# Atelier du GDR MASCOT NUM

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# Dealing with stochastics in optimization problems

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## Introduction

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## The deterministic world

- Mono-objectif constraint optimization
- Multi-objective constraint optimization

## The stochastic world

- What is stochastic ?
- Stochastic Problems
- Stochastic methods

# Mono-objectif constraint optimization

$$\begin{cases} \min_{\boldsymbol{x} \in \mathbb{R}^d} f(x) \\ h_j(\boldsymbol{x}) = 0 \quad j = 1, ..., K_E \\ g_j(\boldsymbol{x}) \leq 0 \quad j = 1, ..., K_I \end{cases}$$

**Goal :**

- Find a feasible point that minimizes the objectif function

**Constraint :**

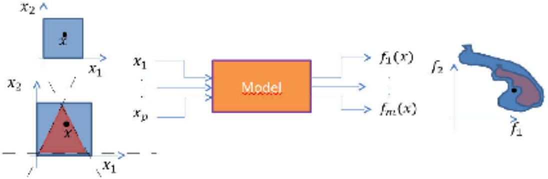
- The objectif function and the constraints are potentially expensive in CPU time to evaluate.

**Examples :**

- Optimal design of a wing with stability constraints
- Placement of a new well in an oil reservoir
- Prediction of extreme scenarios in an oil reservoir

# Multi-objectif optimization

- Consider a numerical simulator taking $d$ scalar input variables and giving $m$ scalar outputs.




**Aim** : Find the input $x$ which leads to the best "compromise" between the outputs

**Constraint** : the objectives functions and the constraints are potentially expensive in CPU time (so we have a limited evaluation budget).

**Examples** : risk and profitability in portfolio management, stiffness and weight in conception, speed and cost in transport, management of software dependencies

# The Multi-Objectif problem

Given

$$(f_i)_{i=1\ldots m} \ m \text{ real scalar functions}$$

gathered in the vector

$$F(\boldsymbol{x}) = (f_1(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x}))$$

Our goal is to minimize

$$\begin{cases} \min\limits_{\boldsymbol{x}\in\mathbb{R}^d} F(\boldsymbol{x}) & \\ h_j(\boldsymbol{x}) = 0 & j = 1, \ldots, K_E \\ g_j(\boldsymbol{x}) \leq 0 & j = 1, \ldots, K_I \end{cases}$$

# But we are not omnipotent/omniscient


Errors occur.

Measurement error can lead to unpredicted behaviours.

# But we are not omnipotent/omniscient

Uncertainties appear at different stages of the optimization problem

**Causes**

- **EPISTEMIC** : **lack of knowledge**, **imprecise** measurements of the model **inputs** or/and **outputs**, modelization error, numerical error ...
- **ALEATORY** : intrinsic to the physics involved, **stochastic codes** ...
- **METHODOLOGICAL CHOICE** : introduction of a probabilistic framework in the resolution method. A way to model our lack of knowledge of the solution and **build a (random) sequence we expect to converge to the solution.**

# Kind of classification

- Non-Stochastic problem + Stochastic method
- Stochastic problem + Non-Stochastic method
- Stochastic problem + Stochastic method
- Non-Stochastic problem + Non-Stochastic method
  $\rightarrow$ deterministic world

# Stochastic problem : introducing uncertainties

Uncertainties appear on the objectif function or/and the constraints

$$\begin{cases} f(\boldsymbol{x}) \\ F(\boldsymbol{x}) \\ g_j(\boldsymbol{x}) \\ h_j(\boldsymbol{x}) \end{cases} \rightarrow \begin{cases} f(\boldsymbol{x}, \boldsymbol{U}) \\ F(\boldsymbol{x}, \boldsymbol{U}) \\ g_j(\boldsymbol{x}, \boldsymbol{U}) \\ h_j(\boldsymbol{x}, \boldsymbol{U}) \end{cases}$$

For example

$$f(\boldsymbol{x} + \boldsymbol{U_{in}}) + \boldsymbol{U}_{out},$$

$$g_j(\boldsymbol{x} + \boldsymbol{U}_{in}) + \boldsymbol{U}_{out},$$

$$h_j(\boldsymbol{x} + \boldsymbol{U}_{in}) + \boldsymbol{U}_{out}$$

**Approach** : find the **best** deterministic world approaching our stochastic world : use the adequate operator.

$$L_1 f(\boldsymbol{x}, \boldsymbol{U}) = \tilde{f}(\boldsymbol{x}), \qquad L_2 g_j(\boldsymbol{x}, \boldsymbol{U}) = \tilde{g}_j(\boldsymbol{x}), \ldots$$

and use your favorite/adapted deterministic optimization method

# Summarizing the distribution

**Approach** : find the **best** deterministic world approaching our stochastic world

$$Lf(\boldsymbol{x}, \boldsymbol{U}) = \tilde{f}(\boldsymbol{x}), \ldots$$

and use your favorite/adapted deterministic optimization method

- What is the "best" ?
- It depends on the question
- 

$$\mathbb{E}(f(\boldsymbol{x}, \boldsymbol{U})), \qquad \mathbb{E}(g_j(\boldsymbol{x}, \boldsymbol{U}))$$

$$\mathbb{E}(f(\boldsymbol{x}, \boldsymbol{U})) \pm 2\sqrt{Var(f(\boldsymbol{x}, \boldsymbol{U}))},$$

$$\mathbb{P}(f(\boldsymbol{x}, \boldsymbol{U}) > s)$$

$$s - \mathbb{P}(g_j(\boldsymbol{x}, \boldsymbol{U}) < 0) < 0$$

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- It depends on the question

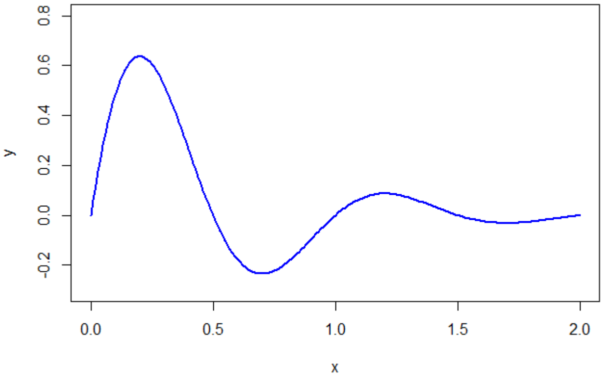
**Scenario approach**

$$\frac{1}{N}\sum_{i=1}^{N} f(\boldsymbol{x}, \boldsymbol{U}_i), \qquad \frac{1}{N}\sum_{i=1}^{N} g_j(\boldsymbol{x}, \boldsymbol{U}_i)$$

$$\max_{i=1,\ldots,N} g_j(\boldsymbol{x}, \boldsymbol{U}_i) < 0 \ldots$$

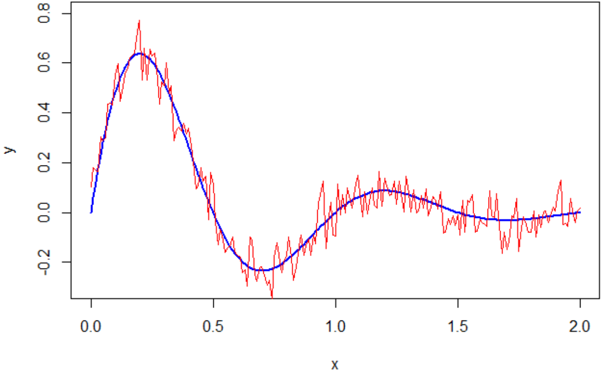
# Illustration

$$f(x) = sin(2\pi x)e^{-2x}$$



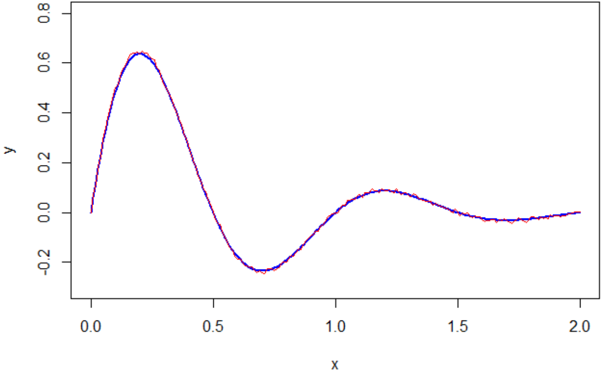
# Illustration : noisy output model

$$f(x,U) = sin(2\pi x)e^{-2x} + U \qquad U \sim \mathcal{N}(0,\sigma^2)$$



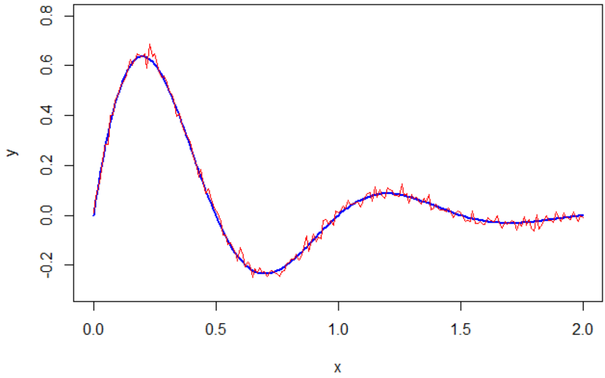
# Illustration : mean of noisy ouput model

$$\mathbb{E}(f(x,U)) = sin(2\pi x)e^{-2x} \qquad U \sim \mathcal{N}(0,\sigma^2)$$



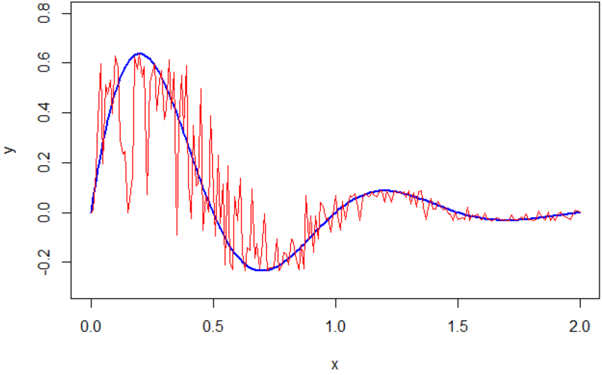
# Illustration : estimated mean of noisy output model

$$\frac{1}{N}\sum_{i=1}^{N} f(x, U_i) \qquad U_i \sim \mathcal{N}(0, \sigma^2) \qquad N \text{ small}$$



# Illustration : noisy input model

$$f(x, U) = sin(2\pi(x + U))e^{-2(x+U)} \qquad U \sim \mathcal{N}(0, \sigma^2)$$



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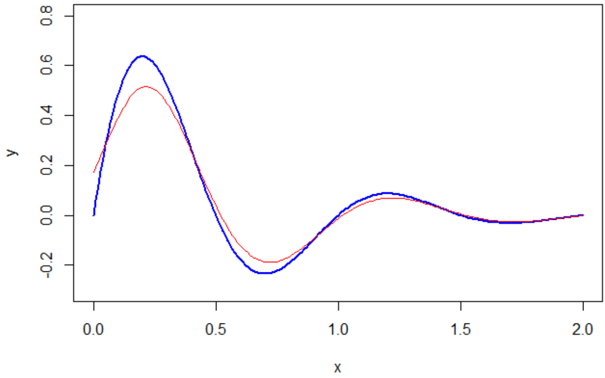

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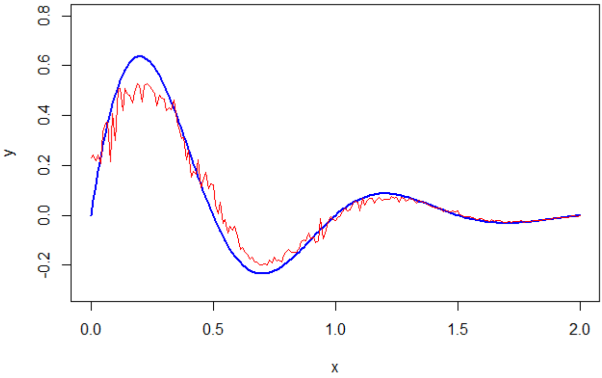
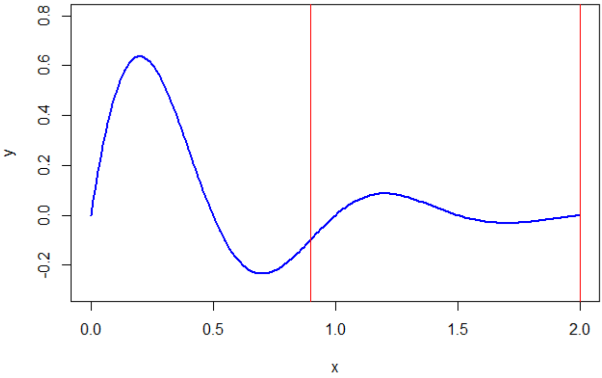


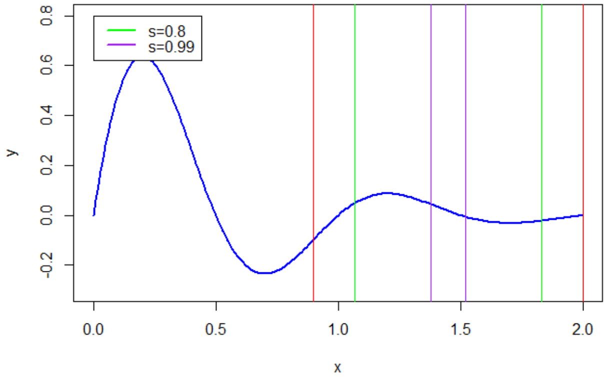
# Illustration : deterministic constraint

$$a < x < b$$



# Illustration : chance constraint

$$\mathbb{P}\big(a < x + U < b\big) > s \qquad U \sim \mathcal{N}(0, \sigma^2)$$

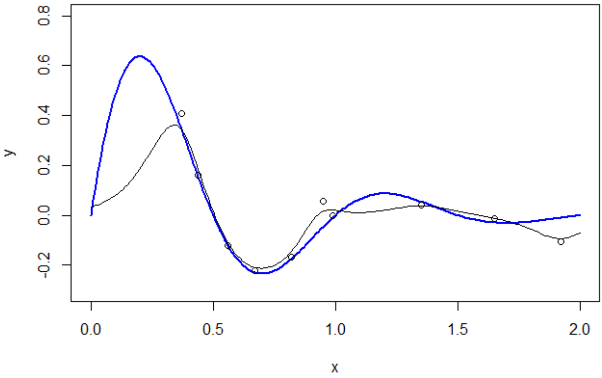


# Stochastic methods I

## Kriging approach

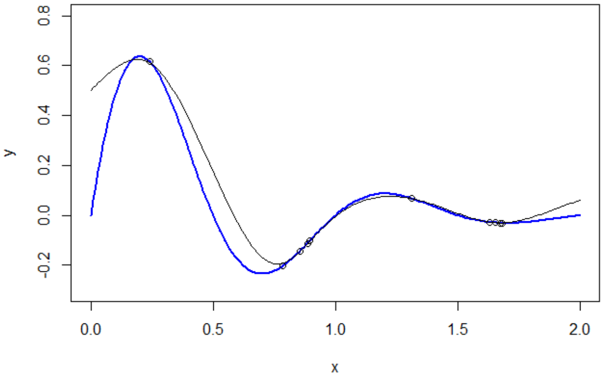
- Consider $x \to f(\boldsymbol{x})$, $(\boldsymbol{x}, \boldsymbol{u}) \to f(\boldsymbol{x}, \boldsymbol{u})$ or $\boldsymbol{x} \to Lf(\boldsymbol{x}, \boldsymbol{U})$ and suppose it is the realisation of a **prior gaussian random process** $Y(\boldsymbol{x}), \ldots$
- sample your function $Y_1, \ldots, Y_N$
- Learn the distribution of the posterior conditional random process $Y(\boldsymbol{x})|Y_1, \ldots, Y_N$
- Use an adequate **summary of the posterior distribution** to find the next best point : **reducing uncertainty or/and converging towards the minimum. Evaluate. Iterate**

## Noisy output



# Stochastic methods I

## Noisy Input



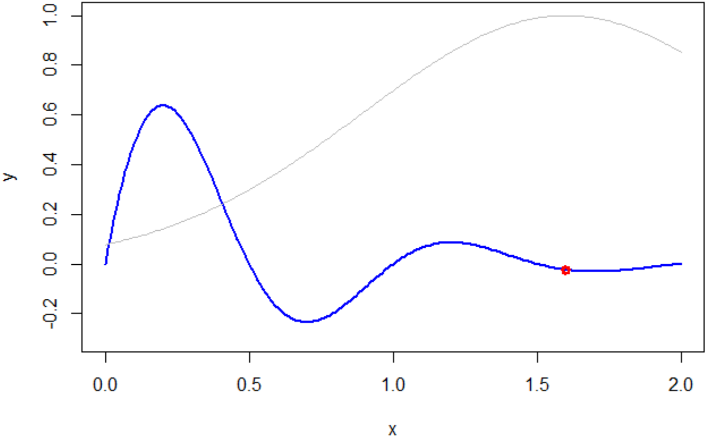
# Stochastic methods II

## Evolutionary approach

- Generate **initial** population ;
- **Select** a part of the population
- **Reproduce** the selected individuals
- **Mutate** the new borns
- **Check** improvement
- **Replace** initial population by new one

# Stochastic methods II

## Evolutionary approach



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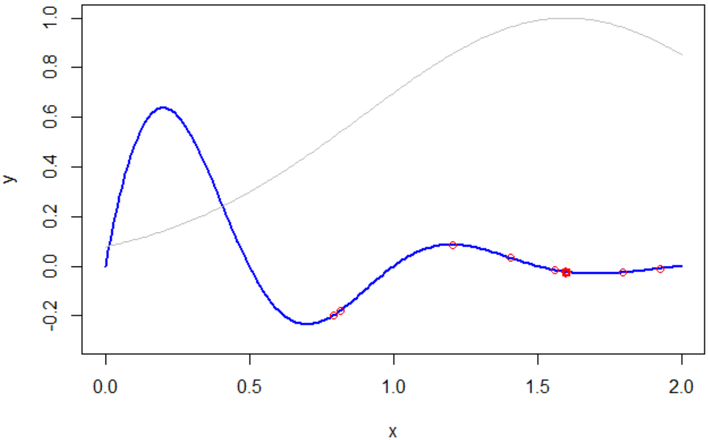

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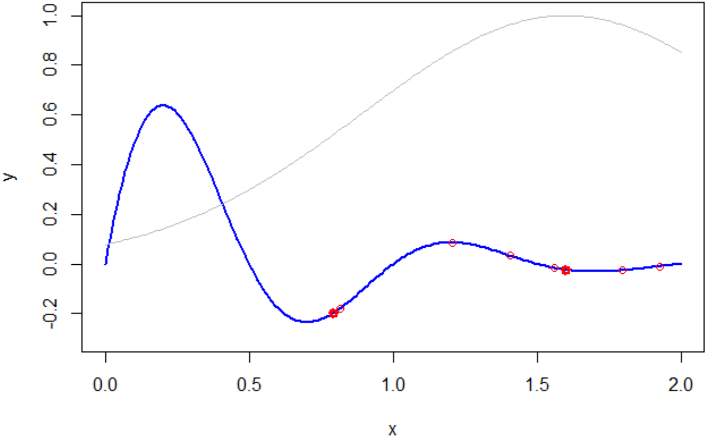

# Stochastic methods II

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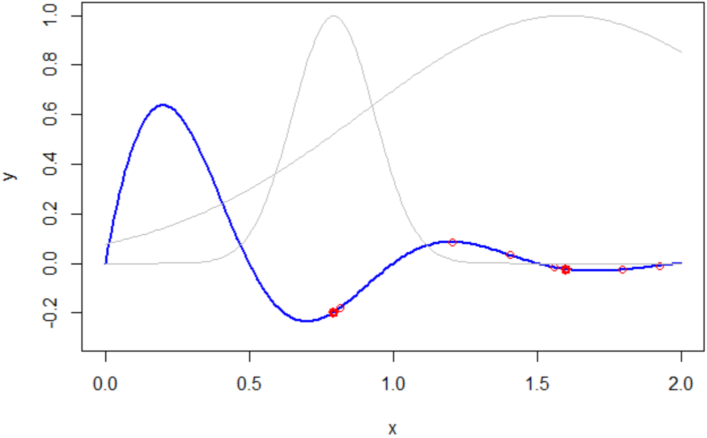
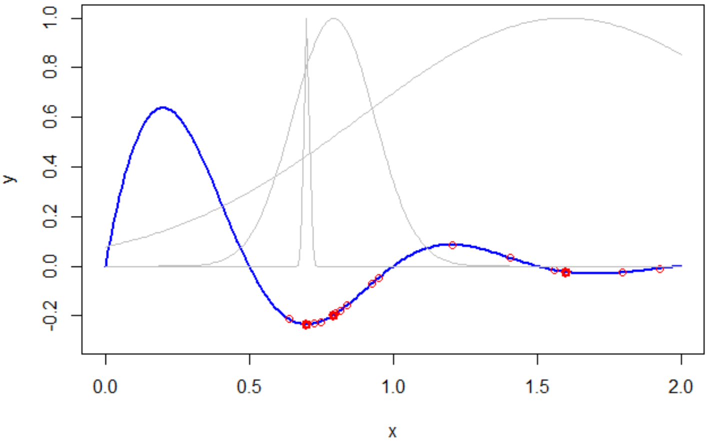


**Evolutionary approach**



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