# (Meta)Modeling with Gaussian processes: An overview

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50èmes journées de statistique

# Outline

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# Metamodeling – Computer experiments

**design**

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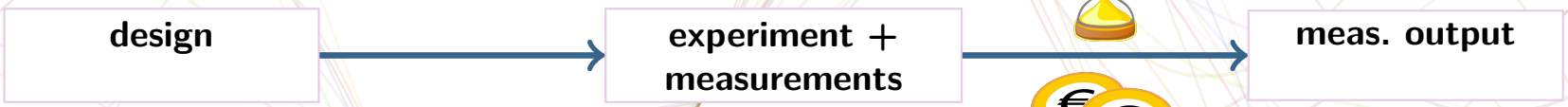
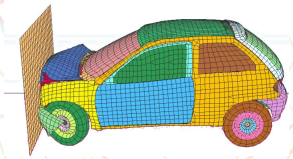


# Metamodeling – Computer experiments



**design**

**experiment + measurements**

**meas. output**

**simulator inputs**
$\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n$

**simulator**
*physical model, numerical methods*

**simulator output**
$f_{\text{sim}}(\mathbf{x}^1), f_{\text{sim}}(\mathbf{x}^2), \ldots, f_{\text{sim}}(\mathbf{x}^n)$

# Metamodeling – Computer experiments

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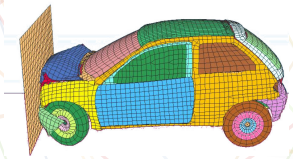

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**metamodel inputs** $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n$ → **metamodel** $y = \mathbf{g}(\mathbf{x})^\top \beta + Z(\mathbf{x})$ → **metamodel output** $\widehat{y}(\mathbf{x}), \ldots$

# Metamodeling – Computer experiments

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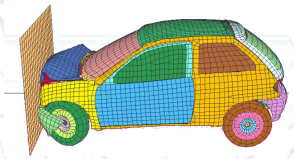
**experiment + measurements**

**meas. output**



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param.

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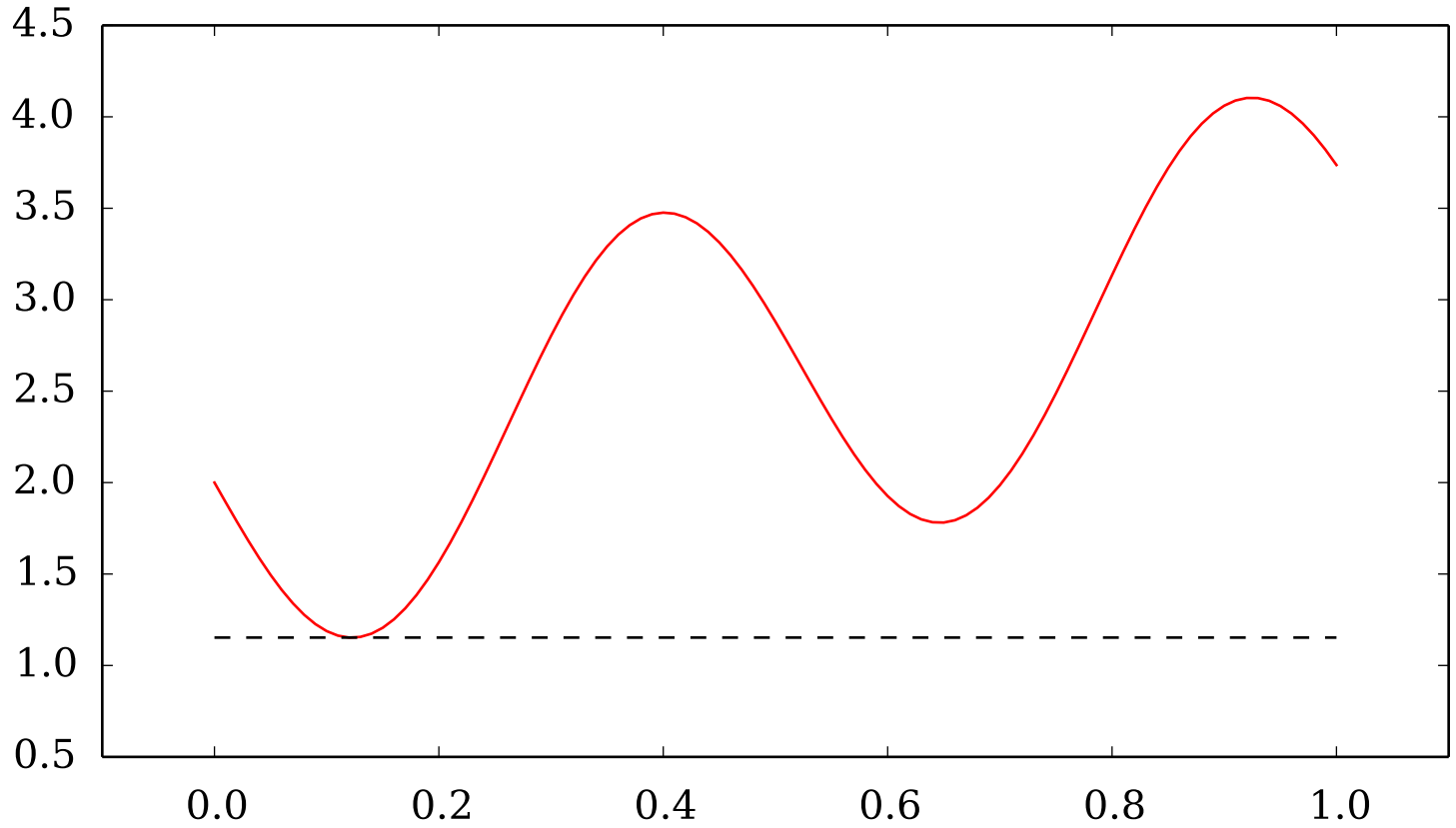
# GP-based optimization

How to find the global minimum of a function... when each evaluation is costly ?



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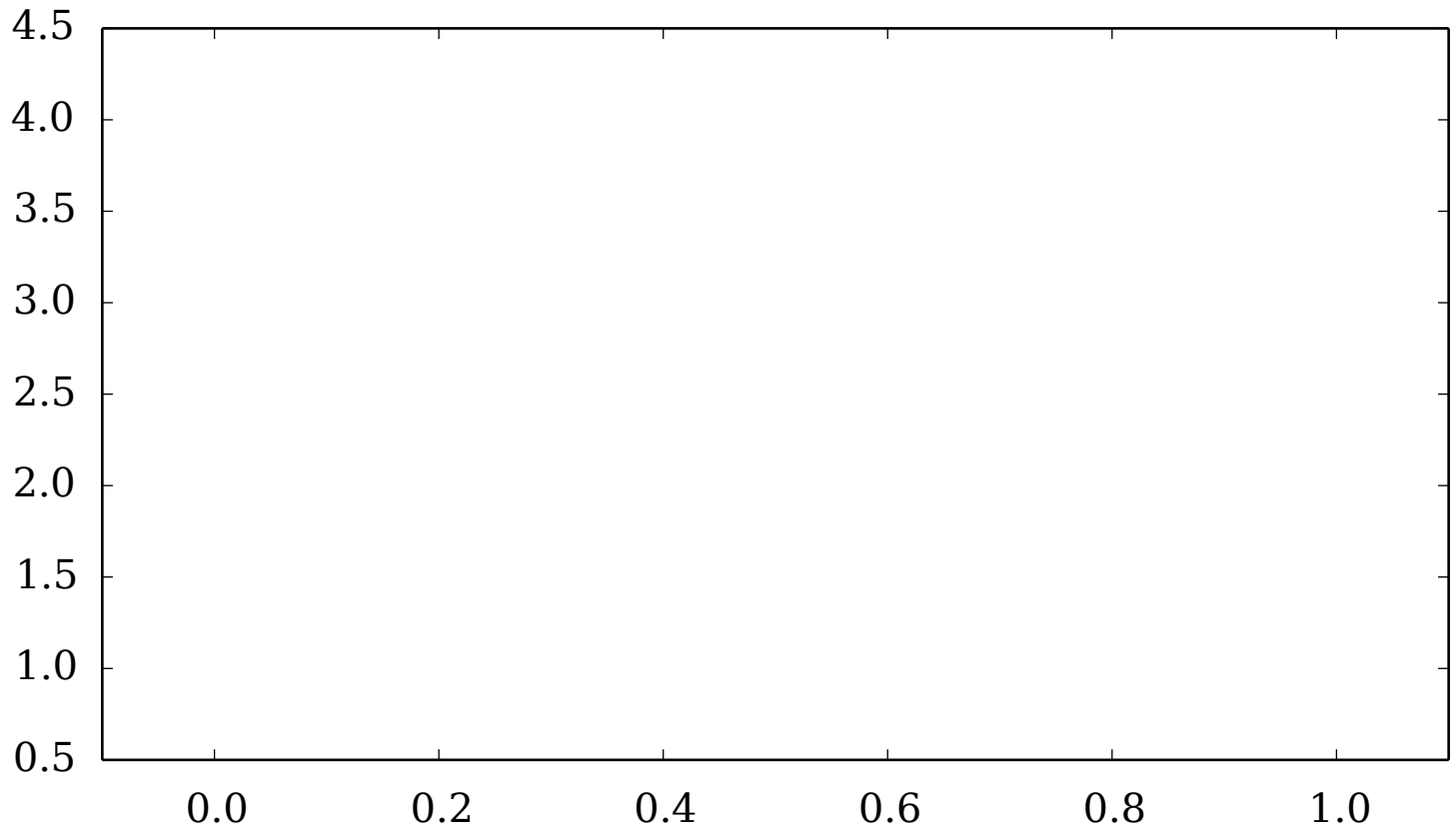

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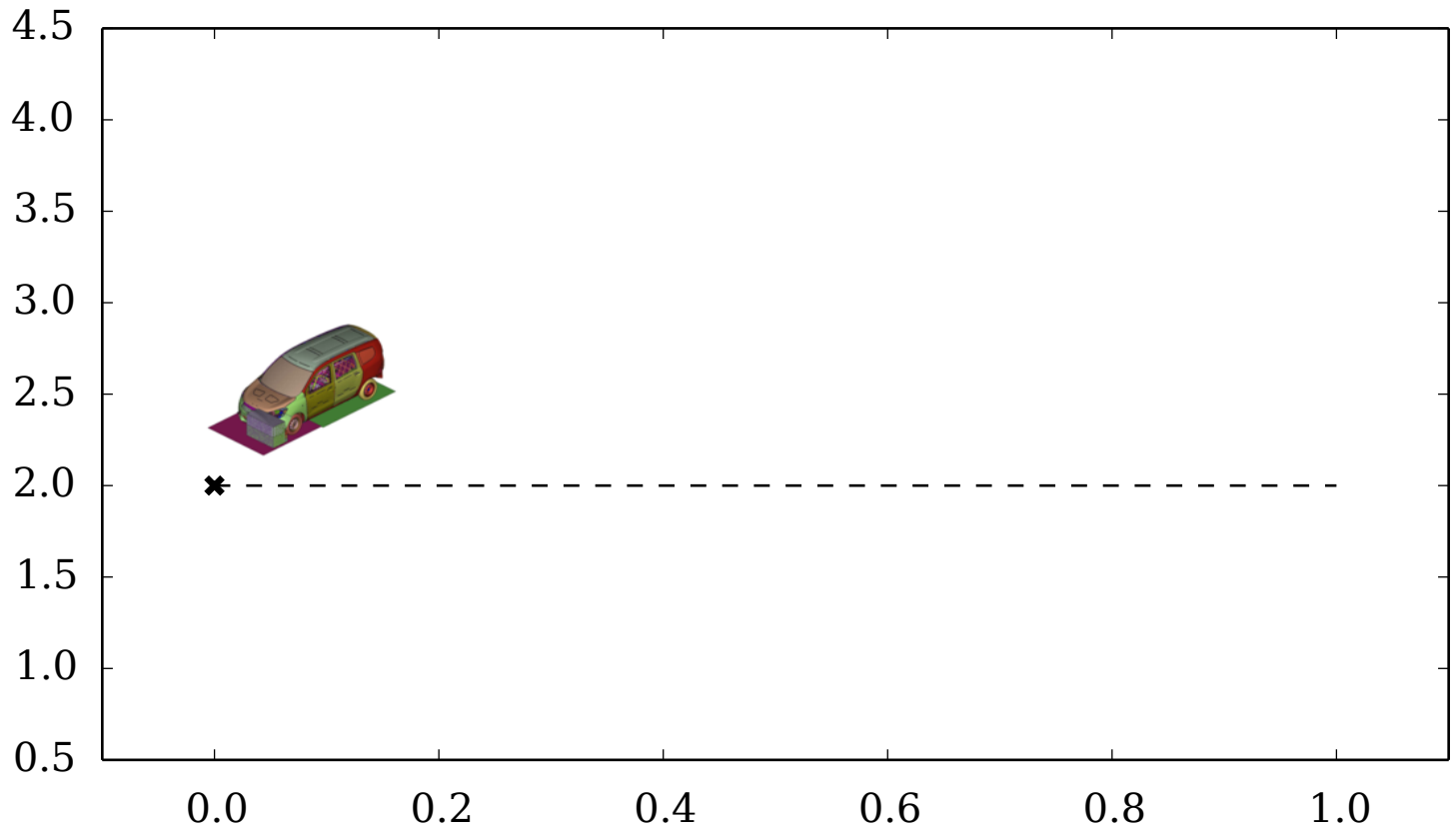

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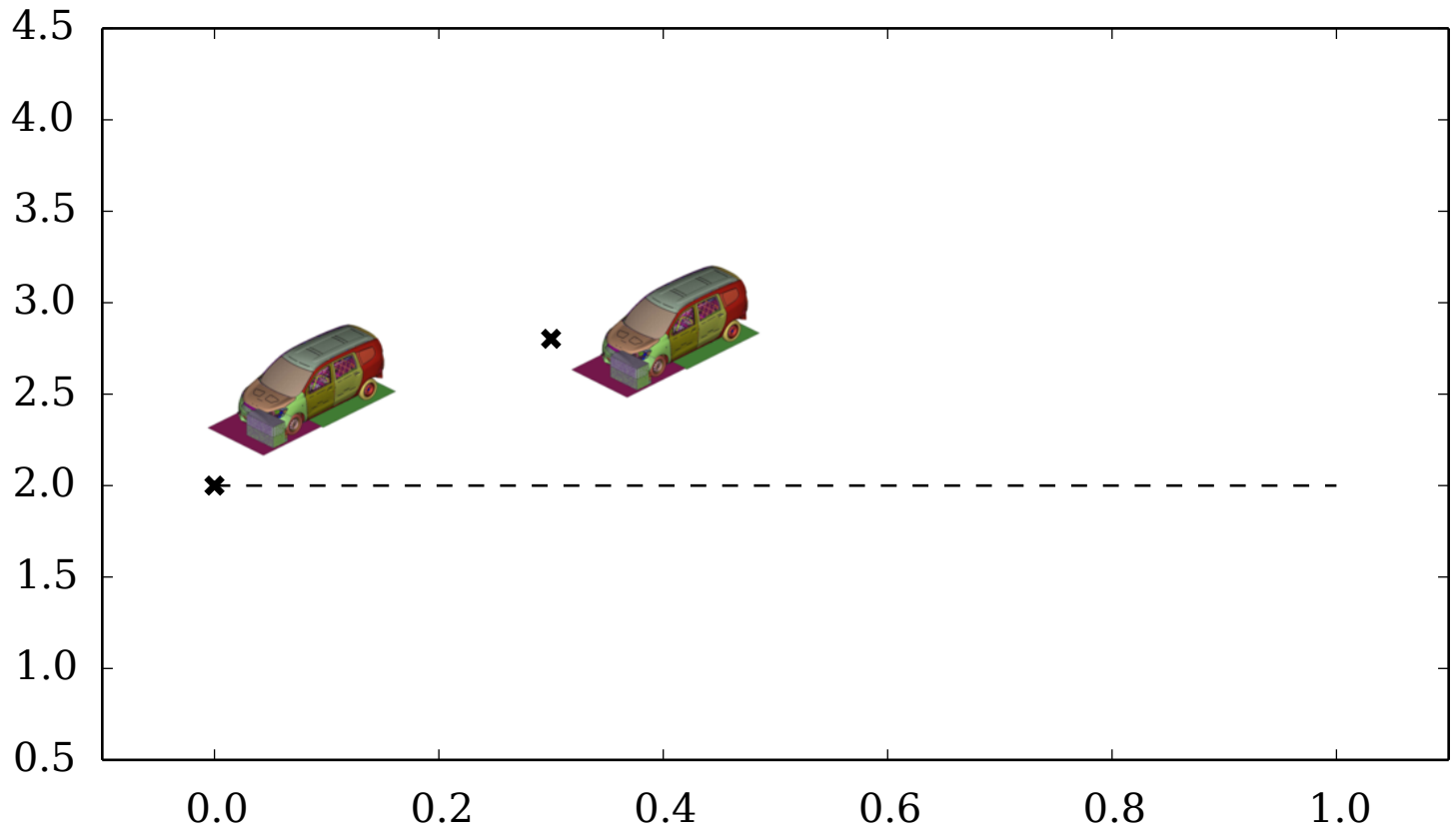

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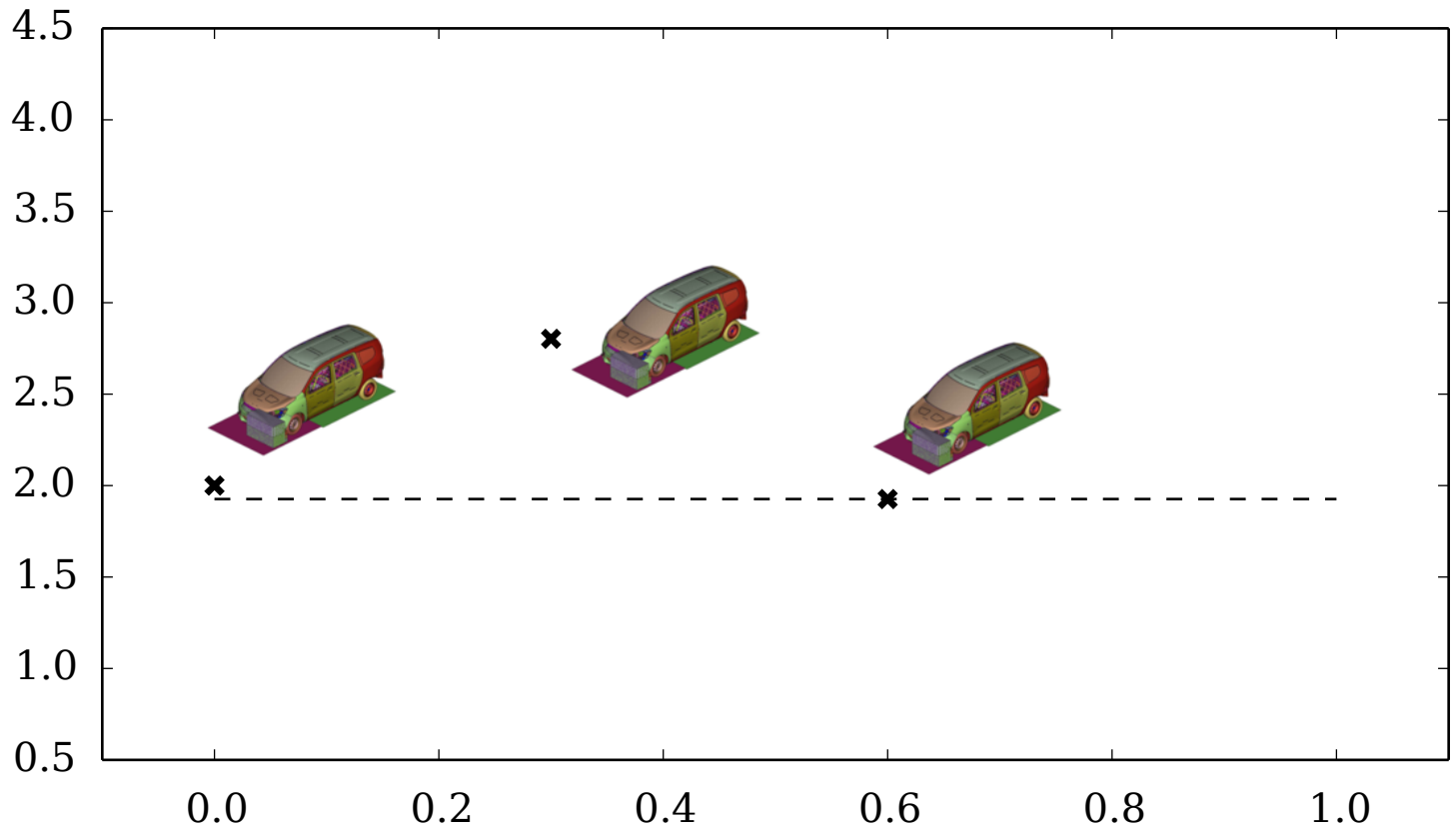

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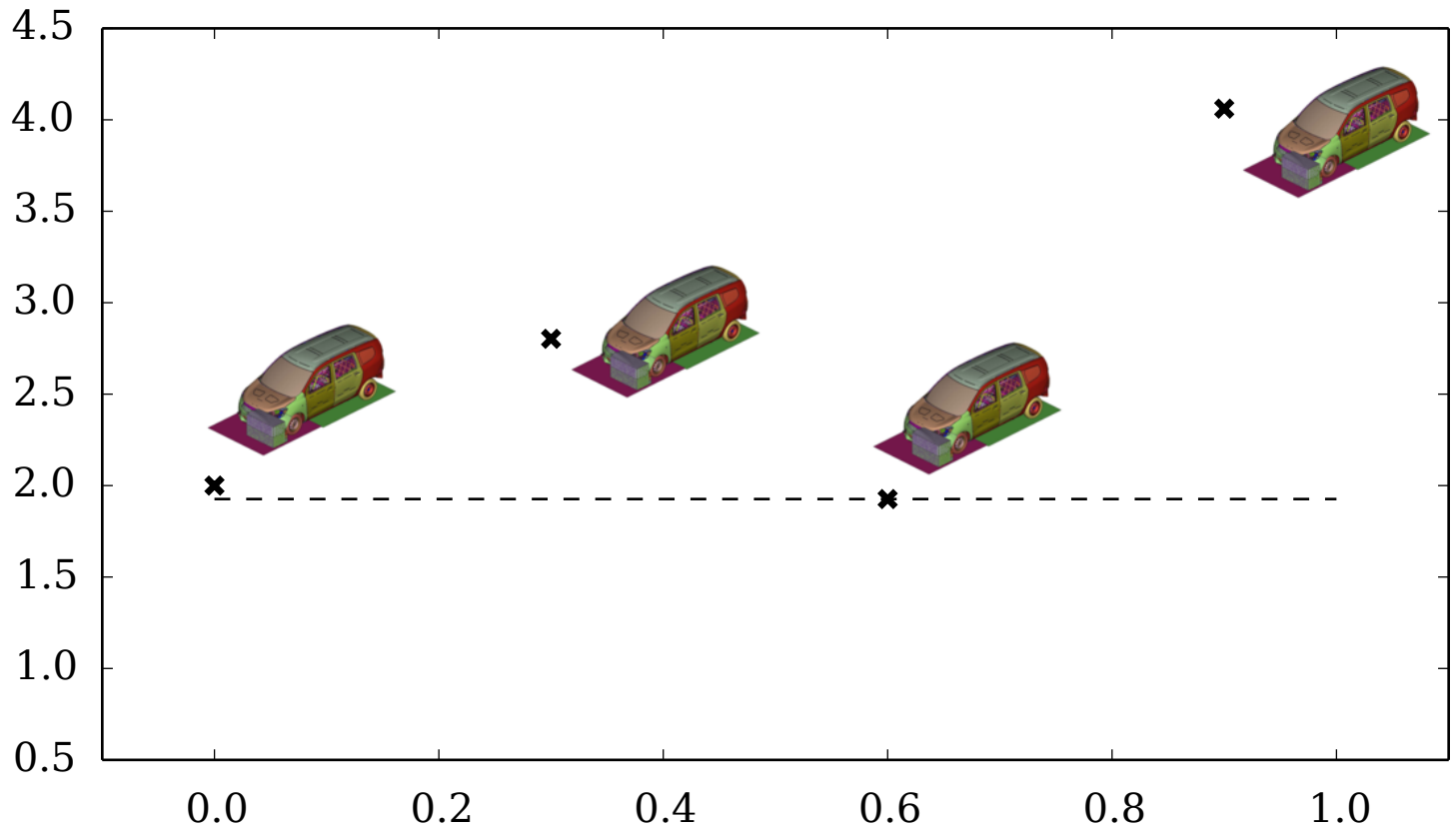
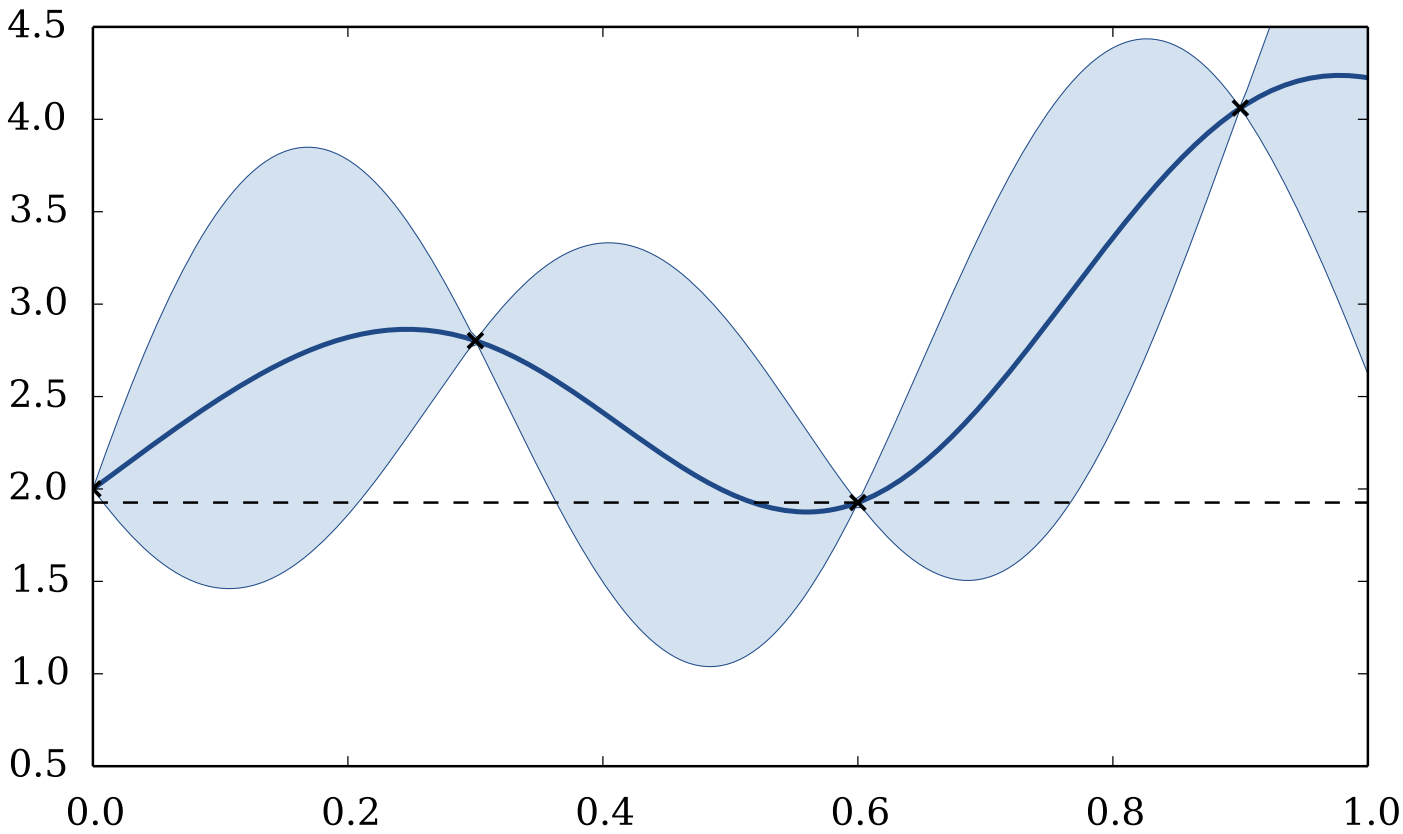


# GP-based optimization

A solution : **GP-based (or "Bayesian") optimization** [Močkus, 1975, Jones et al., 1998]

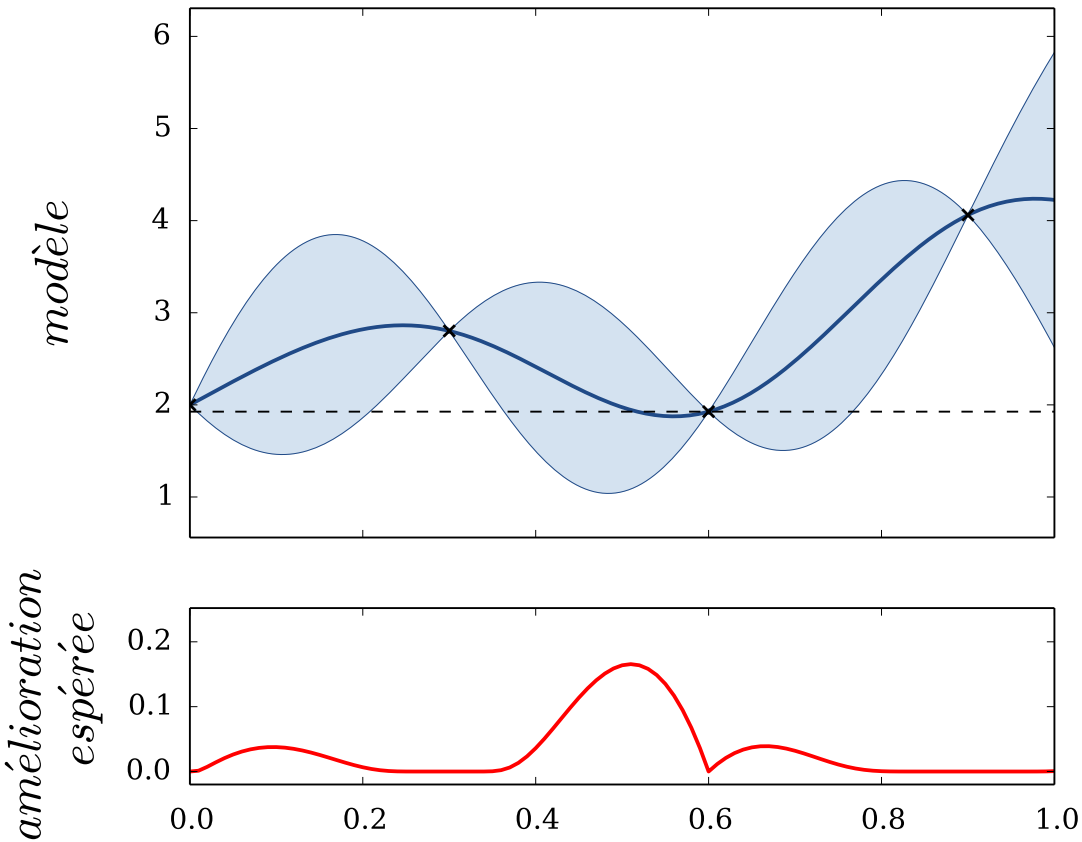
First ingredient : a GP model $Y$



# GP-based optimization

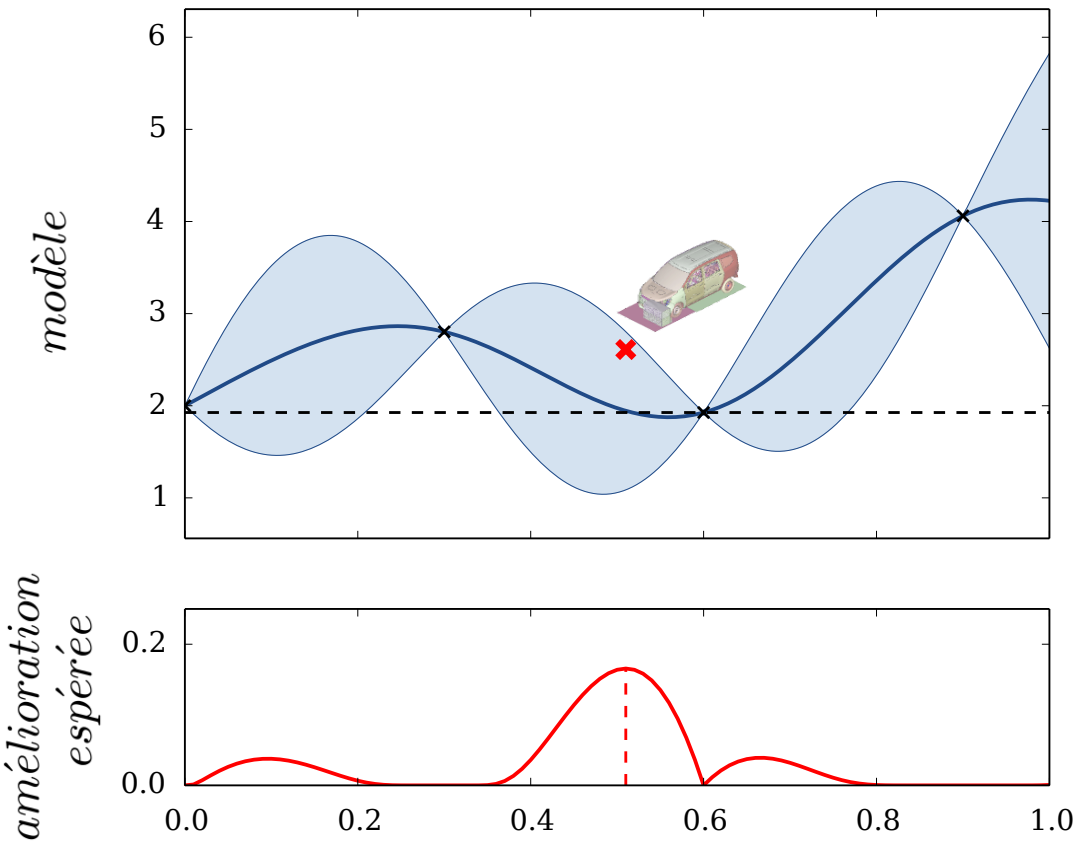
Second ingredient : an **easy-to-compute** criterion **accounting for uncertainty at unknown regions**, e.g. here "expected improvement"

$$EI(x) = \mathrm{E}([f_0 - Y(x)]^+ | Y(x_1), \ldots, Y(x_n)) \qquad f_0 : \textit{ current minimum}$$



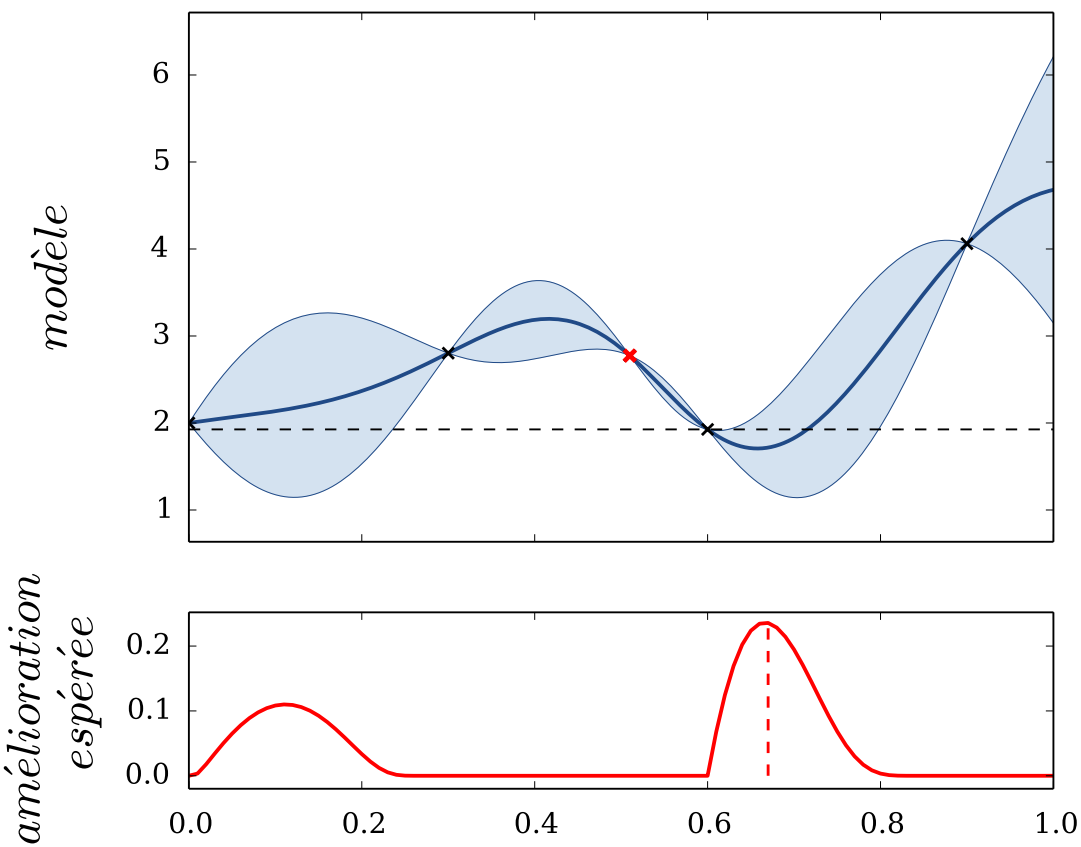
# GP-based optimization

The algorithm (here "EGO") : (1) Find the next point by maximizing the criterion $\rightarrow$ (2) Evaluate the function $\rightarrow$ (3) Update the GP model $\uparrow$



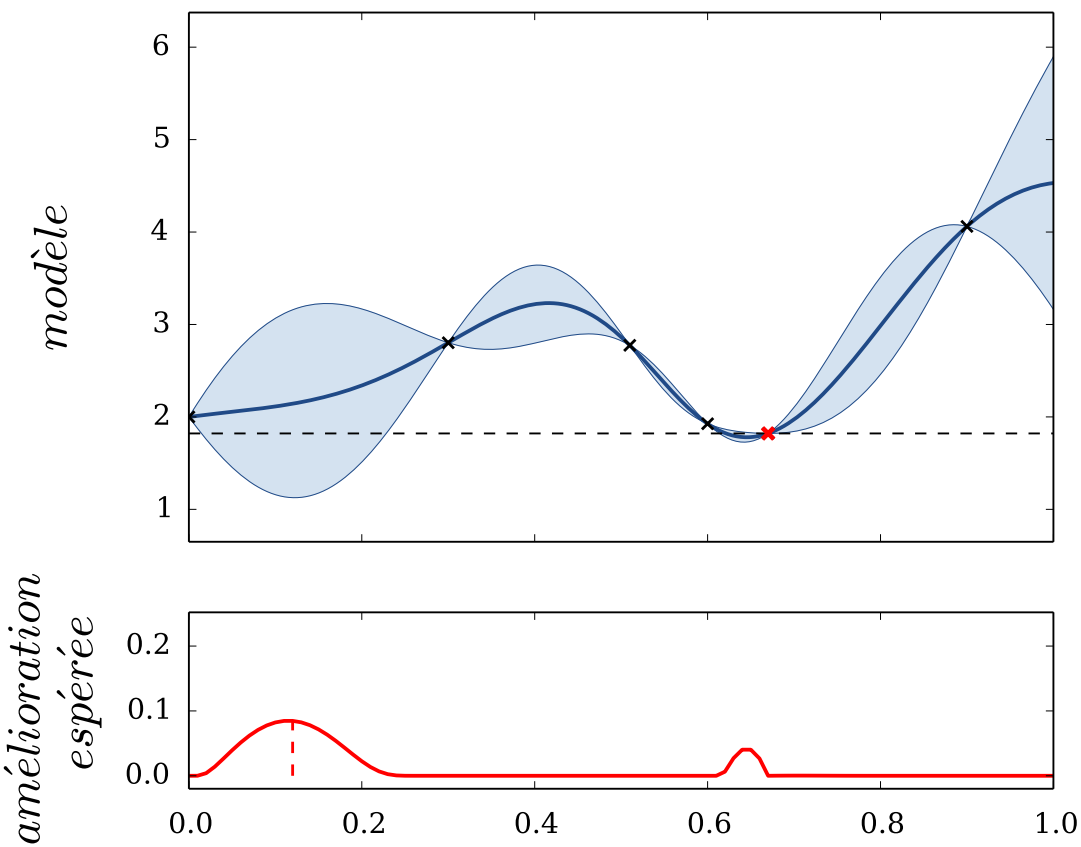
# GP-based optimization

Iteration 2 :



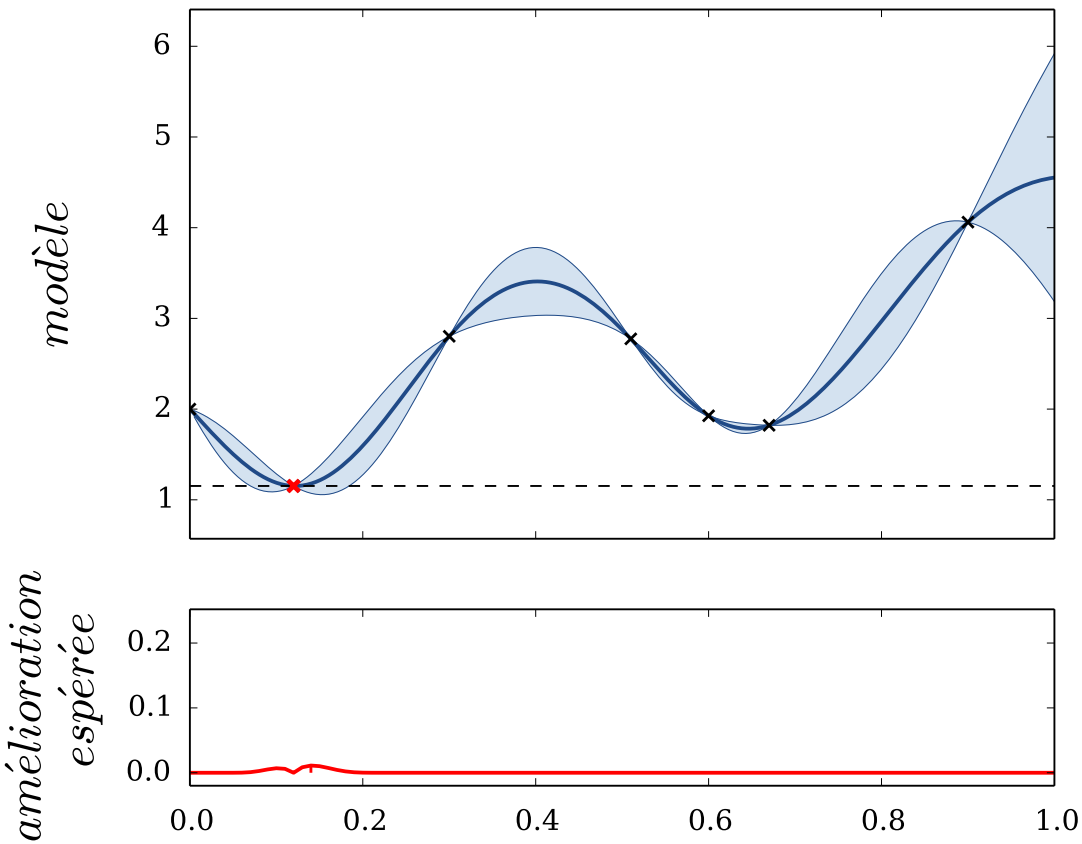
# GP-based optimization

Iteration 3 :



# GP-based optimization

Theory shows that **EGO algorithm provides a dense sequence of points**, up to a slight condition on the kernel used for GPs [Vazquez and Bect, 2010] .

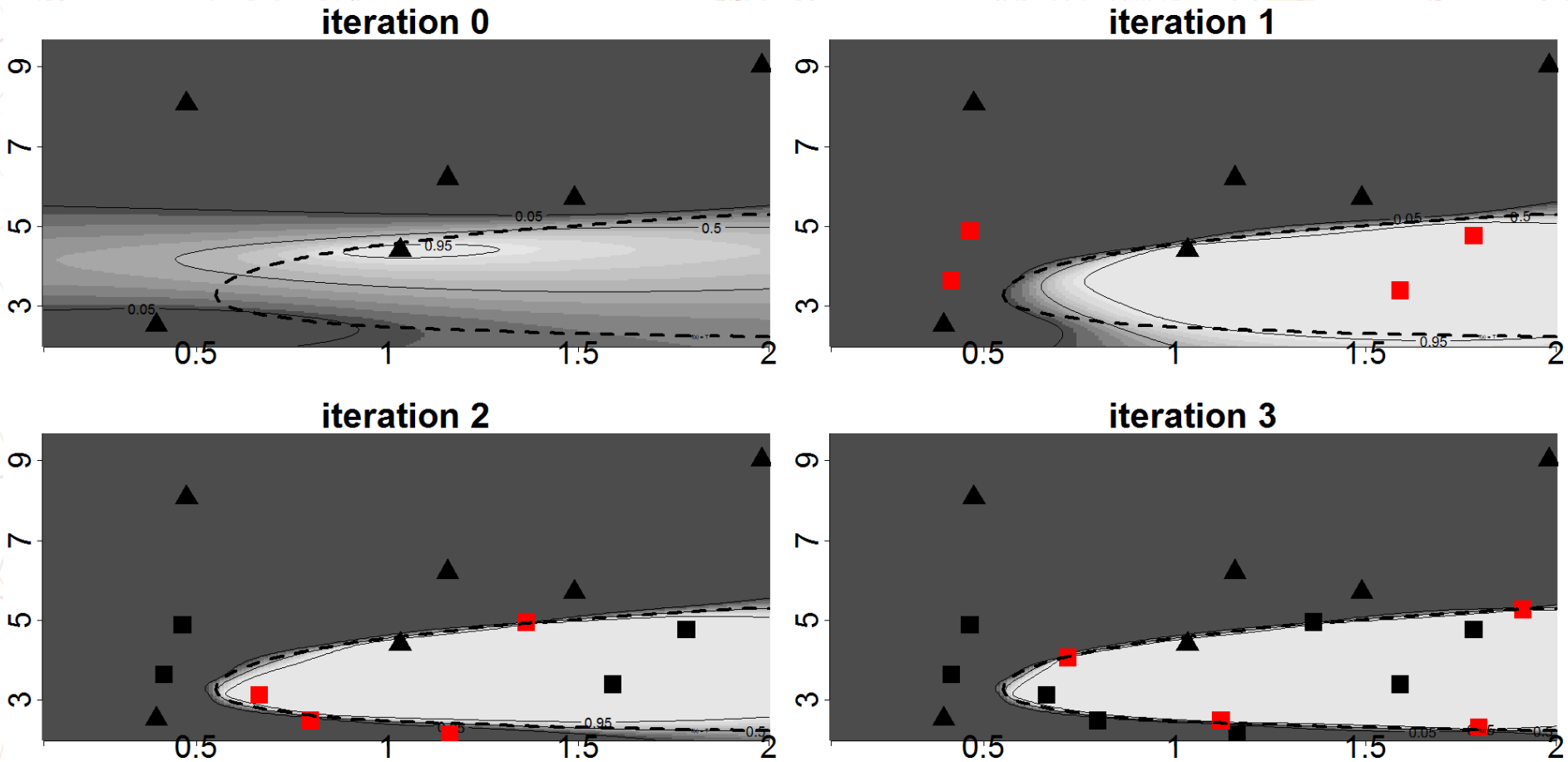


## GP-based inversion

Same receipt for estimating a probability of failure ("SUR" strategy).

See [Chevalier et al., 2014] for details and [Bect et al., 2017] for a convergence analysis with supermartingales.

Illustration : Estimation of the nuclear criticity region $k_{\text{eff}} > 0.95$



# From geostatistics to metamodels

## Time line

- 1951 : Spatial interpolation in geosciences [Krige, 1951]
  $\rightarrow$ "Kriging"
- 1963 : Foundations of geostatistics [Matheron, 1963]
- 1989 : Computer experiments, metamodelling [Sacks et al., 1989]
  $\rightarrow$ Application to dimensions $\geq 4$

## Some books about metamodelling with GPs

- "The Design and Analysis of Computer Experiments" [Santner et al., 2003]
- "Design and Modeling for Computer Experiments" [Fang et al., 2006]
- "Gaussian process for machine learning" [Rasmussen and Williams, 2006]

## Gaussian processes

Gaussian processes are stochastic processes (or random fields) s.t. every finite dimensional distribution is Gaussian. $\rightarrow$ Parameterized by two functions

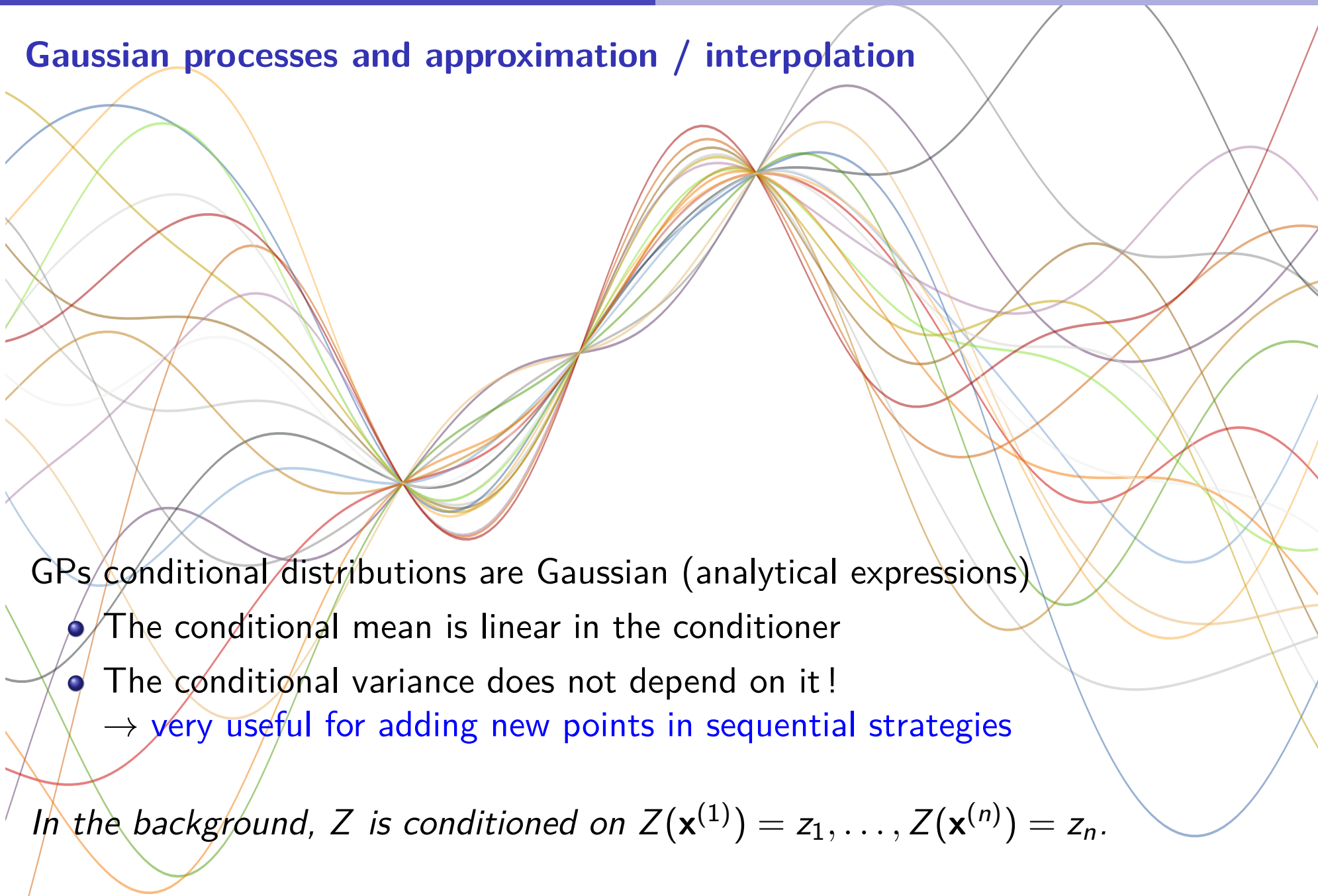
$$Z_{\mathbf{x}} \sim GP(\underbrace{m(\mathbf{x})}_{trend}, \underbrace{k(\mathbf{x}, \mathbf{x}')}_{kernel})$$

- The trend can be any function.
- The kernel is positive semidefinite :

$$\forall n, \alpha_1, \ldots, \alpha_n, \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}, \qquad \sum_{i=1}^{n} \alpha_i \alpha_j k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \geq 0.$$

It contains the spatial dependence.

# Gaussian processes and approximation / interpolation



GPs conditional distributions are Gaussian (analytical expressions)

- The conditional mean is linear in the conditioner
- The conditional variance does not depend on it !
  $\rightarrow$ very useful for adding new points in sequential strategies

*In the background, $Z$ is conditioned on $Z(\mathbf{x}^{(1)}) = z_1, \ldots, Z(\mathbf{x}^{(n)}) = z_n$.*

# Gaussian processes, splines and RKHS

## The 3 faces of a kernel

$GP(0, k(\mathbf{x}, \mathbf{x}')) \quad \Leftrightarrow \quad$ p.s.d. functions $k \quad \Leftrightarrow \quad$ RKHS : $\mathcal{H} = \overline{\text{span}\{k(., \mathbf{x}), \mathbf{x} \in D\}}$

where $\mathcal{H}$ is a "Reproducing Kernel" Hilbert Space with dot product :

$$\langle k(\mathbf{x}, .), k(\mathbf{x}', .) \rangle = k(\mathbf{x}, \mathbf{x}') \qquad (*)$$

*RKHS can be also defined as Hilbert spaces of functions such that evaluations $f \to f(\mathbf{x})$ are continuous : By Riesz theorem, there exists a unique $k(., \mathbf{x})$ s.t.*

$$f(\mathbf{x}) = \langle f, k(., \mathbf{x}) \rangle$$

*Choosing $f = k(., \mathbf{x}')$ gives the reproducing identity (*).*

*Ref : [Aronszajn, 1950], [Berlinet and Thomas-Agnan, 2011].*

# Gaussian processes, splines and RKHS

## Correspondence between interpolation spline and GP conditional mean

**[Kimeldorf and Wahba, 1971]**

The interpolation spline is defined by the functional problem

$$(*) \qquad \min_{h \in \mathcal{H}} \|h\| \qquad s.t. \quad h(\mathbf{x}^{(i)}) = z_i,\ i = 1, \ldots, n$$

If $\mathcal{H}$ is the RKHS of kernel $k$, and if $K = (k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}))_{1 \leq i,j \leq n}$ is invertible, then (*) has a unique solution in the finite dimensional space spanned by the $k(., \mathbf{x}^{(i)})$ :

$$h_{\text{opt}}(\mathbf{x}) = \mathrm{E}\left[ Z_{\mathbf{x}} \,\middle|\, Z(\mathbf{x}^{(i)}) = z_i,\ i = 1, \ldots, n \right]$$

$\rightarrow$ In this sense, GPs are generalizing interpolation splines.

*The first part (reduction to finite dimension) is know as Representer theorem.*

# Playing with kernels

A lot of flexibility can be obtained with kernels !

## Building a kernel from other ones (basic examples)

| | |
|---|---|
| Sum, tensor sum | $k_1 + k_2,\ k_1 \oplus k_2$ |
| Product, tensor product | $k_1 \times k_2,\ k_1 \otimes k_2$ |
| ANOVA | $(1 + k_1) \otimes (1 + k_2)$ |
| Warping | $k(\mathbf{x}, \mathbf{x}') = k_1(f(\mathbf{x}), f(\mathbf{x}'))$ |
| ... | ... |

*See examples in [Rasmussen and Williams, 2006]*... and in this talk !

# Why Gaussian processes are popular in (geo)statistics / machine learning ?

## GP strengths

- Probabilistic models that **traduce spatial dependence**
  $\rightarrow$ provide realistic uncertainty in unvisited area
- **Conditional distributions are analytical**, and the cond. var. is constant
  $\rightarrow$ Useful for prediction and sequential strategies
- **Parameterized by functions** : mean and covariance **(kernel)**
  $\rightarrow$ Flexibility
- At the crossing between **rich mathematical theories**
  $\rightarrow$ Stochastic proc., Reproducing Kernel Hilbert Spaces, Positive Definite Functions

## Aim of this talk

*To illustrate the flexibility of GPs in various (meta)modeling situations.*

# Outline

# Various information... same framework

Question : What is the common point between GPs whose sample paths are...

| | |
|---|---|
| Centered | $\int Z_{\mathbf{x}}\, \mu(d\mathbf{x}) = 0$ |
| Harmonic | $\frac{\partial^2 Z_{\mathbf{x}}}{\partial x_1^2} + \frac{\partial^2 Z_{\mathbf{x}}}{\partial x_2^2} = 0$ |
| Symmetric | $Z_{g.\mathbf{x}} = Z_{\mathbf{x}} \quad \forall g \in G$ |
| Additive | $Z_{\mathbf{x}} = \sum_{j=1}^{d} Z_{x_j}^j$ |
| ... | |

$G$ : Finite group of symmetries.

# Various information... same framework

Answer : The information can be reformulated$^\star$ with a linear operator $T$

| | | |
|---|---|---|
| Centered | $\int Z_{\mathbf{x}}\, \mu(d\mathbf{x}) = 0$ | $T(f) = \int f(\mathbf{x})\, \mu(d\mathbf{x})$ |
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| Symmetric | $Z_{g.\mathbf{x}} = Z_{\mathbf{x}} \quad \forall g \in G$ | $T(f) = f(\mathbf{x}) - \frac{1}{\lvert G\rvert}\sum_{g\in G} f(g.\mathbf{x})$ |
| Additive | $Z_{\mathbf{x}} = \sum_{j=1}^{d} Z^j_{x_j}$ | |

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| Additive | $Z_{\mathbf{x}} = \sum_{j=1}^{d} Z^j_{x_j}$ | $T(f) = f(\mathbf{x}) - \left(m + \sum_{j=1}^{d}(E[f(\mathbf{X})\lvert X_j = x_j] - m)\right)$ |
| ... | | with $m = \mathrm{E}[f(\mathbf{X})]$ and $X_1, \ldots, X_n$ ind. r.v. |

$^\star$ The reformulation is partial for the symmetric condition.

## Two results for GPs constrained by linear equalities [Ginsbourger et al., 2016]

- $Z : GP(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$
- $T$ : linear operator on $Y$ such that $T(m) = 0$ ($+$ integrability condition)

### Argumentwise property for kernels

$T$ can be defined in a unique way on the RKHS corr. to $k$ and

$$\forall \mathbf{x} : T(Z)_{\mathbf{x}} = 0 \quad \Leftrightarrow \quad \forall \mathbf{x}' : T(k(., \mathbf{x}')) = 0$$

*Proof idea :* $Cov(T(Z)_{\mathbf{x}}, Z_{\mathbf{x}'}) = T(Cov(Z_{\mathbf{x}}, Z_{\mathbf{x}'}))$

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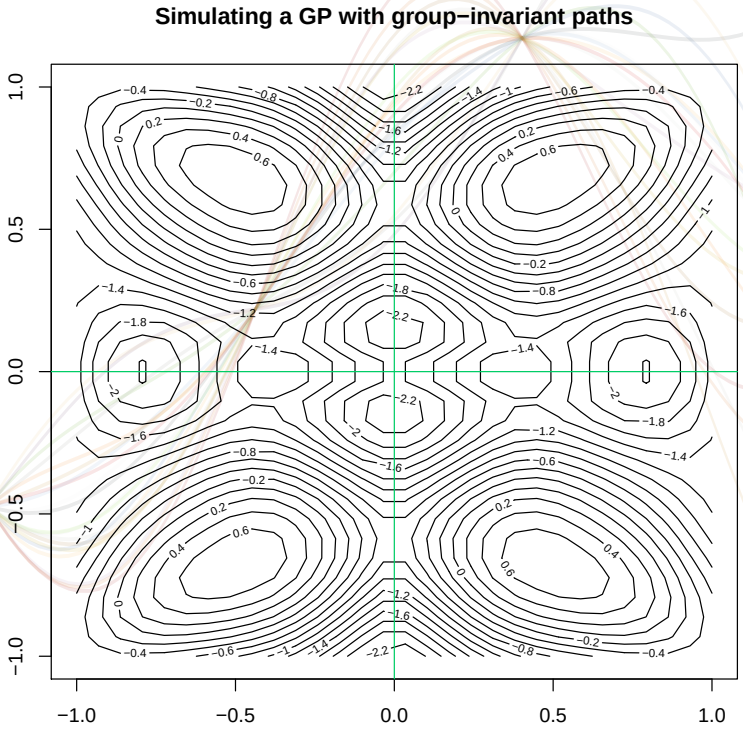
### Inheritance to conditional distributions

Let $Z^c$ the GP $Z$ conditional on $Z_{\mathbf{x}^{(i)}} = z_i$, $i = 1, \ldots, n$. Then

$$\forall \mathbf{x} : T(Z)_{\mathbf{x}} = 0 \quad \Rightarrow \quad \forall \mathbf{x} : T(Z^c)_{\mathbf{x}} = 0$$

*Proof idea : The cond. mean and cond. cov. are linear functions of* $k(., \mathbf{x}')$.

# Illustration : Symmetric GPs




Making new from old : Choose a (non-symmetric) GP $Y$, and define

$$Z_{x_1,x_2} = \sum_{g \in G} Y_{g.\mathbf{x}} = Y_{x_1,x_2} + Y_{-x_1,x_2} + Y_{x_1,-x_2} + Y_{-x_1,-x_2}$$

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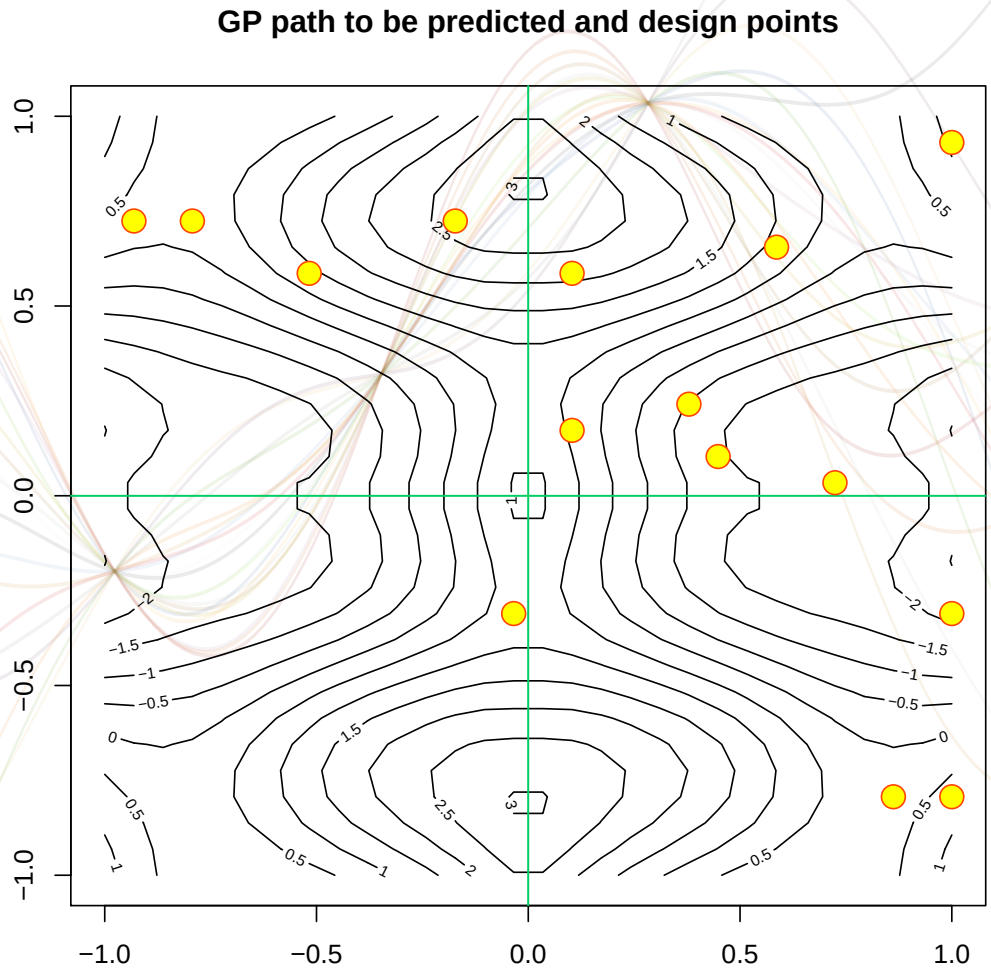

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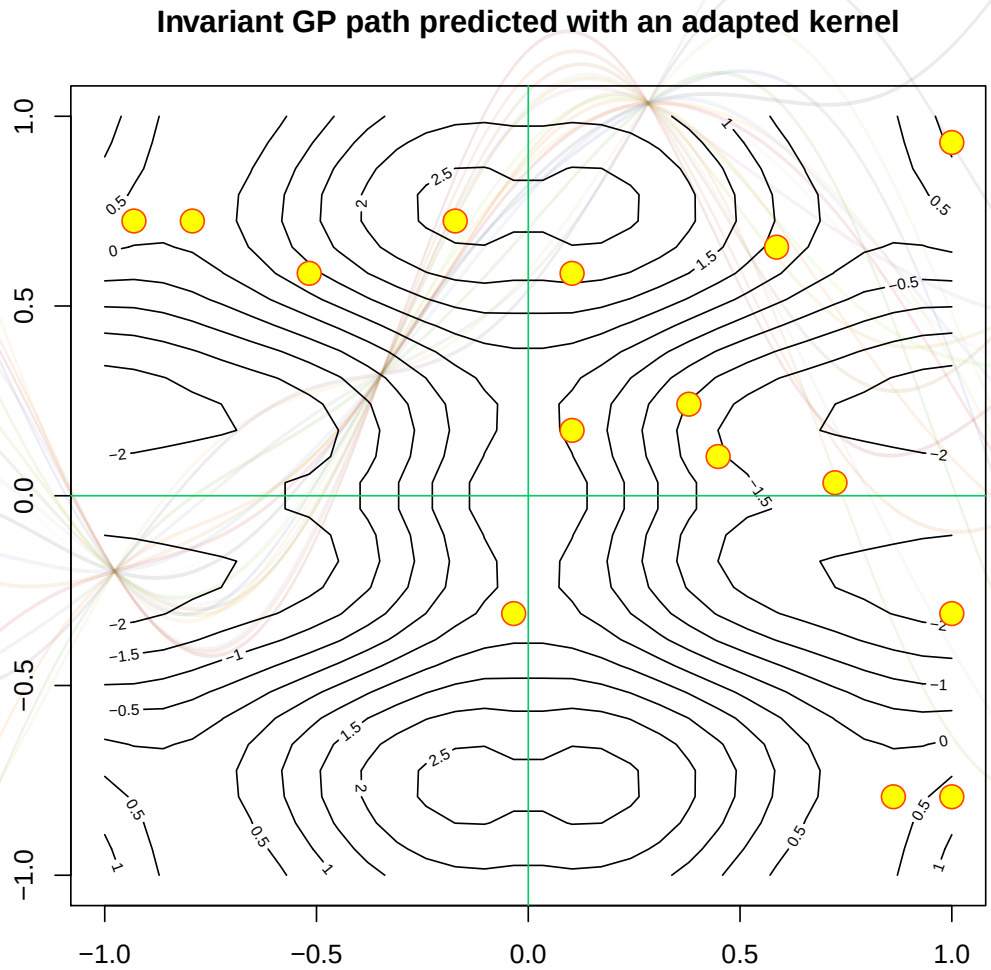

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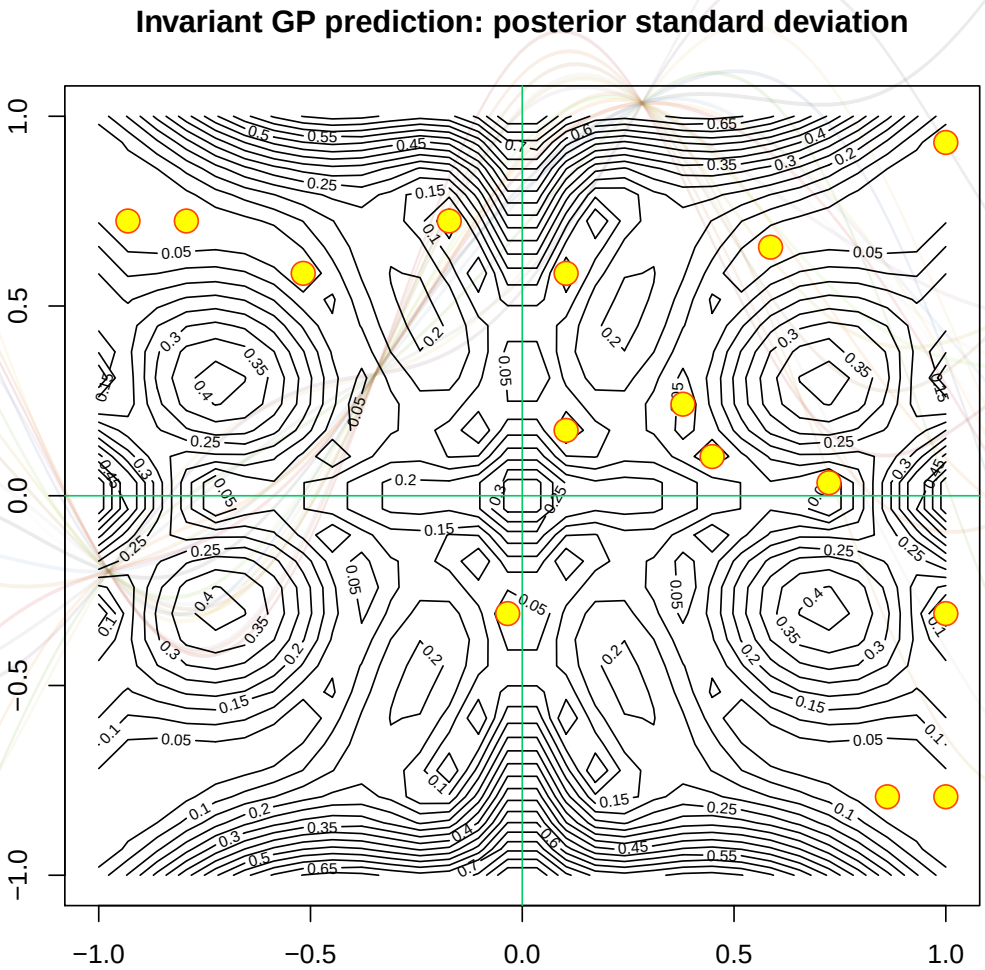
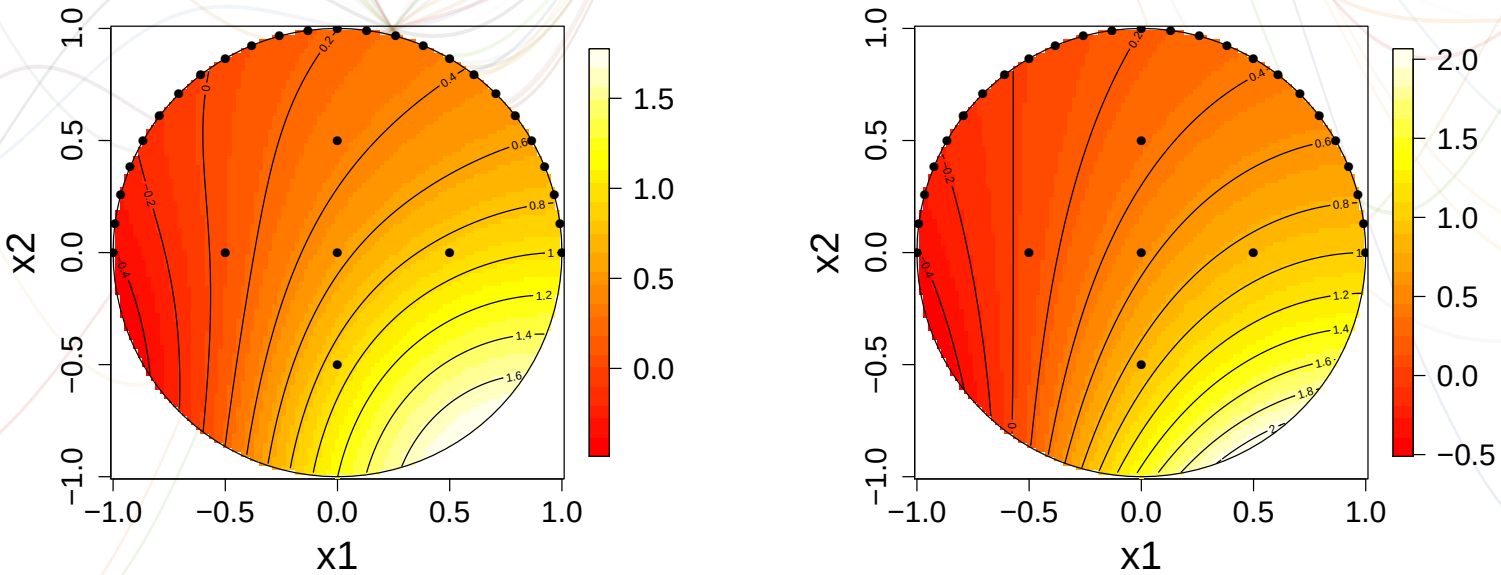


# Illustration : Maximum of a harmonic function [Ginsbourger et al., 2016]

We compare two GPs for predicting the maximum of a 2D harmonic function

Gaussian kernel $$k(\mathbf{x},\mathbf{x}') = \sigma^2 \exp\left(-\frac{(x_1-x_1')^2}{\ell_1^2} - \frac{(x_2-x_2')^2}{\ell_2^2}\right)$$

Harmonic kernel $$k(\mathbf{x},\mathbf{x}') = \sigma^2 \exp\left(\frac{x_1x_1'+x_2x_2'}{\ell^2}\right)\cos\left(\frac{x_2x_1'-x_1x_2'}{\ell^2}\right)$$




Prediction mean – Left : Gaussian kernel ; Right : Harmonic kernel.

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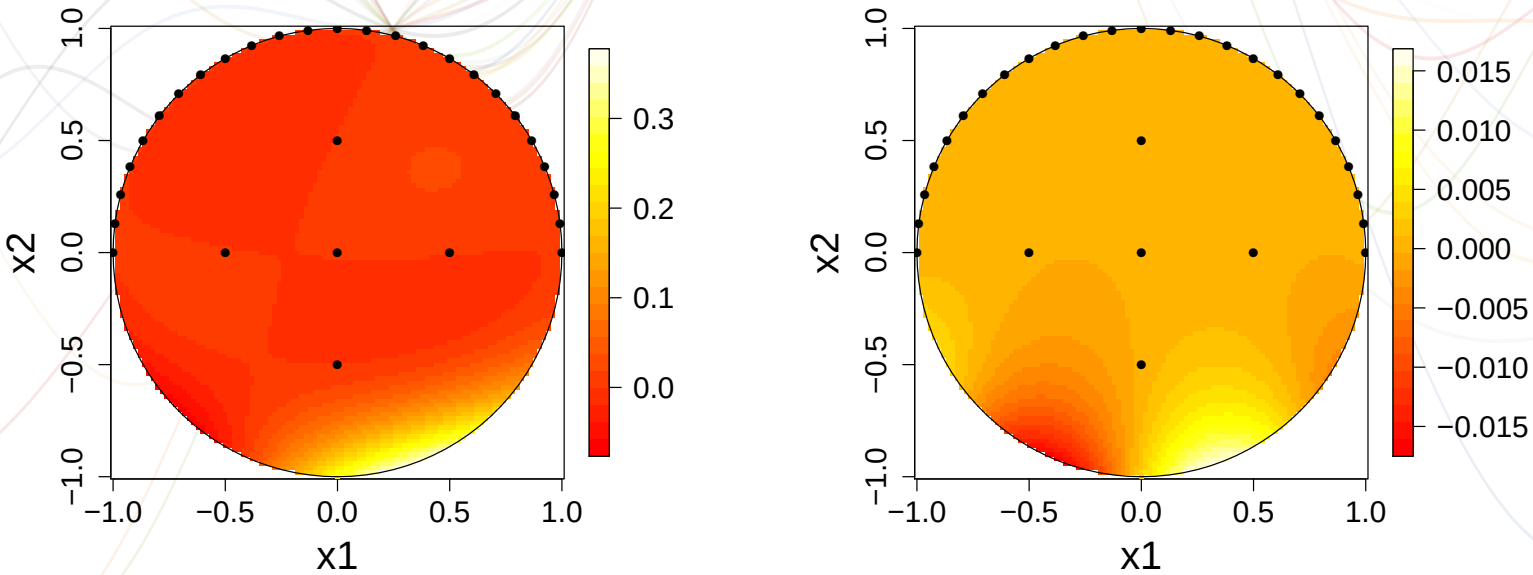


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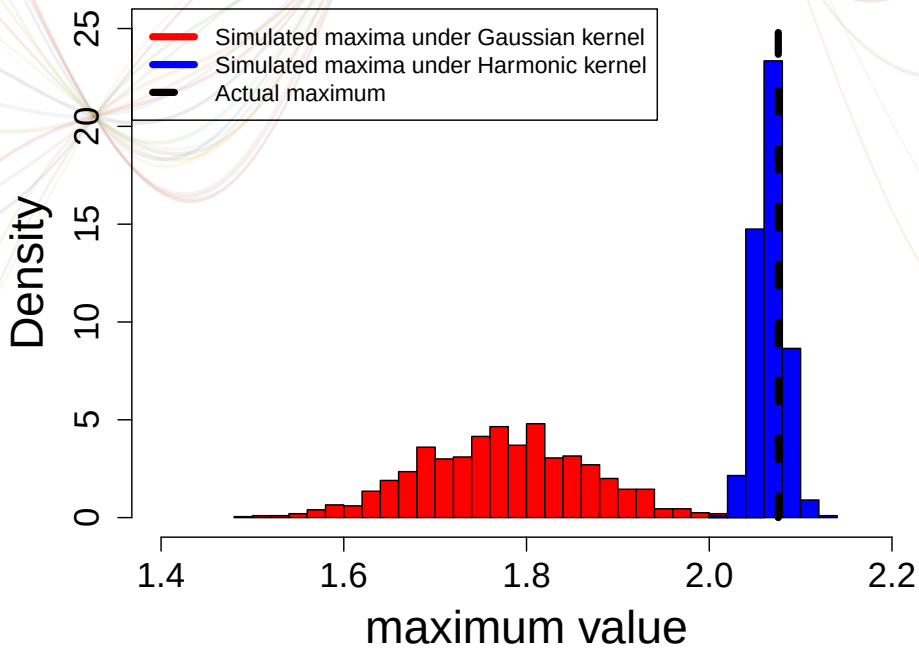
We compare two GPs for predicting the maximum of a 2D harmonic function

Gaussian kernel $$k(\mathbf{x},\mathbf{x}') = \sigma^2 \exp\left(-\frac{(x_1-x_1')^2}{\ell_1^2} - \frac{(x_2-x_2')^2}{\ell_2^2}\right)$$

Harmonic kernel $$k(\mathbf{x},\mathbf{x}') = \sigma^2 \exp\left(\frac{x_1x_1'+x_2x_2'}{\ell^2}\right)\cos\left(\frac{x_2x_1'-x_1x_2'}{\ell^2}\right)$$




Conditional simulations of the maximum under the two GPs.

# GP under linear inequalities : Impact on uncertainty quantification

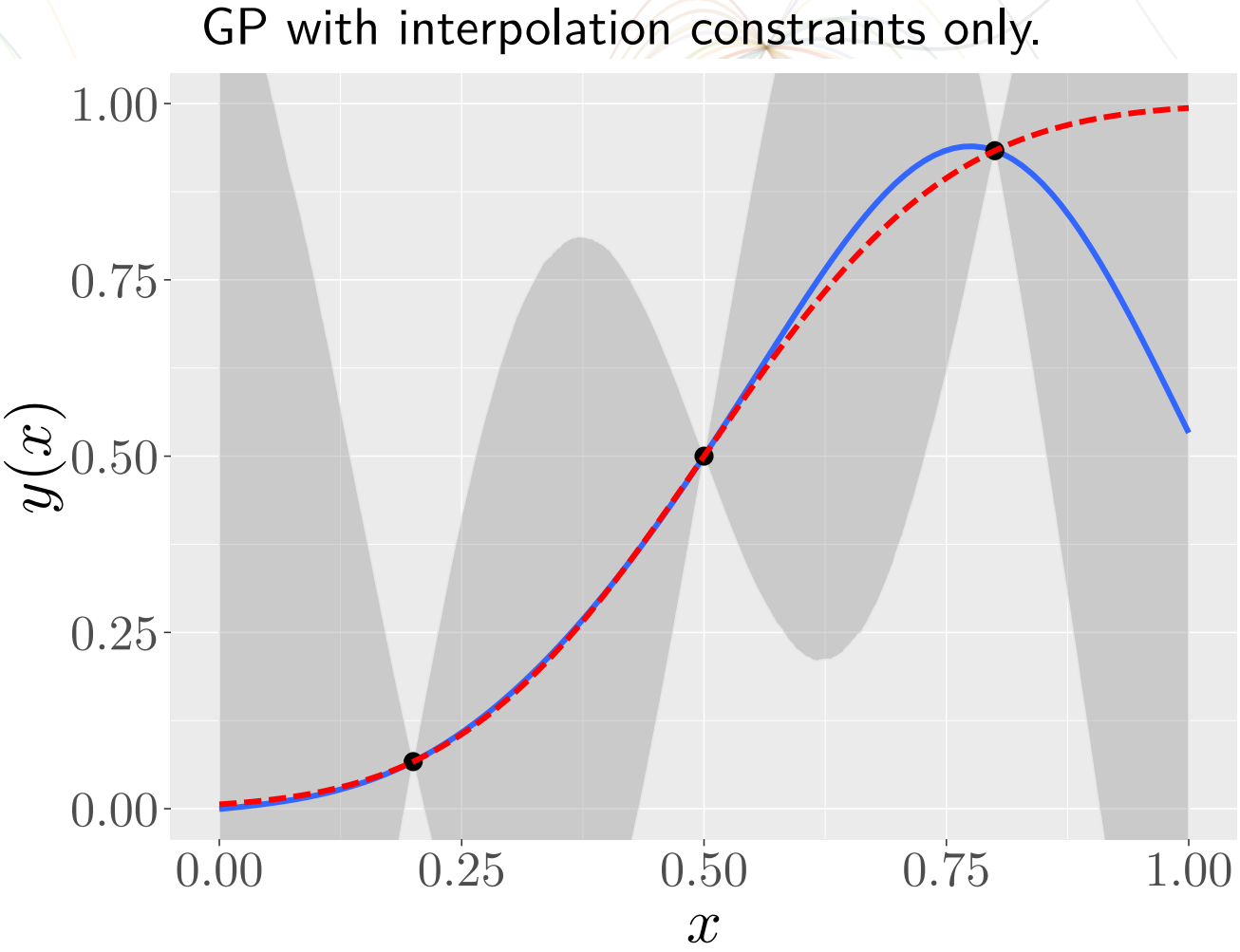



Illustration on a toy example (cdf of a Normal distribution)

# GP under linear inequalities : Impact on uncertainty quantification

GP with boundedness + monotonicity additional constraints.

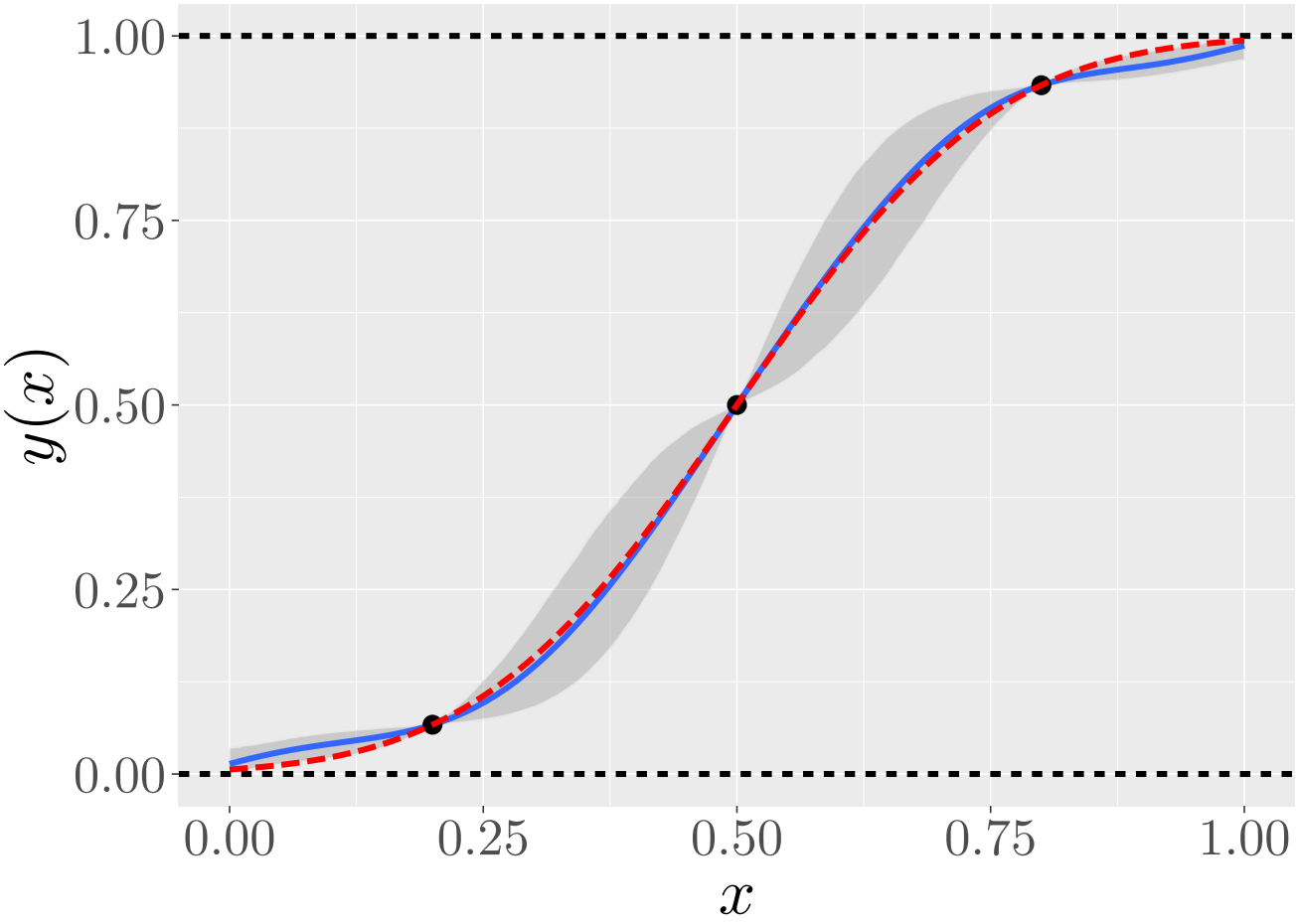



Illustration on a toy example (cdf of a Normal distribution)

# GP and linear inequalities : Some theory

## A finite elements ($P_1$) model for 1D GPs

**[Maatouk and Bay, 2017, López-Lopera et al., 2018]**

Each sample path of a GP $Y$ is approximated by an **affine function**

$$Y_m(x) = \sum_{j=1}^{m} \xi_j \phi_j(x)$$

where $\phi_j$ are "hat" functions and $\boldsymbol{\xi}$ is a Gaussian vector extracted from $Y$

- Key point : Boundedness, monotonicity (and others) for an affine function can be checked only at knots $\rightarrow$ finite number of conditions only

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- Key point : Boundedness, monotonicity (and others) for an affine function can be checked only at knots $\rightarrow$ finite number of conditions only

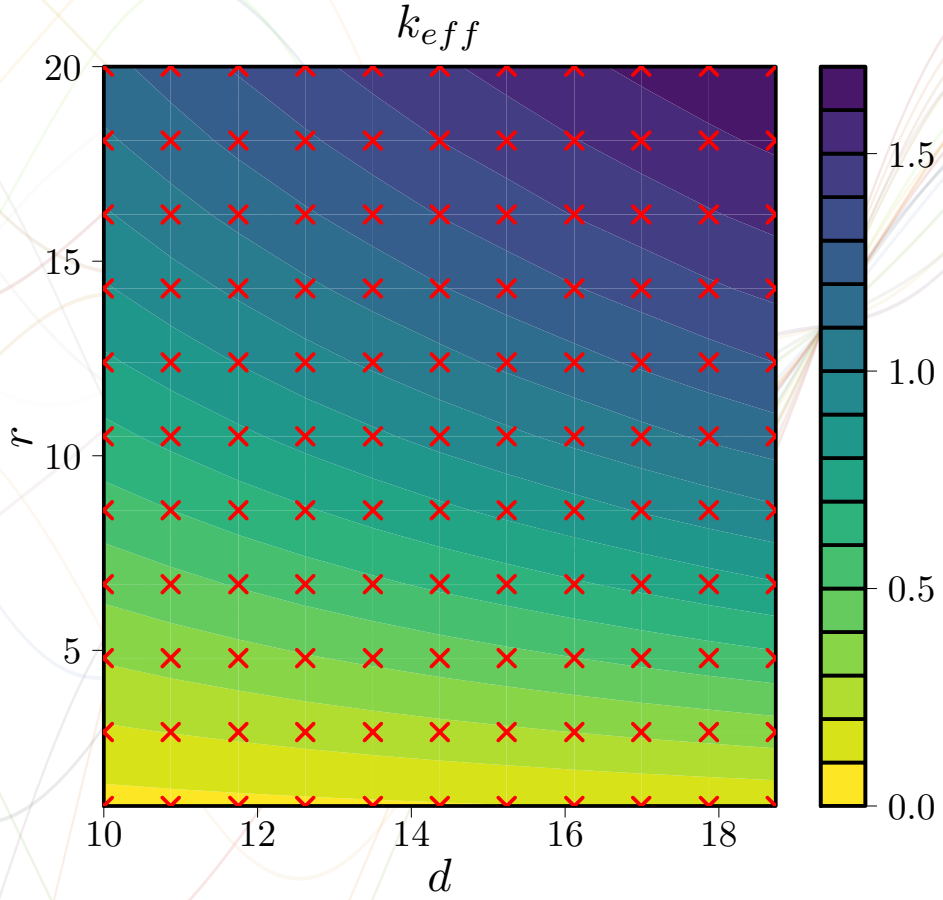
## Correspondence with spline under inequality [Bay et al., 2016]

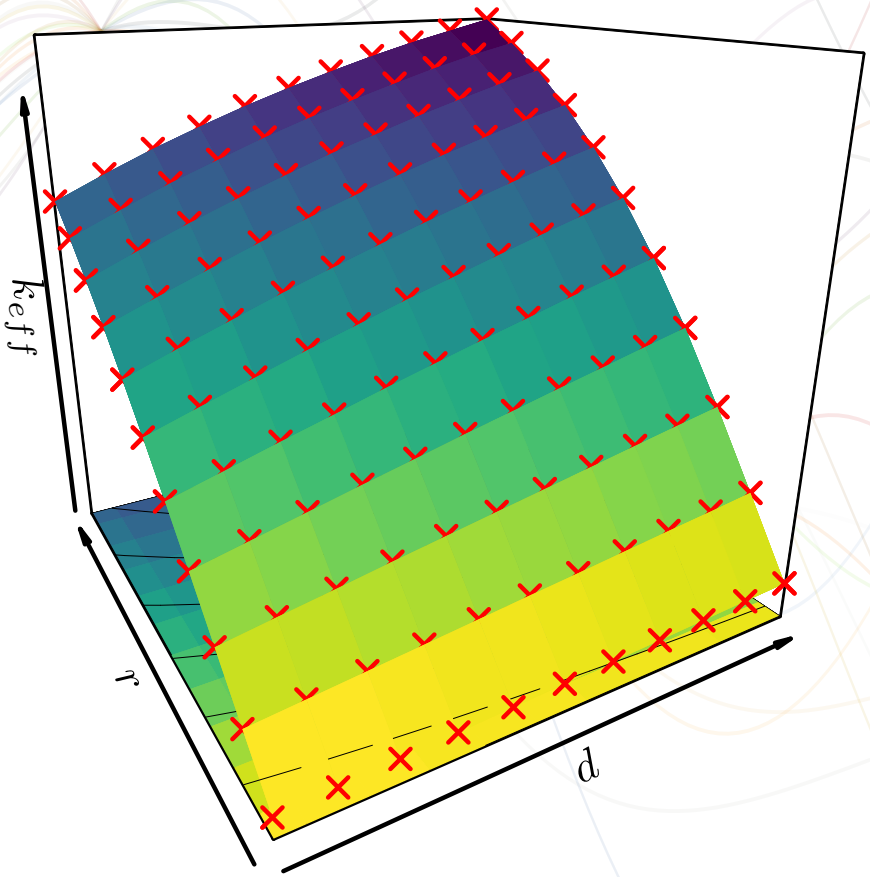
Asymptotically, computing the mode a posteriori of $Y_m$ is equivalent to

$$\min_{f \in \mathcal{H} \cap \mathcal{C}} \|f\| \qquad \text{s.t.} \quad f(x_i) = y_i, \quad (i = 1, \ldots, n)$$

where $\mathcal{C}$ is a convex set of inequalities, and $\mathcal{H}$ is the RKHS associated to $Y$.

# Example of application in 2D

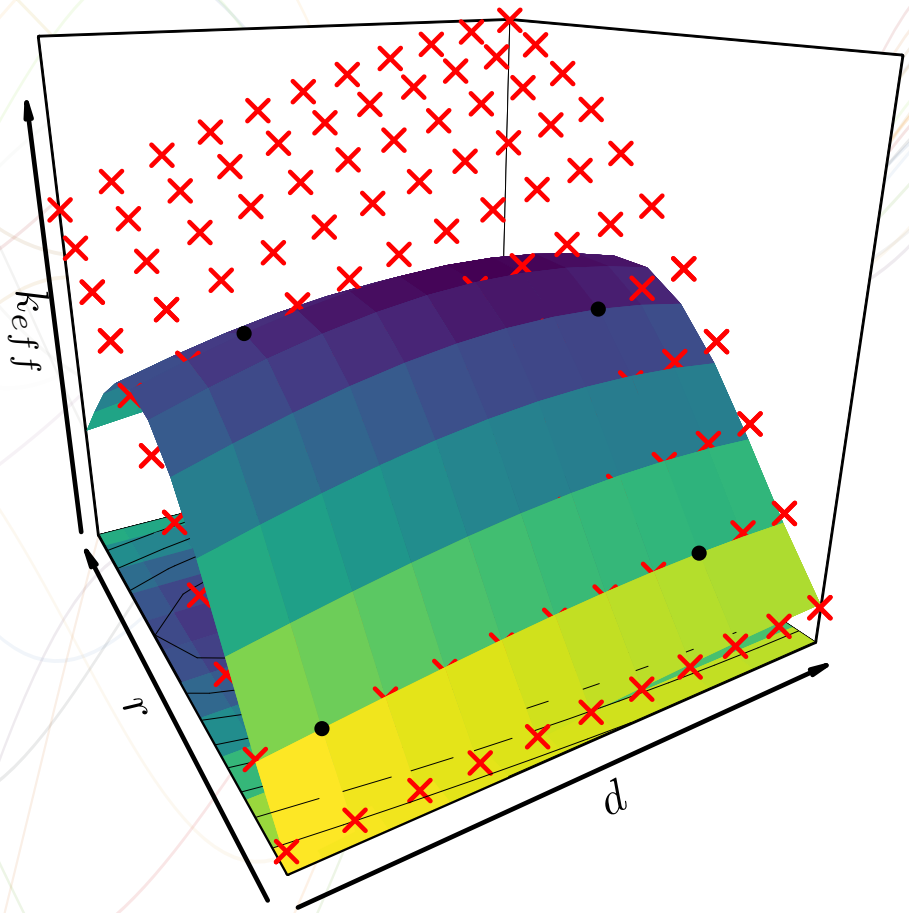


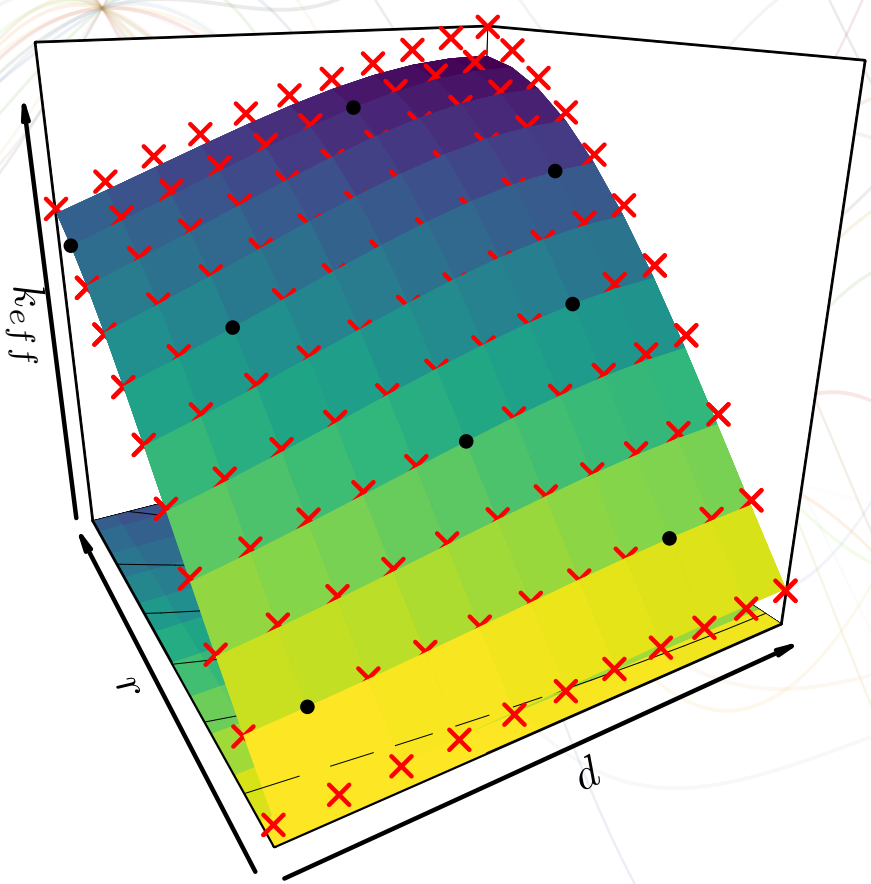




Nuclear criticality safety assessments : IRSN's dataset.

Extra information : $k_{\text{eff}}$ is positive and non-decreasing.

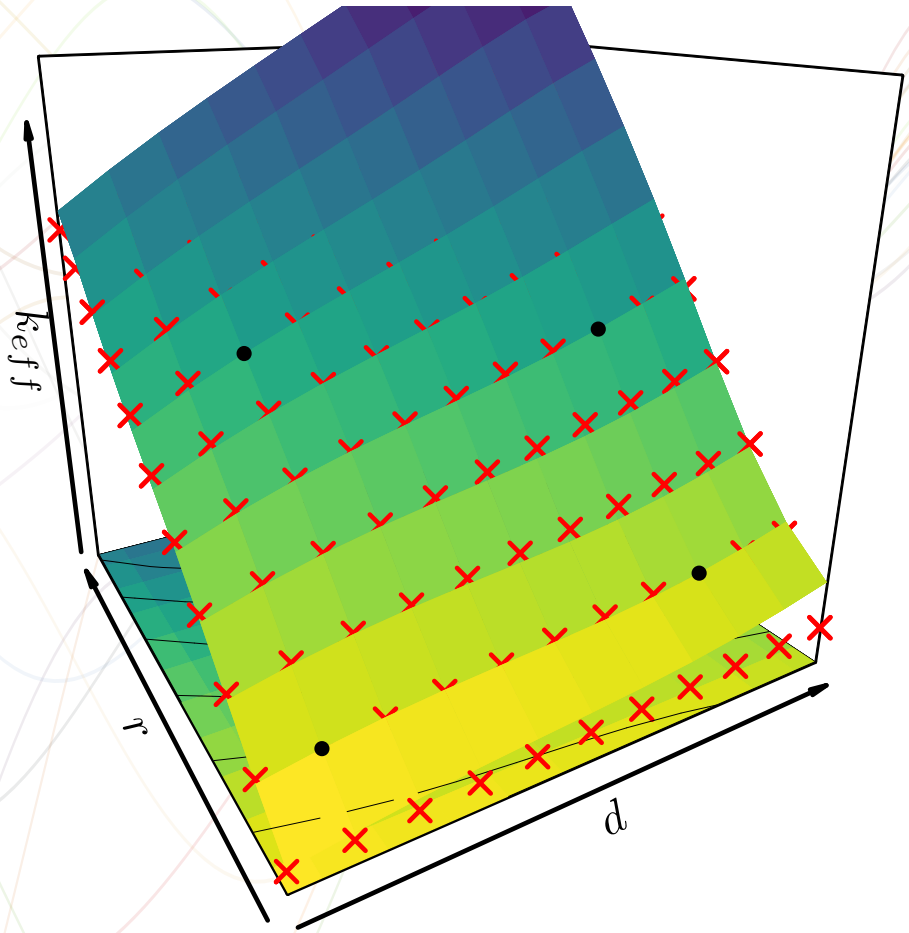
# Example of application in 2D

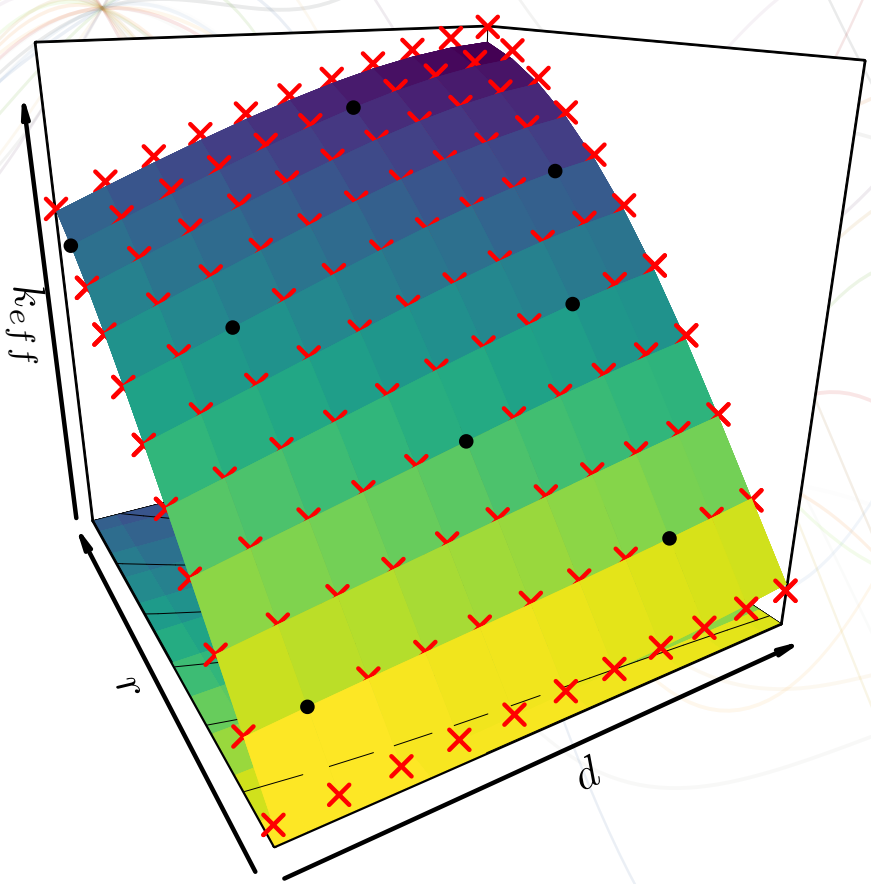



Unconstrained model + MLE.

# Example of application in 2D

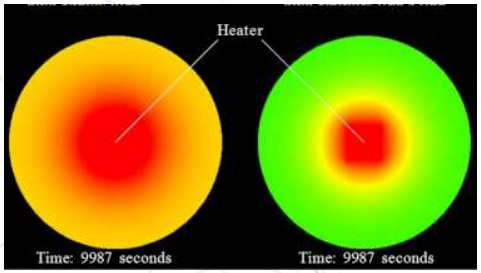


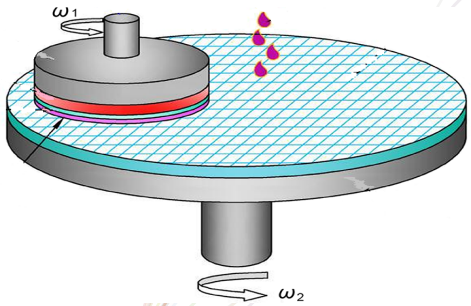

Constrained model + constrained MLE.

# Outline

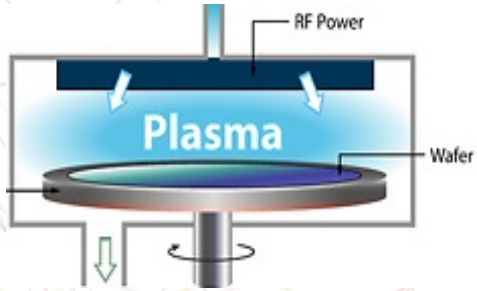
# A motivating industrial context



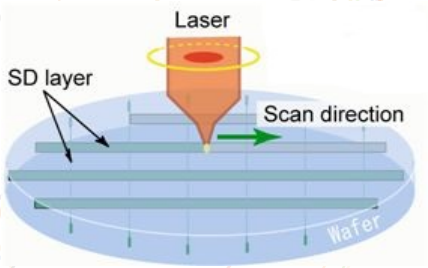

Heating



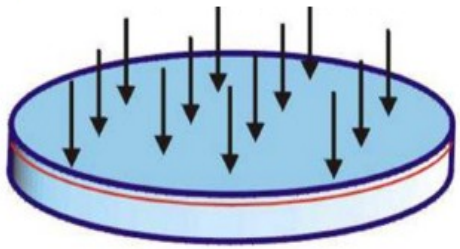

Polishing



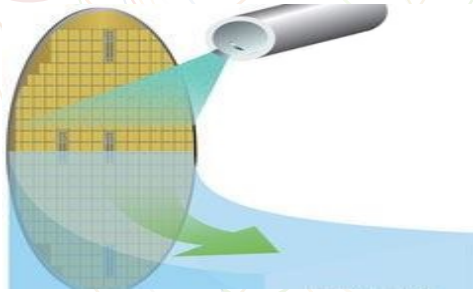

Vapor deposition




Laser processing



Doping



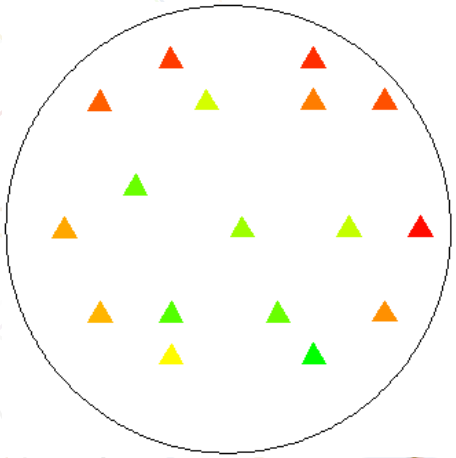
Cleaning

## Surface quality control in microelectronics

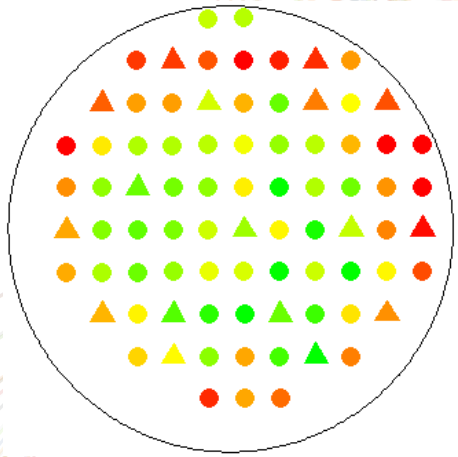
The infinite dimensional problem is made feasible via two steps :

1. *Construction of a spatial interpolation model*
2. Standard quality control of the model parameters

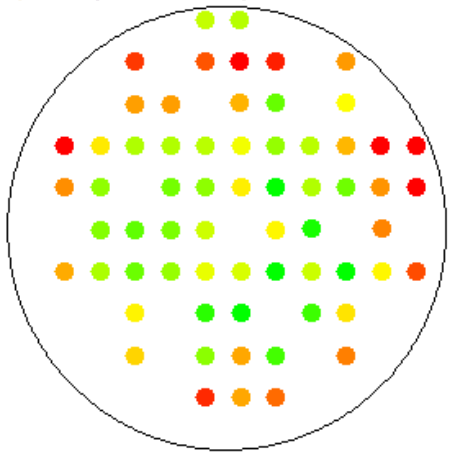
# Zoom on a wafer



DoE



DoE + test set



test set

## Interpolation problem on the unit disk

- The design of experiments (DoE) has 17 fixed (not controllable) points
- Here, presence of strong (but not pure) radial effects

# How to build a GP model on the unit disk ?

## Cartesian GP

Use the restriction of a GP defined on the unit square

$\rightarrow$ "Neighbours" are defined through horizontal and vertical distances

## Polar GP [Padonou and Roustant, 2016]

Combine a GP for the radius (on $[0, 1]$) and a GP for the angle (on the circle)

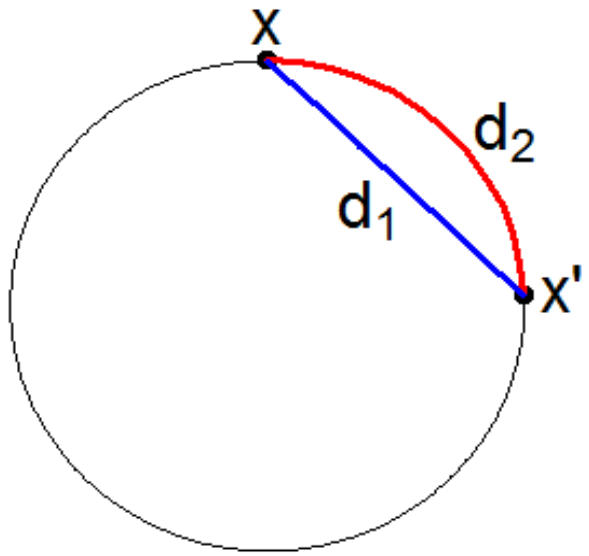
$$Z(x, y) = R(r) * A(\theta)$$

$\rightarrow$ "Neighbours" are defined through radial and angular distances

# How to build a GP model on the unit circle $\mathbb{S}$ ?

## Distances on $\mathbb{S}$

- Chordal distance $d_1$
- Geodesic distance $d_2$

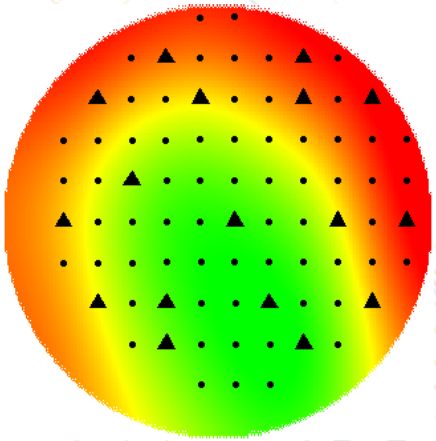



## Stationary (isotropic) kernels on $\mathbb{S} \times \mathbb{S}$

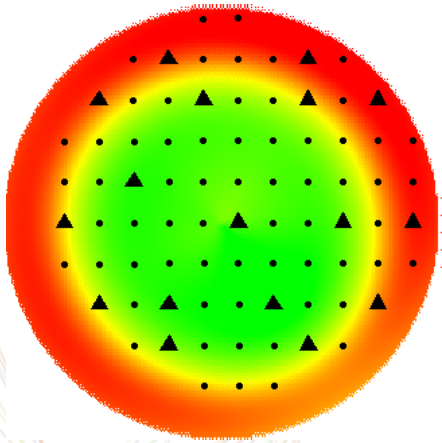
*Examples of construction*

- For $d_1$, just consider the restriction of a 2D isotropic GP to $\mathbb{S}$
- For $d_2$, plug-in $d_2$ into a 1D compactly supported stationary kernel $k(r)$, with support included in $[0, \pi[$

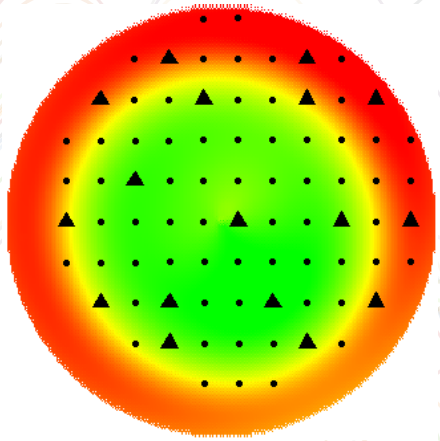
# Results (prediction accuracy)



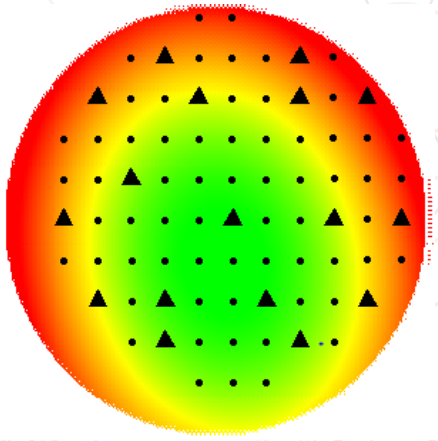
Cartesian GP



Polar GP (chord.)



Polar GP (geo.)



Zernike regression

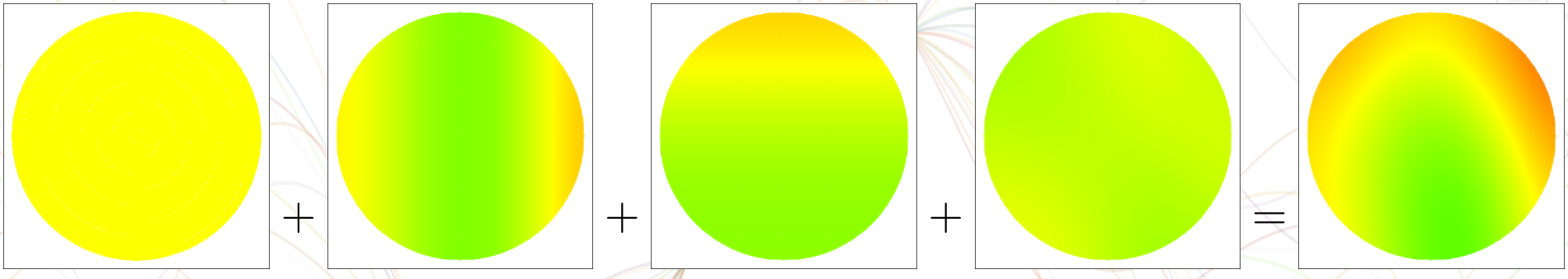
| GP type | Cartesian | | Polar (chordal) | | Polar (geodesic) | |
|---|---|---|---|---|---|---|
| Kernel type | $k_{\text{prod}}$ | $k_{\text{add}}$ | $k_{\text{prod}}$ | $k_{\text{add}}$ | $k_{\text{prod}}$ | $k_{\text{add}}$ |
| RMSE | 0.75 * | 0.77 | 0.69 | 0.60 * | 0.68 | 0.61 * |

Polar GPs better capture the radial pattern

$\Leftarrow$ Parameter estimation detects a strong angular correlation

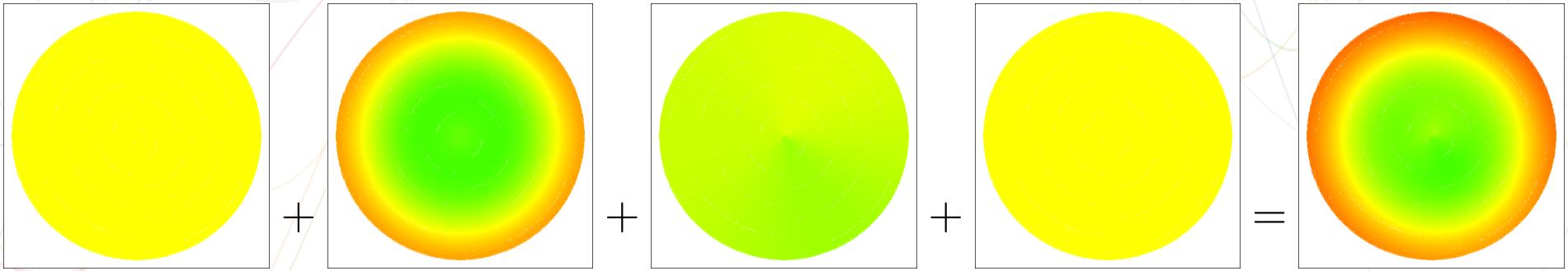
# Results (Hoeffding-Sobol [ANOVA] decomposition)

## Sobol decomposition of the Kriging mean, Cartesian GP, uniform measure over $[-1,1]^2$



| $\mu(x,y)$ | $m_1(x)$ | $m_2(y)$ | $m_{12}(x,y)$ | $m(x,y)$ |
|---|---|---|---|---|
| $-$ | $S = 46$ | $S = 52$ | $S = 2$ | Kriging mean |

## Sobol decomposition of the Kriging mean, polar GP, uniform measure over $\mathcal{D}$

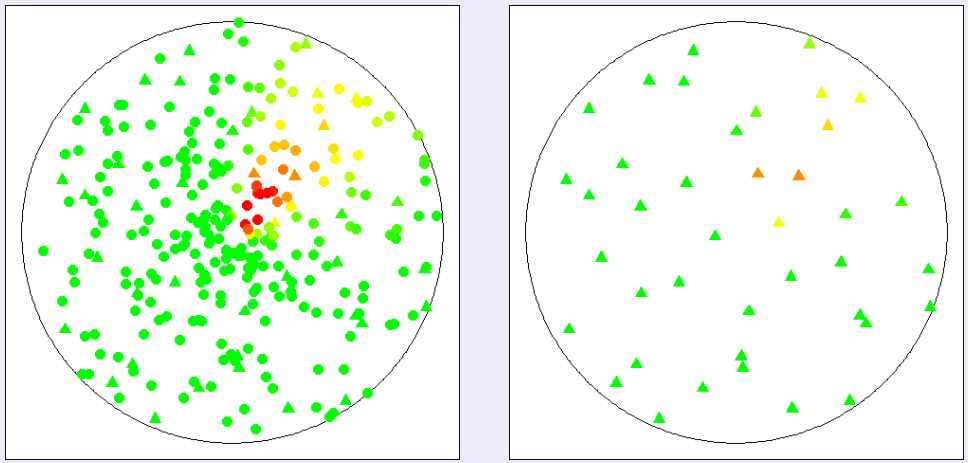


| $\mu(\rho,\theta)$ | $m_1(\rho)$ | $m_2(\theta)$ | $m_{12}(\rho,\theta)$ | $m(\rho,\theta)$ |
|---|---|---|---|---|
| $-$ | $S = 85$ | $S = 8$ | $S = 7$ | Kriging mean |

# Application in environments

## A model of atmospheric dispersion of a greenhouse gas

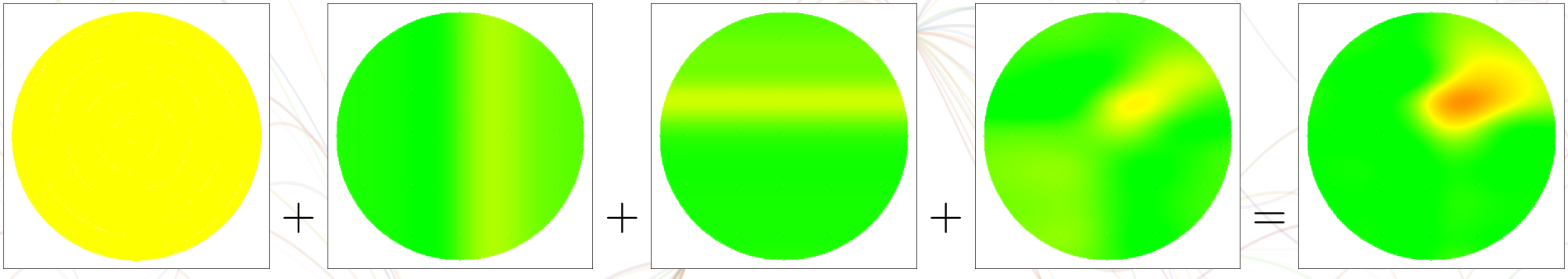
- Complex phenomenon simulated by a computer code [Batton-Hubert et al., 2013]
- Inputs : wind speed (in $[0, v_{\max}]$), wind direction (in $[0, 2\pi]$, directional input)



DoE + test set | DoE

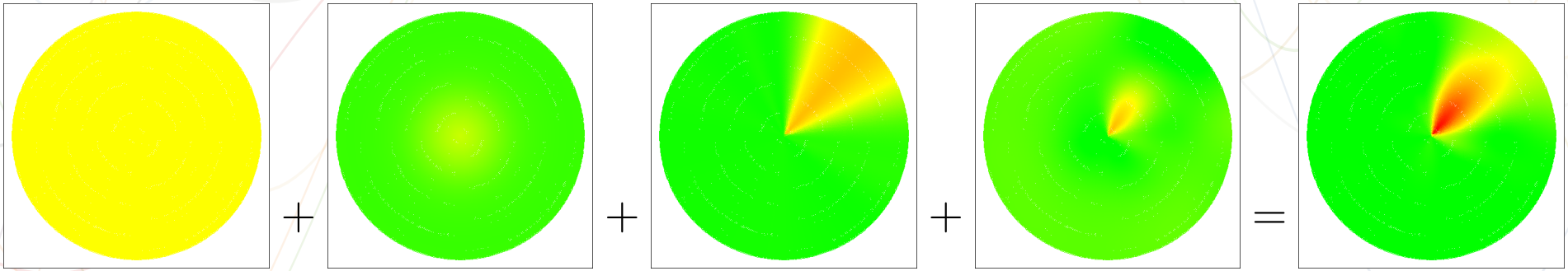
# Results (ANOVA decomposition) [Padonou and Roustant, 2017]

## Sobol decomposition of the Kriging mean, Cartesian GP, uniform measure over $[-1,1]^2$



| $\mu(x,y)$ | $m_1(x)$ | $m_2(y)$ | $m_{12}(x,y)$ | $m(x,y)$ |
|---|---|---|---|---|
| – | $S = 26$ | $S = 29$ | $S = 45$ | Kriging mean |

## Sobol decomposition of the Kriging mean, polar GP, uniform measure over $\mathcal{D}$



| $\mu(\rho,\theta)$ | $m_1(\rho)$ | $m_2(\theta)$ | $m_{12}(\rho,\theta)$ | $m(\rho,\theta)$ |
|---|---|---|---|---|
| – | $S = 6$ | $S = 80$ | $S = 14$ | Kriging mean |

# More about GPs on $d$-dimensional sphere $\mathbb{S}^d$

## Some entries in the literature

- A characterization of isotropic kernels, due to [Schoenberg, 1942]
  - $d = 1$ : $k(\theta) = \sum_{n=0}^{\infty} b_n \cos(n\theta)$ $\quad (b_n \geq 0, \quad \sum_n b_n < +\infty)$
  - $d \geq 2$ : invokes Gegenbauer polynomials.
- A comprehensive review and study by [Gneiting, 2013], among which :
  - Extension of Lévy's theorem : plugging the geodesic distance into a compactly supported 1-dimensional kernel works up to $d \leq 3$
  - Kernels defined with completely monotone functions
- Time-varying GPs on a sphere : see e.g. [Porcu et al., 2016]

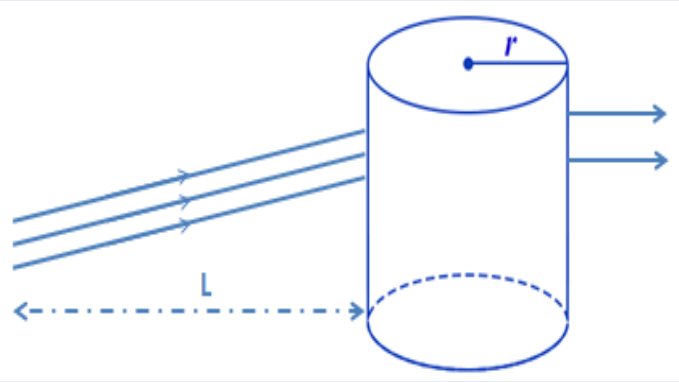
## See also...

- Detecting periodicities in signals with RKHS [Durrande et al., 2016]
- Geodesic GPs to reconstruct free-form surfaces [del Castillo et al., 2015]

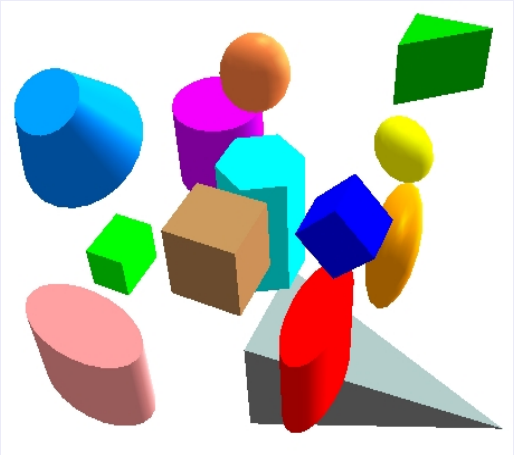
# GP for categorical inputs : groups of levels & trees

## A guiding case study : Nuclear activity quantification

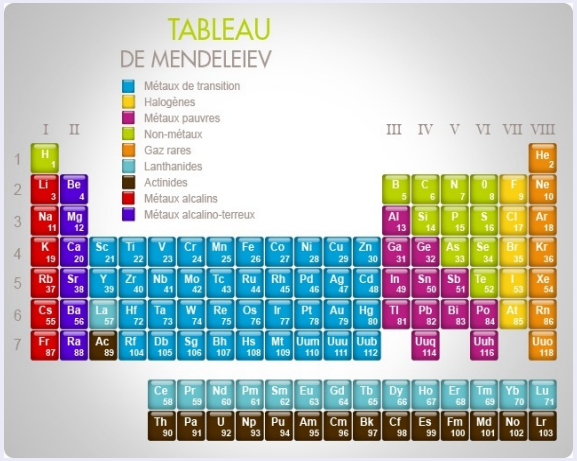
1. Computation using Monte Carlo
2. 4 continuous inputs : $L$, density, mean width, lateral surface
3. 3 categorical inputs : energy, form, chemical element.



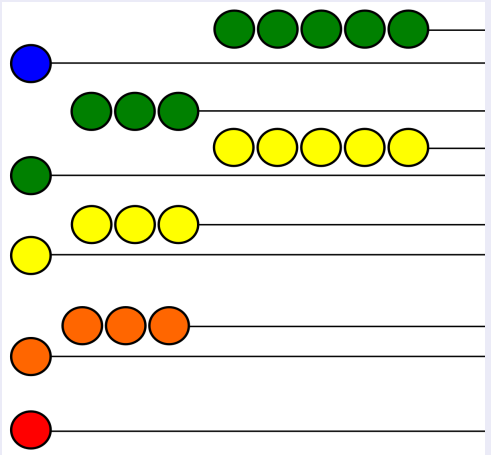

## Specific problem : large number of levels



Form (s, c, p)




$Z \in \{1, \ldots, 94\}$

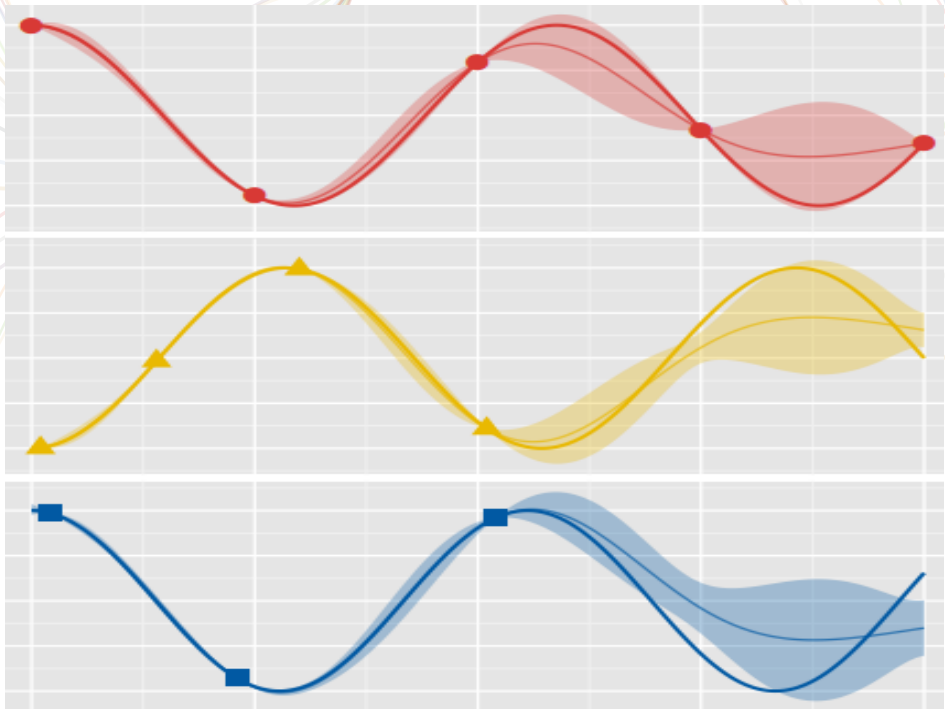


$E \in \{E_1, E_2, E_3, E_4, E_5, E_6\}$

## GP interpretation when no distance is available

A GP for $(x, u) \in [0,1] \times \{"red", "yellow", "blue"\}$ can be defined with :

- a kernel on $[0,1]$, i.e. a **covariance function**
- a kernel on $\{"red", "yellow", "blue"\}$ , i.e. a **covariance matrix**
- a valid operation between them, such as *, $+$, ...



Example : $\mathrm{Cov}(Y(x, "blue"), Y(x', "red")) = k(x, x') \times 0.8$

# GP for categorical inputs : group kernels for partitioned levels

A group kernel is a block covariance matrix

## Block covariance matrix

$$\mathbf{T} = \begin{pmatrix} \mathbf{W}_1 & \mathbf{B}_{1,2} & \cdots & \mathbf{B}_{1,G} \\ \mathbf{B}_{2,1} & \mathbf{W}_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{B}_{G-1,G} \\ \mathbf{B}_{G,1} & \cdots & \mathbf{B}_{G,G-1} & \mathbf{W}_G \end{pmatrix}$$

with constant between-group blocks

## Hierarchical (group/level) process

$$\eta_{g/\ell} = \mu_g + \lambda_{g/\ell}$$

with :

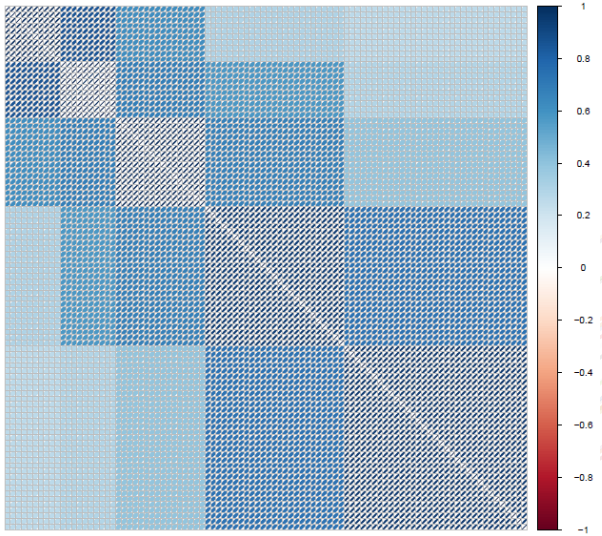
- Gaussian ind. priors for $\boldsymbol{\mu}, \boldsymbol{\lambda}_{g/.}$
- Centering cond. : $\sum_\ell \lambda_{g/\ell} = 0$

## Main results [Roustant et al., 2018]

- Connection with hierarchical GPs : $\mathbf{T} = \mathrm{cov}(\boldsymbol{\eta})$.
- Characterization & parameterization of valid group kernels

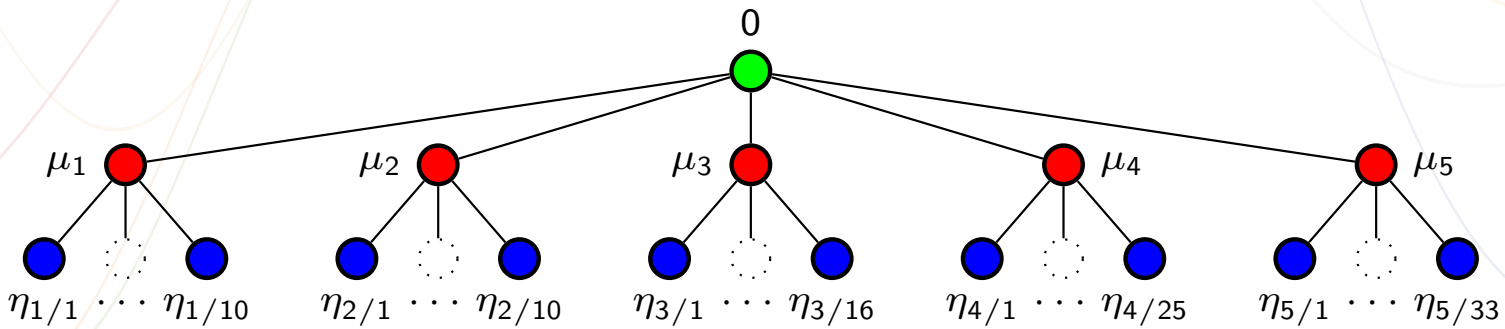
# Result on the case study

For the categorical input 'chemical element', 5 groups are identified by experts
$\rightarrow$ Parsimonious parametrization with only 20 parameters (instead of $94 \times 95/2$)




- 10 between-group covariances
- 5 within-group covariances
- 5 within-group variances

With a stratified LHS design of size $3 \times 94$, the $Q^2$ of the whole model is $> 0.95$

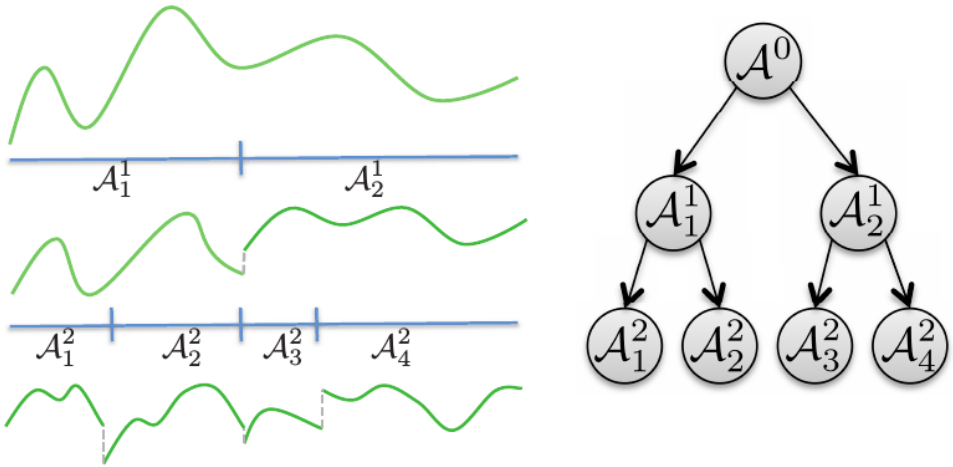


# More on hierarchical GPs

- Wavelet kernels [Amato et al., 2006]
- Treed Gaussian processes [Gramacy, 2007]
- Lattice Kriging [Nychka et al., 2015]
- Multiresolution GPs [Fox and Dunson, 2012]
- Hierarchical GPs [Park and Choi, 2010]
- ...

*Remark : In these models, the children ("details in subareas") are independent conditionaly on the mother ("trend").*

*This was not the case before since children sum to 0 (cond. on the mother).*



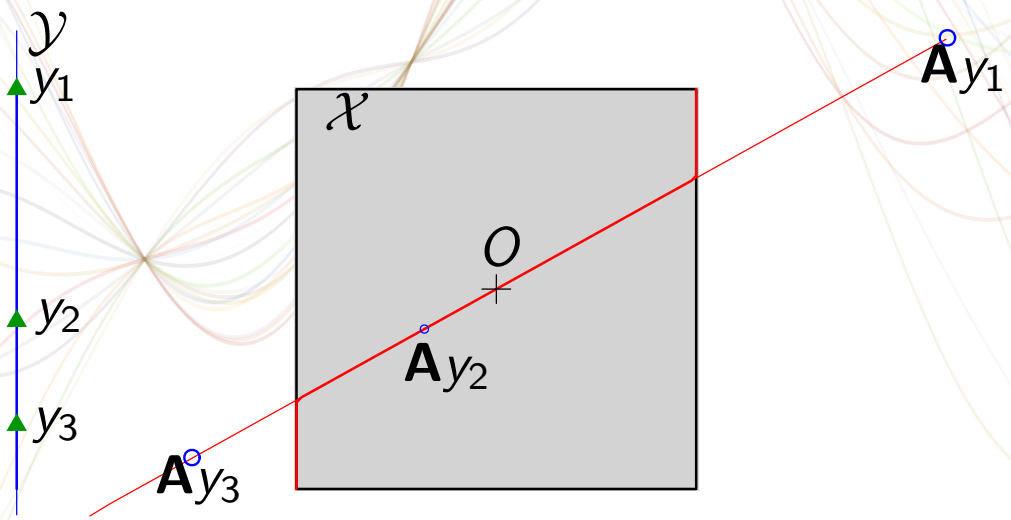

Source : [Fox and Dunson, 2012], Figure 2.

# Outline

# Random EMbedding Bayesian Optimization (REMBO, [Wang et al., 2013] )

**Hypothesis** $(\mathcal{H})$ : Only $d_e \ll D$ of the $D$ variables of $f$ are influential

**Principle** : Embed $\mathcal{Y} \subset \mathbb{R}^d$ to $\mathcal{X}$ ($d \ll D$) with a random matrix of normals.

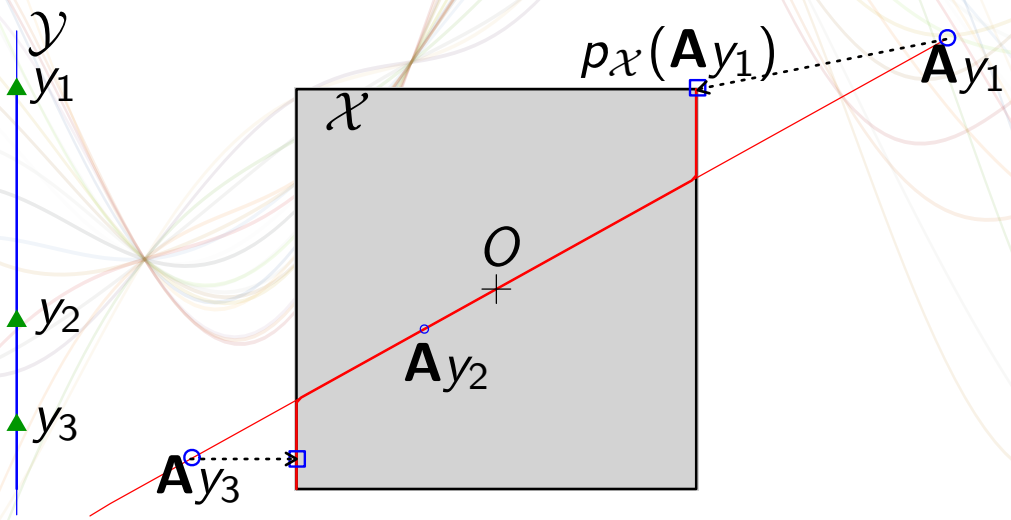



A convex projection on $\mathcal{X}$, $p_{\mathcal{X}}$, is applied to points mapped outside of $\mathcal{X}$.

# Random EMbedding Bayesian Optimization (REMBO, [Wang et al., 2013] )

**Hypothesis** $(\mathcal{H})$ : Only $d_e \ll D$ of the $D$ variables of $f$ are influential

**Principle** : Embed $\mathcal{Y} \subset \mathbb{R}^d$ to $\mathcal{X}$ ($d \ll D$) with a random matrix of normals.



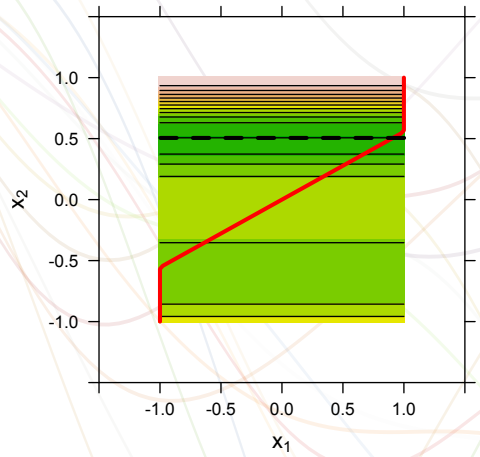

A convex projection on $\mathcal{X}$, $p_{\mathcal{X}}$, is applied to points mapped outside of $\mathcal{X}$.

# REMBO principle

**Interest** : Optimization of $f$ is carried out on

$$g : \begin{array}{ccc} \mathcal{Y} \subset \mathbb{R}^d & \to & \mathbb{R} \\ \mathbf{y} & \mapsto & f(p_{\mathcal{X}}(\mathbf{A}\mathbf{y})) \end{array}$$

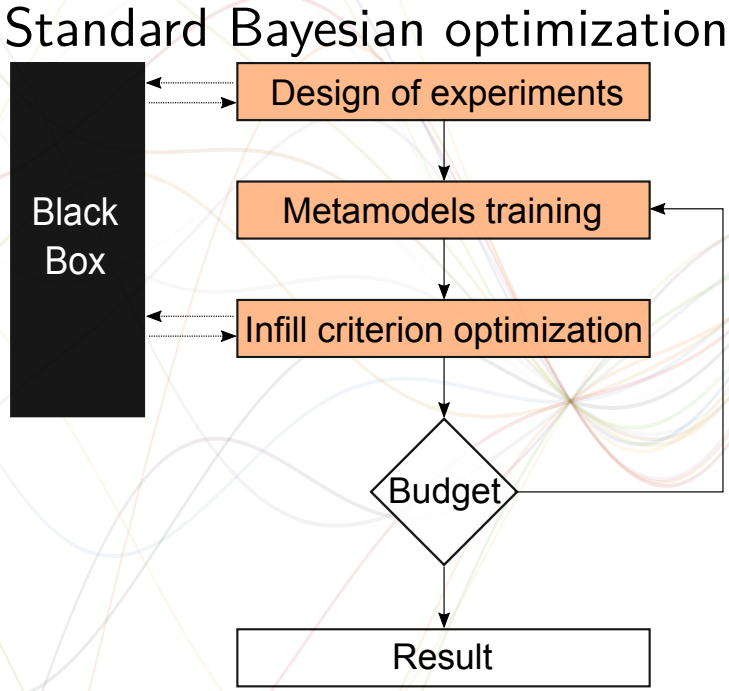
$\to$ Much smaller search space




**Theorem**

If $\mathcal{Y} \supset \mathcal{B}(0, d/\varepsilon)$ and under $(\mathcal{H})$, finding $\mathbf{y}^* \in \mathcal{Y}$ such that $g(\mathbf{y}^*) = \min f$ has a solution with probability at least $(1 - \varepsilon)$.

# REMBO procedure for a costly function $f$




Orange : dimension $D$

Yellow : dimension $d$ or $D$

Green : dimension $d$

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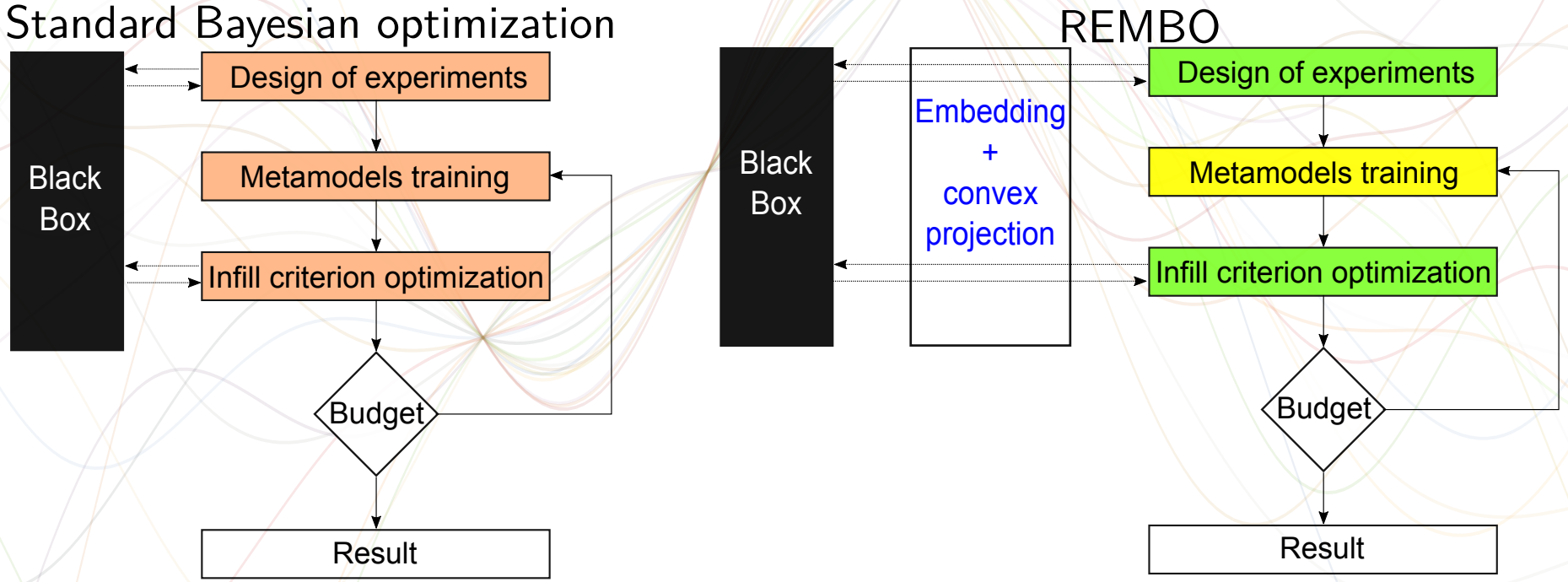


Orange : dimension $D$

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# Choice of the covariance kernel for sequential optimization

**Main issue** : Incorporating high-dimensional information on $f$ via a kernel

[Wang et al., 2013] proposed two covariance kernels :

- kernel defined between projections in $\mathcal{X}$,
  e.g. $k_{\mathcal{X}}(\mathbf{y}, \mathbf{y'}) = exp(-\frac{\|p_{\mathcal{X}}(\mathbf{Ay}) - p_{\mathcal{X}}(\mathbf{Ay'})\|_D^2}{2l^2})$
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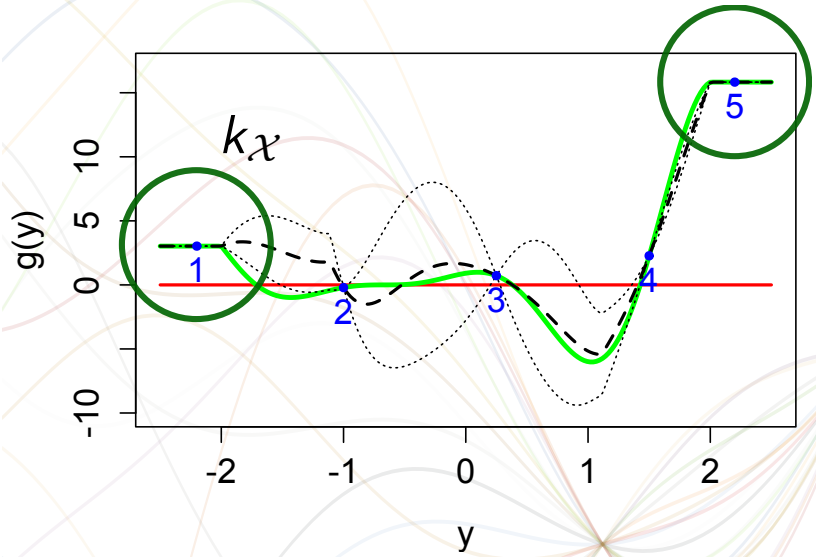
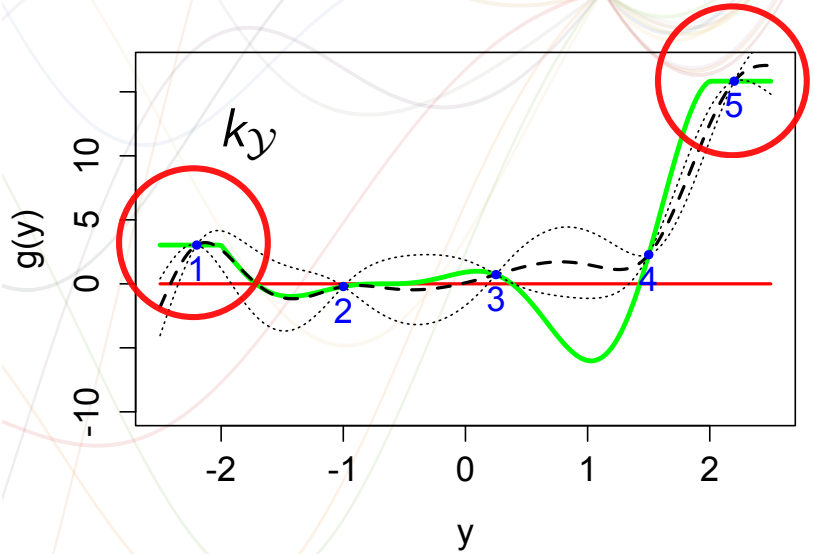
  - kriging in dimension $D$

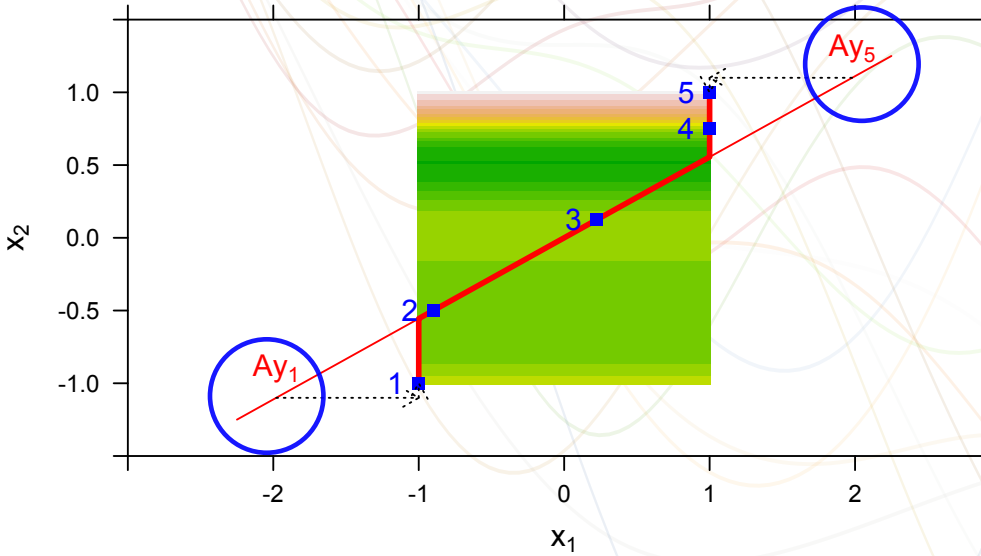
- kernel defined between points of $\mathcal{Y}$,
  e.g. $k_{\mathcal{Y}}(\mathbf{y}, \mathbf{y'}) = exp(-\frac{\|\mathbf{y} - \mathbf{y'}\|_d^2}{2l^2})$
  - kriging in dimension $d$
  - suffers from non-injectivity of the mapping

# Illustration : GP predictions with $k_{\mathcal{X}}$ and $k_{\mathcal{Y}}$



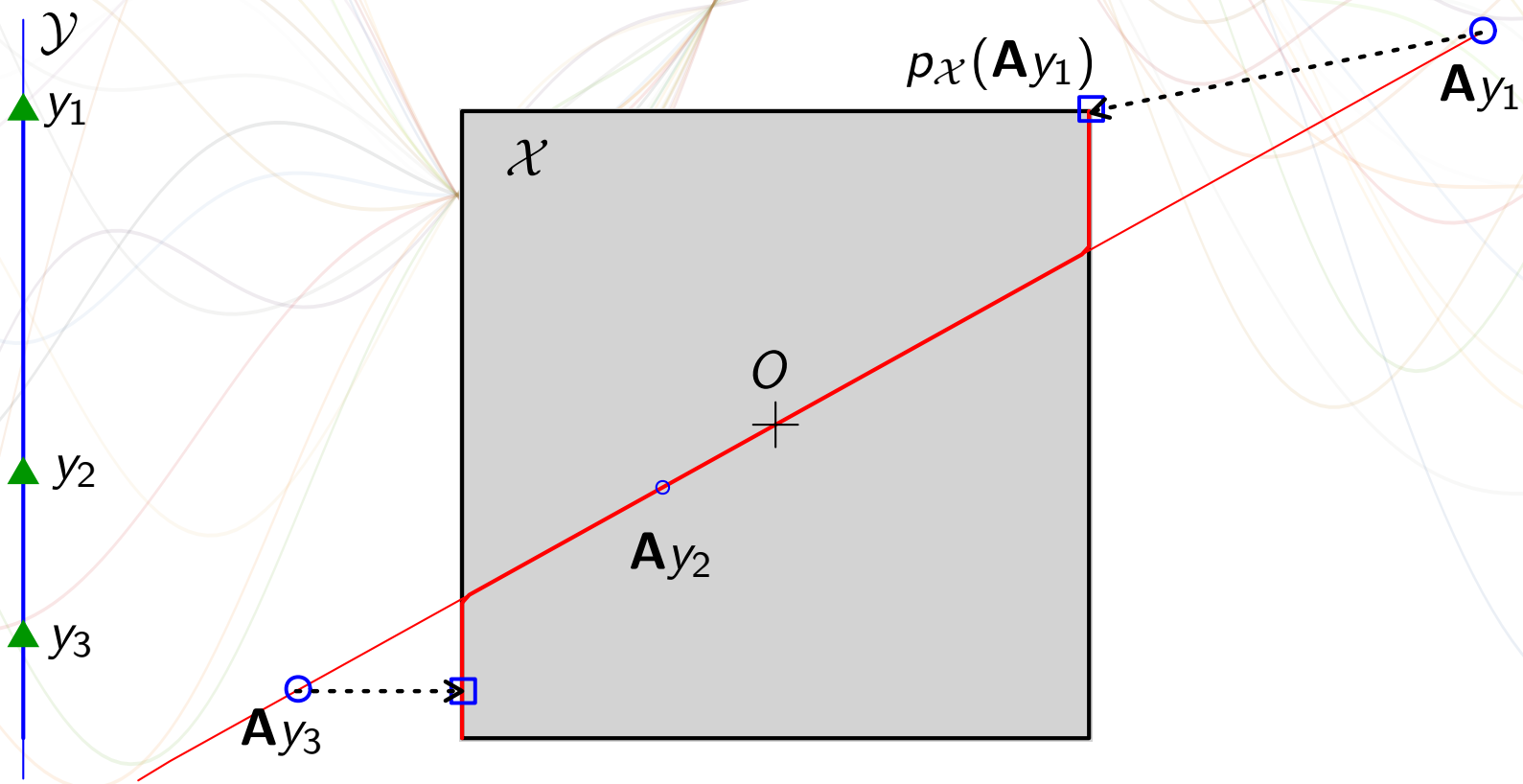

$$\mathcal{Y} = [-2.5, 2.5],\ \mathcal{X} = [-1, 1]^2$$




$$\mathbf{A} = [0.9, 0.5]^T$$

# Towards a new kernel : new mapping [Binois et al., 2015]

**Aim** : accounting for real distances within a low-dimensional kernel



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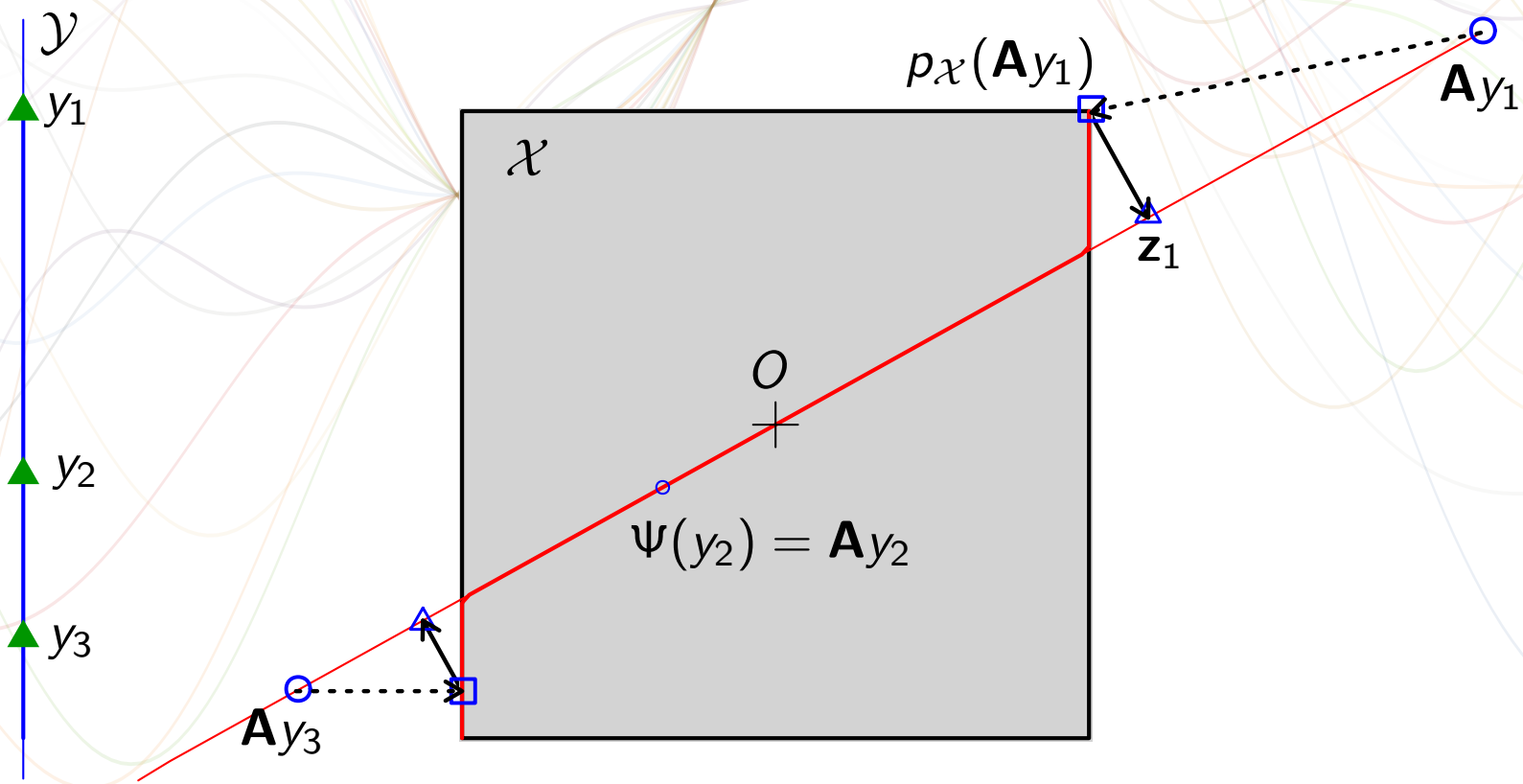

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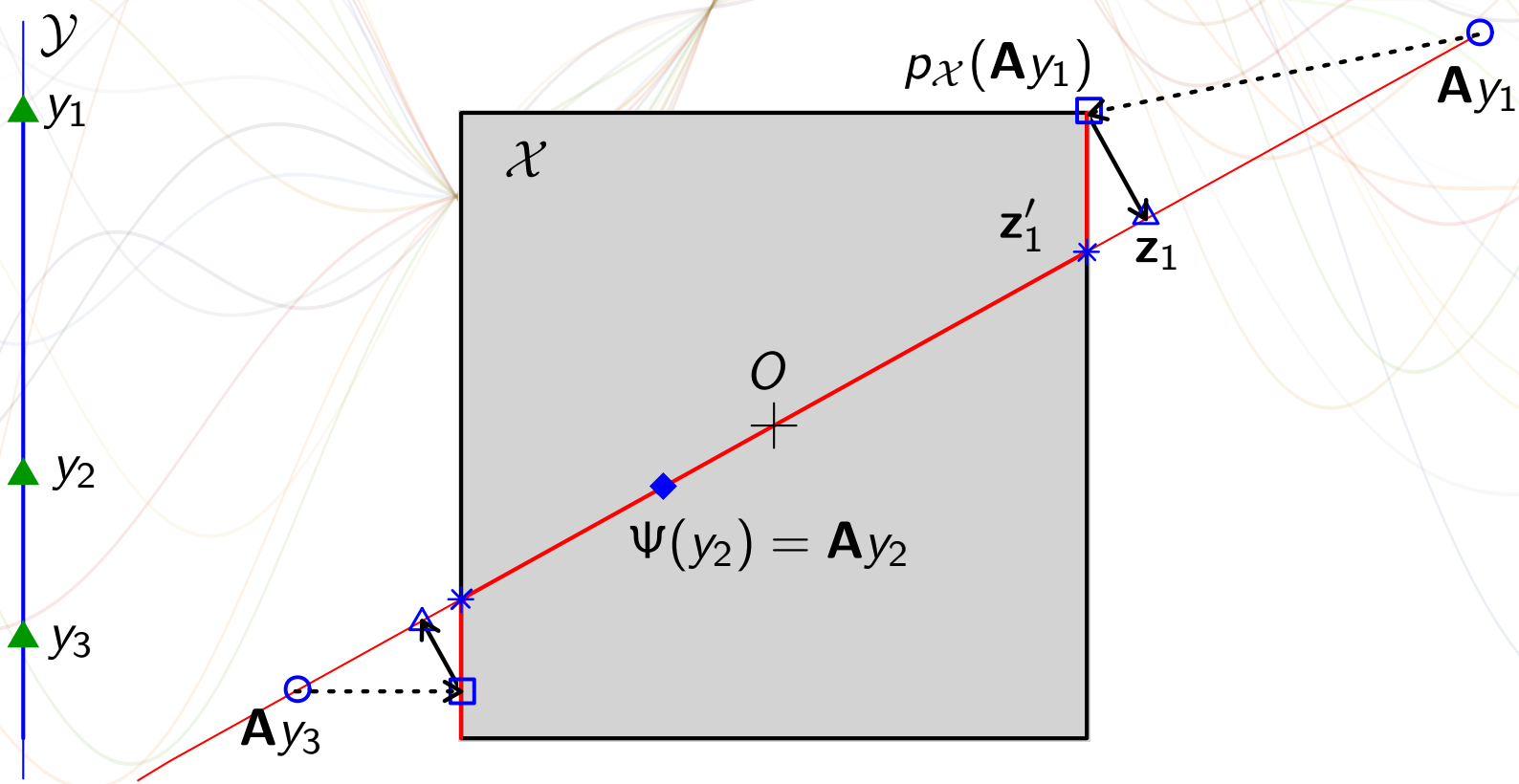

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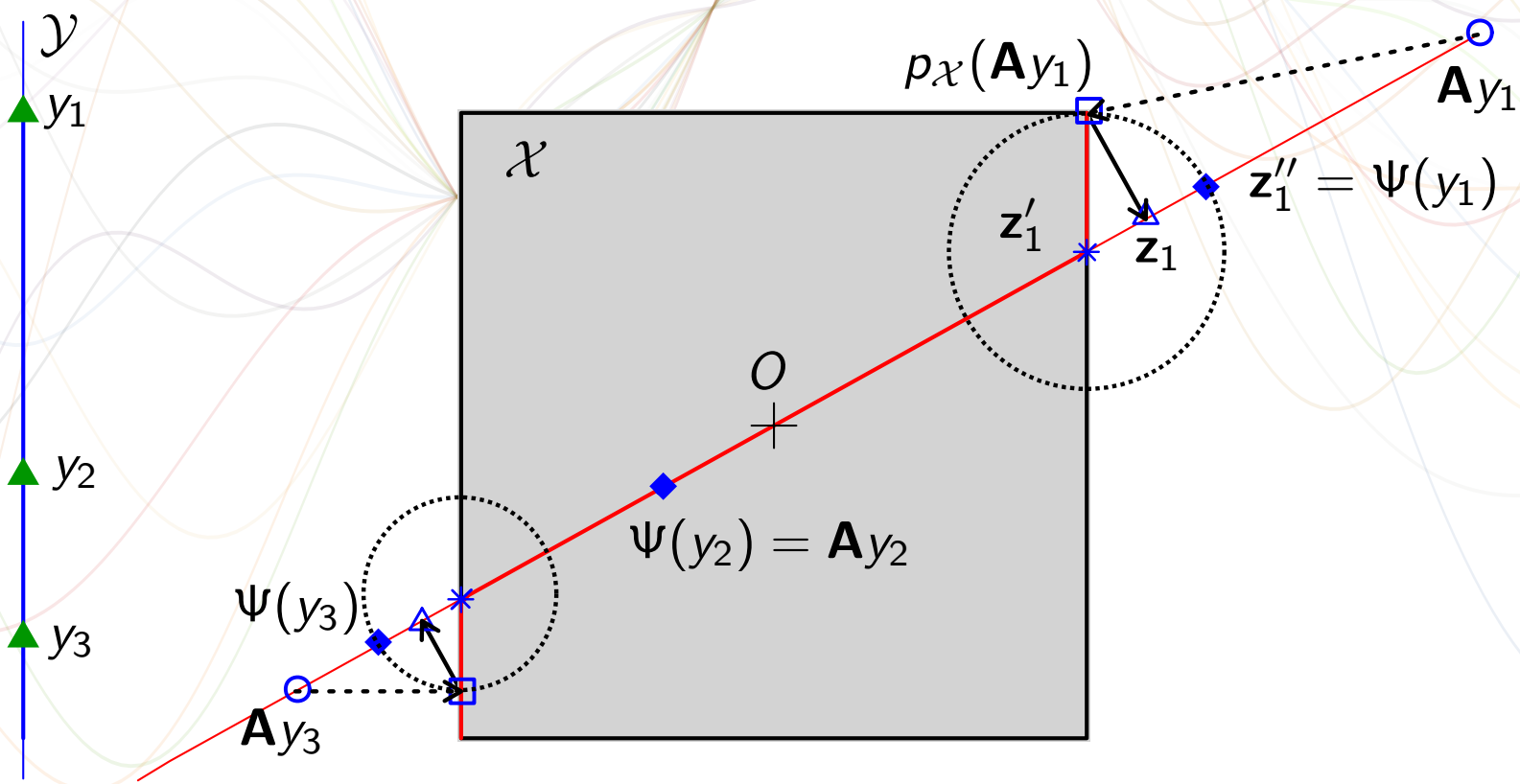

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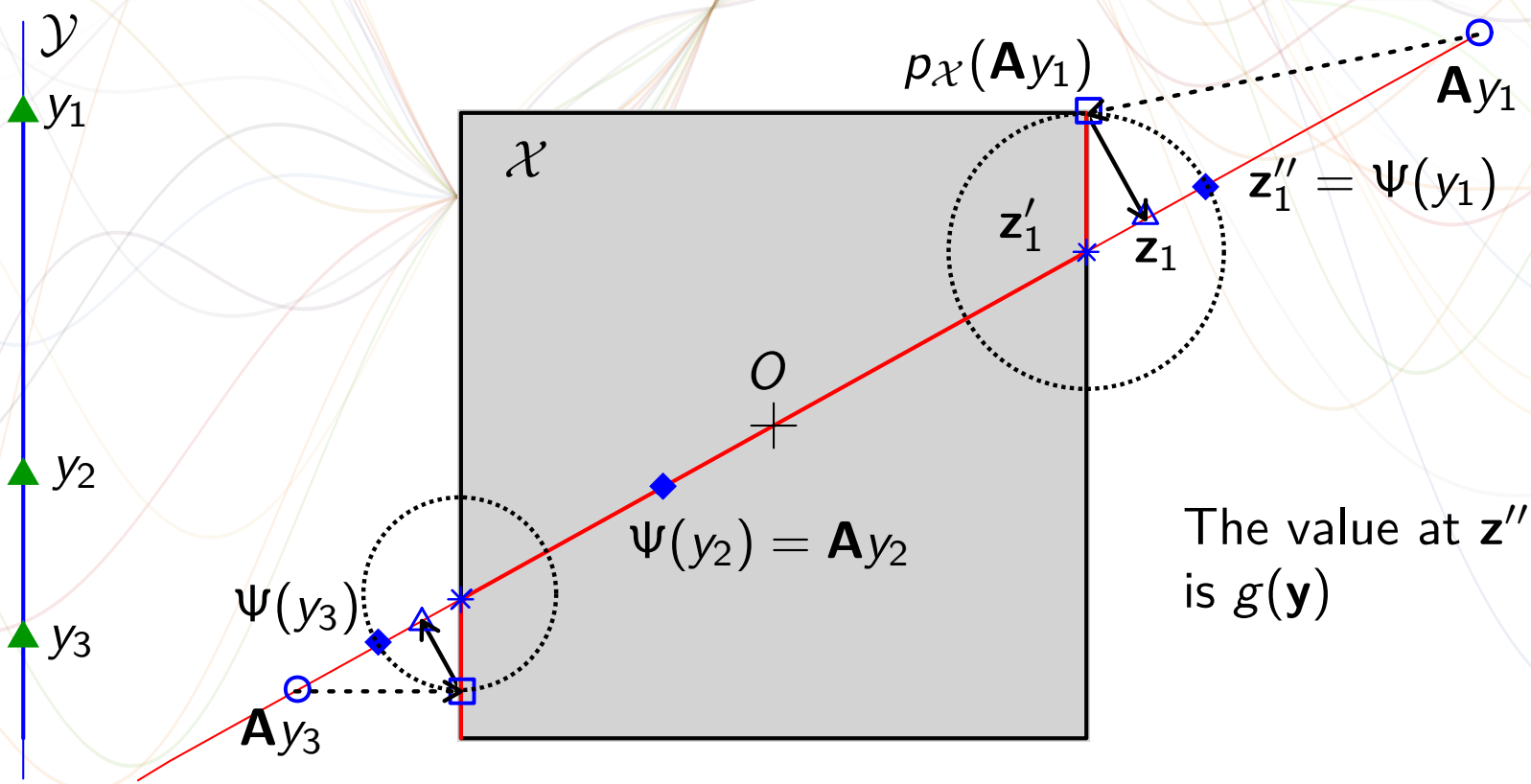
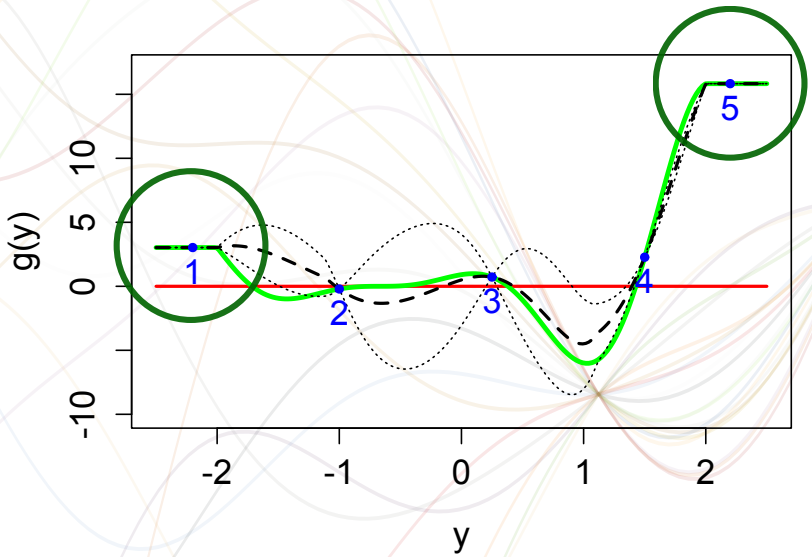



The value at $\mathbf{z}''=\Psi(\mathbf{y})$ is $g(\mathbf{y})$

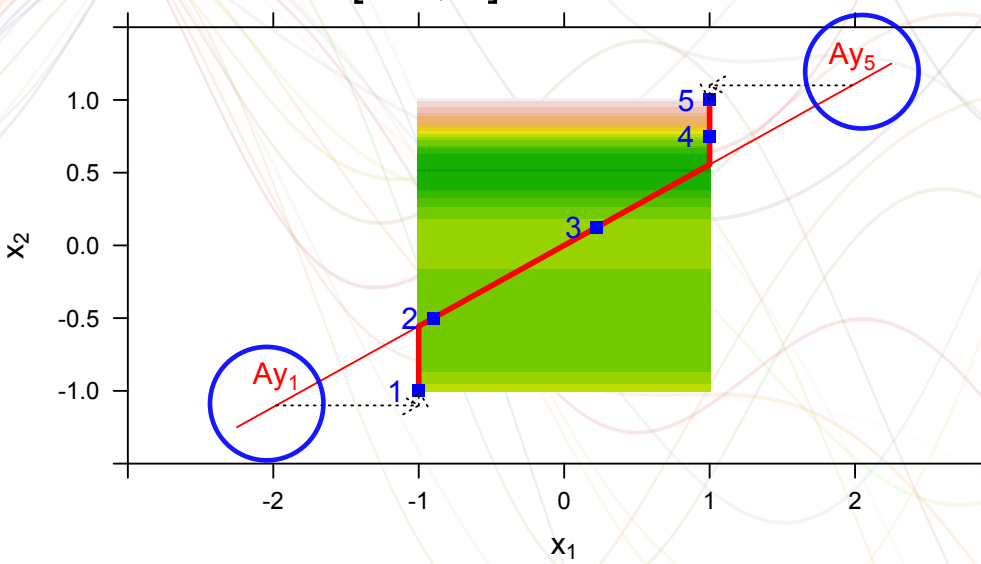
# Illustration : GP predictions with $k_\Psi$

$$\mathbf{A} = [0.9, 0.5]^T$$

$\mathcal{Y} = [-2.5, 2.5]$




$\mathcal{X} = [-1, 1]^2$

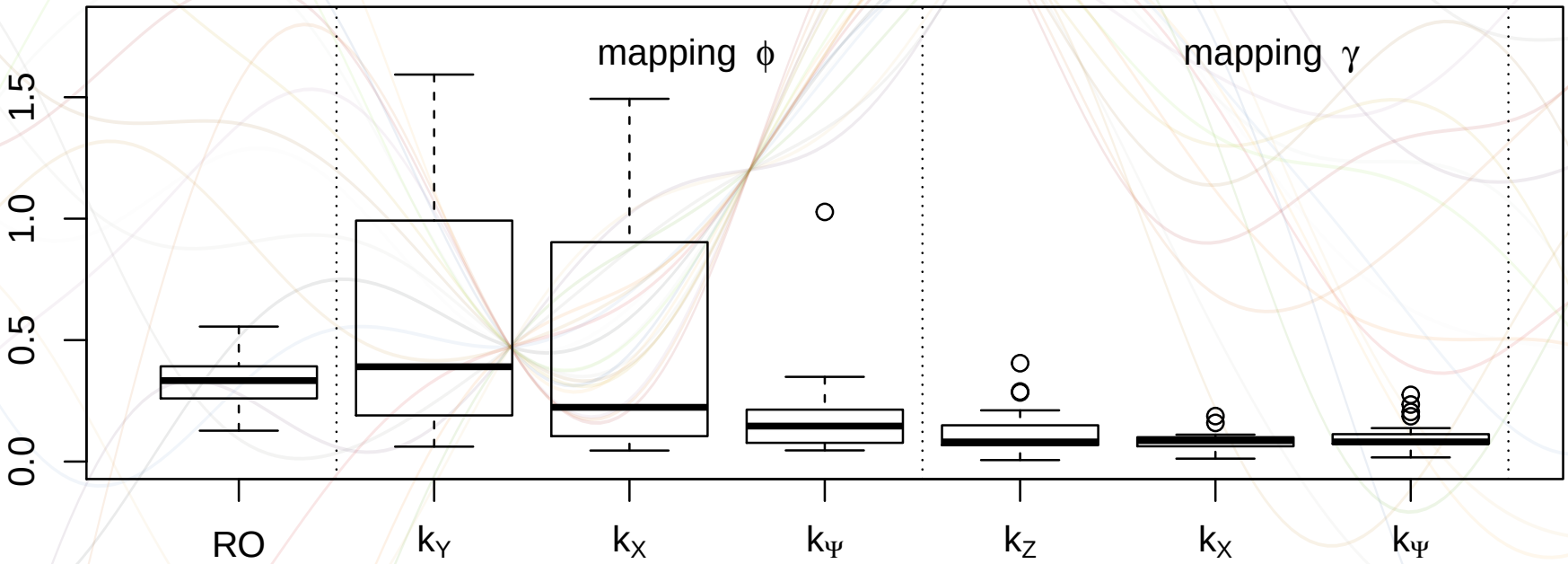



Warped kernel,

e.g. $k_\Psi(\mathbf{y}, \mathbf{y'}) = exp(-\frac{\|\Psi(\mathbf{y}) - \Psi(\mathbf{y}')\|_d^2}{2l^2})$

# An example of optimization performance in 50 dim. [Binois et al., 2018]

Hartman 6 function, $d = 6$, $D = 50$, 250 evaluations over 25 runs, optimality gap :




RO : Random optimization
$\phi(y)$ : embedding from $\mathcal{Y} = [-\sqrt{d}, \sqrt{d}]^d$ to $\mathcal{X}$
$\gamma(z)$ : embedding from $\mathcal{B} \subseteq Ran(\mathbf{A})$ to $\mathcal{X}$.

# Outline

# Some conclusions

- We illustrated the versatility of GPs on small data (metamodeling)
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- There is a florishing literature on GPs for big data :
  - neural networks for GPs : deep GPs
  - scalable GPs with variational inference
  - ...
- What statisticians & mathematicians can add more
  - A better theoretical understanding (e.g. convergence results on EGO)
  - Connections with math. theory (e.g. here : spline and inequalities)
  - Different point of views (e.g. identifiability "vs" prediction only)
  - ...

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- All collaborators involved in the presented works !


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