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## Uncertainty

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# UNCERTAINTY

**Master Class 2020 – LGC**

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# UNCERTAINTY



*"The only certainty is uncertainty"*

~ Pliny the Elder (AD 23/24 – 79)

"Gaius Plinius Secundus (AD 23/24–79), called Pliny the Elder (/ˈplɪni/), was a Roman author, **a naturalist** and natural philosopher, a naval and army commander of the early Roman Empire, and a friend of emperor Vespasian. He wrote the encyclopedic *Naturalis Historia* (Natural History), which became an editorial model for encyclopedias. He spent most of his spare time **studying, writing, and investigating natural and geographic phenomena** in the field." (Quoted source: Wikipedia)

# UNCERTAINTY

## A fact of nature

**Field observations, i.e. "real data" are uncertain, always !**

Scientists and engineers use real data in order to derive working solutions to real-world problems. Uncertainties are therefore inevitable in science and engineering.

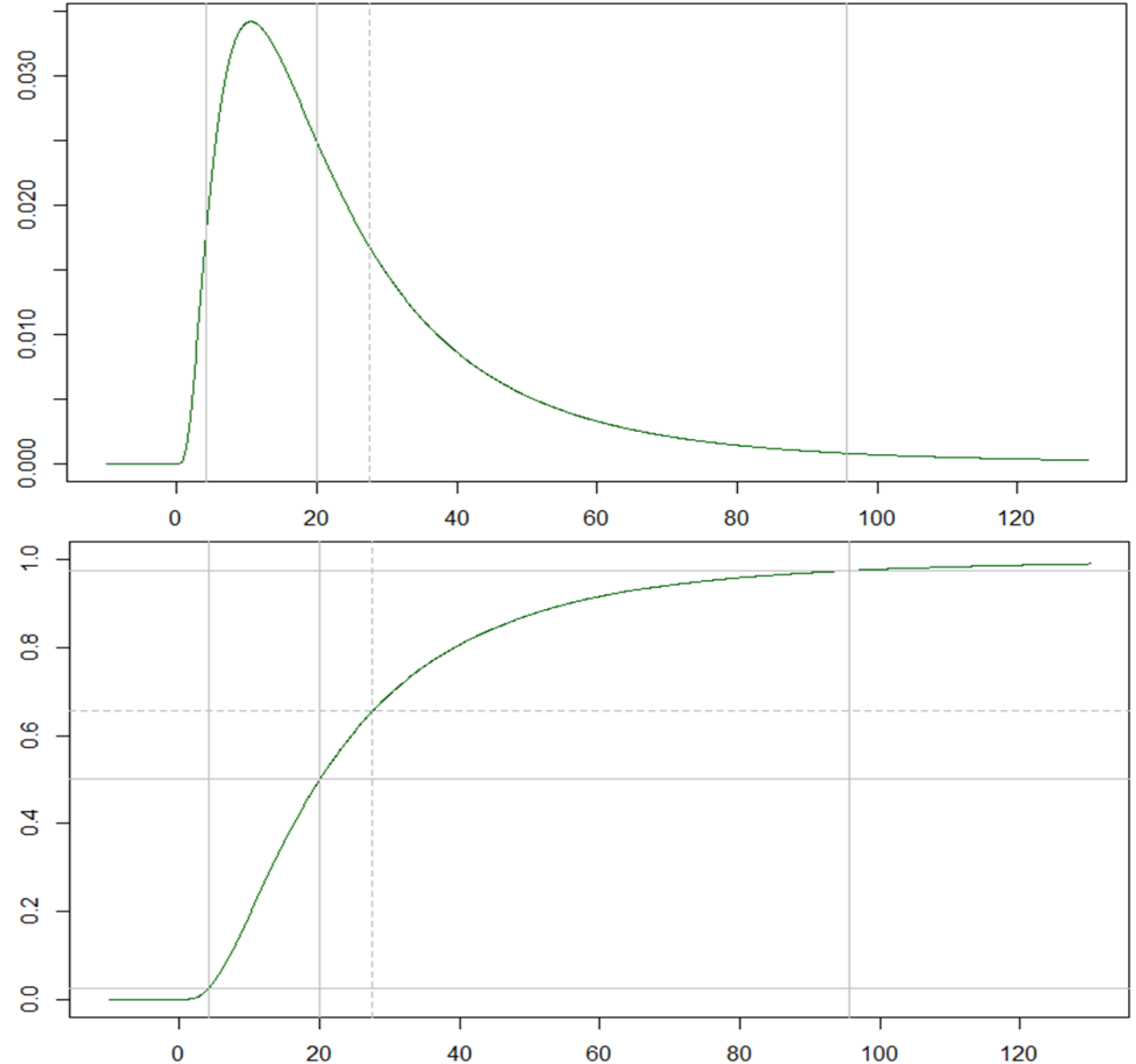
**No real data should be trusted nor reported without error bars !**

Real data can be abstracted as random variables (r.v.), which are characterized fully by probability distribution functions.

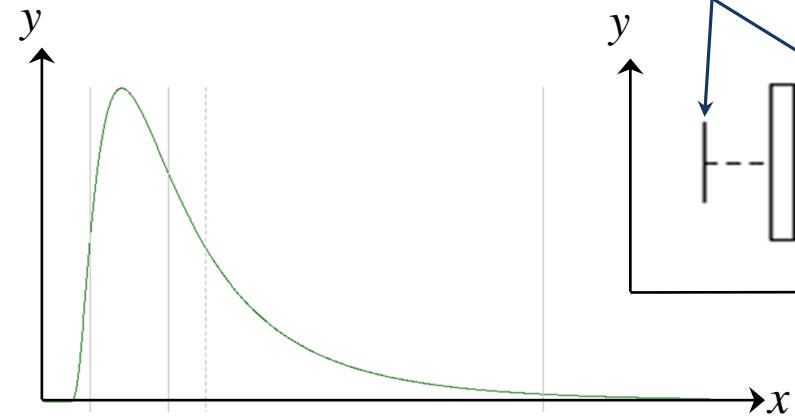
Once a probability distribution function is assigned to a variable of interest, all is known about the said variable.

**Error bars are estimated from the r.v.'s probability distribution function**

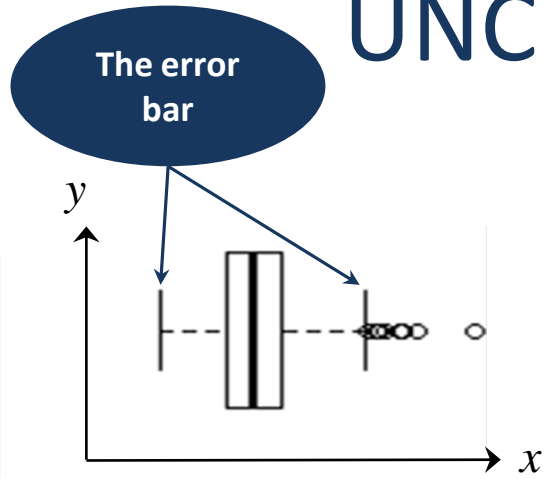
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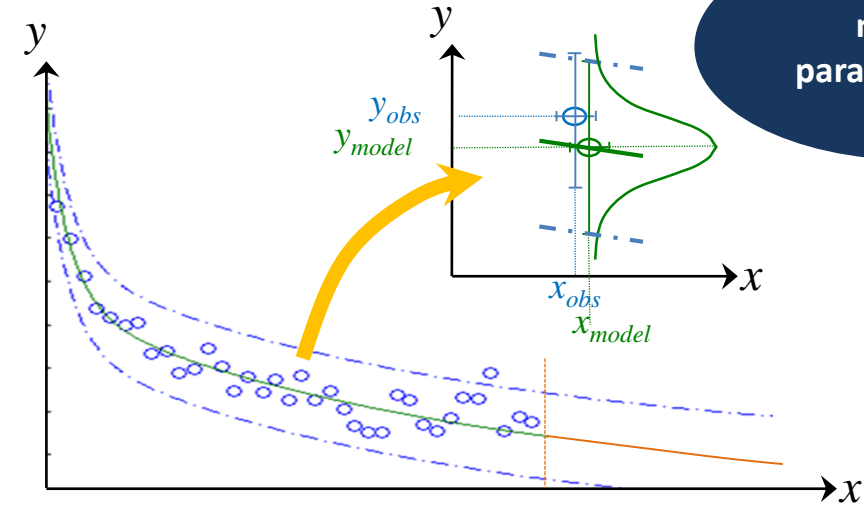
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An observation

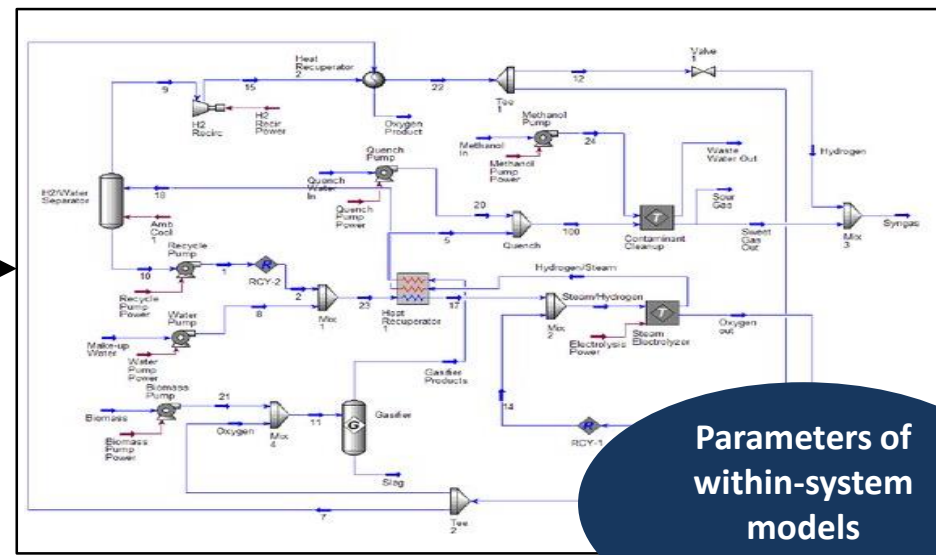
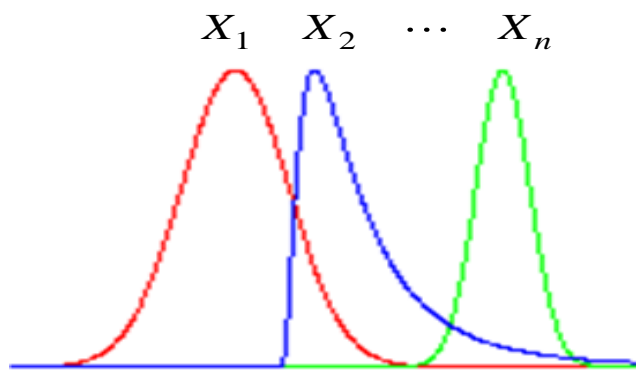


The error bar



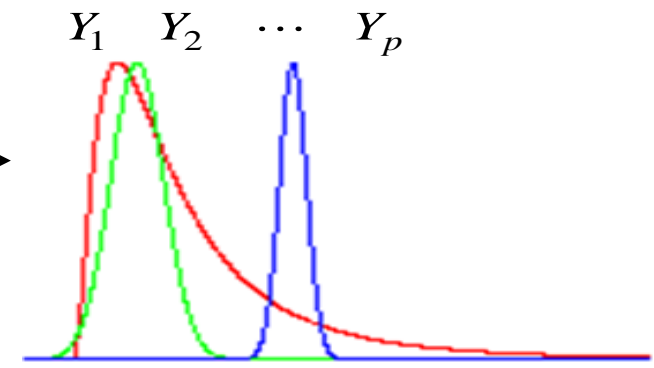
A model

Estimated models parameters are r.v.



A system

Parameters of within-system models are often r.v.



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## Computational statistics

- **Computational statistics** merges statistics with numerical methods.
- Computational statistics' methods and tools make analysis and manipulation of statistical data possible without mastering the (elitist) art of formal statistical (paper-and-pencil) derivations, i.e. without a formal mathematician training in statistics (up to a point...).
- Statistical analyses and calculations can now be performed using dedicated and easily accessible computing tools.
- Such tools offer powerful capabilities for visualizing statistical data and results. "Graphical statistics" makes statistical concepts (distribution functions, confidence intervals, inference testing,...) easier to understand.

### **Draw your statistics !**

- That said, it remains essential to understand statistical concepts in order to make a sound use of computational statistics and carry out quality analysis of real data.

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## Computational statistics tools



- Primary function : statistical data manipulation, analysis, modelling and visualisation
- Now a full-fledged scientific computing tool
- Free, all platforms (<https://www.r-project.org/>)
- Large and growing community of users and developers (<https://www.r-bloggers.com/>) and a myriad of dedicated self-learning websites and textbooks.

- Recommended GUI : RStudio (<http://www.rstudio.com/>)



- Interactive web applications with Shiny (<https://shiny.rstudio.com/>)



- Notebooks

- MExcel<sup>®</sup> interoperability with BERT (<https://oatao.univ-toulouse.fr/24353/>)



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## An unworthy illustrative example

$$\text{model: } Y = 48 \frac{X_1 X_2 X_3}{X_4 X_5}$$

i	$X_i$ (obs.)	$\Delta X_i$
1	0.5	0.001
2	0.05	0.0002
3	5.5	0.28
4	0.0544	0.0005
5	18.7	0.28

$$\Rightarrow Y = 6.49 \pm \Delta Y$$

## Monte-Carlo solution

- Hyp. :  $X_i$ 's are normally distributed
- Hyp. :  $\Delta X_i$ 's are given at the 99.73% confidence level
- Monte-Carlo simulation:
  - Select a sample size, say  $n = 10^6$
  - Generate  $n$  sets  $[X_1, \dots, X_5]$  by random sampling
  - Calculate  $n$  values of  $Y$  using the model equation
  - Analyse the statistics of the  $n \times Y$  values

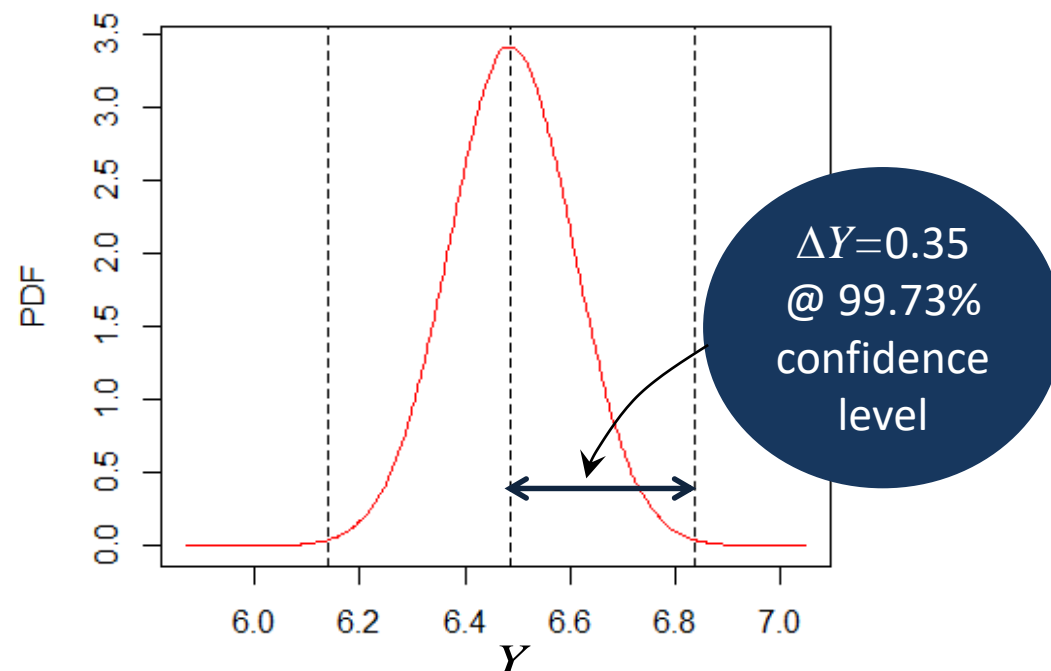


## Paper-and-pencil solution

- By propagation of variance (simple derivation, but derivation nonetheless, just making a point here...)

$$\Delta Y = Y \sqrt{\sum_{i=1}^5 \left( \frac{\Delta X_i}{X_i} \right)^2} = 0.35$$

- Is this derivation correct? Are there underlying assumptions? Is there a confidence associated?



## An unworthy illustrative example

$$\text{model: } Y = 48 \frac{X_1 X_2 X_3}{X_4 X_5}$$

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- Is this derivation correct? What are the underlying assumptions? Is there a confidence associated?

```

library(mvtnorm)
meanX<-c(0.5,0.05,5.5,0.0544,18.7) #  $X_i$ 
deltaX<-c(1e-3,2e-4,2.8e-1,5e-4,2.8e-1) #  $\Delta X_i$ 
n<-1e6 # Monte-Carlo sample size
prob<-0.9973 # Confidence associated with  $\Delta X$ 
varX<-diag((deltaX/qnorm(1-(1-prob)/2))^2) #  $X \sim \text{Normal}$ 
Xsim<-rmvnorm(n,mu=X,sigma=varX) # generate  $n \times [X_1, \dots, X_5]$ 
Ysim<-48*Xsim[,1]*Xsim[,2]*Xsim[,3]/(Xsim[,4]*Xsim[,5]) # generate  $n \times Y$ 
q <- quantile(ecdf(Ysim), probs=c((1- prob)/2,1-(1- prob)/2)) # quantiles
Ysimpdf <- density(Ysim) # PDF
print(paste("deltaY=",q[2]-mean(Ysim)))
plot(Ysimpdf$x, Ysimpdf$y, type="l", col="red", ylab="PDF", xlab="Y")
abline(v=c(mean(Ysim), q), lty="dashed")
    
```

⇒

Sensitivity analysis of hypotheses

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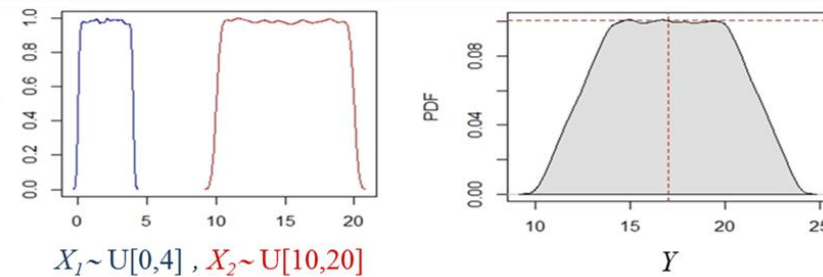
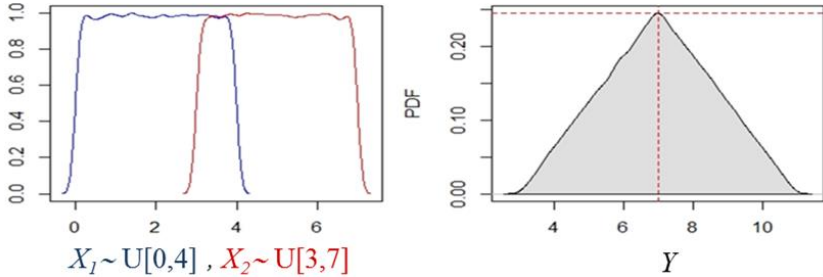
## A worthier illustrative example

$X_1$  and  $X_2$  are uniform random variables.

What is the uncertainty  $\Delta Y$  of  $Y = X_1 + X_2$  ?

What is the distribution of  $Y$  ?

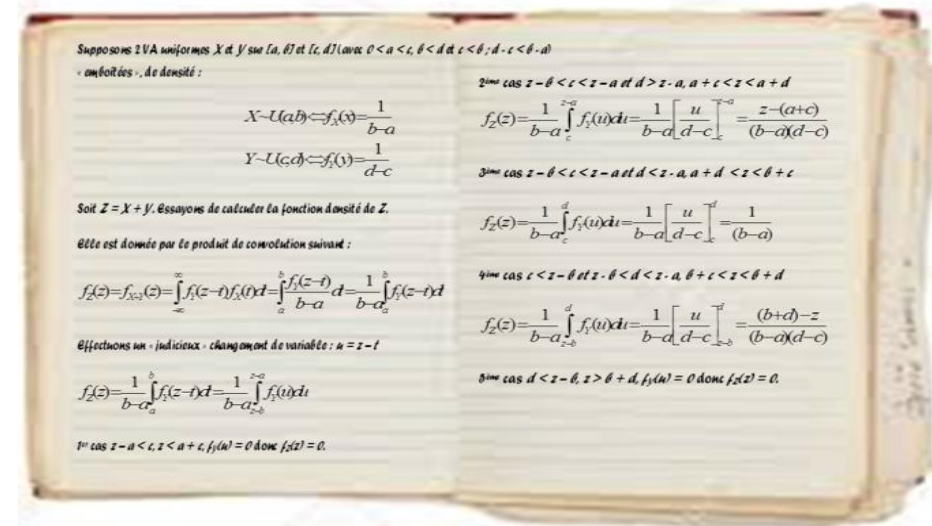
### Monte-Carlo solution



Quantiles, uncertainties and distribution function parameters can be estimated numerically from a **Monte-Carlo sample**. Here, trapezoid[10,13,22,24].

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### Paper-and-pencil solution



- Let us now consider the situation where the r.v. have different distributions? What would the uncertainty  $\Delta Y$  be in this case ? The distribution of  $Y$  ?

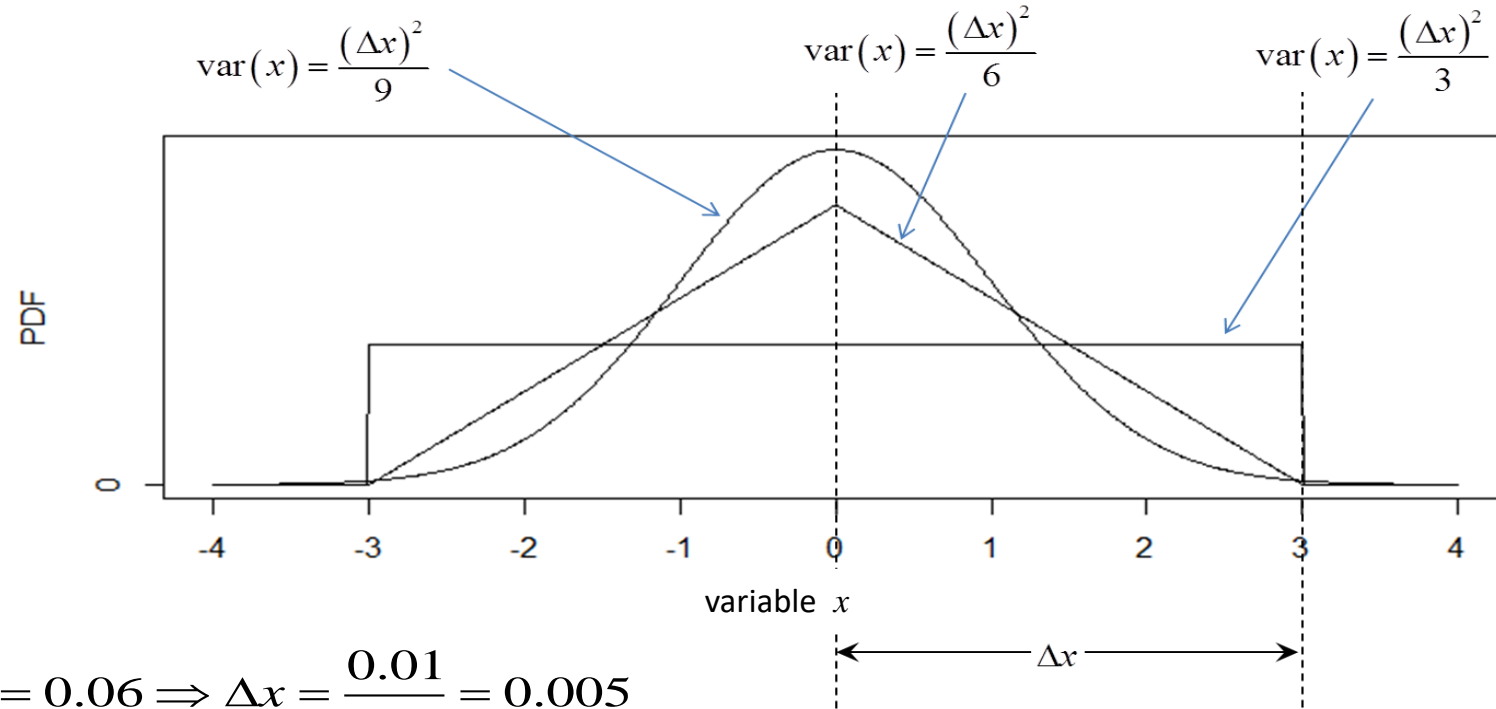
$$\text{model: } Y = 48 \frac{X_1 X_2 X_3}{X_4 X_5}$$

**Which pathway would you rather walk ?**

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## Standards

**Ref. : Guide for Uncertainty Measurement (norme ISO GUM) / Guide pour l'expression de l'incertitude de mesure - Annex F: Practical guidance on evaluating uncertainty components. (2008 versions: [EN](#) / [FR](#))**



- Significant figures :  $x = 0.06 \Rightarrow \Delta x = \frac{0.01}{2} = 0.005$

- A prudent solution when one does not know the statistical distribution from which an observation is drawn is to use the triangular isosceles distribution.

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## Generation of correlated random variables

Model parameters are always correlated !

- Their correlation comes from the model equation itself.

$$\text{Example: } \hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{\beta}_2 X^2$$

- Model parameters are correlated through a **variance-covariance matrix**

- Taking the correlation of model parameters into account, with their variance-covariance matrix, is critical when using a model in a **sensitivity analysis**.

- Example shows the output of a **Monte-Carlo simulation** (sample size = 10,000 ) for 3 normally distributed r.v., with and without correlation.

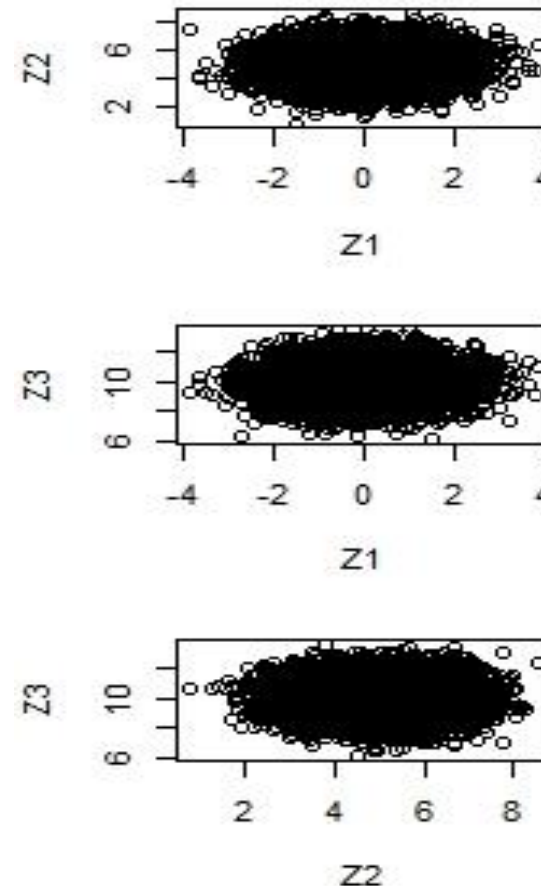
$$X_1 \sim N(0, \sqrt{3}); X_2 \sim N(5, \sqrt{2}); X_3 \sim N(10, 1)$$

- This can be done with any type of r.v.

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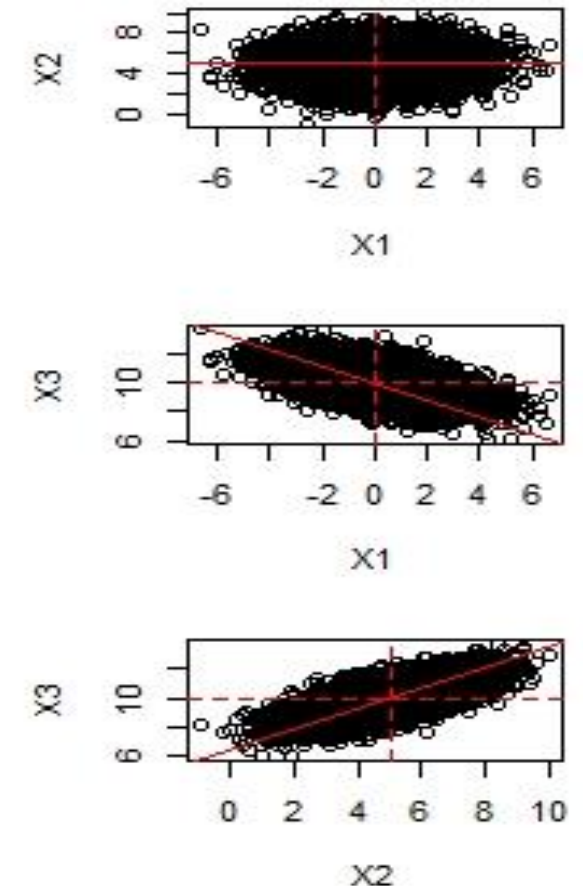
Uncorrelated r.v.

$$\Sigma = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



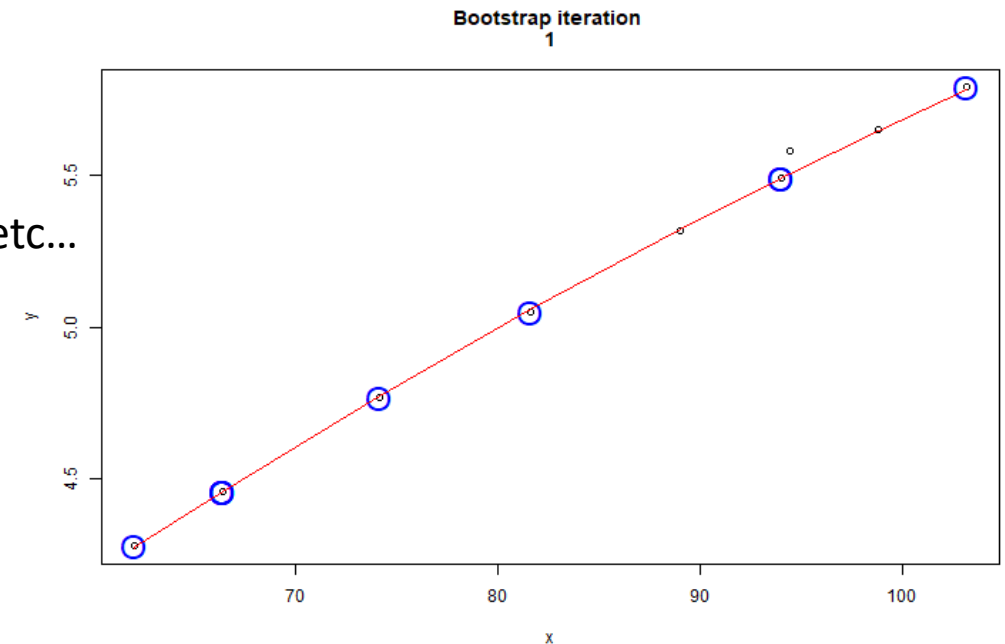
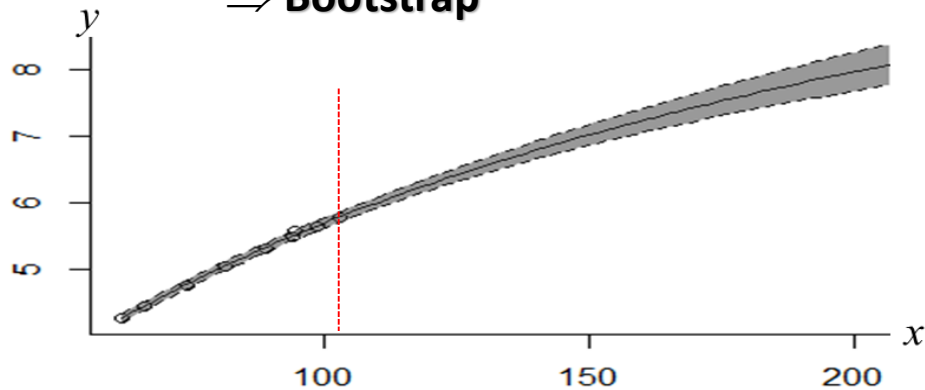
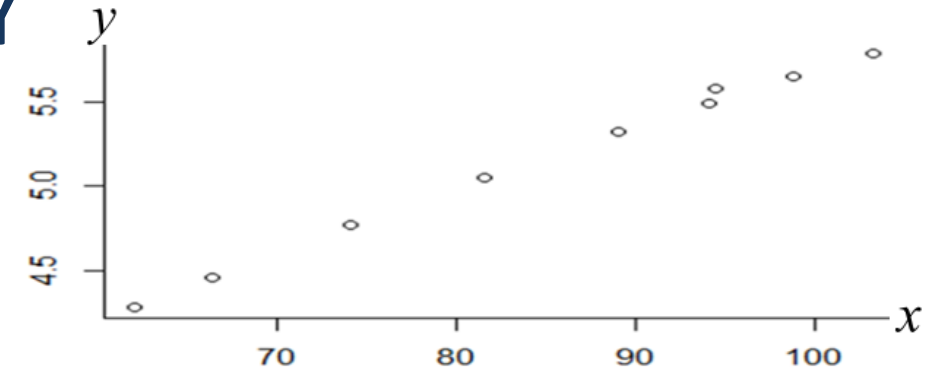
Correlated r.v.

$$\Sigma = \begin{pmatrix} 3 & 0 & -1 \\ 0 & 2 & 1 \\ -1 & 1 & 1 \end{pmatrix}$$



# UNCERTAINTY

- **One set** of observations  $(x,y)$
- Consider the simplest of cases, i.e. independent identically distributed (i.i.d.) Normal r.v.  $\Rightarrow$  estimation of model parameters (expected values and uncertainties) and model confidence/prediction intervals by least-squares estimation.
  - Linear models with errors in  $Y$  only  
 $\Rightarrow$  analytical solutions exist
  - Linear models with errors in  $X$  and  $Y$ , non-linear models  
 $\Rightarrow$  numerical solutions only
    - $\Rightarrow$  Levenberg-Marquardt, Simulated annealing, etc...
    - $\Rightarrow$  **Bootstrap**



- Broad applicability of the **bootstrap method** to estimation problems in engineering systems' analysis

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# UNCERTAINTY

## Wrap-up

- Uncertainty is a fact of life, and uncertainties are inevitable in science and engineering.
- Computational statistics brings analysis of real data at your fingertips, **with uncertainties !**
- **Today's keywords** : Uncertainty; Random variable; Probability distribution function; Monte-Carlo method; Sensitivity analysis; Bootstrap; Variance-covariance matrix; Computational statistics; **R**

## Last words

- **Quality data are priceless !**
- With data analysis, and particularly with computational statistics, **take nothing for granted !** Always question hypotheses and test them.
- **Outliers are your worst foes !**
  - Detection of outliers / Sampling, data collection and manipulation
- **Small number of observations (sample size)**

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