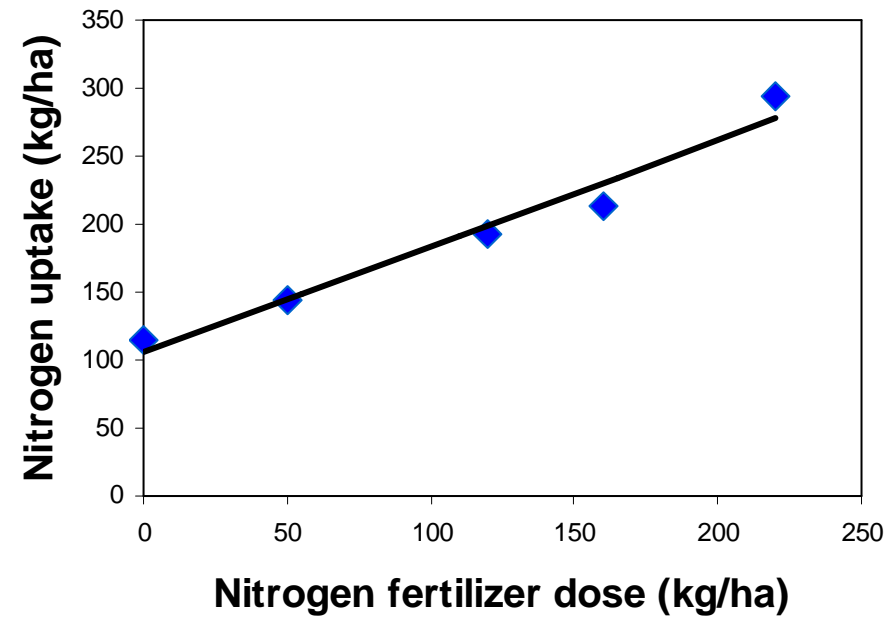
that is

$$\hat{\theta}_2 = \frac{\sum_{i=1}^N (y_i - \bar{Y})(x_i - \bar{X})}{\sum_{i=1}^N (x_i - \bar{X})^2}$$

$$\hat{\theta}_1 = \bar{Y} - \hat{\theta}_2 \bar{X}.$$



Here, with our 5 measurements, we got  $\hat{\theta}_1 = 106.01 \text{ kg.ha}^{-1}$   
 $\hat{\theta}_2 = 0.78 \text{ kg.kg}^{-1}$



## Step 4. Are these estimators accurate?

$$E\left[\left(\hat{\theta} - \theta\right)^2\right] = \left[E\left(\hat{\theta}\right) - \theta\right]^2 + \text{var}\left(\hat{\theta}\right)$$

**Mean squared  
error**

**Bias<sup>2</sup>**

**Variance**

## Step 4. Are these estimators accurate?

### a. Theoretical aspect

« Under some assumptions, these estimators are ***unbiased*** and with ***minimum variances*** among the unbiased estimators ».

Assumptions are:

- ***independance*** of the model errors,
- ***homogeneity*** of the model error variances.

## Step 4. Are these estimators accurate?

### b. Variances of the estimators

Estimation of  $\text{var}(\hat{\theta})$  from the data

$$\sqrt{\text{var}(\hat{\theta}_1)} = 11.99 \text{ kg.ha}^{-1}$$

$$\sqrt{\text{var}(\hat{\theta}_2)} = 0.09 \text{ kg.kg}^{-1}$$

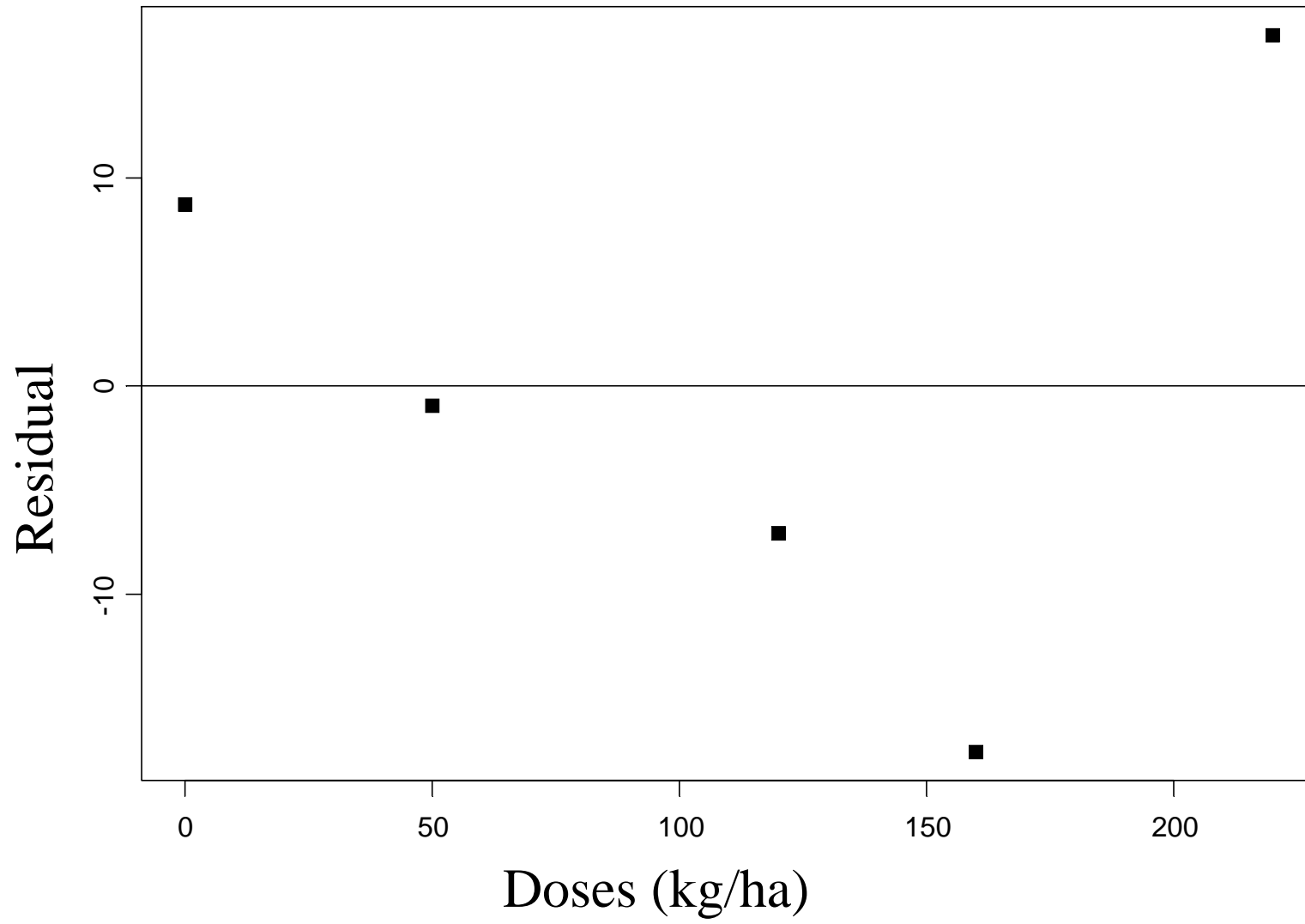


**Step 4. Are these estimators accurate?**

**c. Analysis of the residuals**

$$r_i = y_i - (\hat{\theta}_1 + \hat{\theta}_2 x_i), \quad i = 1, \dots, 5$$

Useful to check the independance of the model errors and  
variance homogeneity



## R code

```
DOSE<-c(0,50,120,160,220)
```

```
NABS<-c(114.75,144.0,192.38,213,294.16)
```

```
DATA<-data.frame(DOSE,NABS)
```

```
Fit<-lm(NABS~DOSE,data=DATA)
```

```
print(summary(Fit))
```

```
plot(DOSE,Fit$residuals,ylab="Residual",ylab="Dose",pch=15)
```

```
abline(0,0)
```

# Comments on the first two problems

## Four steps

- 1. Which parameters?**
- 2. What kind of information?**
- 3. Which estimation method?**
- 4. Accuracy of the parameter estimators?**

# Comments on the first two problems

## It was easy because

- Linear model:  $\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_p x_p$ 
  - Analytic relationships between estimators and data
- Number of data > Number of parameters
- Only one type of measurements
- No prior information about parameter values
- Softwares are available for the computations (SAS, R, ModelMaker...).

# It can be much more difficult

- Non linear models:  $\neq \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_p x_p$ 
  - No analytic relationship between the estimators and the data
- The number of data can be low compared to the number of parameters
- Complex dataset
  - several types of observations, correlated observations
- Prior information about parameter values

## A much more difficult problem !

- Non linear model
- Many parameters
- Prior information
- Several types of measurements collected in several plots

# Problem C

## *Estimation of the parameters of a model simulating winter wheat growth between January and May*

*(Jeuffroy et Recous, 1999)*

### State variables simulated at a daily time step

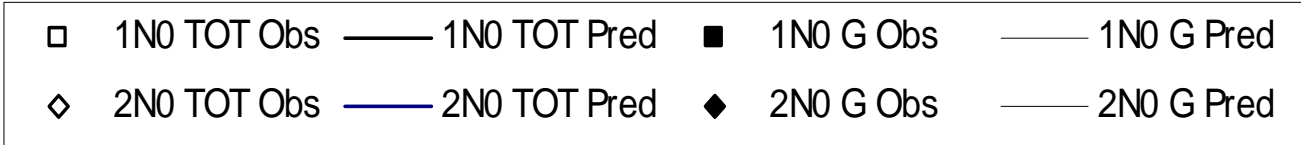
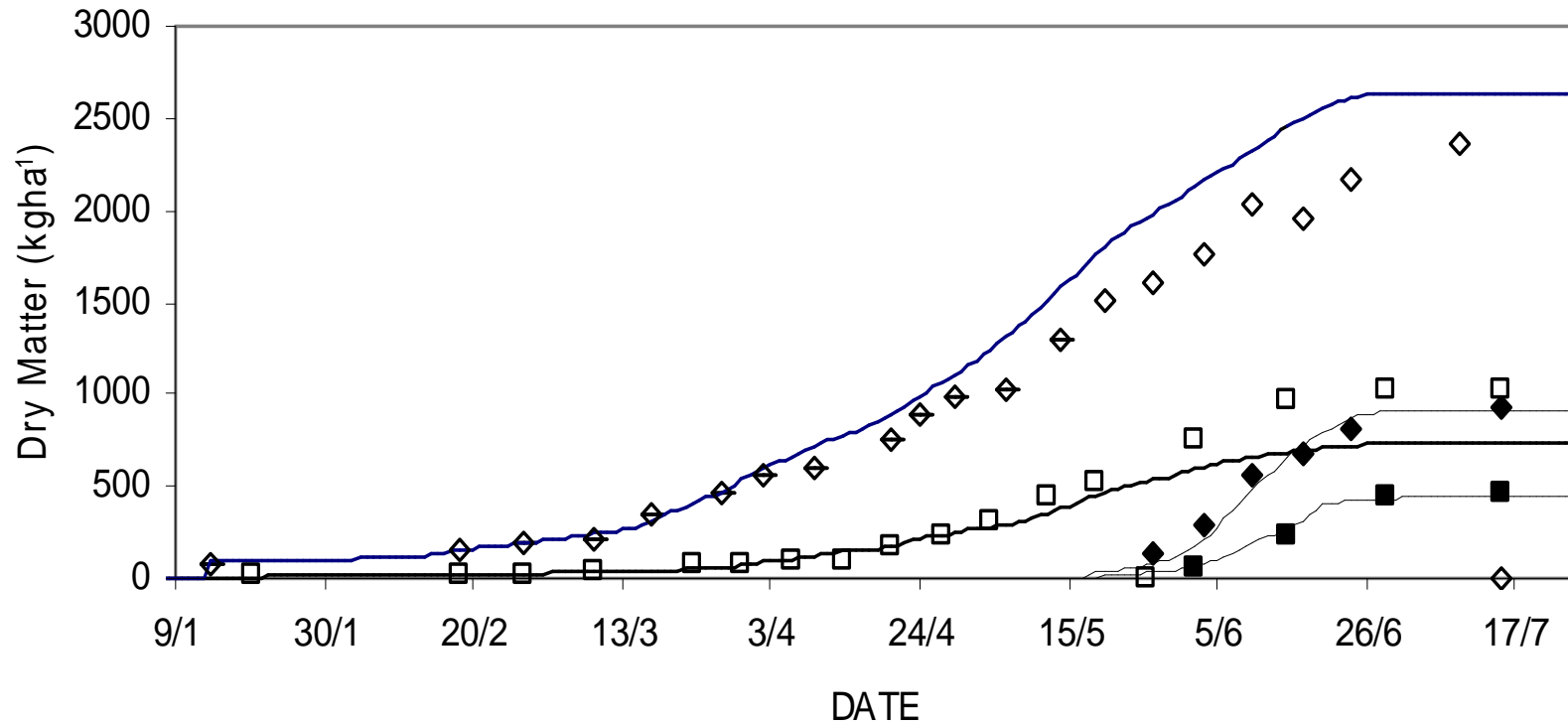
- Crop above-ground biomass (dry matter) (kg/ha) →  $MS_t$
- Nitrogen uptake (kg/ha), →  $QN_t$
- Leaf Area Index →  $LAI_t$

### Input variables:

- Global daily radiation →  $RG_t$
- Average daily temperature, →  $T_t$
- Initial values of biomass and nitrogen uptake →  $MS_0, QN_0$



# Simulations of wheat biomass using the AZODYN dynamic crop model



# Problem C

## Few model equations

$$MS_j = MS_{j-1} + (E_{b\max} \times ft_{j-1} \times Ei_{j-1} \times C \times RG_{j-1})$$

$$Ei_{j-1} = E_{i\max} \left[ 1 - \exp(-K \times LAI_{j-1}) \right]$$

$$LAI_{j-1} = D \times QNc_{j-1}$$

$$MS_j = MS_{j-1} + \left\{ E_{b\max} \times C \times E_{i\max} \left[ 1 - \exp(-K \times D \times QNc_{j-1}) \right] \times ft_{j-1} \times RG_{j-1} \right\}$$

# 18 parameters

Parameter	Meaning	Initial value	Range
Ebmax	Efficiency of radiation conversion	3.3 g/MJ	1.8-4
K	Coefficient of radiation extinction	0.72	0.6-0.8
D	Ratio LAI / Critical nitrogen uptake	0.028	0.02-0.045
Vmax	Maximum rate of nitrogen uptake	0.5 kg/ha/dj	0.2-0.7
C	PAR/RG	0.48	
Tmin	Minimum temperature for photosynthesis	0 °C	
Topt	Optimum temperature for photosynthesis	15 °C	
Tmax	Maximum temperature for photosynthesis	40 °C	
Eimax	Efficiency of radiation interception	0.96	
Tep-flo	Time between two stages	150 dj	
E		1.55 t/ha	
F		4.4 %	
G		5.35 %	
H		-0.442	
L		2 t/ha	
M		6 %	
N		8.3 %	
P		-0.44	

# The two expressions of a dynamic model

## 1: Dynamic system model

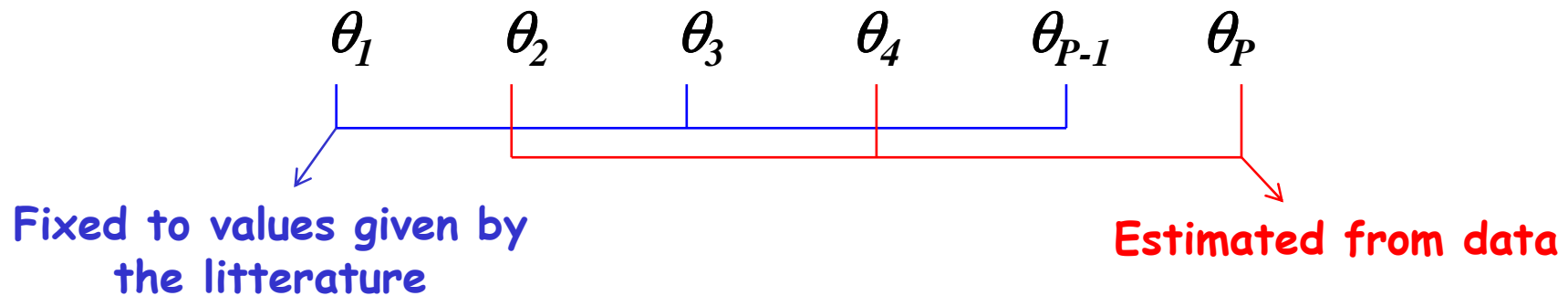
$$MS_t = MS_{t-1} + g(X_{t-1}; \theta)$$

## 2: Response model

$$MS_t = f(t, X; \theta)$$

## Step 1. Which parameters?

A subset of parameters must be selected



- **Numerical problems if all the parameters are estimated**
- **Not a good idea anyway**
  - High estimator variances
  - High prediction errors

## **New issue: How to select the subset of parameters**

- i. from the literature**
- ii. by analyzing the model equations**
- iii. by sensitivity analysis**
- iv. from data**

## i. from the literature

« Determine the parameters whose values are not well known ».

### **Drawbacks :**

- can be quite subjective
- the available papers are not always relevant

ii. by analyzing the model equations

« Identify the parameters which cannot be simultaneously estimated »



$$MS_j = MS_{j-1} + (E_{b\max} \times ft_{j-1} \times Ei_{j-1} \times C \times RG_{j-1})$$

$$Ei_{j-1} = E_{i\max} \left[ 1 - \exp(-K \times LAI_{j-1}) \right]$$

$$LAI_{j-1} = D \times QNc_{j-1}$$

$$MS_j = MS_{j-1} + \left\{ E_{b\max} \times C \times E_{i\max} \left[ 1 - \exp(-K \times D \times QNc_{j-1}) \right] \times ft_{j-1} \times RG_{j-1} \right\}$$

**Case 1: only observed values of MS are available**

**Case 2: observed values of MS and LAI are available**

$$MS_j = MS_{j-1} + (E_{b\max} \times ft_{j-1} \times Ei_{j-1} \times C \times RG_{j-1})$$

$$Ei_{j-1} = E_{i\max} \left[ 1 - \exp(-K \times LAI_{j-1}) \right]$$

$$LAI_{j-1} = D \times QNc_{j-1}$$

$$MS_j = MS_{j-1} + \left\{ E_{b\max} \times C \times E_{i\max} \left[ 1 - \exp(-K \times D \times QNc_{j-1}) \right] \times ft_{j-1} \times RG_{j-1} \right\}$$

### **Case 1: only observed values of MS are available**

- the 3 parameters  $E_{b\max}, C, E_{i\max}$

It is not possible to estimate simultaneously

- the 2 parameters  $K, D$

### **Case 2: observed values of MS and LAI are available**

It is not possible to estimate simultaneously the 3 parameters  $E_{b\max}, C, E_{i\max}$

### iii. by sensitivity analysis

« Select the parameters that strongly influence the model outputs »

#### **Drawbacks:**

A sensitivity threshold must be defined.

Does not prevent from lack of identifiability .

## iv. from data

« Select the parameters leading to the best model predictions »

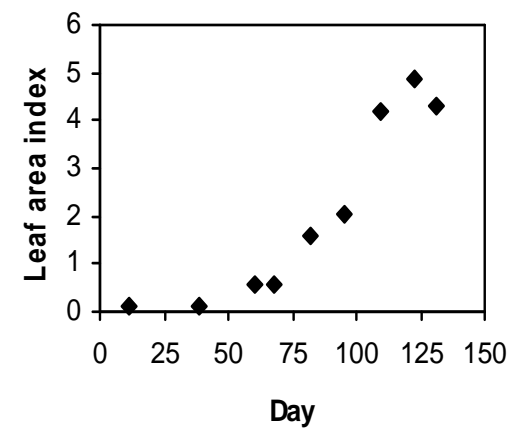
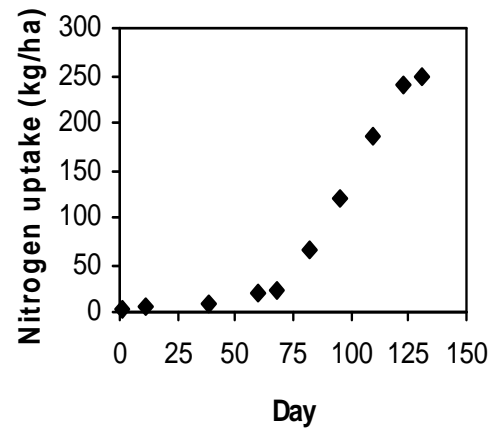
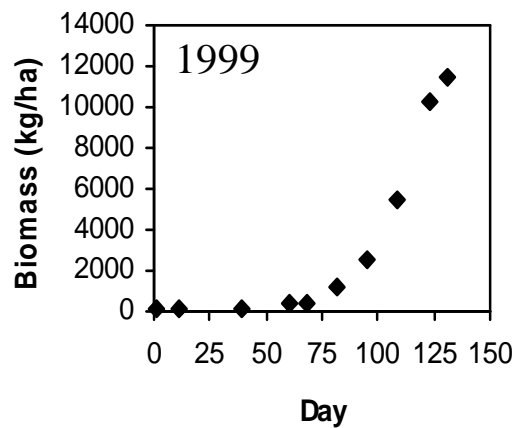
Number of estimated parameters	MSEPCv
1	MSEP <sub>1</sub>
2	MSEP <sub>2</sub>
3	MSEP <sub>3</sub>
...	...
P	MSEP <sub>P</sub>

## Step 1. Which parameters?

- **13 parameters** were fixed to values provided by the literature.
- **One parameter** was fixed after an analysis of the model equation.
- **Four parameters** were estimated from data:  $E_{BMAX}$ ,  $D$ ,  $K$  and  $V_{MAX}$

## Step 2. What kind of information?

- Measurements of wheat **biomass**, of **leaf area index** and of **nitrogen uptake** for one site (Grignon) and 6 years.
- Ten dates of measurement each year.
- Three replicates at each date. Replicates were averaged.



## Step 3. Which estimation method?

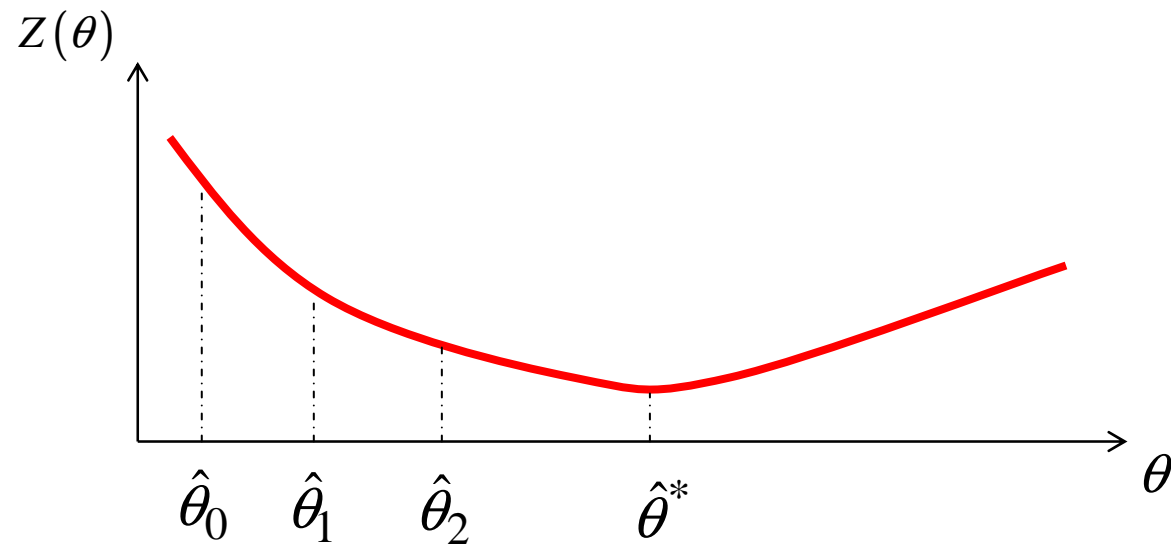
### 1st option: Ordinary least squares

Find  $\theta$  minimizing: 
$$Z(\theta) = \sum_{i=1}^N [y_i - f(t_i, x_i; \theta)]^2$$

#### **Difficulties:**

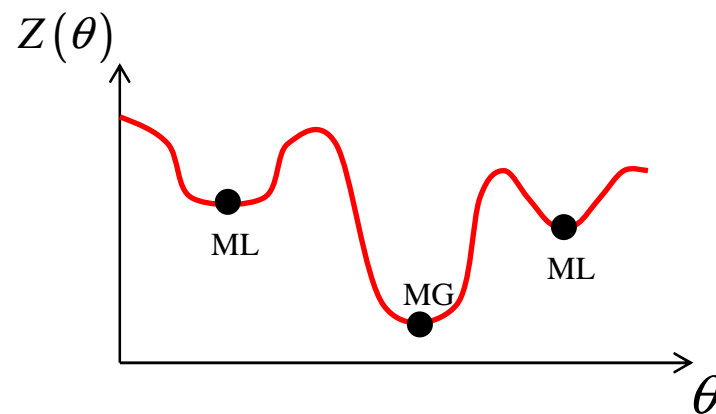
- non linear model
- no analytical expression for the estimators

## Minimization using an iterative algorithm





## Local optimum, global optimum



**→ Try several starting values !**

## Practical considerations

- Several programs were developed to implement this kind of algorithm (SAS, R, MatLab, Fortran, C++...)
- They use the following entries:
  - data
  - a model equation,
  - initial parameter values.
- The output is a set of estimated parameter values.

## Step 3. Which estimation method?

### **1st option: Ordinary least squares**

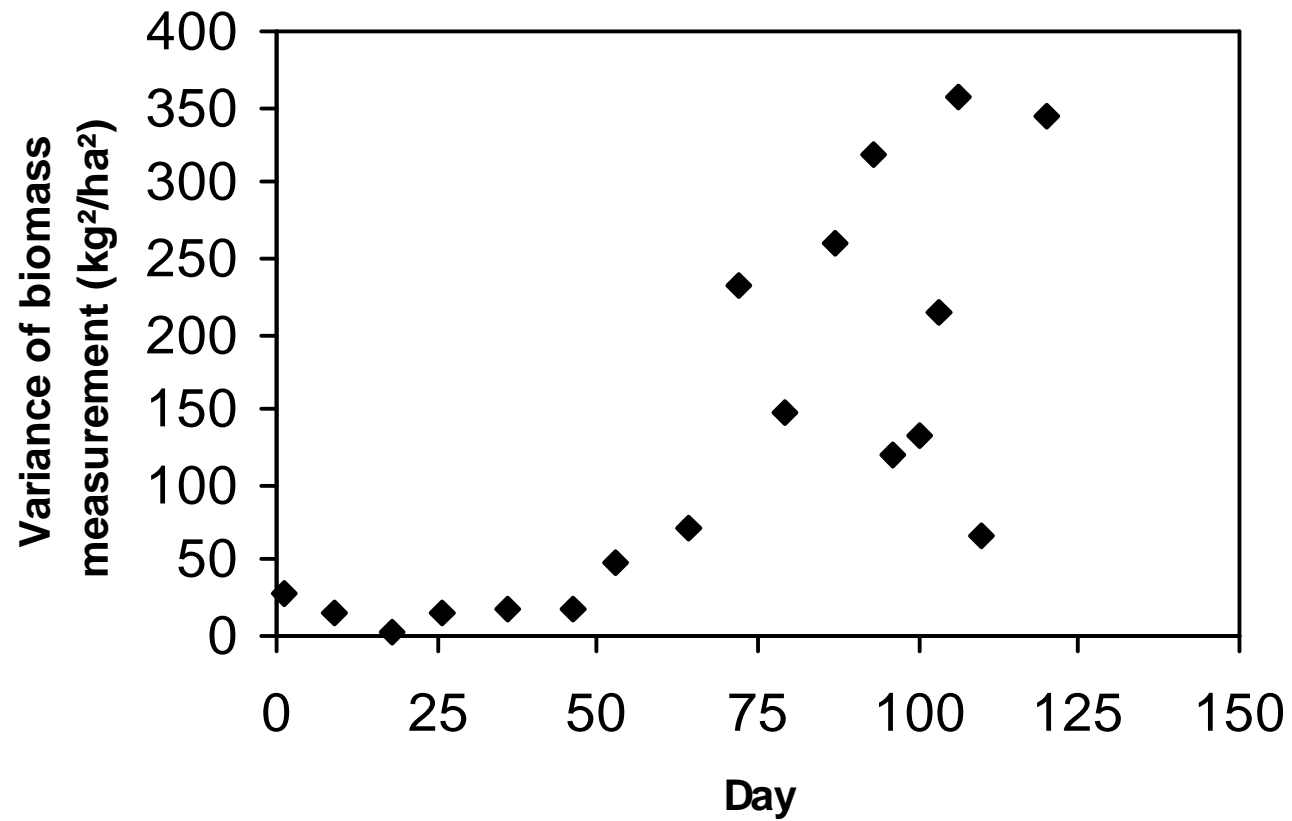
Find  $\theta$  minimizing:

$$Z(\theta) = \sum_{i=1}^N [y_i - f(t_i, x_i; \theta)]^2$$

This method performs well when the model error variances are constant

This is not very realistic here.

Here, the variances of the observations are variable



## Step 3. Which method?

### 2nd option: Weighted least squares

Find the value of  $\theta$  minimizing:

$$Z(\theta) = \sum_{i=1}^N \frac{[y_i - f(t_i, x_i; \theta)]^2}{\sigma_i^2}$$

$$\text{with } \hat{\sigma}_i^2 = \frac{1}{K(K-1)} \sum_{k=1}^K (y_{ik} - y_i)^2$$

## Weighted least squares

minimizing

$$Z_{MCP}(\theta) = \sum_{i=1}^6 \sum_{j=1}^{10} \frac{\left[ y_{ij}^{MS} - f^{MS}(t_j, x_i; \theta) \right]^2}{\hat{\sigma}_{MS.ij}^2} + \sum_{i=1}^6 \sum_{j=1}^{10} \frac{\left[ y_{ij}^N - f^N(t_j, x_i; \theta) \right]^2}{\hat{\sigma}_{N.ij}^2} + \sum_{i=1}^6 \sum_{j=1}^{10} \frac{\left[ y_{ij}^L - f^L(t_j, x_i; \theta) \right]^2}{\hat{\sigma}_{L.ij}^2}$$

$$\hat{\sigma}_{MS.ij}^2 = \frac{1}{K(K-1)} \sum_{k=1}^K \left[ y_{ijk}^{MS} - y_{ij}^{MS} \right]^2$$

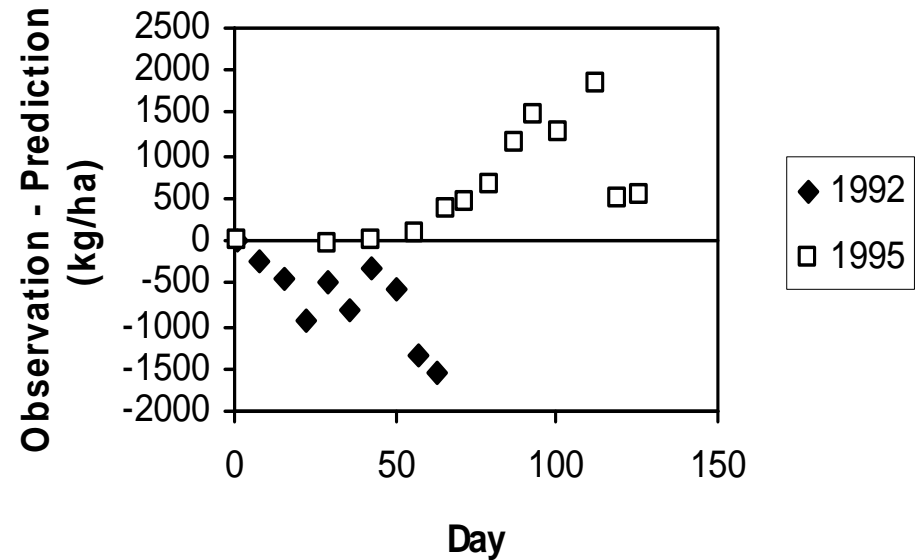
## Results of step 3: weighted least square estimates of the 4 model parameters

Parameter	Initial value	Estimated value
$E_{\text{BMAX}}$ (g/MJ)	3.3	3.29 (0.11)
D	0.028	0.037 (0.06)
K	0.72	0.74 (0.001)
$V_{\text{MAX}}$ (kg/ha/dj)	0.5	0.38 (0.02)

## Step 4. Are these estimators accurate?

Model residuals

**Residuals are not  
independent**



### Methods for taking correlations into account

- Generalized least squares
- Mixed models



# Four estimation problems

**Pb.A: One parameter**

**Pb.B: Linear with 2 parameters**

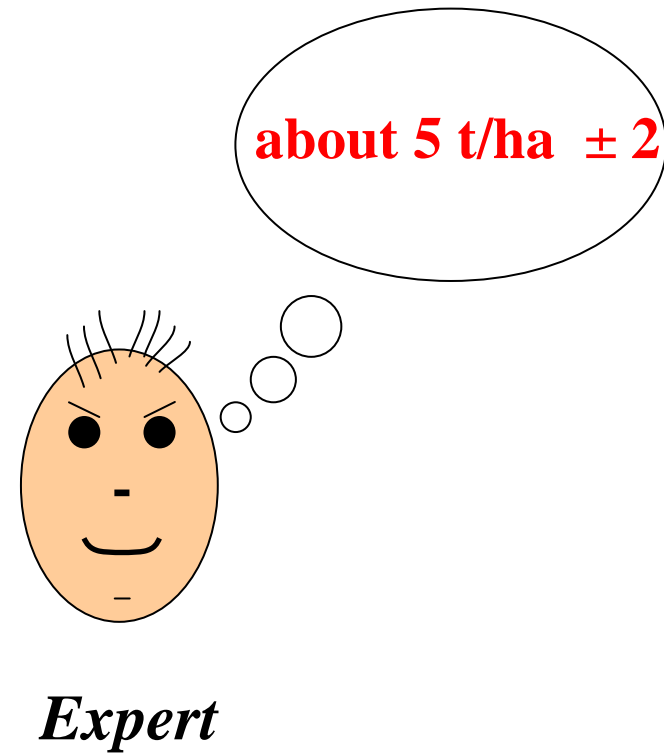
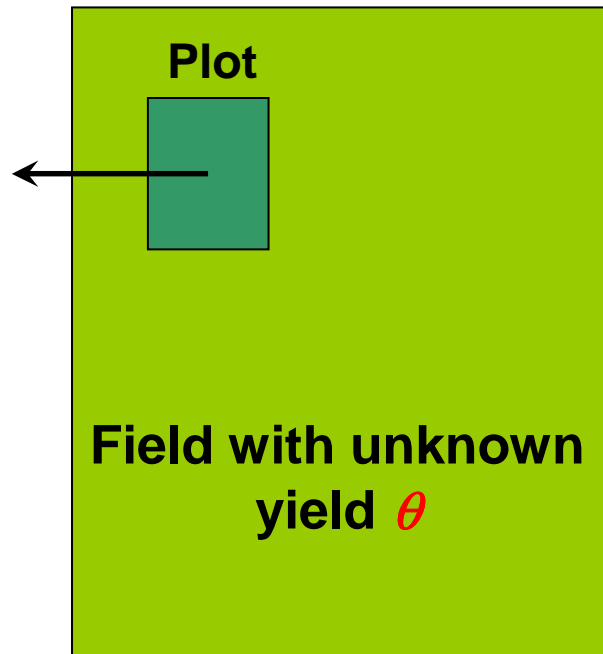
**Pb.C: Non linear with 18 parameters**

**Pb.D: Estimation from data and prior information**

# Problem D

Estimation of crop yield  $\theta$  by combining a measurement with expert knowledge

Measurement  
 $y = 9 \text{ t/ha} \pm 1$



# Bayesian method

**The Bayesian estimation methods allow one to combine information from different sources to estimate unknown parameters**

## **Basic principles:**

- Both data and external information (prior) are used
- Computations are based on the Bayes theorem
- Parameters are defined as random variables

# Bayes' theorem for model parameters

$\theta$ : vector of parameters.

$y$ : vector of observations

$P(\theta)$ : prior distribution of the parameter values.

$P(y | \theta)$ : likelihood function.

$P(\theta | y)$ : posterior distribution of the parameter values.

$$P(\theta|y) = \frac{P(y|\theta)P(\theta)}{\int_{\theta} P(y|\theta)P(\theta)}$$

often difficult to compute

# How to proceed for estimating the parameters of models

We proceed in three steps:

Step 1: Definition of the *prior distribution*.

Step 2: Definition of the *likelihood function*.

Step 3: Computation of the *posterior distribution* using Bayes' theorem.

## Three distributions in Bayes' theorem

- **Prior parameter distribution** = probability distribution describing our initial knowledge about parameter values

$$P(\theta)$$

- **Likelihood function** = function relating data to parameters

$$P(y|\theta)$$

- **Posterior parameter distribution** = probability distribution summarizing our final state of knowledge about parameters

$$P(\theta|y)$$

**Measurements**

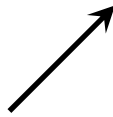


**Bayesian method**



**Posterior  
distribution of  
parameter values**

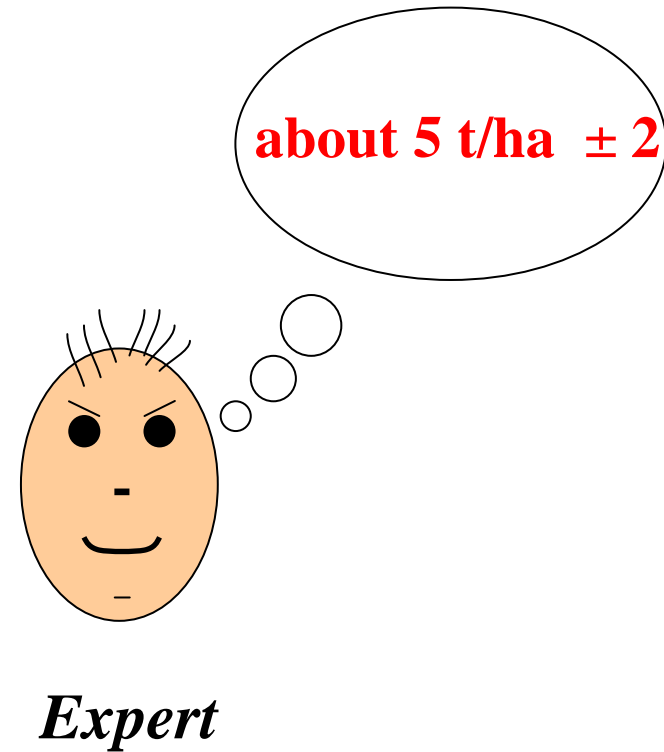
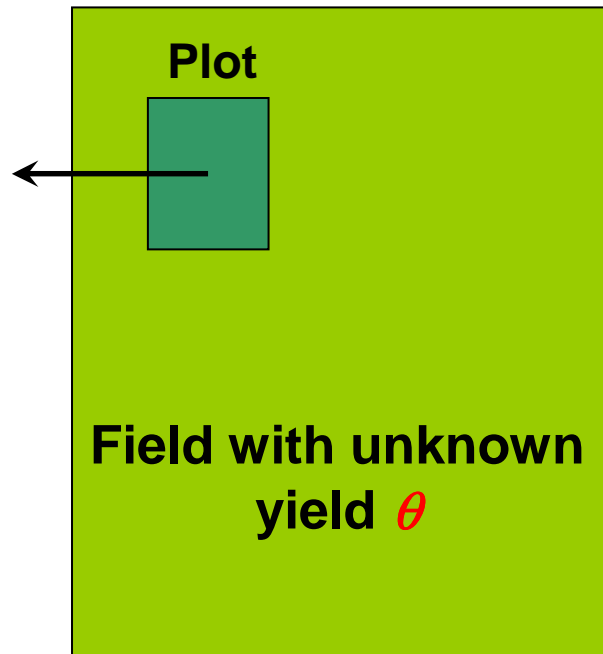
**Prior distribution of  
parameter values**



# Our problem

Estimation of crop yield  $\theta$  by combining a measurement with expert knowledge

*Measurement*  
 **$y = 9 \text{ t/ha} \pm 1$**





## Prior distribution

- It describes our belief about the parameter values **before** we observe the measurements.
- It is based on past studies, expert knowledge, and literature.

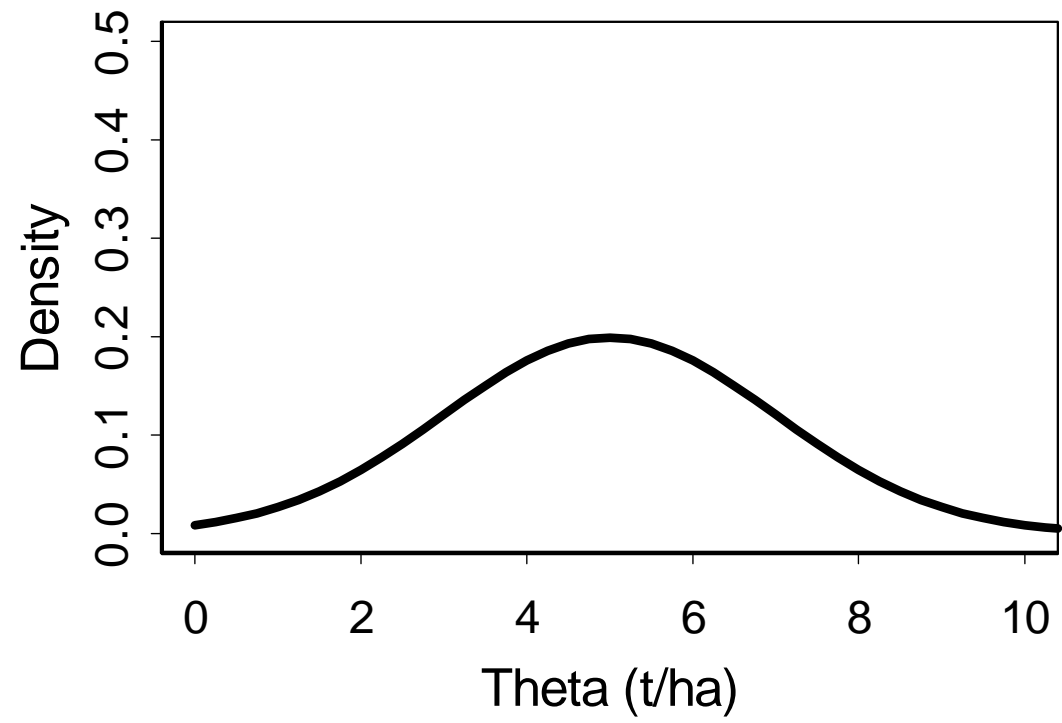
## Definition of a prior distribution for our problem

$$\theta \sim N(\mu, \tau^2)$$

$$P(\theta) = \frac{1}{\sqrt{2\pi\tau^2}} \exp\left[-\frac{(\theta - \mu)^2}{2\tau^2}\right] = \frac{1}{\sqrt{2\pi} \cdot 2} \exp\left[-\frac{(\theta - 5)^2}{2 \times 4}\right]$$

- Normal probability distribution.
- Expected value equal to 5 t/ha.
- Standard error equal to 2 t/ha

## Plot of the prior distribution



## Statistical model and likelihood function

$$y = \theta + \varepsilon \quad \text{with } \varepsilon \sim N(0, \sigma^2)$$

$$y | \theta \sim N(\theta, \sigma^2)$$

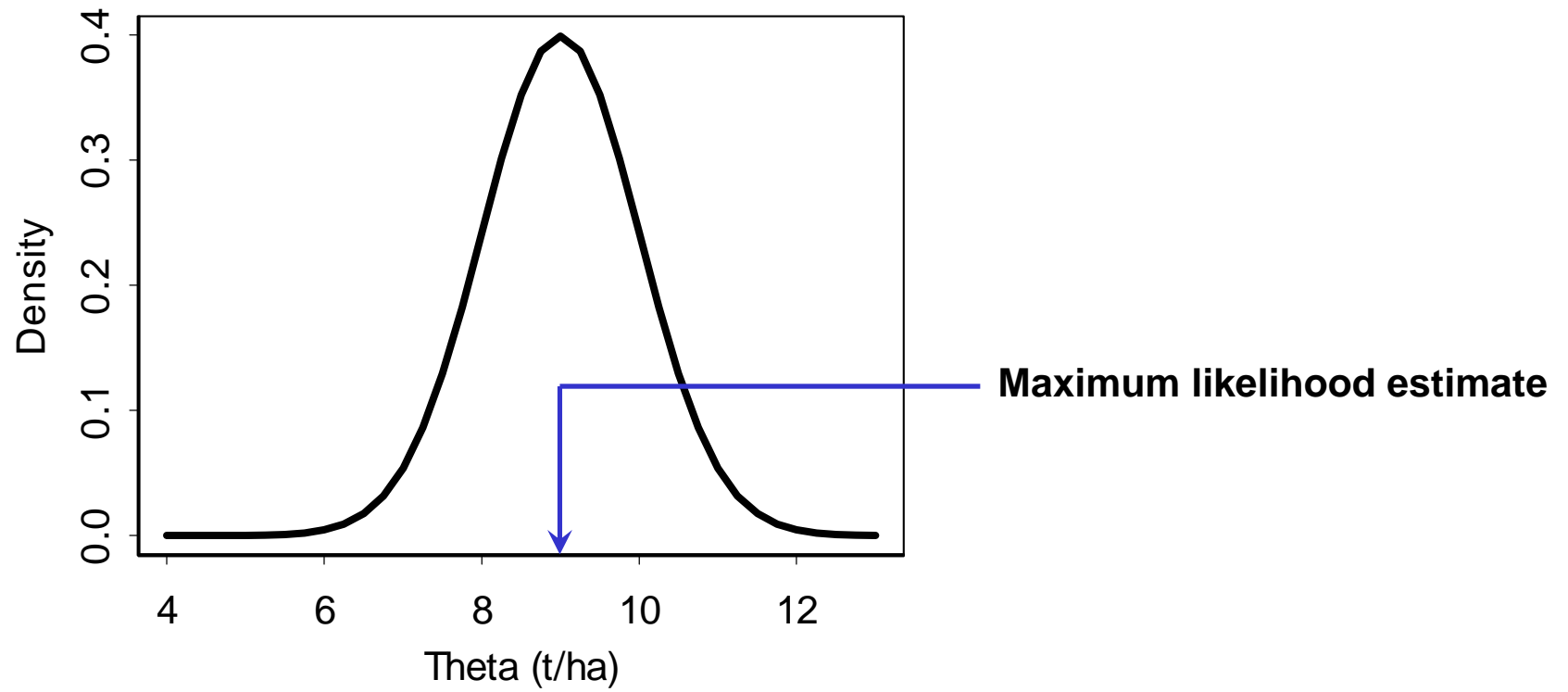
## Definition of a likelihood function

$$y | \theta \sim N(\theta, \sigma^2)$$

$$P(y|\theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y-\theta)^2}{2\sigma^2}\right] = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{(9-\theta)^2}{2}\right]$$

- Normal probability distribution.
- Measurement  $y$  assumed unbiased and equal to 9 t/ha.
- Standard error  $\sigma$  assumed equal to 1 t/ha

## Definition of a likelihood function



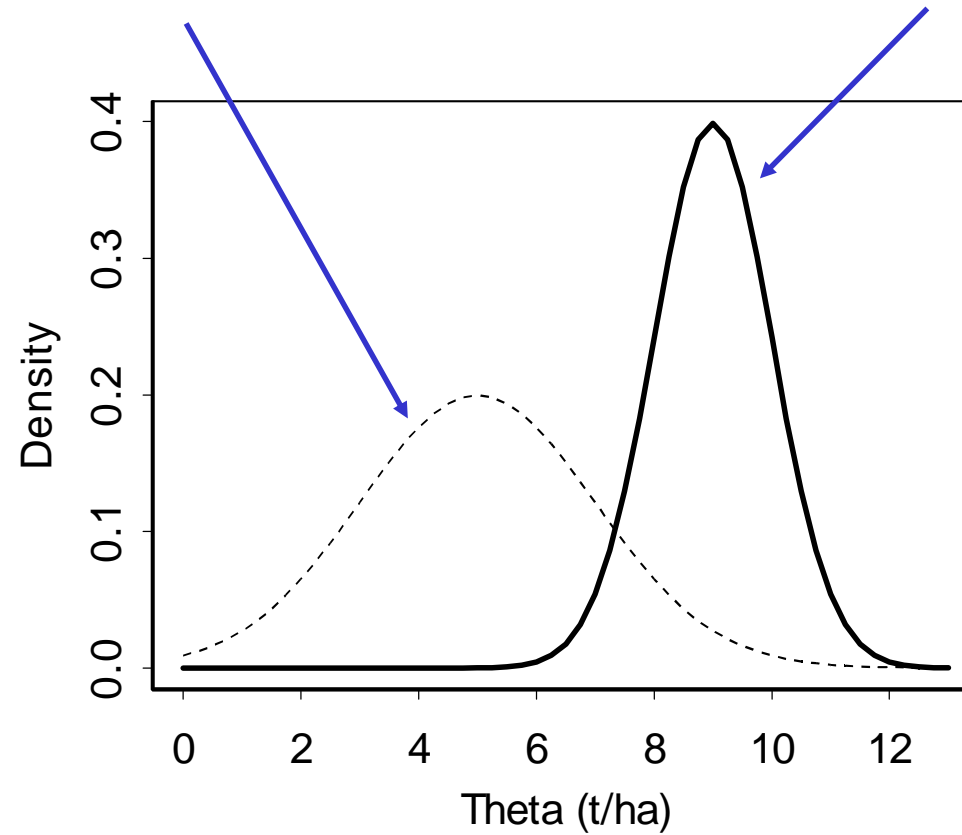
## Maximum likelihood

Likelihood functions are also used by frequentist to implement the *maximum likelihood method*.

The maximum likelihood estimator is the value of  $\theta$  maximizing  $P(y | \theta)$ .

**Prior probability distribution**

**Likelihood function**





## Example (continued)

### Analytical expression of the posterior distribution

$$\theta | y \sim N(\mu_{post}, \tau_{post}^2)$$

$$\mu_{post} = (1 - w) \times \mu + w \times y = 8.2$$

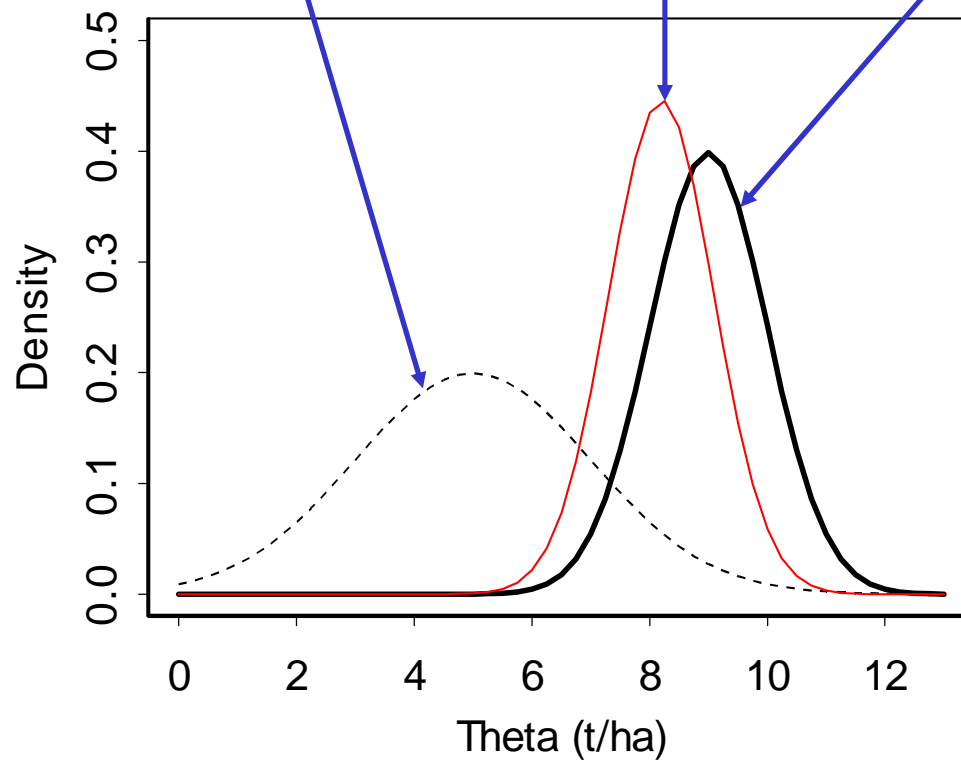
$$\tau_{post}^2 = (1 - w) \times \tau^2 = 0.8$$

$$w = \frac{\tau^2}{\tau^2 + \sigma^2} = \frac{4}{5}$$

**Prior probability distribution**

**Posterior probability distribution**

**Likelihood function**



## Discussion of the posterior distribution

1. Result is a probability **distribution** (posterior distr.)
2. Posterior mean is **intermediate** between prior mean and observation.
3. Weights depend on prior variance and measurement error.
4. Posterior variance is **lower** than both prior variance and measurement error variance.
5. A full distribution was derived from only **one data**

## Frequentist *versus* Bayesian

Bayesian analysis introduces an element of **subjectivity**:  
*the prior distribution.*

But its representation of the uncertainty is **easy** to understand

- the uncertainty is assessed conditionally to the observations,
- the calculations are straightforward when the posterior distribution is known.

## Practical considerations

- The analytical expression of the posterior distribution can be derived for simple applications.
- For complex problems, the posterior distribution must be **approximated**
  - Markov chain Monte Carlo algorithms (MCMC)
  - Importance sampling
- Softwares were recently developed for running MCMC (WinBUGS, JAGS...)

## **Conclusion. Proceed in four steps**

### **1. How many and which parameters should be estimated?**

- In simple models, all parameters.
- In complex models, parameters must be selected.

### **2. What kind of information is available?**

- Data
- Prior information (expert knowledge, literature etc.)

### **3. Which estimation method?**

- Ordinary least squares,
- Weighted/Generalized least squares,
- Bayesian method

### **4. What is the accuracy of the parameter estimator?**

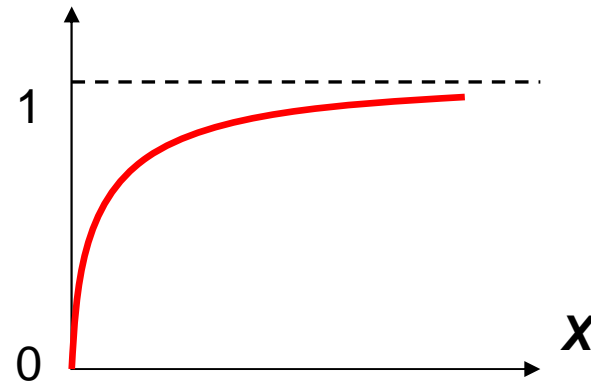
- Theoretical consideration, variances, residuals.

# Exercise

## Estimation of the parameter of a non linear model using a Bayesian method

- Non linear model predicting relative yield as a function of a factor  $x$  (amount of soil mineral N)

$$f(x, \theta) = [1 - \exp(-\theta \times x)]$$



- One parameter  $\theta$ : the growth rate

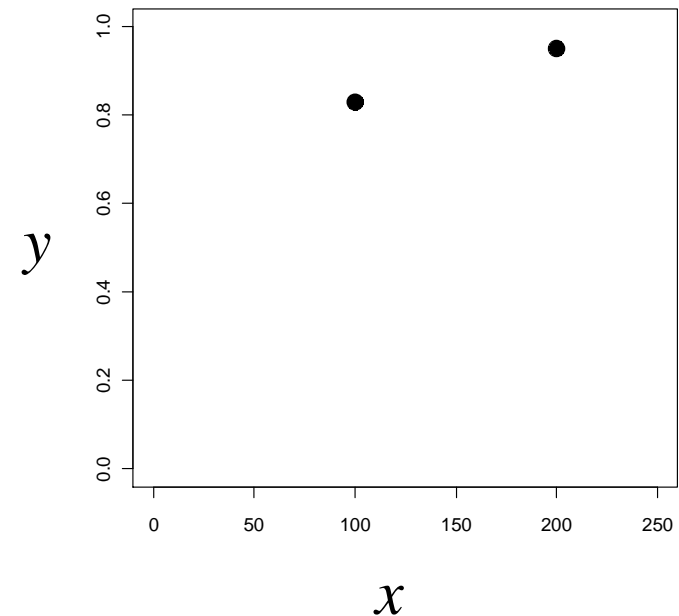


# Data

Two measurements of relative yield  $y_1$  and  $y_2$  are available:

$$y_1 = 0.83 \text{ for } x_1 = 100 \text{ kg/ha}$$

$$y_2 = 0.95 \text{ for } x_2 = 200 \text{ kg/ha}$$



# Questions

- Estimate the parameter by ordinary least squares
- Estimate the parameter by using a Bayesian method

# Ordinary least squares

```
x<-c(100, 200)
```

```
y<-c(0.83, 0.95)
```

```
TAB<-data.frame(x,y)
```

```
x<-c(100, 200)
```

```
y<-c(0.83, 0.95)
```

```
TAB<-data.frame(x,y)
```

```
Fit<-nls(y~1-exp(-Theta*x), data=TAB, start=list(Theta=0.05), trace=T)
```

```
print(summary(Fit))
```

```
> Fit<-nls(y~1-exp(-Theta*x), data=TAB, start=list(Theta=0.05), trace=T)
0.02914996 : 0.05
0.001751208 : 0.01959284
0.001160448 : 0.01897615
0.0005836208 : 0.01810939
0.0003974804 : 0.01732987
0.0003974661 : 0.01733614
0.0003974661 : 0.01733635
```

```
> print(summary(Fit))
```

Formula:  $y \sim 1 - \exp(-\text{Theta} * x)$

Parameters:

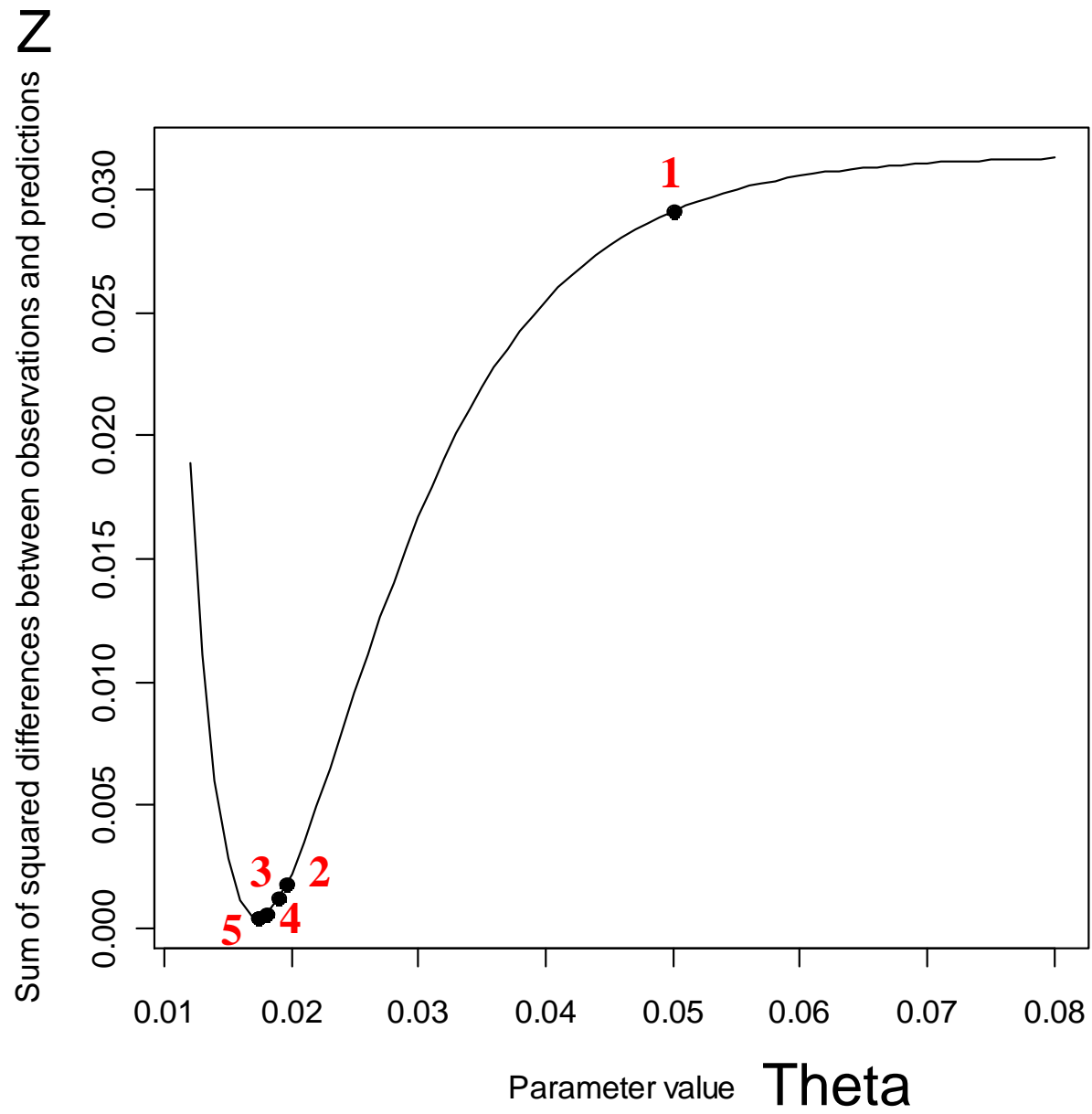
	Estimate	Std. Error	t value	Pr(> t )
Theta	0.017336	0.001064	16.29	0.039 *

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.01994 on 1 degrees of freedom

Number of iterations to convergence: 6



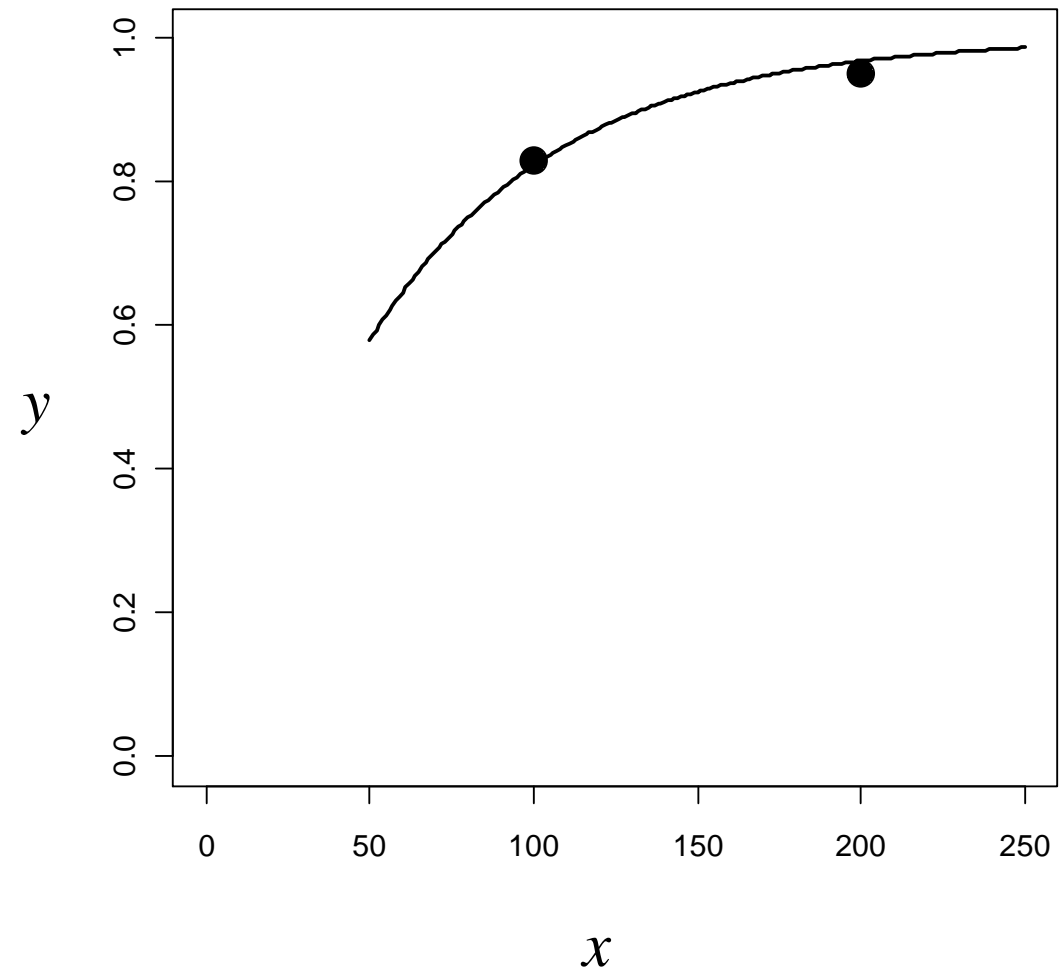
```
X.vec<-50:250
```

```
Y.vec<-1-exp(-coef(Fit)[1]*X.vec)
```

```
plot(x,y, xlim=c(0, 250), pch=19, cex=2, ylim=c(0,1))
```

```
lines(X.vec, Y.vec, lwd=2)
```

$$\hat{\theta} = 0.0173$$





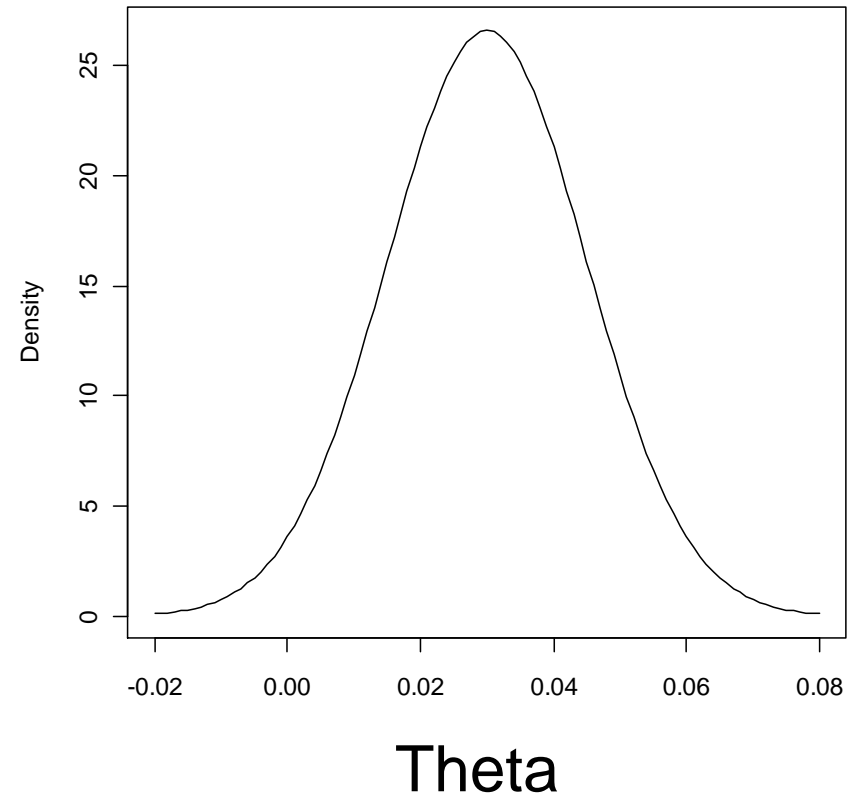
# **A Bayesian approach**

## Prior distribution

Assume that the prior distribution is defined from expert knowledge as:

$$\theta \sim N(\mu, \tau^2)$$

$$\theta \sim N(0.03, 0.015^2)$$



## Data

- Two measurements of relative yield  $y_1$  and  $y_2$  are available:

$$y_1 = 0.83 \text{ for } x_1 = 100 \text{ kg/ha,}$$

$$y_2 = 0.95 \text{ for } x_2 = 200 \text{ kg/ha.}$$

# Statistical model

The statistical model is defined as

$$y = f(x, \theta) + \varepsilon$$

$$\varepsilon \sim N(0, \sigma^2)$$

with independence between the two values of  $\varepsilon$

# Likelihood

$$P(y_1, y_2 | \theta) = P(y_1 | \theta) \times P(y_2 | \theta)$$

$$\begin{aligned} &= \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{[y_1 - f(x, \theta)]^2}{2\sigma^2}\right\} \times \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{[y_2 - f(x, \theta)]^2}{2\sigma^2}\right\} \\ &= \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{[y_1 - (1 - \exp(-\theta \times x_1))]^2}{2\sigma^2}\right\} \times \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{[y_2 - (1 - \exp(-\theta \times x_2))]^2}{2\sigma^2}\right\} \end{aligned}$$

**We assume that  $\sigma$  is known and equal to 0.02.**

# Importance sampling

**Step 0:** Use the prior distribution as the proposal distribution.

$$g(\theta) = N(0.03, 0.015^2).$$

**Step 1:** Generate  $N$  parameter values  $\theta_1, \theta_2, \dots, \theta_N$ .

**Step 2:** Calculate a « weight » for each parameter value  $w_1, w_2, \dots, w_N$ .

The weight is equal to the likelihood value,  $w_i = P(y_1 | \theta_i) \times P(y_2 | \theta_i)$

$$w_i = \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{[Y_1 - (1 - \exp(-\theta_i \times X_1))]^2}{2\sigma^2}\right\} \times \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{[Y_2 - (1 - \exp(-\theta_i \times X_2))]^2}{2\sigma^2}\right\}$$

**Step 3:** Calculate normalized weights  $w_1^*, \dots, w_N^*$ .

$$w_i^* = \frac{w_i}{\sum_{i=1}^N w_i}$$

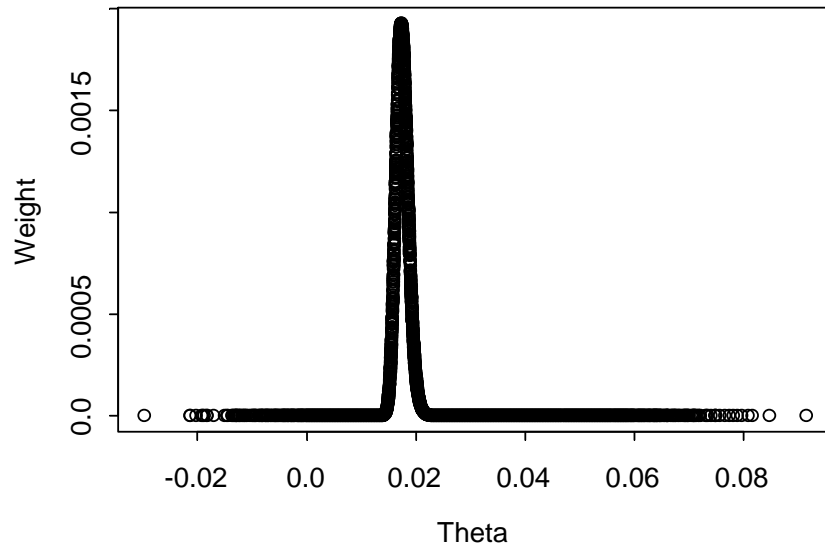
**Step 4:** Use the sample of parameter values and the normalized weights to approximate the posterior distribution.

# Implementation

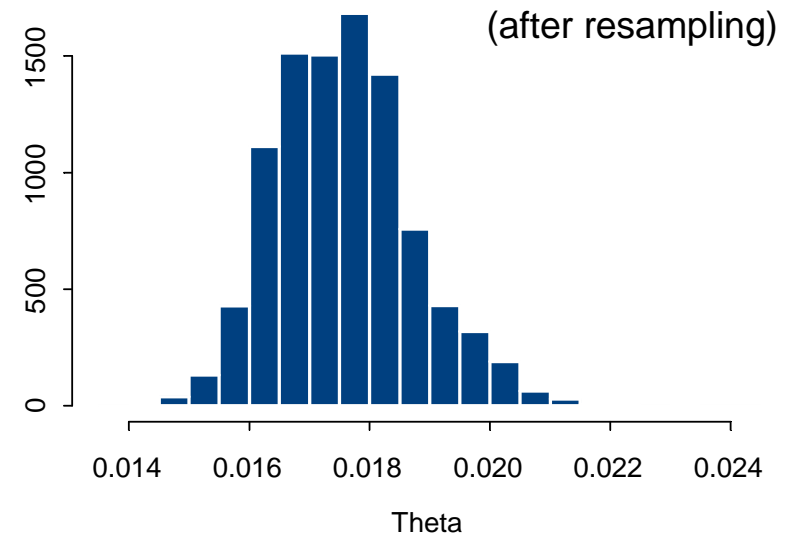
- The algorithm is implemented with the R function ISgrowth.txt.
- You can run it yourself and modify it for other models

# Results obtained with $N=10000$

Plot of normalized weights



Parameter values drawn from posterior



**Estimated posterior mean: 0.0176**

**Estimated posterior standard deviation:  $1.17 \cdot 10^{-3}$**



## Which value for $N$ ?

- The algorithm is run five times (with different seeds) for two different  $N$  values:

$N=100$

$N=10000$

- The posterior mean and posterior variance are computed after each run.
- The stability of the result is analyzed.

## How many simulations ?

N	Run	Posterior mean	Posterior standard deviation
100	1	0.0178	9.99E-04
100	2	0.0173	9.48E-04
100	3	0.0173	1.10E-03
100	4	0.0176	1.04E-03
100	5	0.0176	9.91E-04
10000	1	0.0176	1.17E-03
10000	2	0.0176	1.14E-03
10000	3	0.0176	1.17E-03
10000	4	0.0176	1.14E-03
10000	5	0.0176	1.14E-03

**The estimation of the posterior mean is very accurate with  $N=10000$ .**