Introduction to Gaussian Process Surrogate Models

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Introduction to Gaussian Process Surrogate models

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`http://github.com/NicolasDurrande/intro_to_GPs_with_R`

Statistical models in engineering and physics?

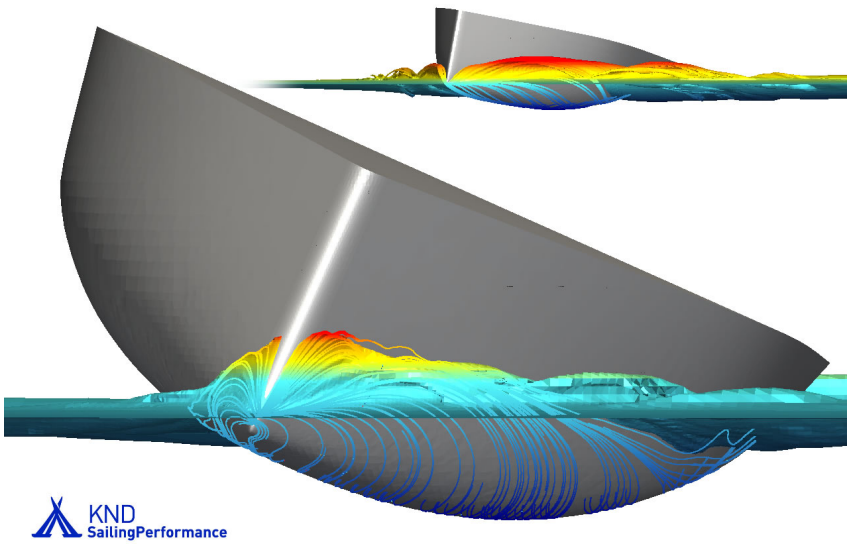
There is a wide variety of situations where getting data about a system performance can be extremely expensive:

- real world experiments in particular
  - destructive tests
  - prototyping
- and even numerical experiments (e.g. non linear, with uncertainties, ...): Numerical experiments are less expensive but can be very time consuming! (expl.: 15 min / execution, 5 parameters, a grid with 10 levels, total time $= 10^5 \times 15$ min $>$ 2 years and 10 months)

Example: boat hull design

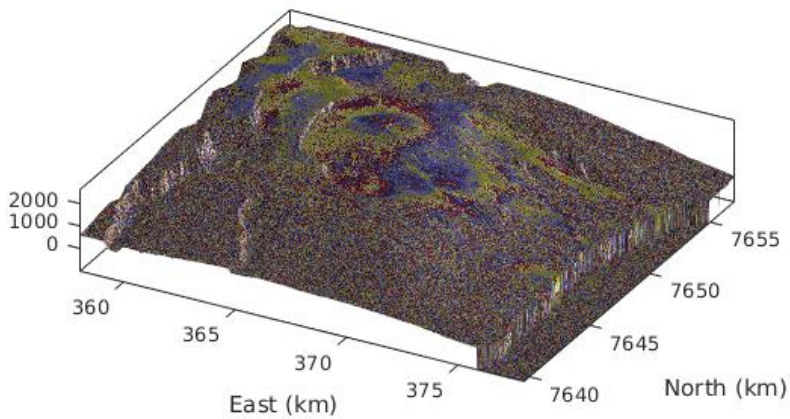
real

numerical



Example: volcano internal structure identification

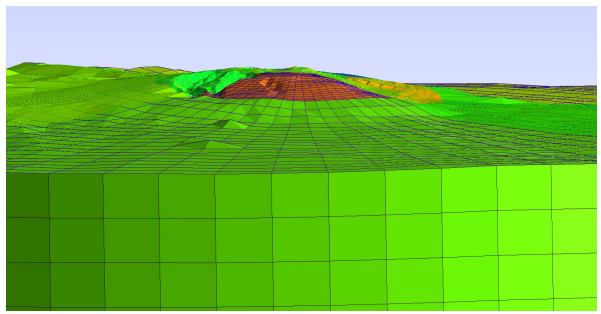
real



Range change measured prior to the May 2016 Piton de la Fournaise eruption. It may correspond to a source inflation + a stratisfied atmospheric signal.

(thanks J.-L. Froger)

numerical



Finite elements mesh of the Piton de la Fournaise.

(thanks V. Cayol)

In all these cases, the quantity of interest (drag, misfit ...) can be seen as a function of the input parameters

$$y = f(X)$$

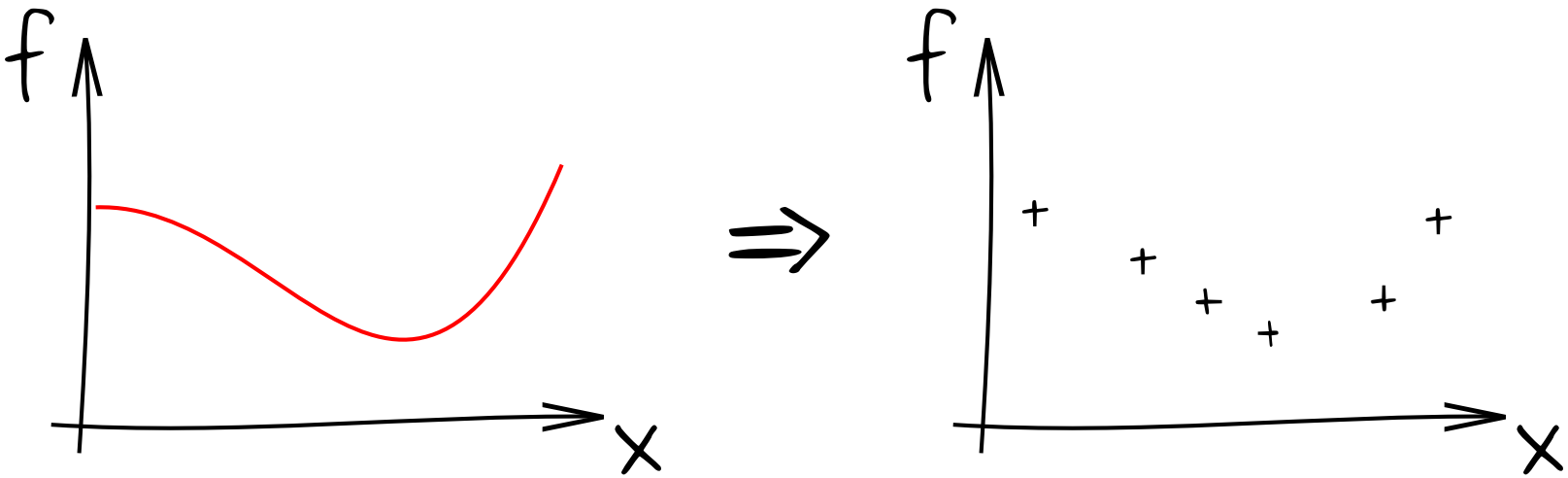
where f is a **costly to evaluate function**.

In the following, we will assume that

- $X \in \mathbb{R}^d$: There are d input variables,
- $y \in \mathbb{R}$: The output is a scalar.

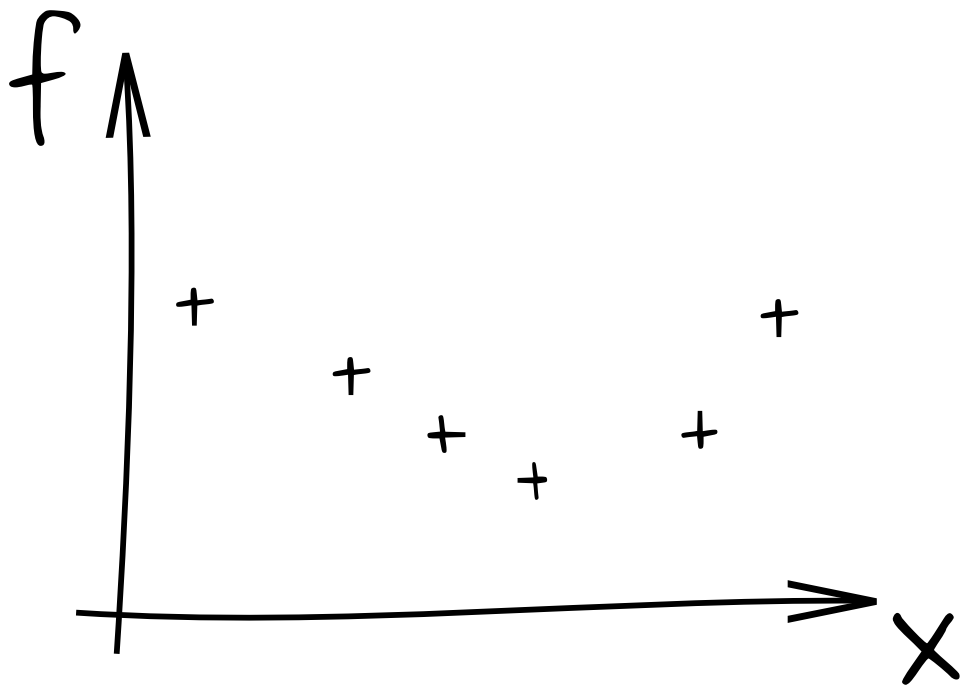
The fact that f is **costly to evaluate** changes a lot of things...

1. Representing the function is not possible...



The fact that f is **costly to evaluate** changes a lot of things...

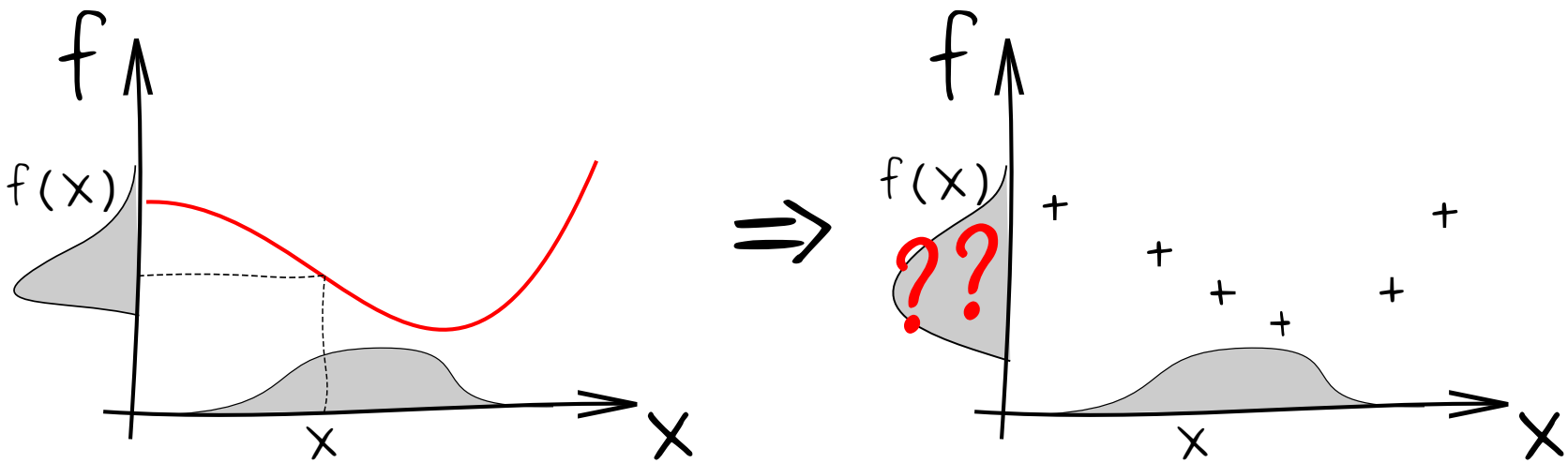
2. Computing integrals is not possible...



What is the mean value of f?

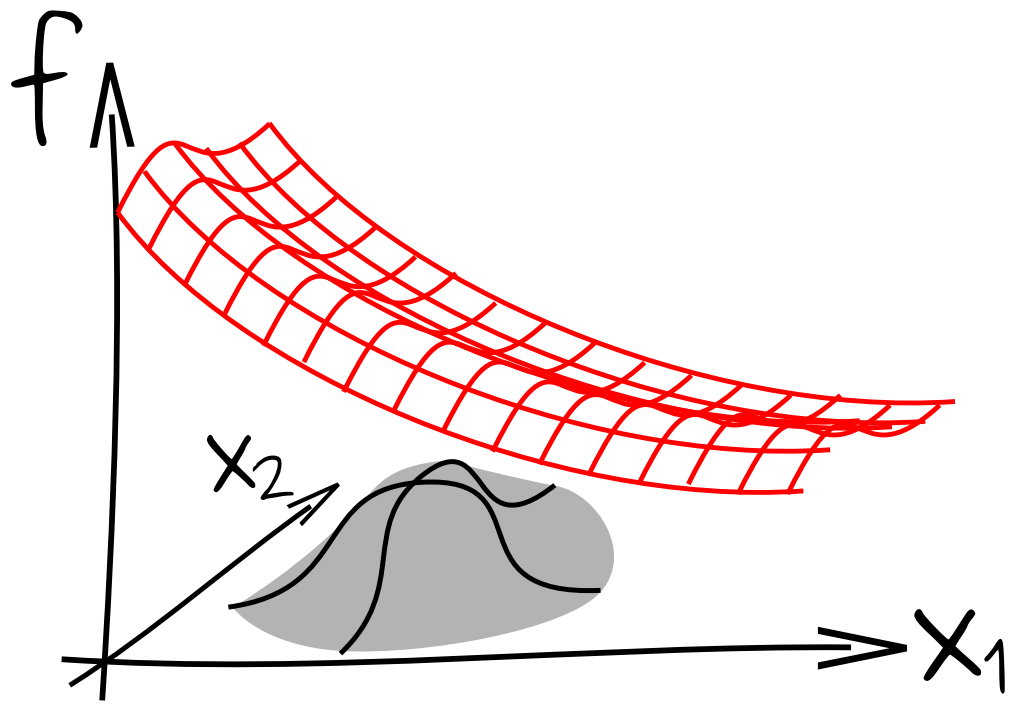
The fact that f is **costly to evaluate** changes a lot of things...

3. Uncertainty propagation is not possible...



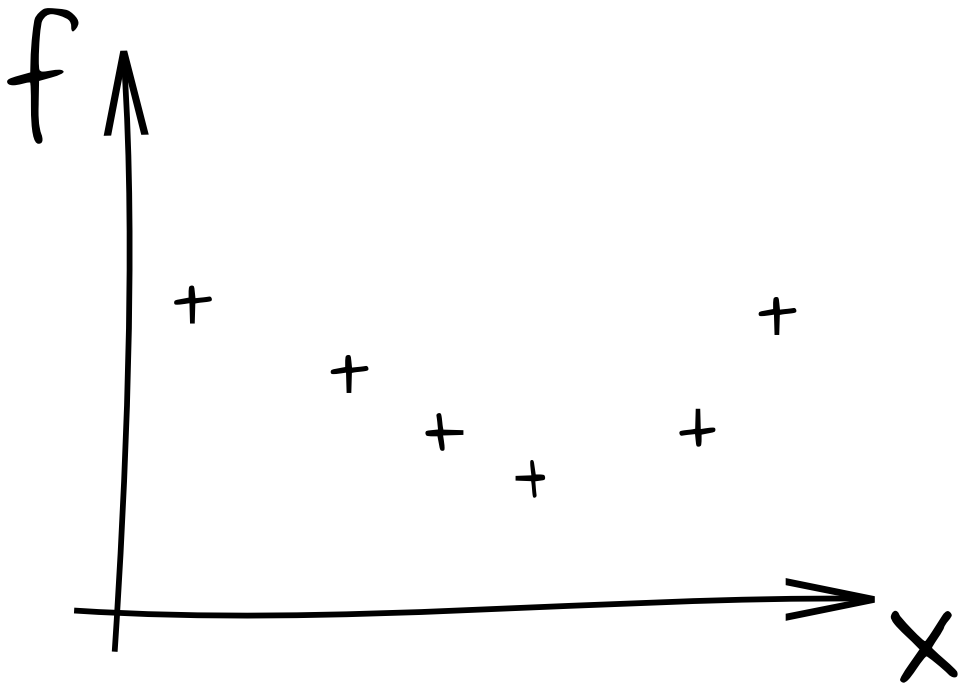
The fact that f is **costly to evaluate** changes a lot of things...

4. Sensitivity analysis is not possible...

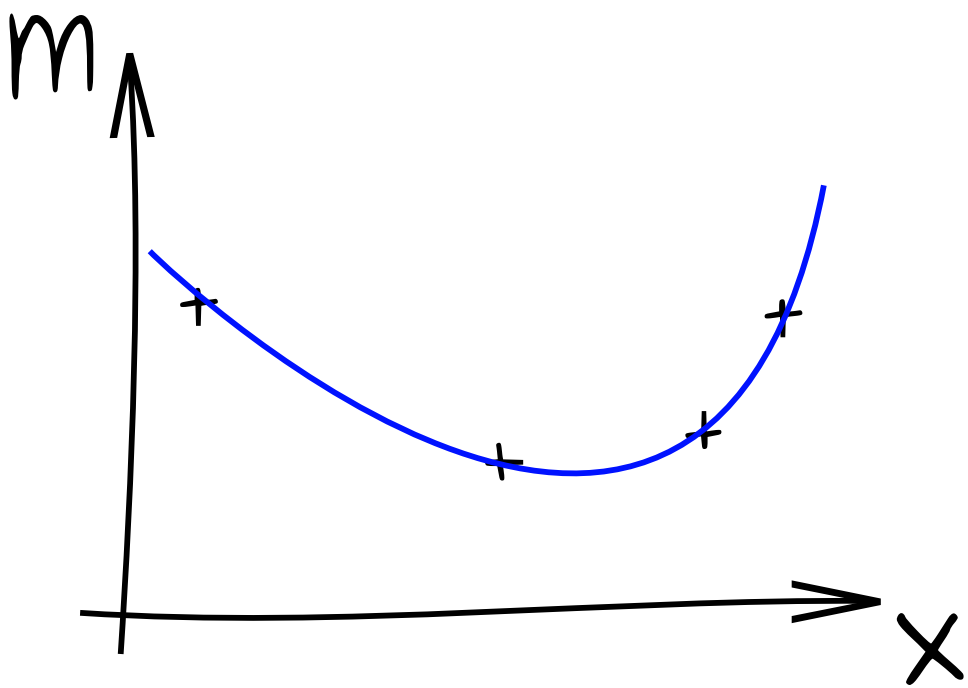


The fact that f is **costly to evaluate** changes a lot of things...

5. Optimisation is also tricky...

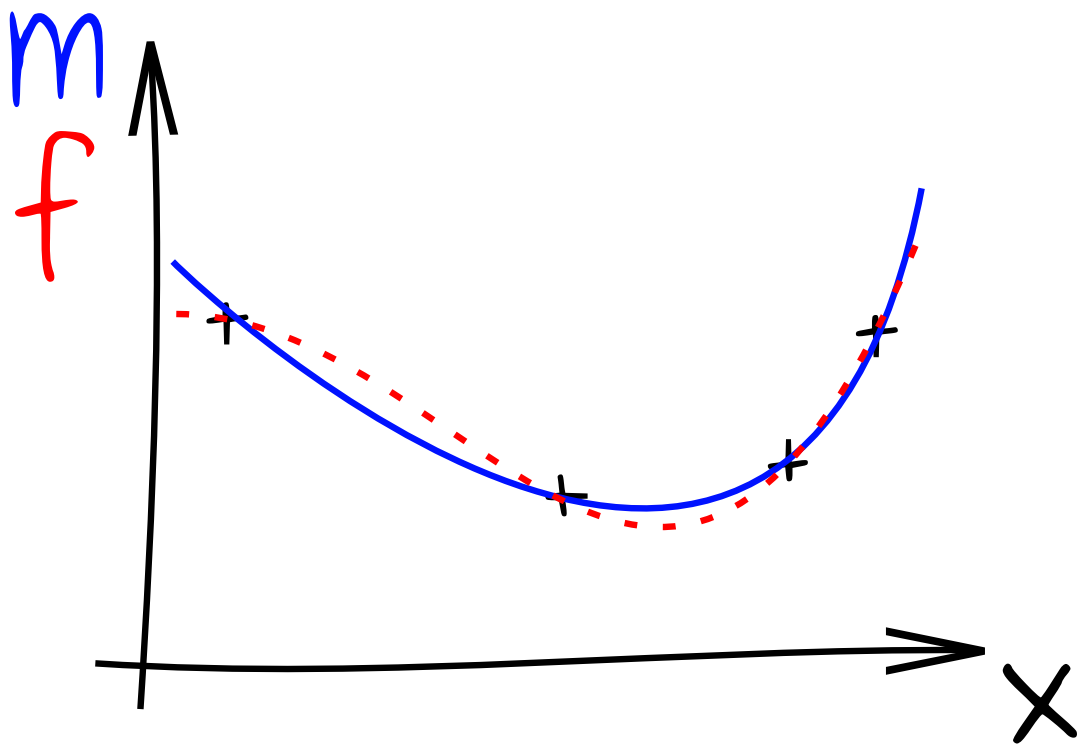


The principle of statistical modelling is to use the data to build a mathematical approximation of the function.

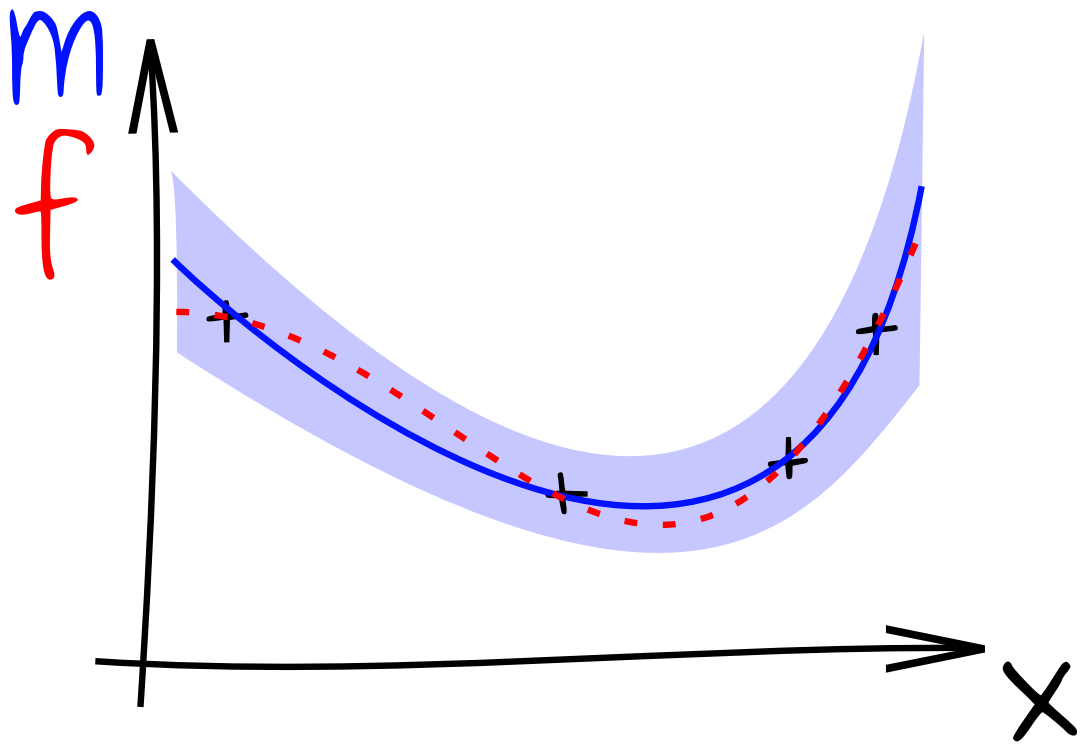


The model can then be used to answer all previous questions

Of course, there is a difference between f and m...



Why **statistical models**?
We want to be able to quantify the model error:



The confidence intervals can be used to obtain a **measure of uncertainty on the value of interest**.

In the sequel, we will use the following notations :

- The set of observation points will be represented by a $n \times d$ matrix $X = (X_1, ..., X_n)^t$
- The vector of observations will be denoted by F : $F_i = f(X_i)$ (or $F = f(X)$).

There are many surrogate methods available on the market

- Linear regression
- Smoothing splines
- Gaussian process regression
- Neural Networks
- ...

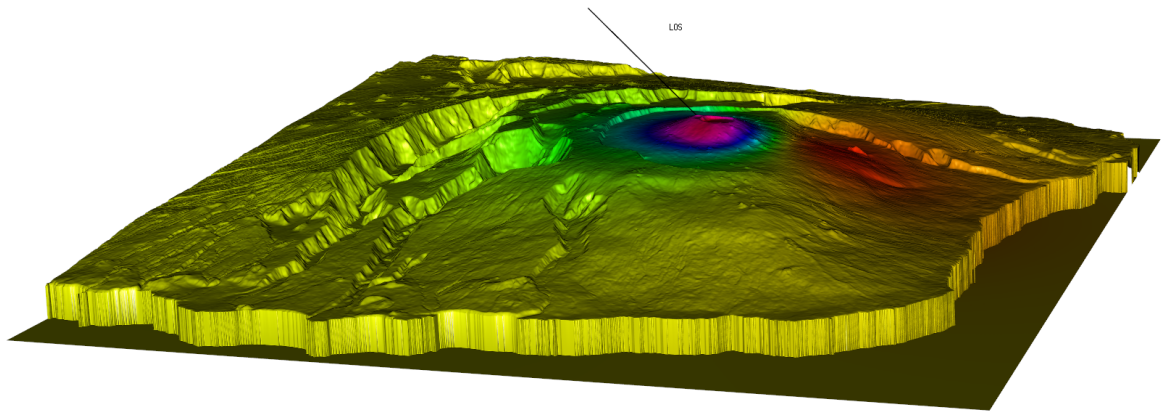
In this course we will focus on **Gaussian Process Regression**.

(This notation may a few times be ambiguous as X will also denote the random variable associated to x but the context should allow understanding)

Two breadcrumb examples related to the **identification of a spherical magma reservoir from measured displacements** along a satellite line of sight:

1) the processing of surface measures for *i)* reconstructing missing measures and *ii)* denoising,

2) minimizing the missfit between a Mogi model of a spherical reservoir and the surface measures.



Misfit minimization problem:

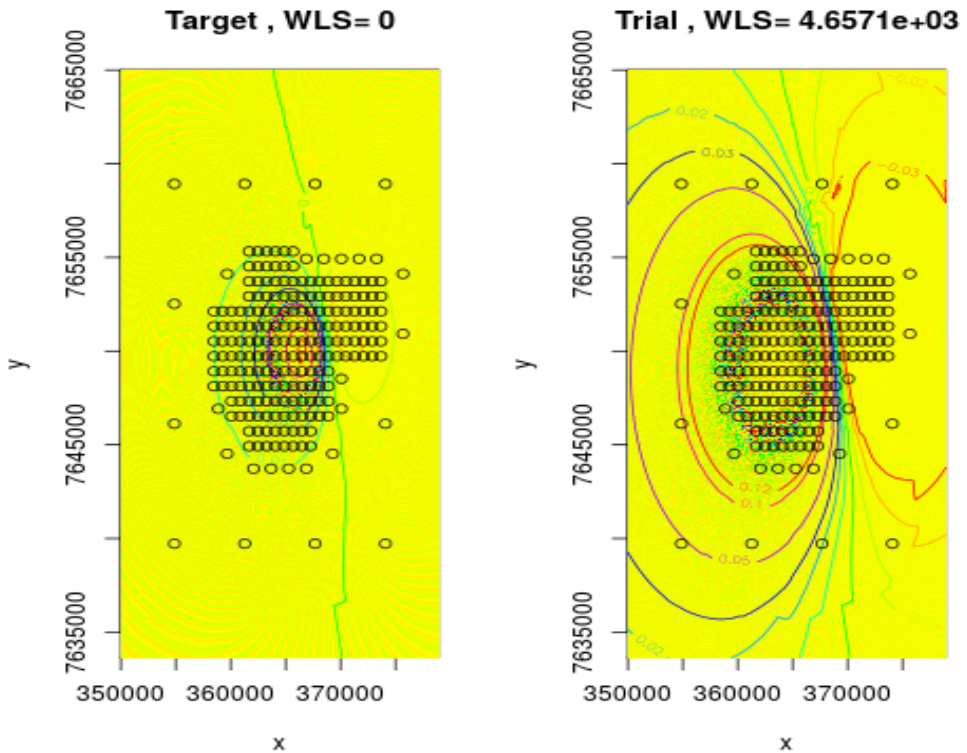
$$\min_{x \in [x^L, x^U] \subset \mathbb{R}^d} f(x) \quad \text{where the misfit is}$$

$$f(x) = \frac{1}{2}(U(x) - U^m)^\top C^{-1}(U(x) - U^m)$$

- U^m: $m \times 1$ displacements projected on the line of sight.
- $U(x)$: $m \times 1$ Mogi model displacements projected on the line of sight.
- x: identification variables, the coordinates, radius and overpressure of a spherical magma reservoir, $x = \{xs, ys, zs, a, p\}$, resp.
- C: $m \times m$ covariance matrix of the measures.

Misfit minimization problem:

$\Rightarrow$ demo with `plots_3d_full_grid.R`



The bullets are the $m = 220$ measure locations (under-sampled from the full grid with the quadtree method).
target reservoir (left): $xs = 367000$, $ys = 7650300$, $zs = 0$ (UTM m), $a = 500$ m, $p = 20$ MPa.
trial reservoir (right): $xs = 365000$, $ys = 7649800$, $zs = -2000$ (UTM m), $a = 500$ m, $p = 300$ MPa.

Gaussian Process Regression

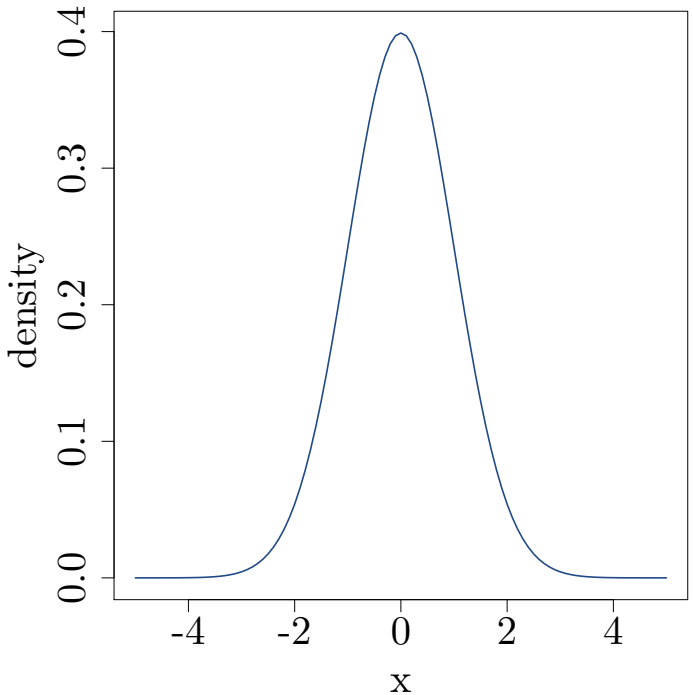
This section is organised in 3 subsections:

1. Univariate and multivariate normal distributions
2. Gaussian processes
3. Gaussian process regression

1D normal distribution

We say that $X \sim \mathcal{N}(\mu, \sigma^2)$ if it has the following pdf:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



The distribution is characterised by

mean: $\mu = \mathrm{E}[X]$

variance: $\sigma^2 = \mathrm{E}[X^2] - \mathrm{E}[X]^2$

One fundamental property: a linear combination of independant normal distributed random variables is still normal distributed.

Multivariate normal distribution

Definition

We say that a vector $Y = (Y_1, \ldots, Y_n)^t$ follows a multivariate normal distribution if any linear combination of Y follows a normal distribution:

$$\forall \alpha \in \mathbb{R}^n,\ \alpha^t Y \sim \mathcal{N}$$

The distribution of a Gaussian vector is characterised by

- a **mean vector** $\mu = \mathrm{E}[Y]$
- a **covariance matrix** $\Sigma = \mathrm{E}[YY^t] - \mathrm{E}[Y]\,\mathrm{E}[Y]^t$

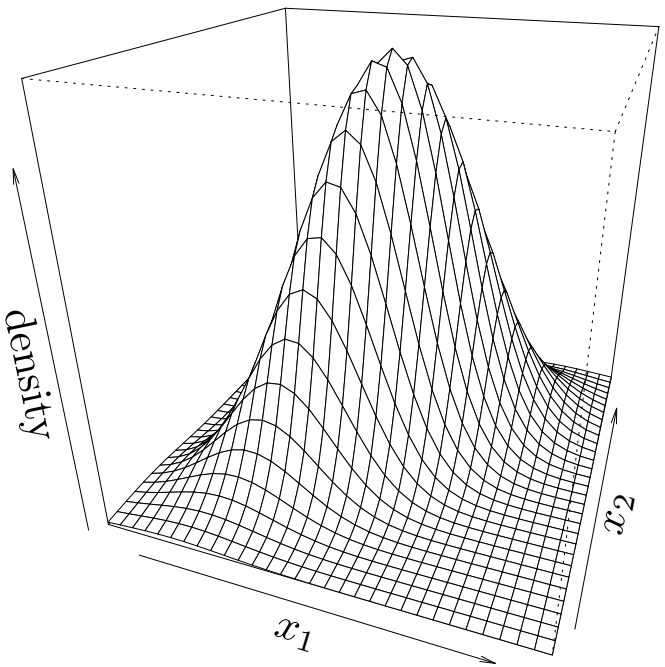
Property:

A covariance matrix is

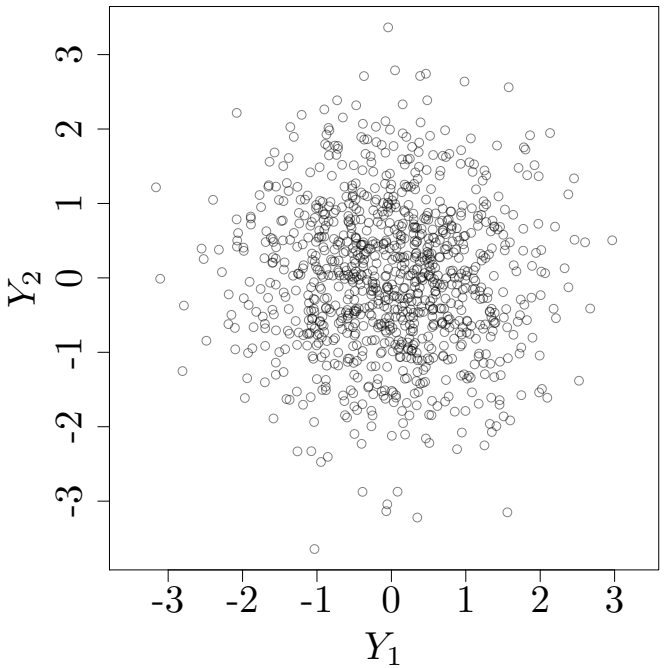
- symmetric $K_{i,j} = K_{j,i}$
- positive semi-definite $\forall \alpha \in \mathbb{R}^n, \alpha^t K \alpha \geq 0$.

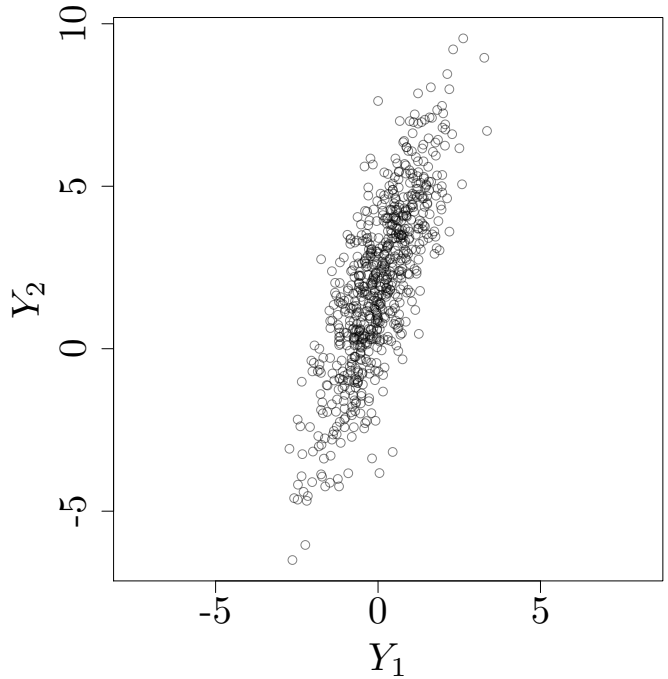
The density of a multivariate Gaussian is:

$$f_Y(x) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu)^t K^{-1}(x-\mu)\right).$$



Samples from a multivariate normal



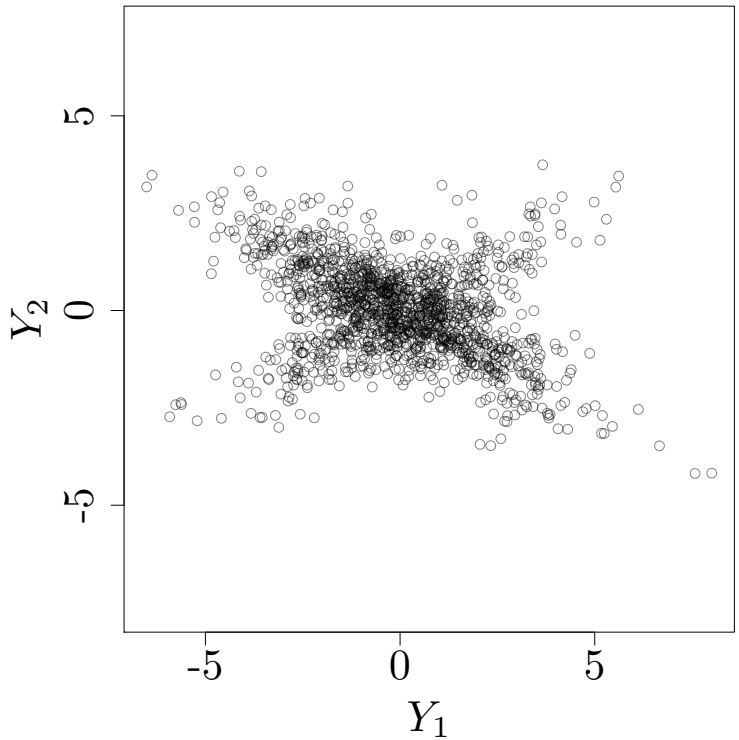


Exercise

- For $X = (X_1, \ldots, X_n)$ with X_i independent and $\mathcal{N}(0, 1)$, and a $n \times n$ matrix A, what is the distribution of AX?
- For a given covariance matrix K and independent $\mathcal{N}(0, 1)$ samples, how can we generate $\mathcal{N}(\mu, K)$ random samples?

$\Rightarrow$ R demo

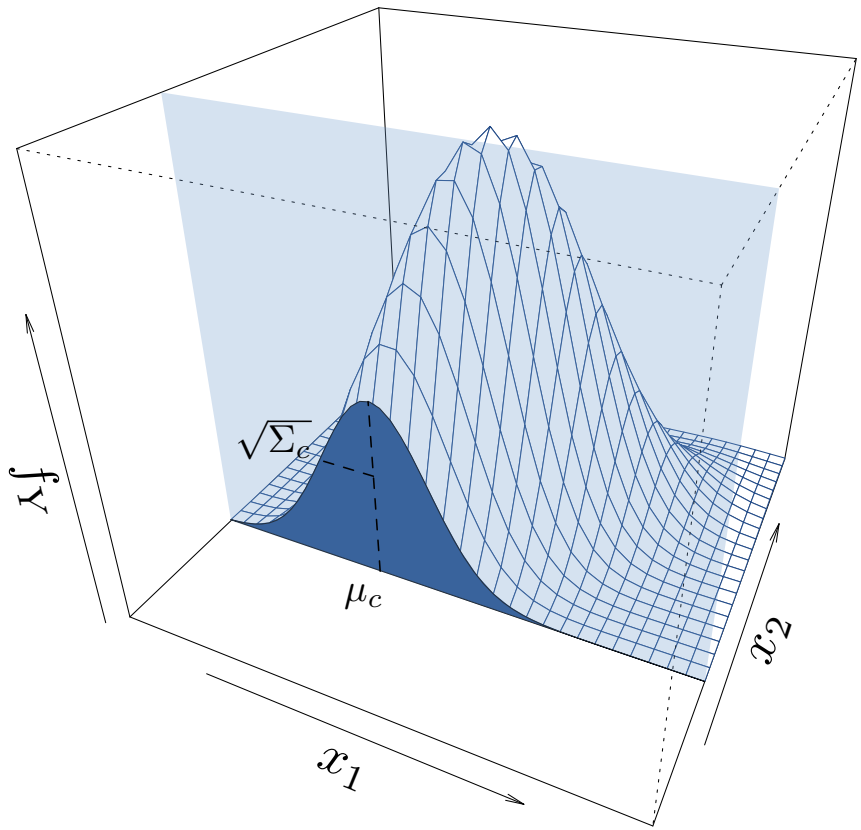
Counter example



Y_1 and Y_2 are normally distributed but **the couple** (Y_1, Y_2) **is not**.

Conditional distribution

2D multivariate Gaussian conditional distribution:



The conditional distribution is still Gaussian!

Conditional distribution

Let (Y, Z) be a Gaussian vector (Y and Z may both be vectors) with mean $(\mu_Y, \mu_Z)^t$ and covariance matrix

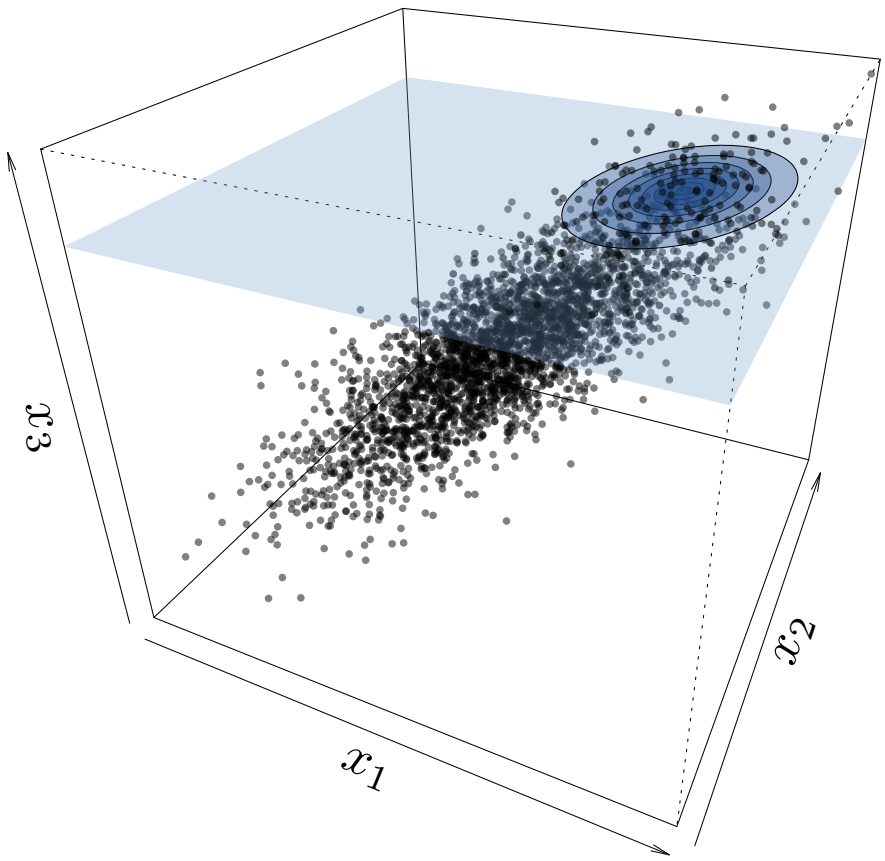
$$\begin{pmatrix} \text{cov}(Y,Y) & \text{cov}(Y,Z) \\ \text{cov}(Z,Y) & \text{cov}(Z,Z) \end{pmatrix}.$$

The conditional distribution of Y knowing Z is still multivariate normal $Y|Z \sim \mathcal{N}(\mu_{cond}, \Sigma_{cond})$ with

$$\mu_{cond} = \text{E}[Y|Z] = \mu_Y + \text{cov}(Y,Z)\,\text{cov}(Z,Z)^{-1}(Z - \mu_Z)$$
$$\Sigma_{cond} = \text{cov}[Y,Y|Z] = \text{cov}(Y,Y) - \text{cov}(Y,Z)\,\text{cov}(Z,Z)^{-1}\,\text{cov}(Z,Y)$$

3D Example

3D multivariate Gaussian conditional distribution:



2. Gaussian processes

The multivariate Gaussian distribution can be generalised to random processes:

Definition

A random process Z over $D \subset \mathbb{R}^d$ is said to be Gaussian if

$$\forall n \in \mathbb{N}, \forall x_i \in D, (Z(x_1), \ldots, Z(x_n)) \text{ is a Gaussian vector.}$$

The distribution of a GP is fully characterised by:

- its mean function m defined over D
- its covariance function (or kernel) k defined over $D \times D$: $k(x, y) = \text{cov}(Z(x), Z(y))$

We will use the notation $Z \sim \mathcal{N}(m(.), k(.,.))$.

Let's look at the sample paths of a Gaussian Process!

$\Rightarrow$ Shiny App:

`https://github.com/NicolasDurrande/shinyApps`

In order to simulate sample paths from a GP $Z \sim \mathcal{N}(m(.), k(.,.))$, we consider the samples discretised on a fine grid.

Exercise: Simulating sample paths

Let X be a set 100 regularly spaced points over the input space of Z.

- What is the distribution of $Z(X)$?
- How to simulate samples from $Z(X)$?

A kernel satisfies the following properties:

- It is symmetric: $k(x, y) = k(y, x)$
- It is positive semi-definite (psd):

$$\forall n \in \mathbb{N}, \forall x_i \in D, \forall \alpha \in \mathbb{R}^n, \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j k(x_i, x_j) \geq 0$$

Furthermore any symmetric psd function can be seen as the covariance of a Gaussian process. This equivalence is known as the Loeve theorem.

There are a lot of functions that have already been proven psd:

constant	$k(x,y) = \sigma^2$
white noise	$k(x,y) = \sigma^2 \delta_{x,y}$
Brownian	$k(x,y) = \sigma^2 \min(x,y)$
exponential	$k(x,y) = \sigma^2 \exp\left(-\lvert x-y\rvert/\theta\right)$
Matern 3/2	$k(x,y) = \sigma^2 \left(1+\lvert x-y\rvert\right) \exp\left(-\lvert x-y\rvert/\theta\right)$
Matern 5/2	$k(x,y) = \sigma^2 \left(1+\lvert x-y\rvert/\theta + 1/3\lvert x-y\rvert^2/\theta^2\right) \exp\left(-\lvert x-y\rvert/\theta\right)$
squared exponential	$k(x,y) = \sigma^2 \exp\left(-(x-y)^2/\theta^2\right)$
$\vdots$	

The parameter σ^2 is called the **variance** and θ the **length-scale**.

$\Rightarrow$ Shiny App

Here is a list of the most common kernels in higher dimension:

constant	$k(x,y) = \sigma^2$
white noise	$k(x,y) = \sigma^2 \delta_{x,y}$
exponential	$k(x,y) = \sigma^2 \exp\left(-\|\|x-y\|\|_\theta\right)$
Matern 3/2	$k(x,y) = \sigma^2 \left(1+\sqrt{3}\|\|x-y\|\|_\theta\right) \exp\left(-\sqrt{3}\|\|x-y\|\|_\theta\right)$
Matern 5/2	$k(x,y) = \sigma^2 \left(1+\sqrt{5}\|\|x-y\|\|_\theta + \frac{5}{3}\|\|x-y\|\|_\theta^2\right) \exp\left(-\sqrt{5}\|\|x-y\|\|_\theta\right)$
Gaussian	$k(x,y) = \sigma^2 \exp\left(-\frac{1}{2}\|\|x-y\|\|_\theta^2\right)$

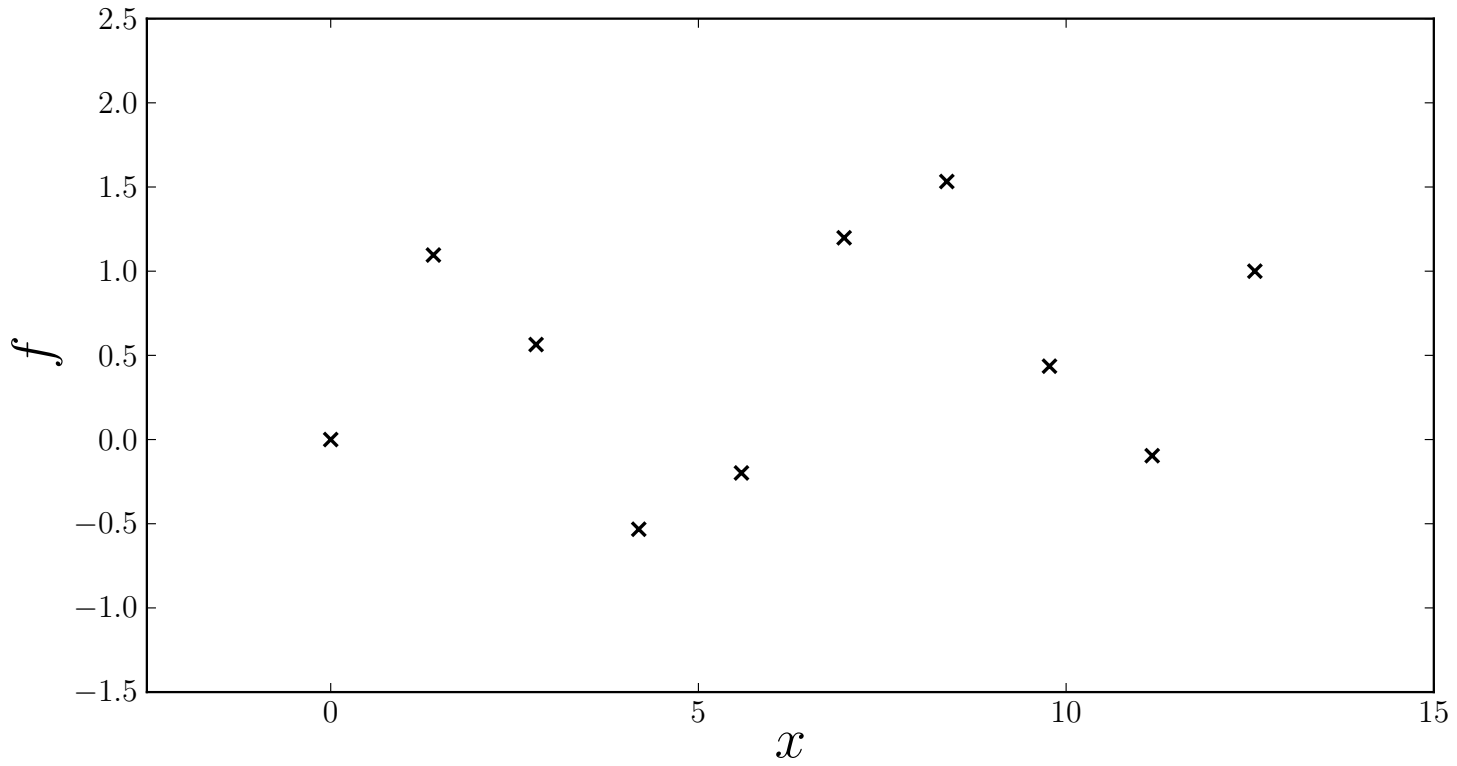
where

$$||x-y||_\theta = \left(\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{\theta_i^2}\right)^{1/2}.$$

$\Rightarrow$ R demo

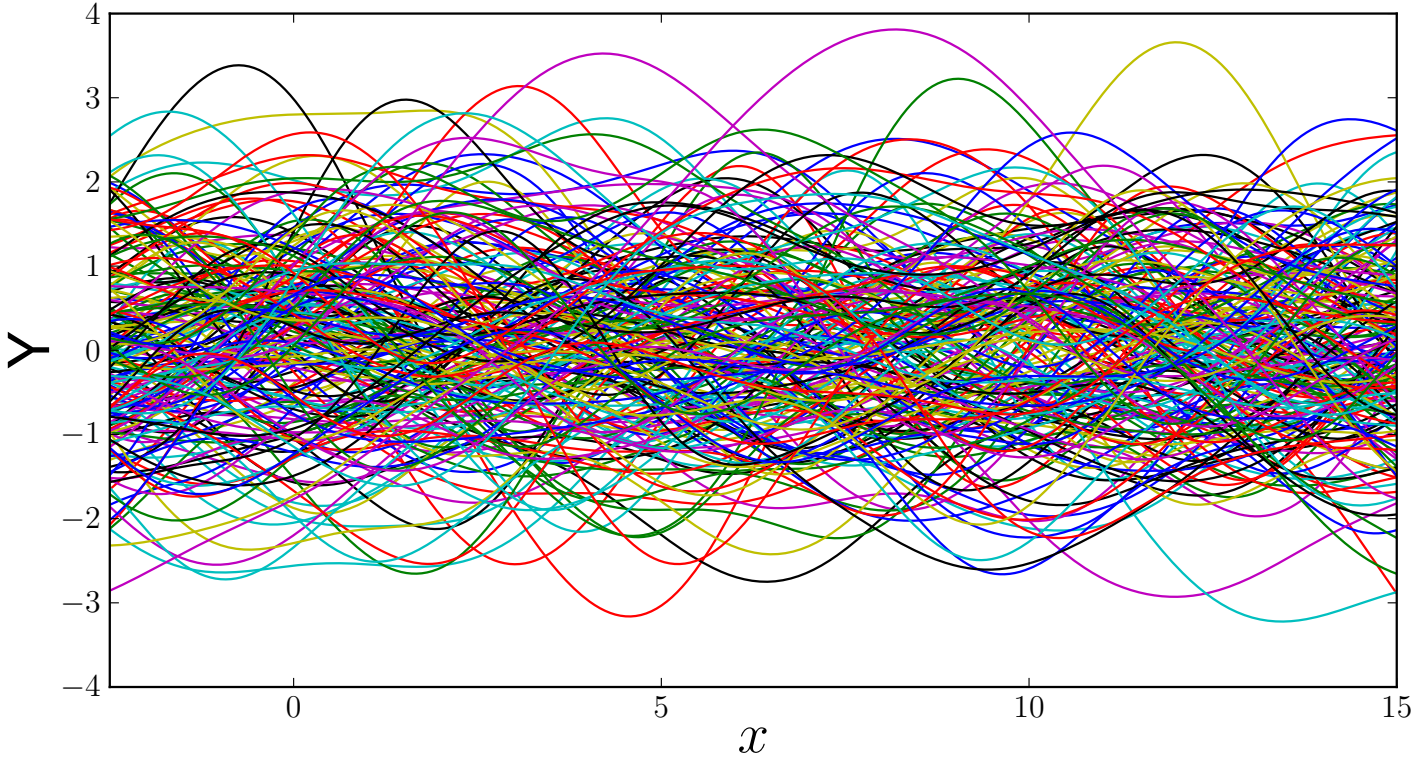
3. Gaussian process regression

We assume we have observed a function f for a set of points $X = (X_1, \ldots, X_n)$:



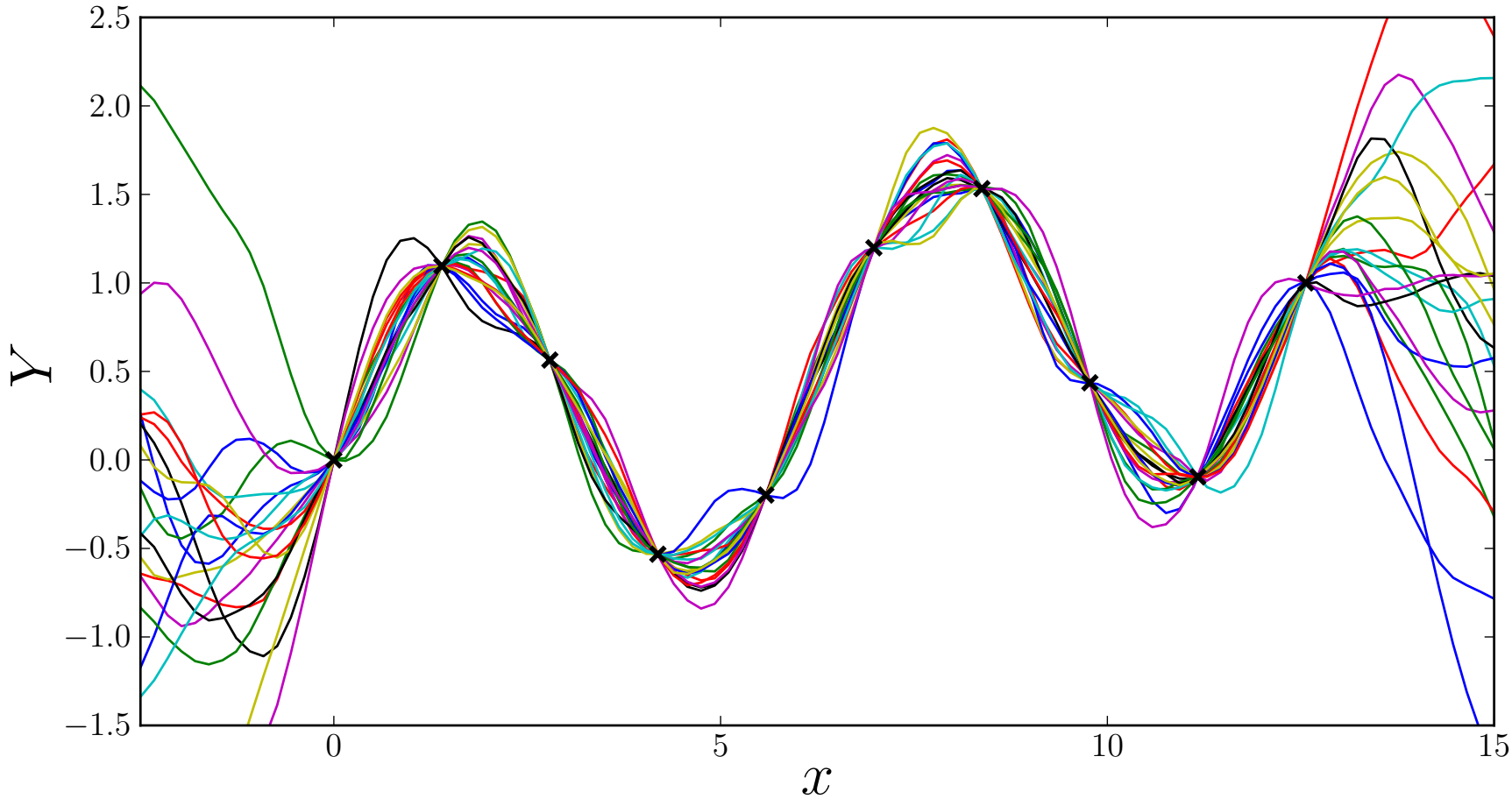
The vector of observations is $F = f(X)$ (ie $F_i = f(X_i)$).

Since f in unknown, we make the general assumption that it is the sample path of a Gaussian process $Z \sim \mathcal{N}(0, k)$:

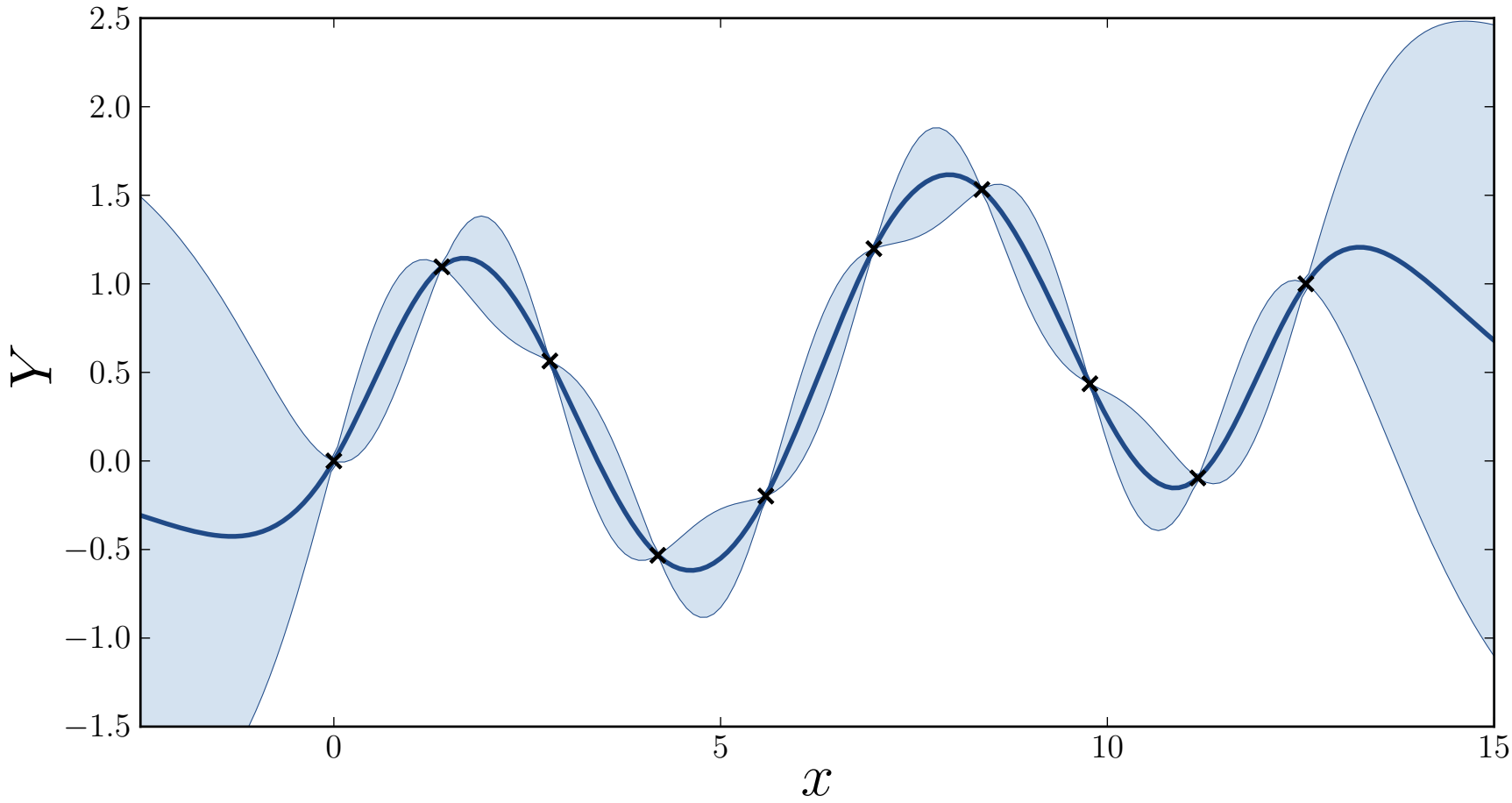


What would be the next step?

If we remove all the samples that do not interpolate we obtain:



It can summarized by a mean function and 95% confidence intervals.



In practice, the conditional distribution can be obtained analyticaly:

By definition, $(Z(x), Z(X))$ is multivariate normal so we know the distribution of $Z(x)|Z(X) = F$ is $\mathcal{N}(m(.), c(.,.))$ with:

$$\begin{aligned} m(x) &= \mathrm{E}[Z(x)|Z(X)=F] \\ &= k(x,X)k(X,X)^{-1}F \\ c(x,y) &= \mathrm{cov}[Z(x), Z(y)|Z(X)=F] \\ &= k(x,y) - k(x,X)k(X,X)^{-1}k(X,y) \end{aligned}$$

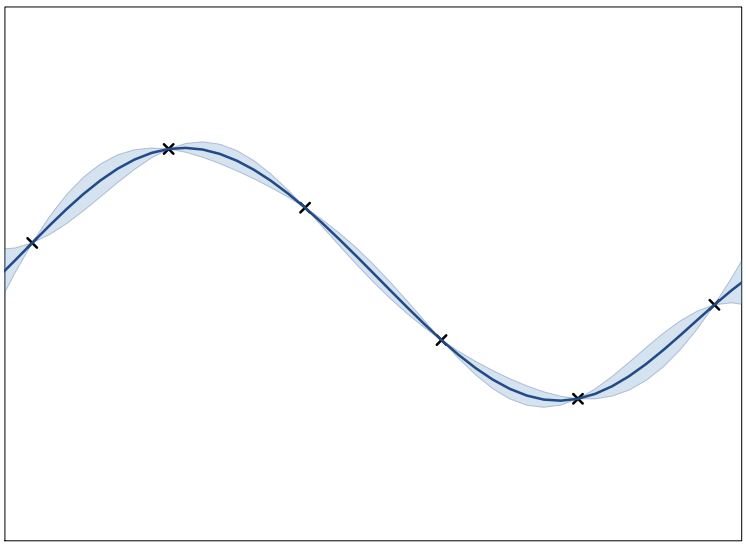
A few remarkable properties of GPR models

- They (can) interpolate the data-points
- The prediction variance does not depend on the observations
- The mean predictor does not depend on the variance parameter
- They (usually) come back to zero when we are far away from the observations.

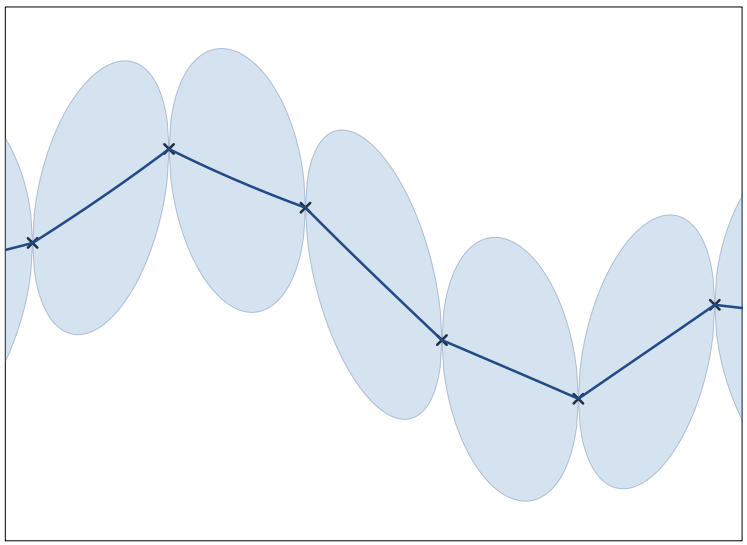
Can we prove them?

Changing the kernel has a huge impact on the model:

Gaussian kernel:

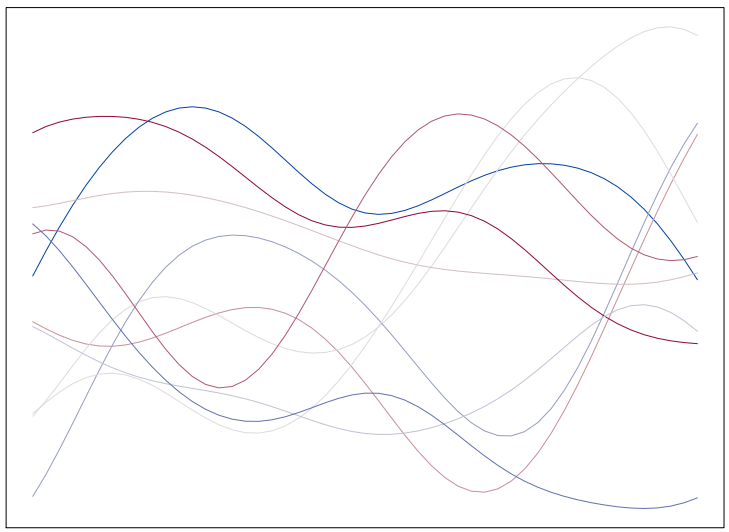


Exponential kernel:

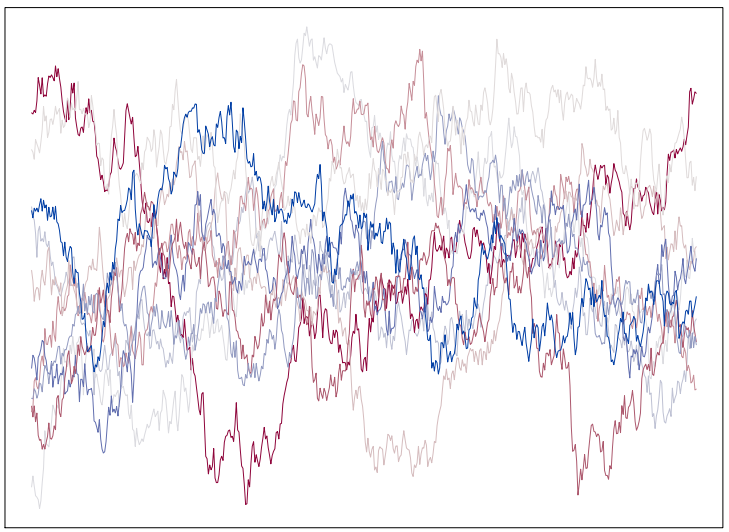


This is because changing the kernel means changing the prior on f

Gaussian kernel:

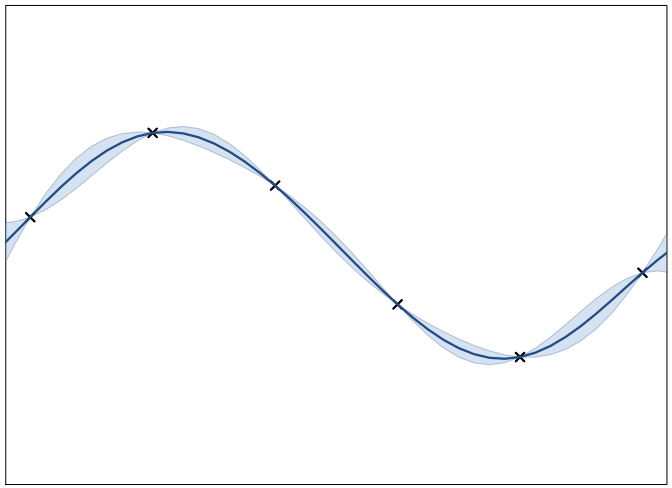


Exponential kernel:

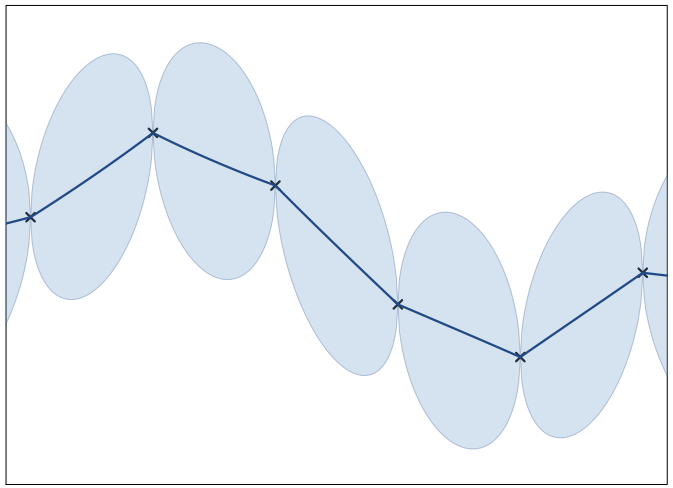


There is no kernel that is intrinsically better... it depends on data!

Gaussian kernel:



Exponential kernel:

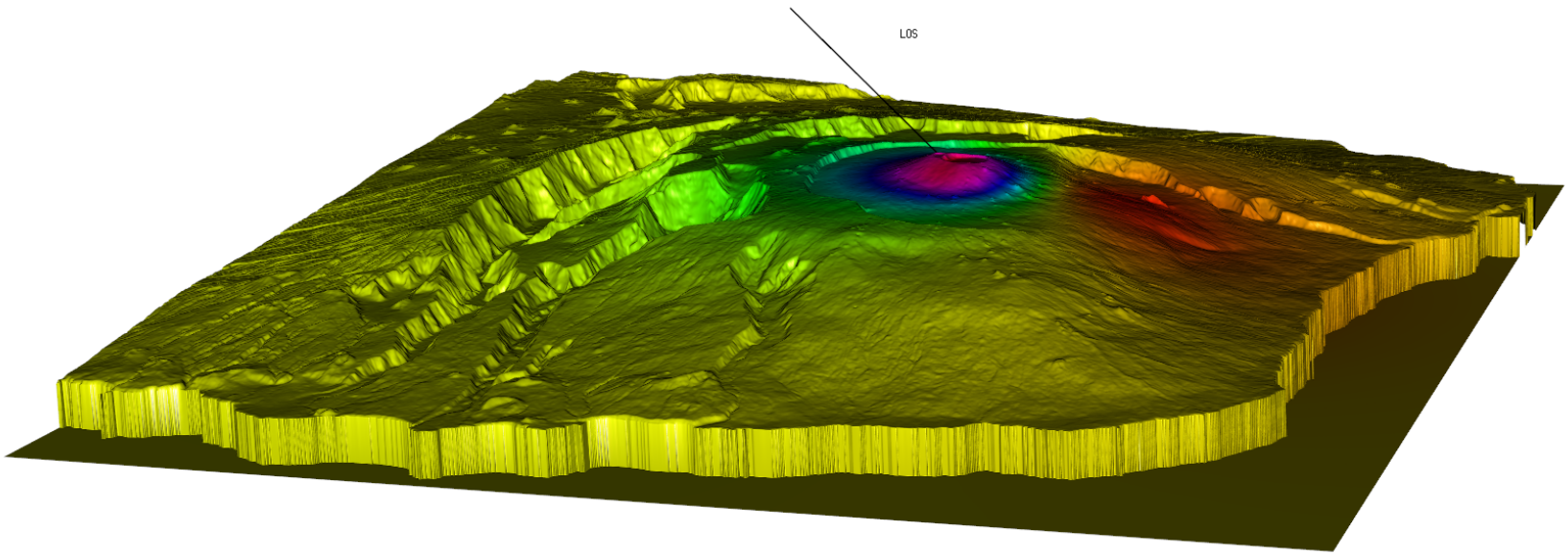


The kernel has to be chosen accordingly to our prior belief on the behaviour of the function to study:

- is it continuous, differentiable, how many times?
- is it stationary ?
- ...

Example

Let's recreate the map of displacements using a subset of the data



$\Rightarrow$ R demo

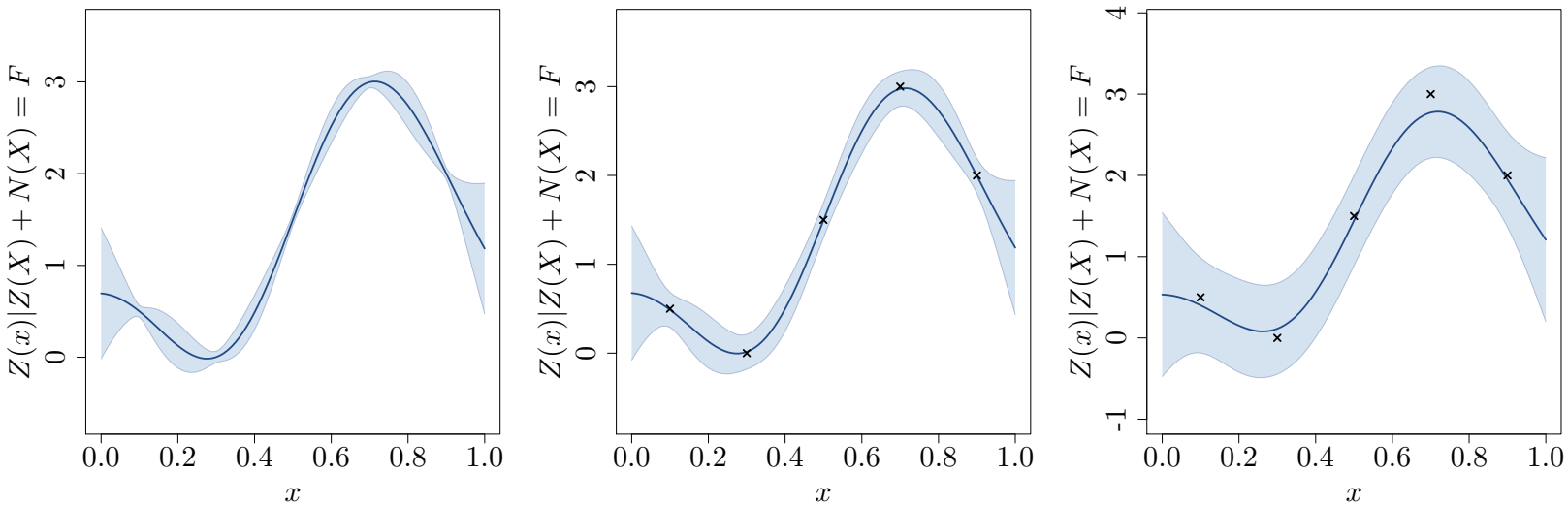
We are not always interested in models that interpolate the data. For example, if there is some observation noise: $F = f(X) + \varepsilon$. Let

N be a process $\mathcal{N}(0, n(.,.))$ that represent the observation noise. The expressions of GPR with noise are

$$\begin{aligned} m(x) &= \mathrm{E}[Z(x)|Z(X) + N(X)=F] \\ &= k(x,X)(k(X,X) + n(X,X))^{-1}F \end{aligned}$$

$$\begin{aligned} c(x,y) &= \mathrm{cov}[Z(x), Z(y)|Z(X) + N(X)=F] \\ &= k(x,y) - k(x,X)(k(X,X) + n(X,X))^{-1}k(X,y) \end{aligned}$$

Examples of models with observation noise for $n(x, y) = \tau^2 \delta_{x,y}$:



The values of τ^2 are respectively 0.001, 0.01 and 0.1.

Parameter estimation

We have seen previously that the choice of the kernel and its parameters have a great influence on the model.

In order to choose a prior that is suited to the data at hand, we can consider:

- minimising the model error
- Using maximum likelihood estimation

We will now detail the second one.

Definition

The **likelihood** of a distribution with a density f_X given some observations $X_1, \ldots, X_p$ is:

$$L = \prod_{i=1}^{p} f_X(X_i)$$

This quantity can be used to measure the adequacy between observations and a distribution.

In the GPR context, we often have only **one observation** of the vector F. The likelihood is then:

$$L = f_{Z(X)}(F) = \frac{1}{(2\pi)^{n/2}|k(X,X)|^{1/2}} \exp\left(-\frac{1}{2}F^t k(X,X)^{-1}F\right).$$

It is thus possible to maximise L – or $\log(L)$ – with respect to the kernel's parameters in order to find a well suited prior.

$\Rightarrow$ R demo

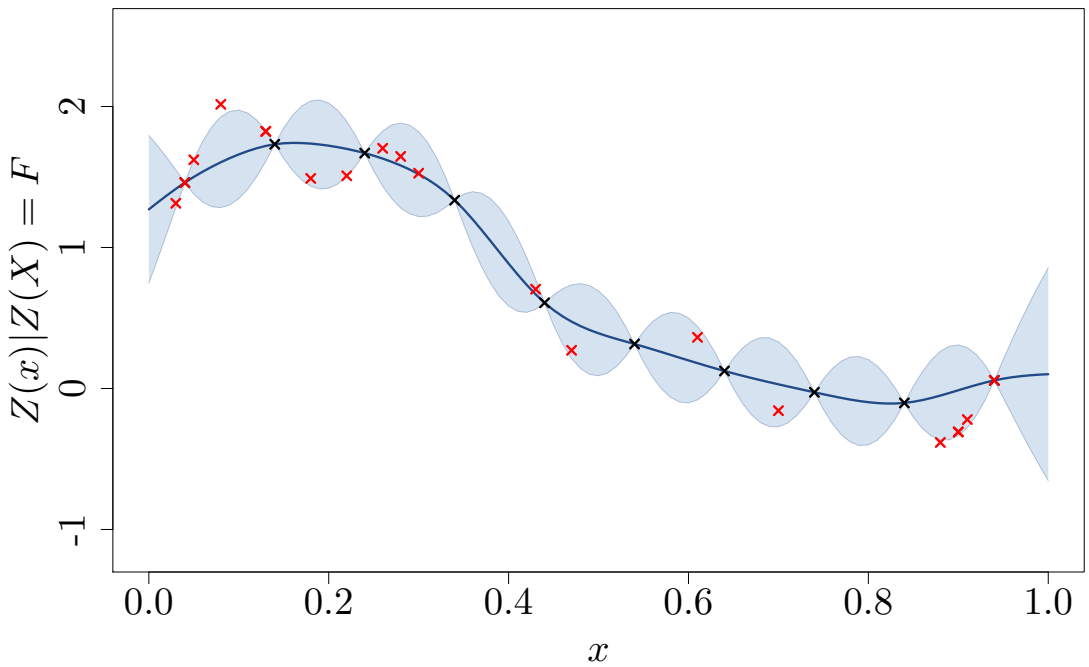
Model validation

We have seen that given some observations $F = f(X)$, it is very easy to build lots of models, either by changing the kernel parameters or the kernel itself.

The interesting question now is to know how to get a good model. To do so, we will need to answer the following questions:

- What is a good model?
- How to measure it?

The idea is to introduce new data and to compare the model prediction with reality



Since GPR models provide a mean and a covariance structure for the error they both have to be assessed.

Let X_t be the test set and $F_t = f(X_t)$ be the associated observations.

The accuracy of the mean can be measured by computing:

$$\text{Mean Square Error} \qquad MSE = \text{mean}((F_t - m(X_t))^2)$$

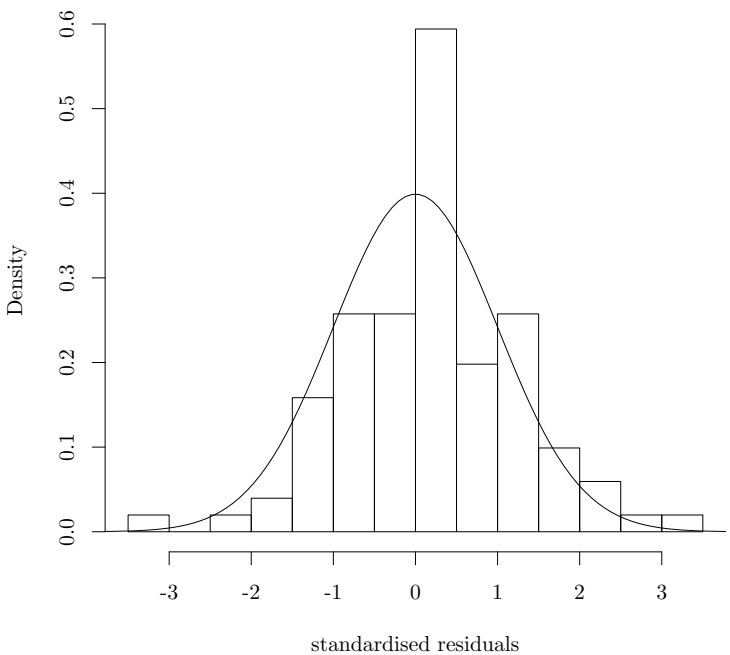
$$\text{A "normalised" criterion} \qquad Q_2 = 1 - \frac{\sum (F_t - m(X_t))^2}{\sum (F_t - \text{mean}(F_t))^2}$$

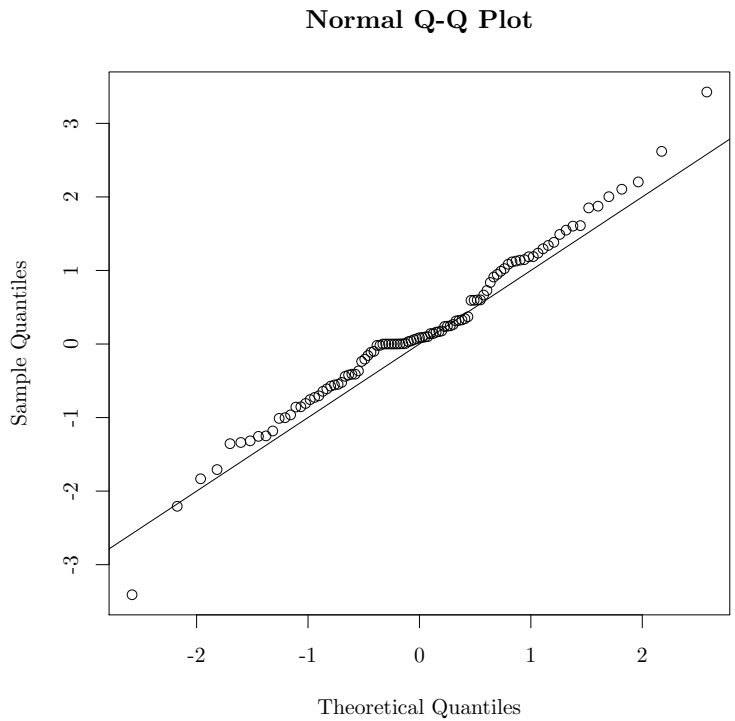
On the above example we get $MSE = 0.038$ and $Q_2 = 0.95$.

The predicted distribution can be tested by normalising the residuals.

According to the model, $F_t \sim \mathcal{N}(m(X_t), c(X_t, X_t))$.

$c(X_t, X_t)^{-1/2}(F_t - m(X_t))$ should thus be independents $\mathcal{N}(0, 1)$:





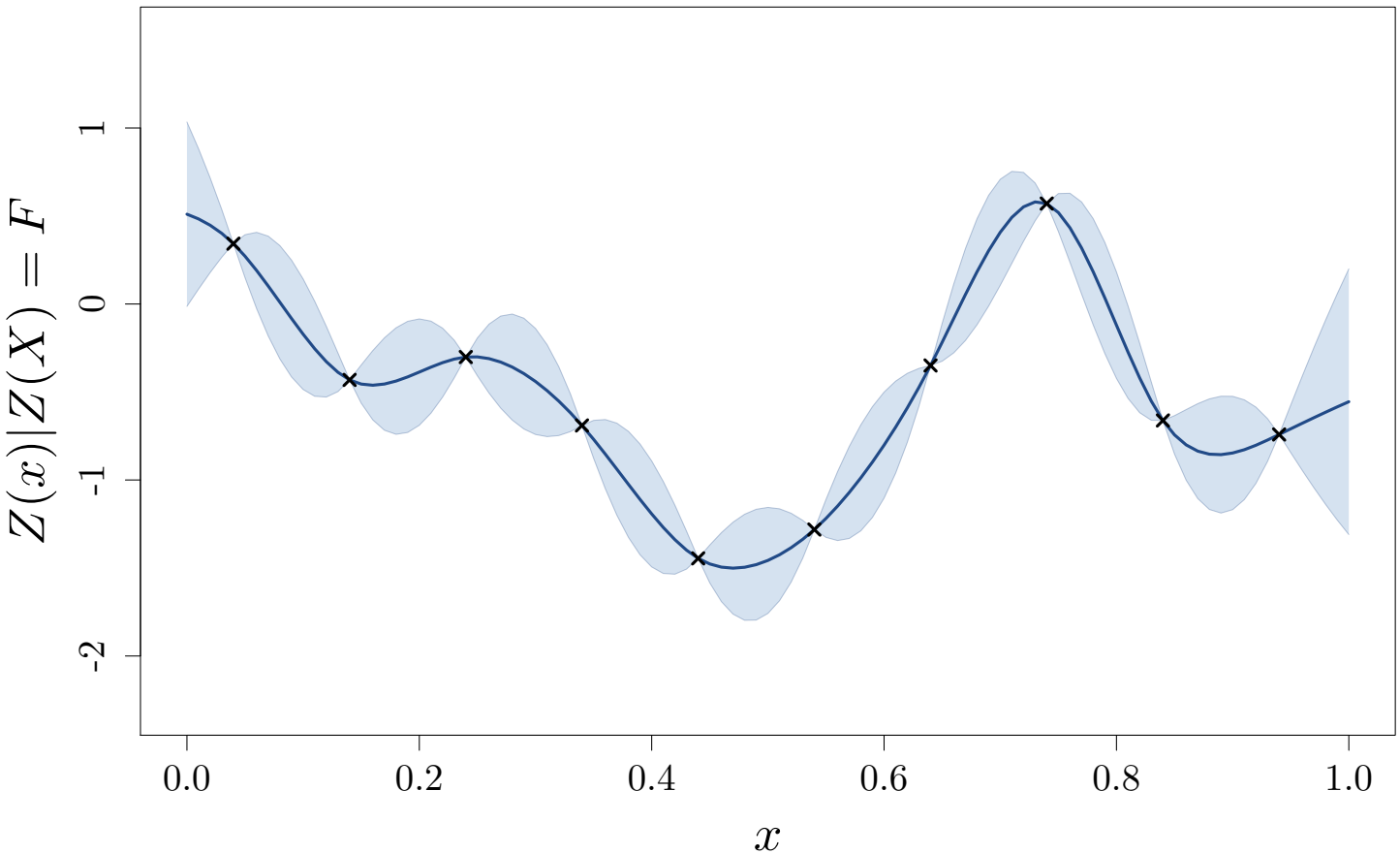
When no test set is available, another option is to consider cross validation methods such as leave-one-out.

The steps are:

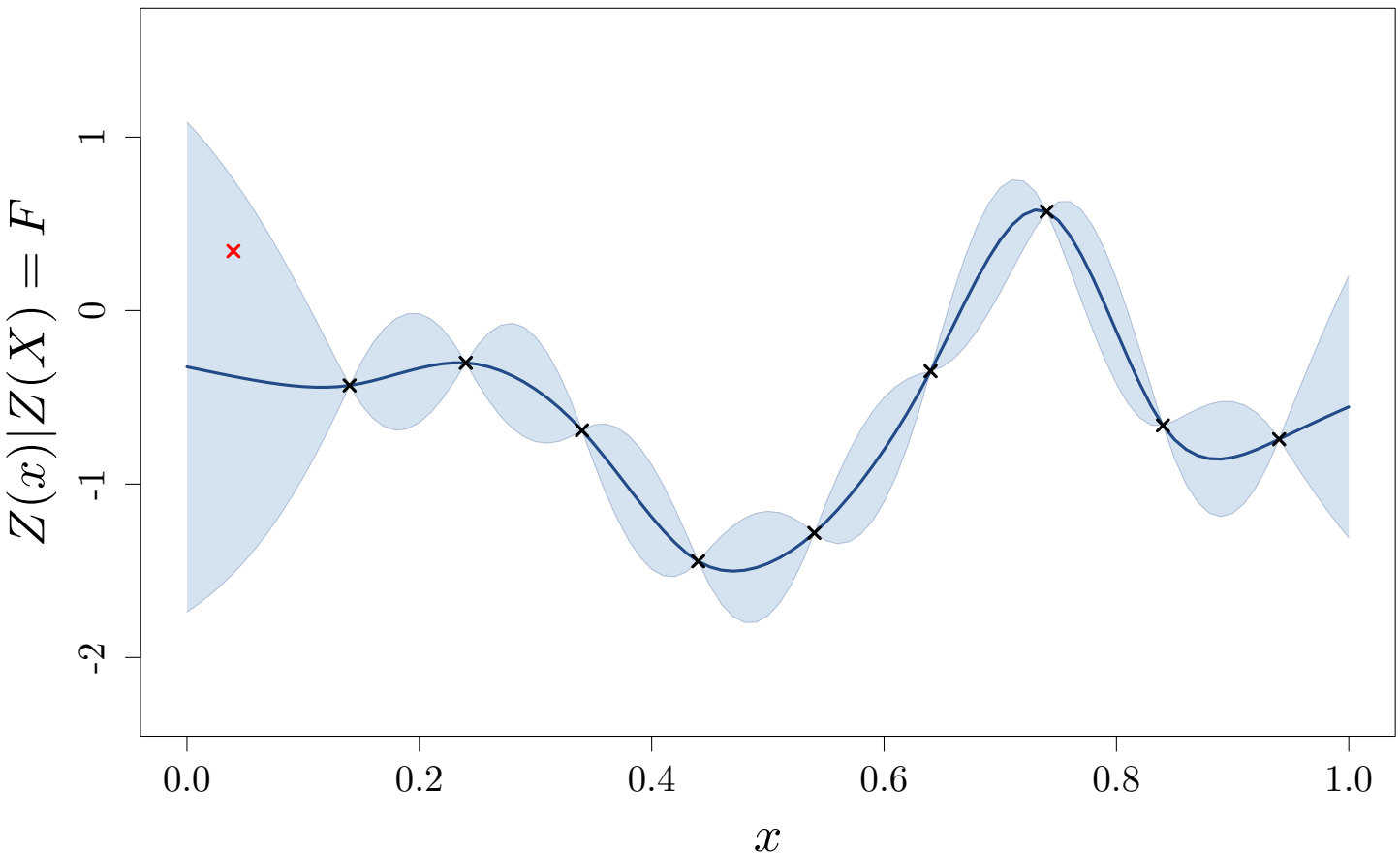
1. build a model based on all observations except one
2. compute the model error at this point

This procedure can be repeated for all the design points in order to get a vector of error.

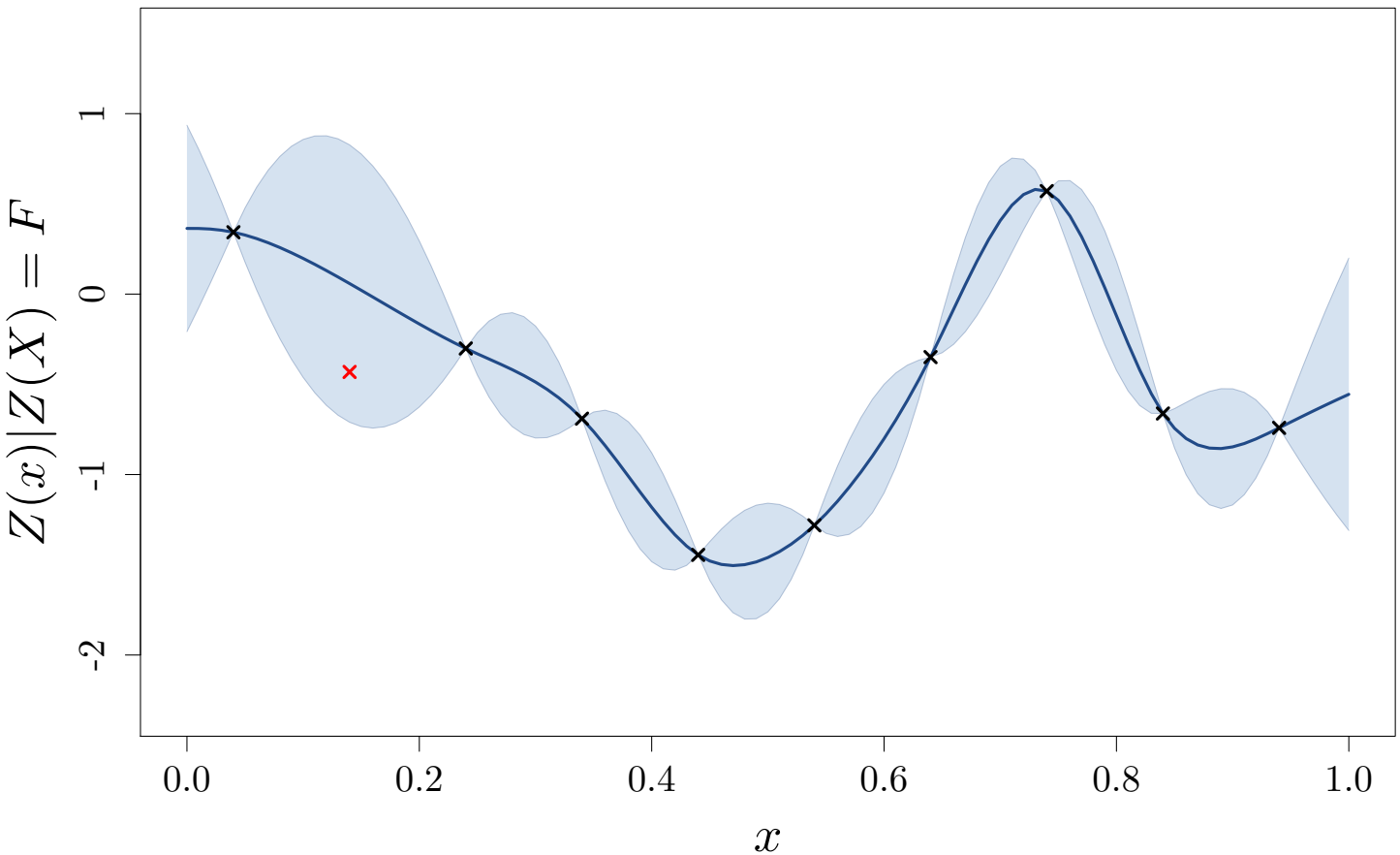
Model to be tested:



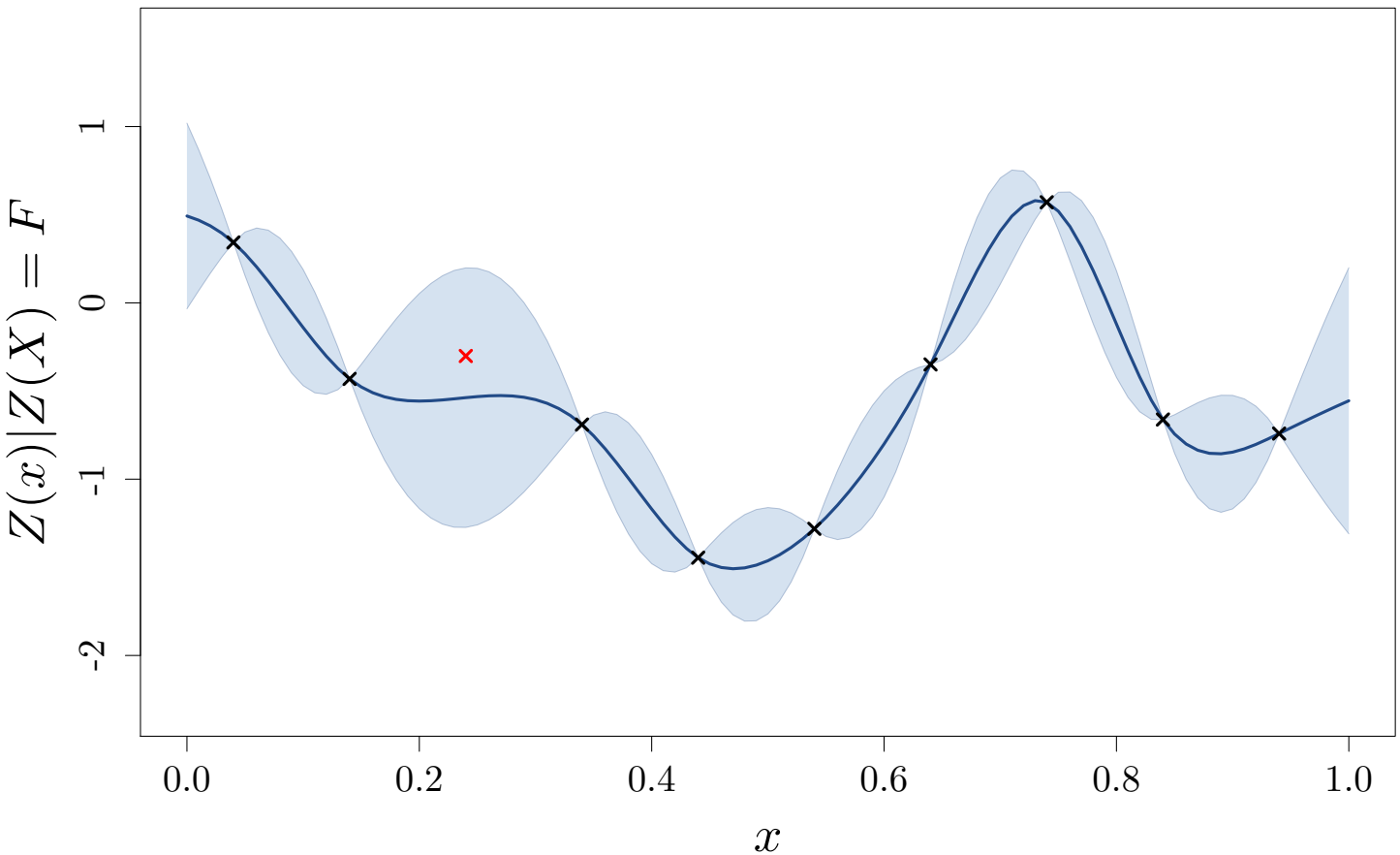
Step 1:



Step 2:



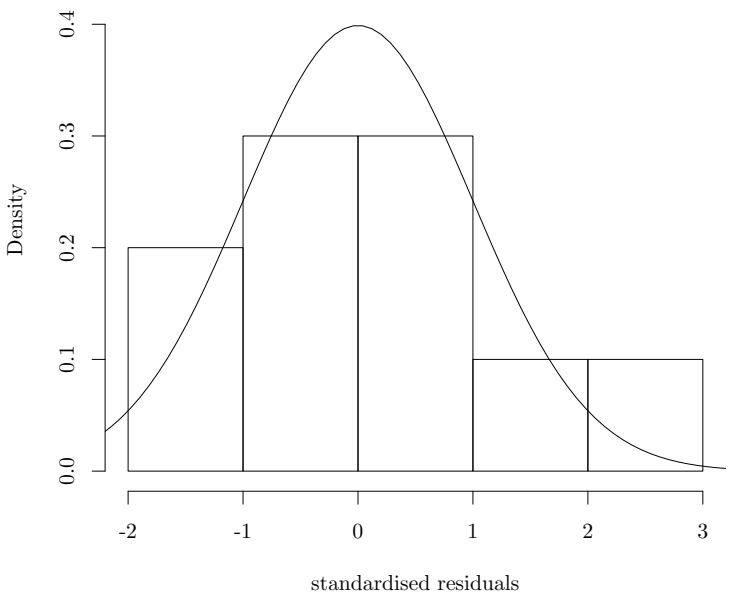
Step 3:

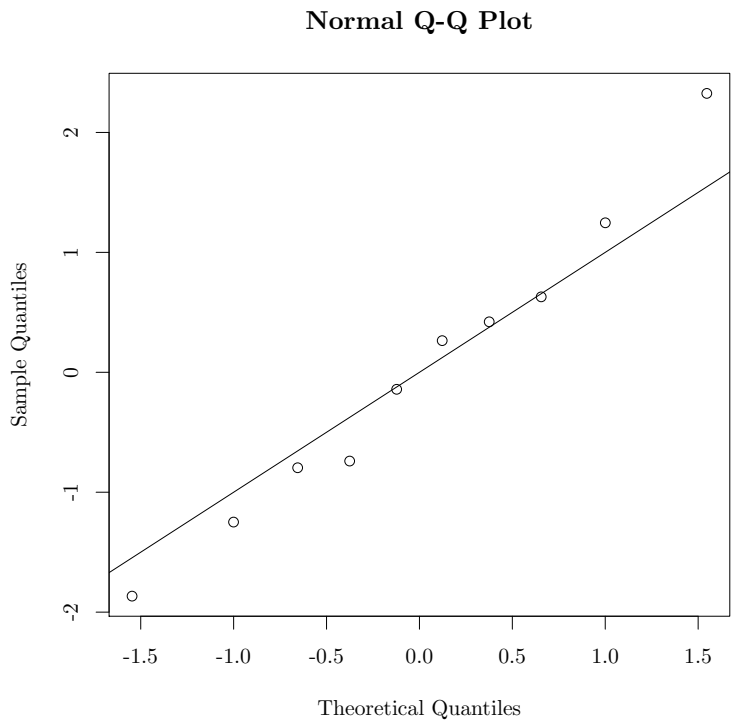


We finally obtain:

$$MSE = 0.24 \text{ and } Q_2 = 0.34.$$

We can also look at the residual distribution. For leave-one-out, there is no joint distribution for the residuals so they have to be standardised independently.





Kernel Design

Making new from old: Many operations can be applied to psd functions while retaining this property

Kernels can be:

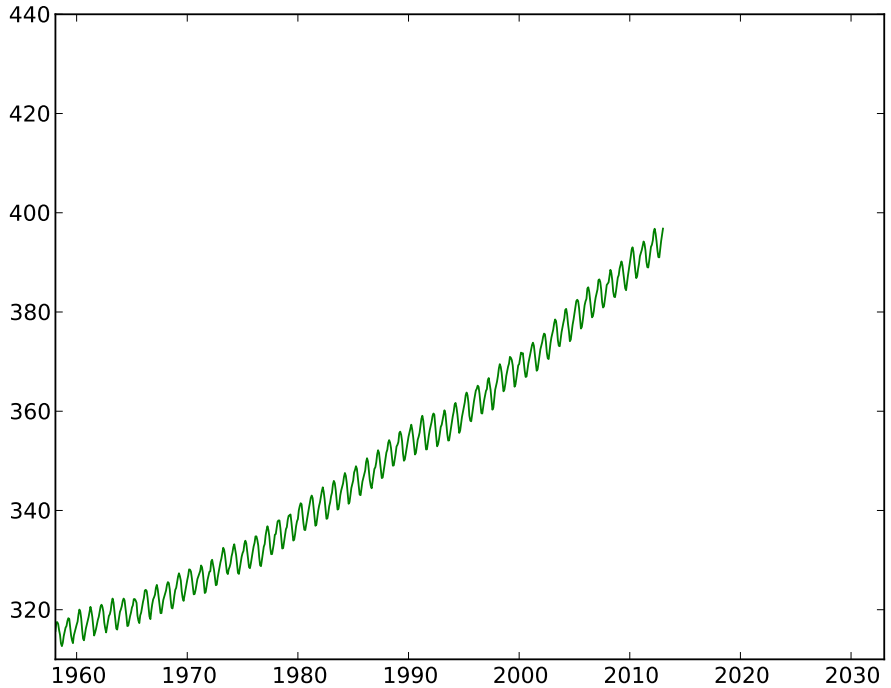
- Summed together
  - On the same space $k(x, y) = k_1(x, y) + k_2(x, y)$
  - On the tensor space $k(x, y) = k_1(x_1, y_1) + k_2(x_2, y_2)$
- Multiplied together
  - On the same space $k(x, y) = k_1(x, y) \times k_2(x, y)$
  - On the tensor space $k(x, y) = k_1(x_1, y_1) \times k_2(x_2, y_2)$
- Composed with a function
  - $k(x, y) = k_1(f(x), f(y))$

How can this be useful?

Sum of kernels over the same space

Example (The Mauna Loa observatory dataset)

This famous dataset compiles the monthly CO_2 concentration in Hawaii since 1958.

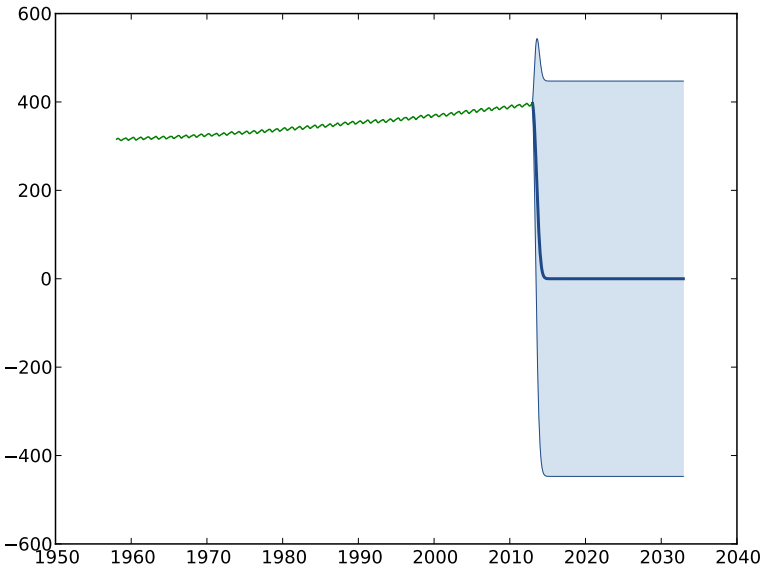


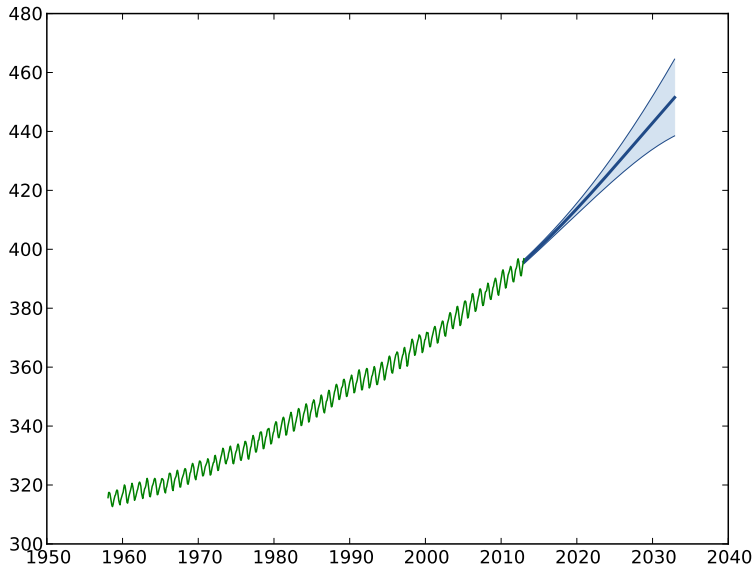
Let's try to predict the concentration for the next 20 years.

Sum of kernels over the same space

We first consider a squared-exponential kernel:

$$k_{se}(x, y) = \sigma^2 \exp\left(-\frac{(x-y)^2}{\theta^2}\right)$$





The results are terrible!

Sum of kernels over the same space

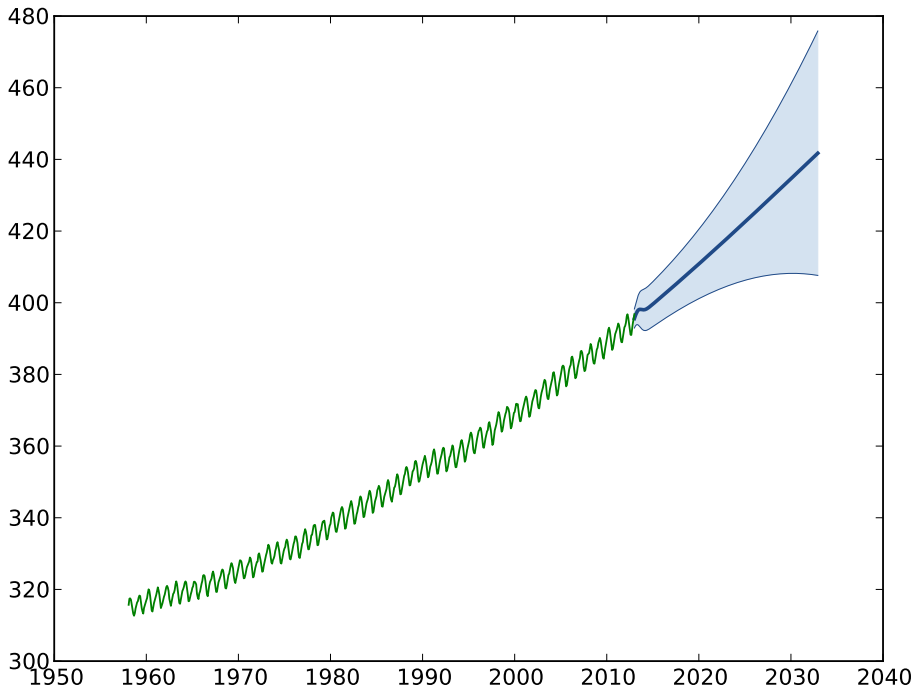
What happen if we sum both kernels?

$$k(x, y) = k_{se1}(x, y) + k_{se2}(x, y)$$

Sum of kernels over the same space

What happen if we sum both kernels?

$$k(x, y) = k_{se1}(x, y) + k_{se2}(x, y)$$



The model is drastically improved!

Sum of kernels over the same space

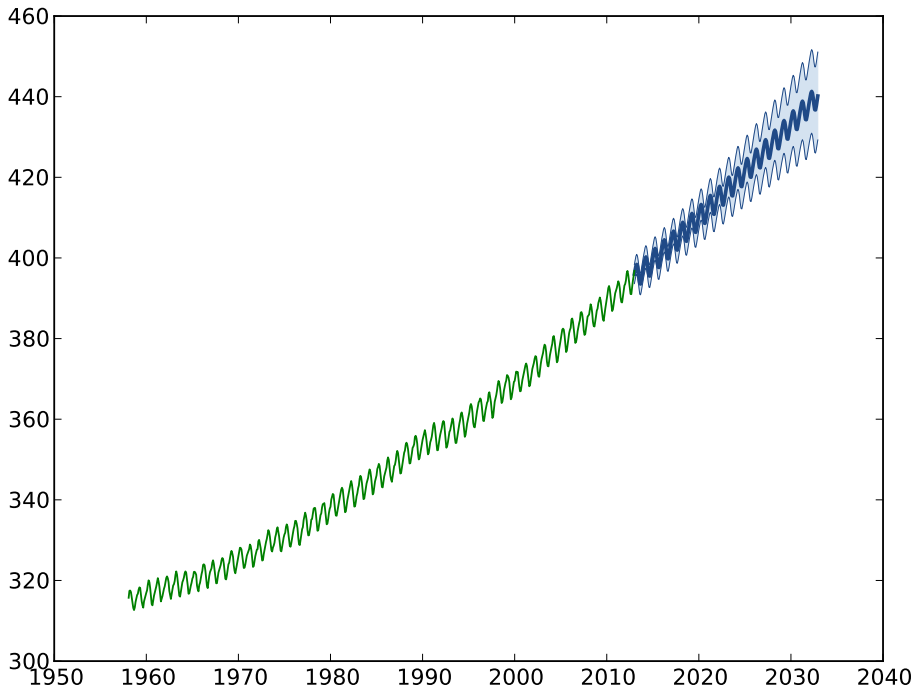
We can try the following kernel:

$$k(x, y) = \sigma_0^2 x^2 y^2 + k_{se1}(x, y) + k_{se2}(x, y) + k_{per}(x, y)$$

Sum of kernels over the same space

We can try the following kernel:

$$k(x, y) = \sigma_0^2 x^2 y^2 + k_{se1}(x, y) + k_{se2}(x, y) + k_{per}(x, y)$$



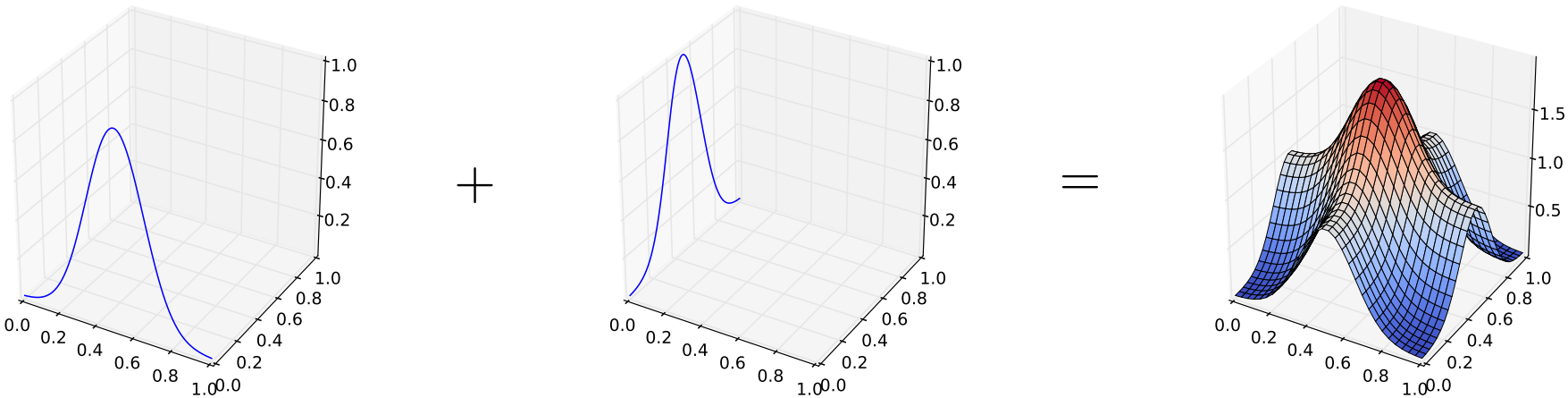
Once again, the model is significantly improved.

Sum of kernels over tensor space

Property

$$k(x, y) = k_1(x_1, y_1) + k_2(x_2, y_2)$$

is valid covariance structure.

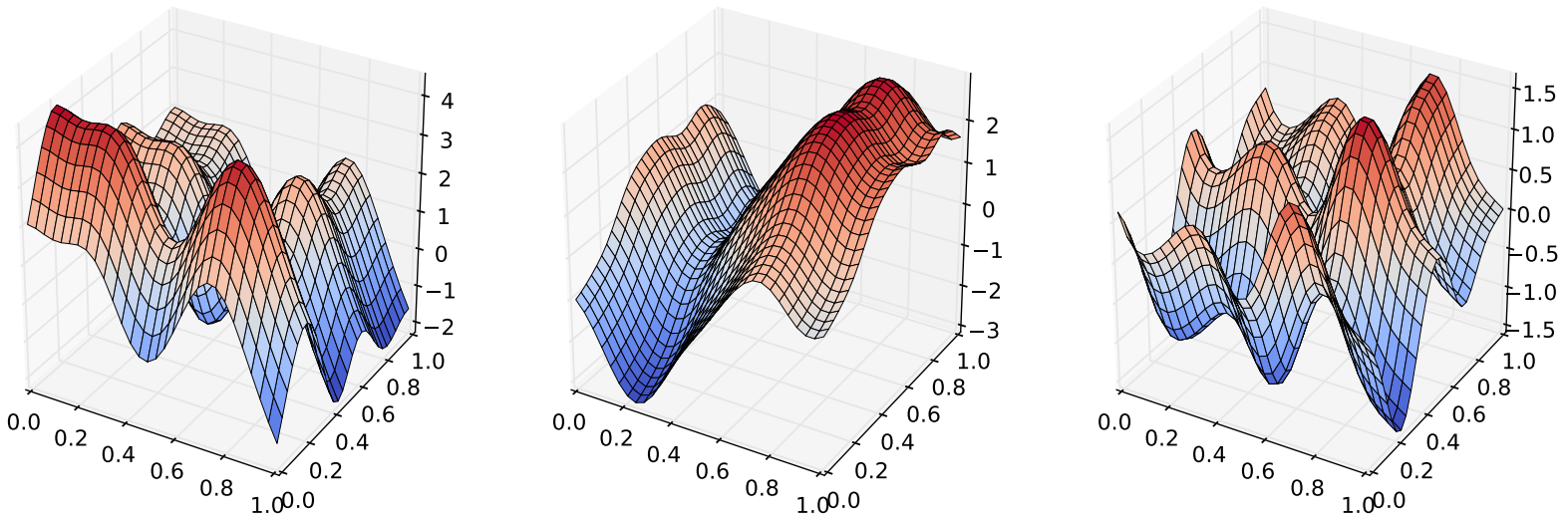


Remark: From a GP point of view, k is the kernel of

$$Z(x) = Z_1(x_1) + Z_2(x_2)$$

Sum of kernels over tensor space

We can have a look at a few sample paths from Z:



$\Rightarrow$ They are additive (up to a modification)

Tensor Additive kernels are very useful for

- Approximating additive functions
- Building models over high dimensional inputs spaces

Product over the same space

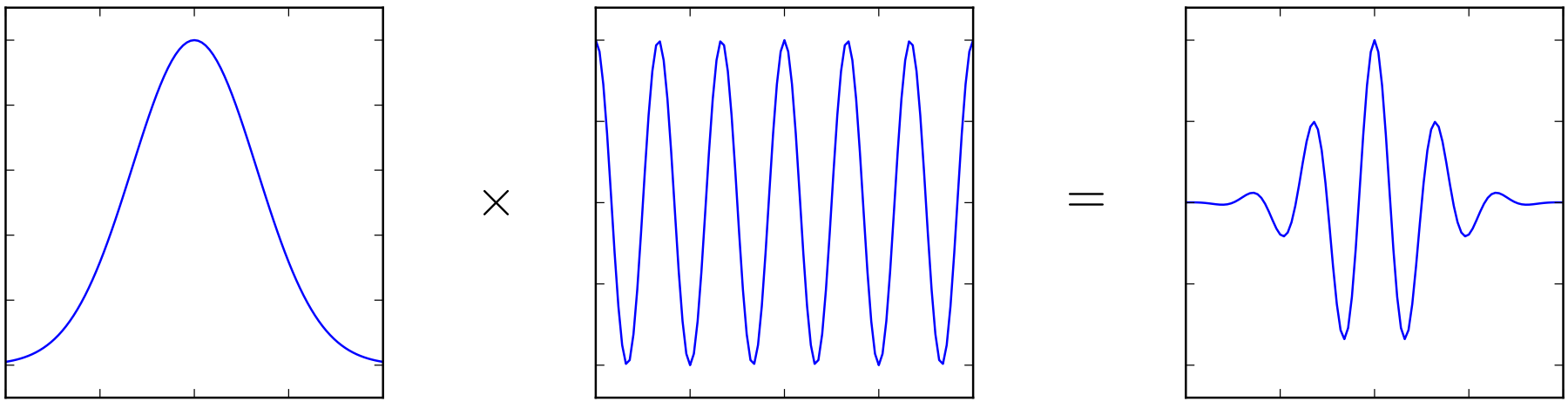
Property

$$k(x, y) = k_1(x, y) \times k_2(x, y)$$

is valid covariance structure.

Example

We consider the product of a squared exponential with a cosine:



Product over the tensor space

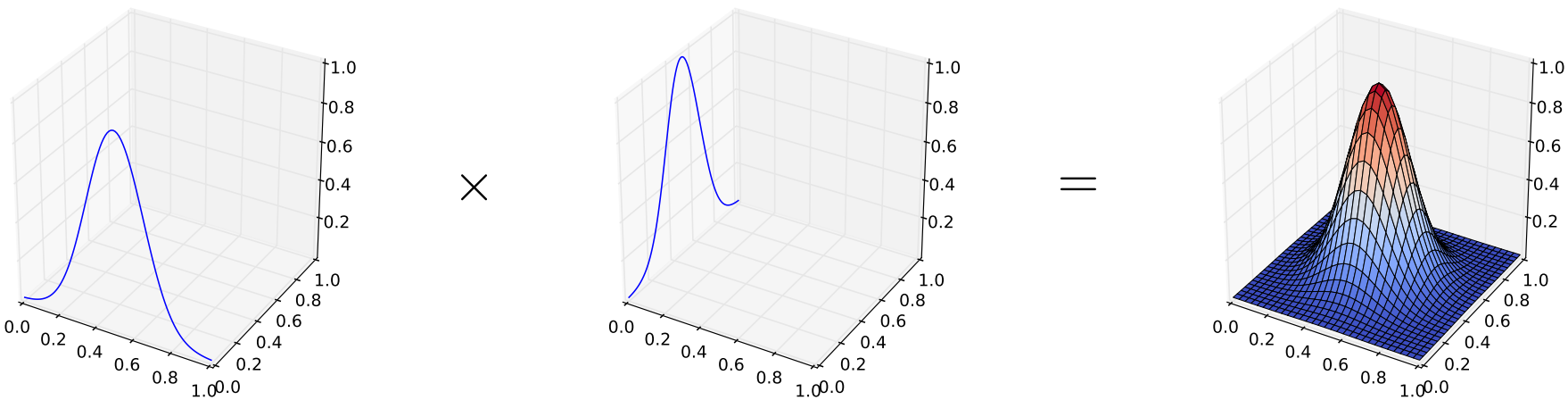
Property

$$k(x, y) = k_1(x_1, y_1) \times k_2(x_2, y_2)$$

is valid covariance structure.

Example

We multiply 2 squared exponential kernel



Calculation shows this is the usual 2D squared exponential kernel.

Composition with a function

Property

Let k_1 be a kernel over $D_1 \times D_1$ and f be an arbitrary function $D \to D_1$, then

$$k(x, y) = k_1(f(x), f(y))$$

is a kernel over $D \times D$.

proof

$$\sum\sum a_i a_j k(x_i, x_j) = \sum\sum a_i a_j k_1(\underbrace{f(x_i)}_{y_i}, \underbrace{f(x_j)}_{y_j}) \geq 0$$

Remarks:

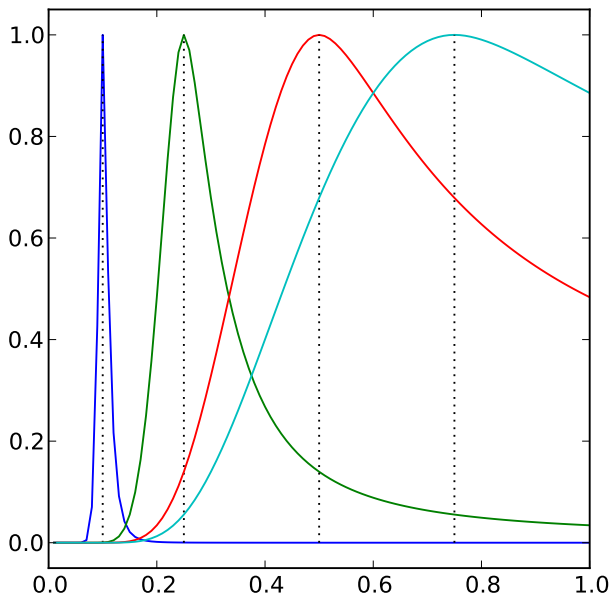
- k corresponds to the covariance of $Z(x) = Z_1(f(x))$
- This can be seen as a (non-linear) rescaling of the input space

Example

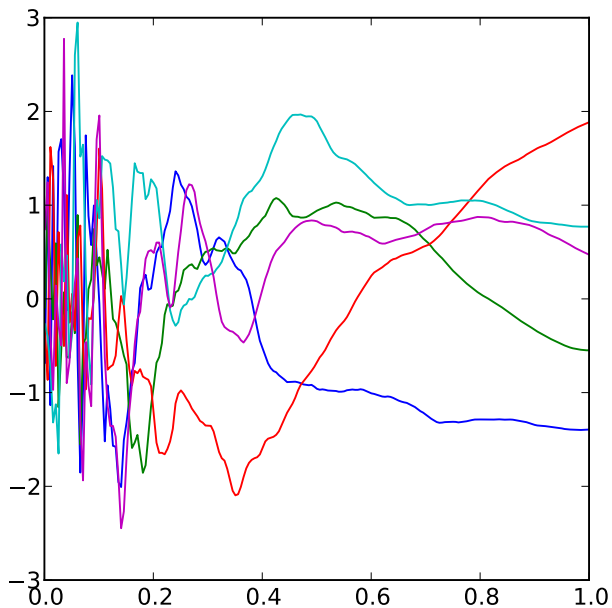
We consider $f(x) = \frac{1}{x}$ and a Matérn 3/2 kernel $k_1(x, y) = (1 + |x - y|)e^{-|x-y|}$.

We obtain:

Kernel



Sample paths



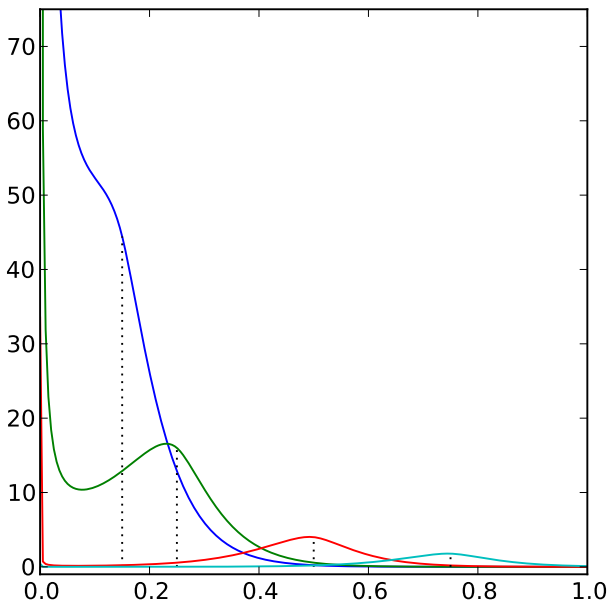
All these transformations can be combined!

Example

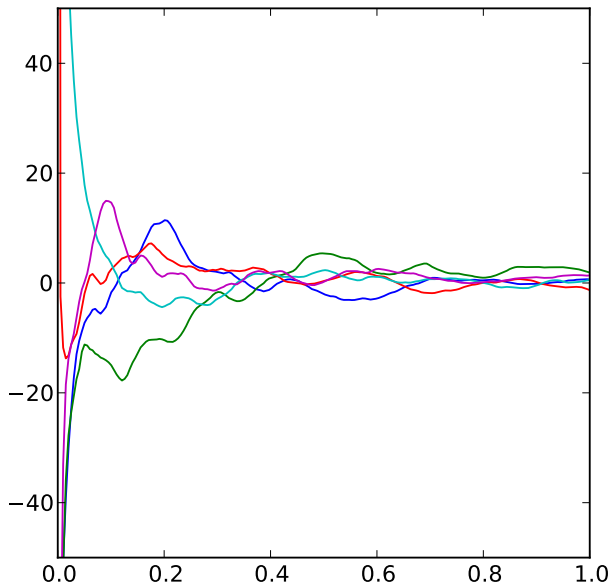
$k(x, y) = f(x)f(y)k_1(x, y)$ is a valid kernel.

This can be illustrated with $f(x) = \frac{1}{x}$ and $k_1(x, y) = (1 + |x - y|)e^{-|x-y|}$:

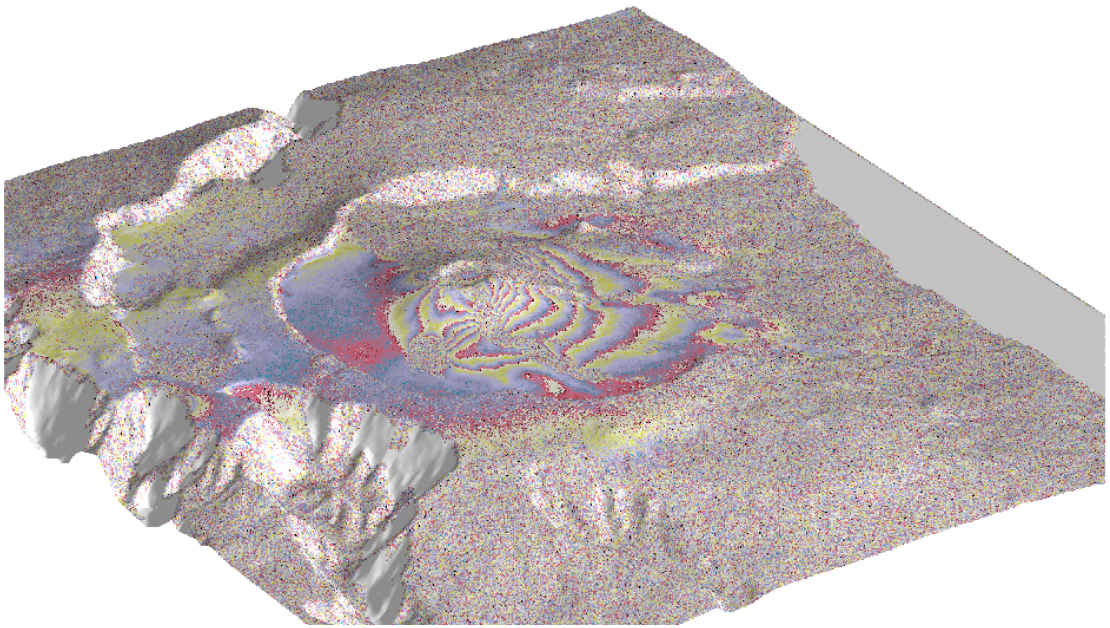
Kernel



Sample paths



Example



$\Rightarrow$ R demo

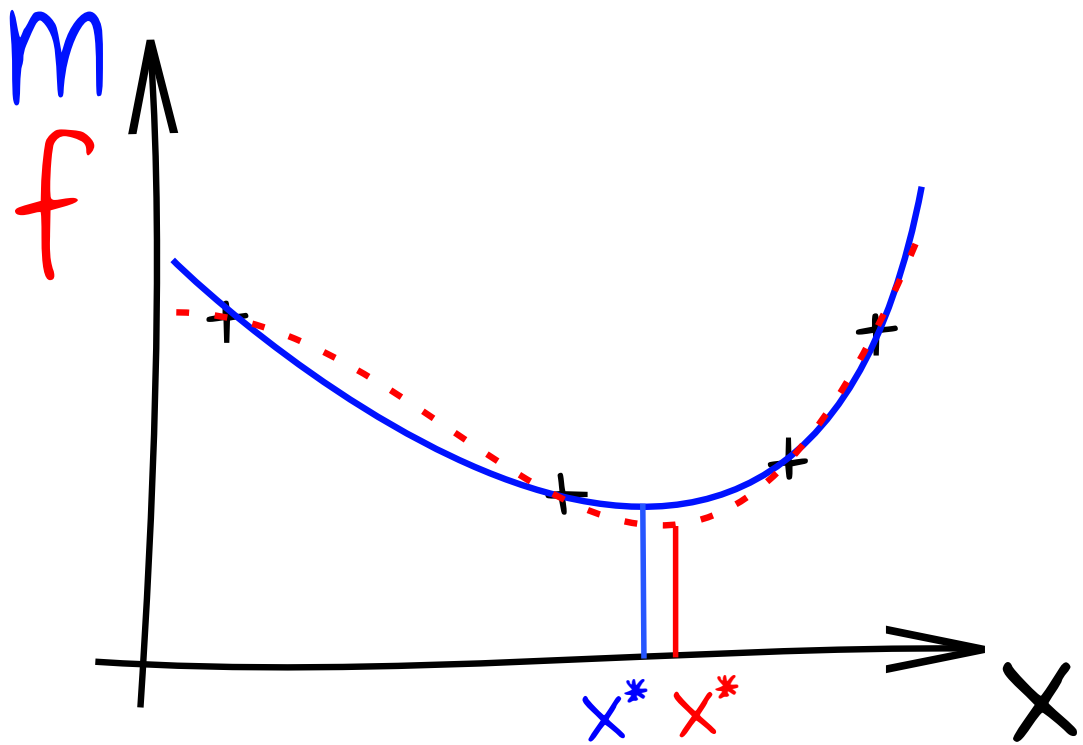
Other kernel design methods

There are two other popular methods for kernel design:

- Bochner Theorem
  There is an equivalence between positive measures and stationnary positive definite functions.
- Linear operators
  If the function to approximate has particular properties that can be obtained via a linear transform, it is possible to build a GP with the wanted properties. For example, one can build symmetric GPs or GPs with integral equal to zero.

Model based optimization methods

If the number of function evaluations are limited, we can run the optimization on the model instead of running it directly on the function

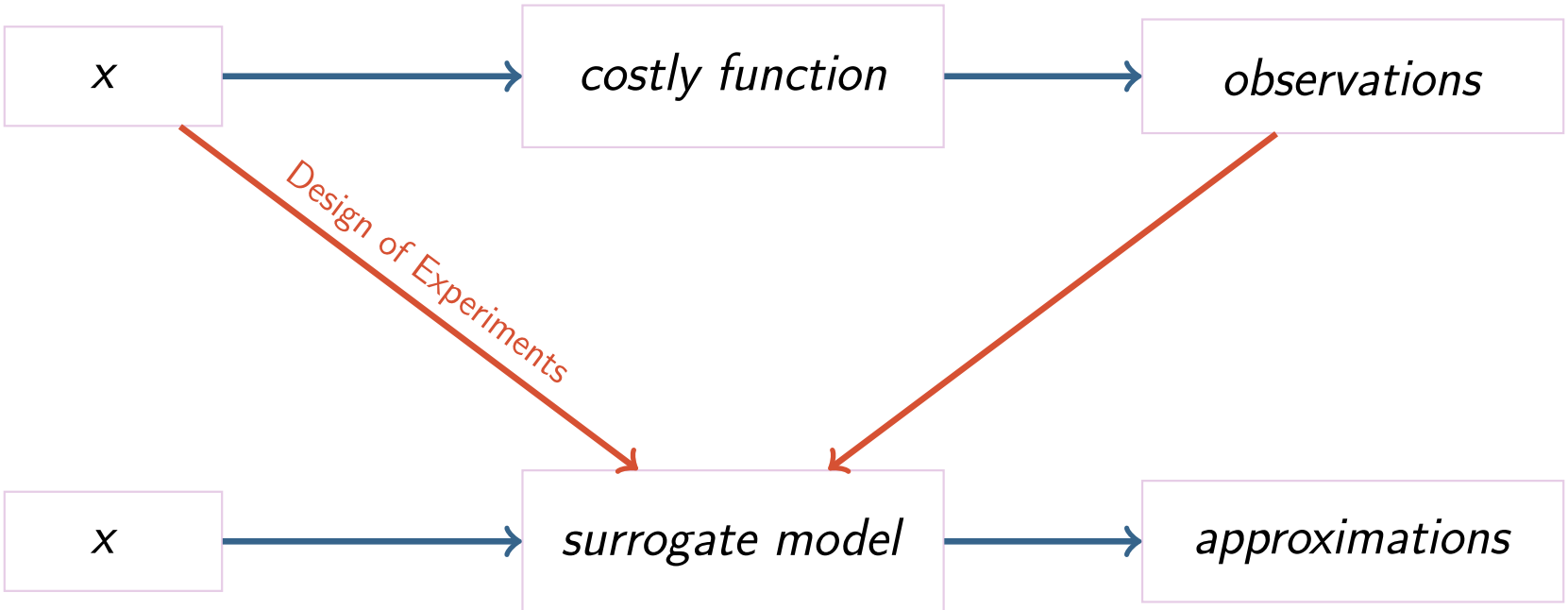


In the end, we hope that:

$$\text{argmin}(m) \approx \text{argmin}(f)$$

$$\min(m) \approx \min(f)$$

Overall framework



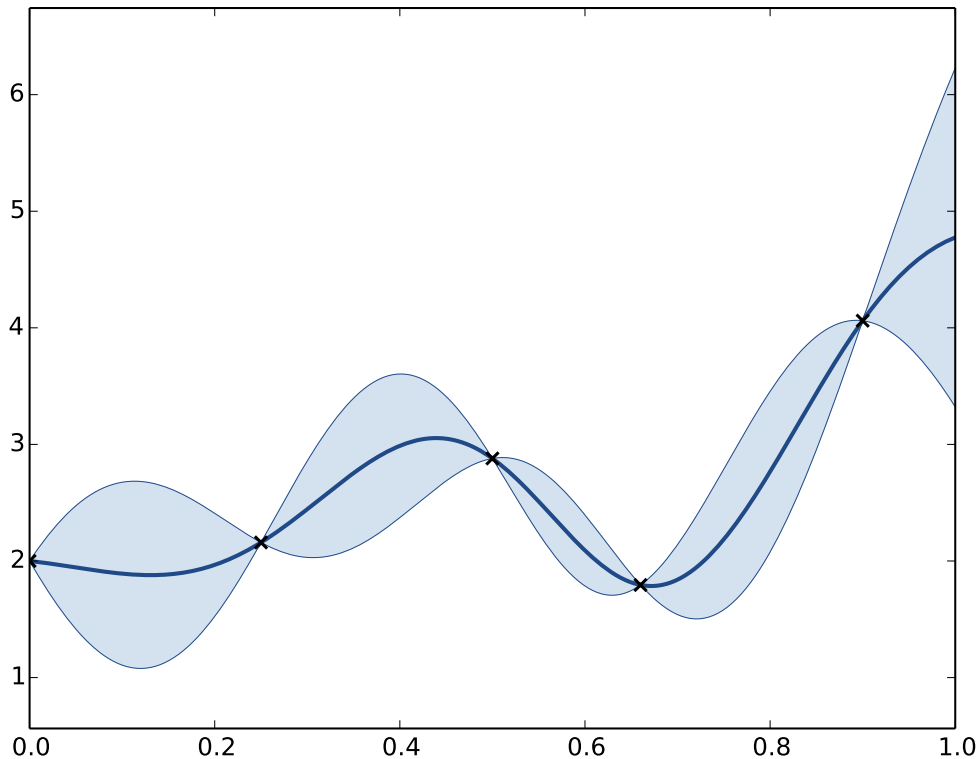
In practice, it is risky to take decisions based only on the model...

On the other hand, the model can be used to guide us in the search for the optimum.

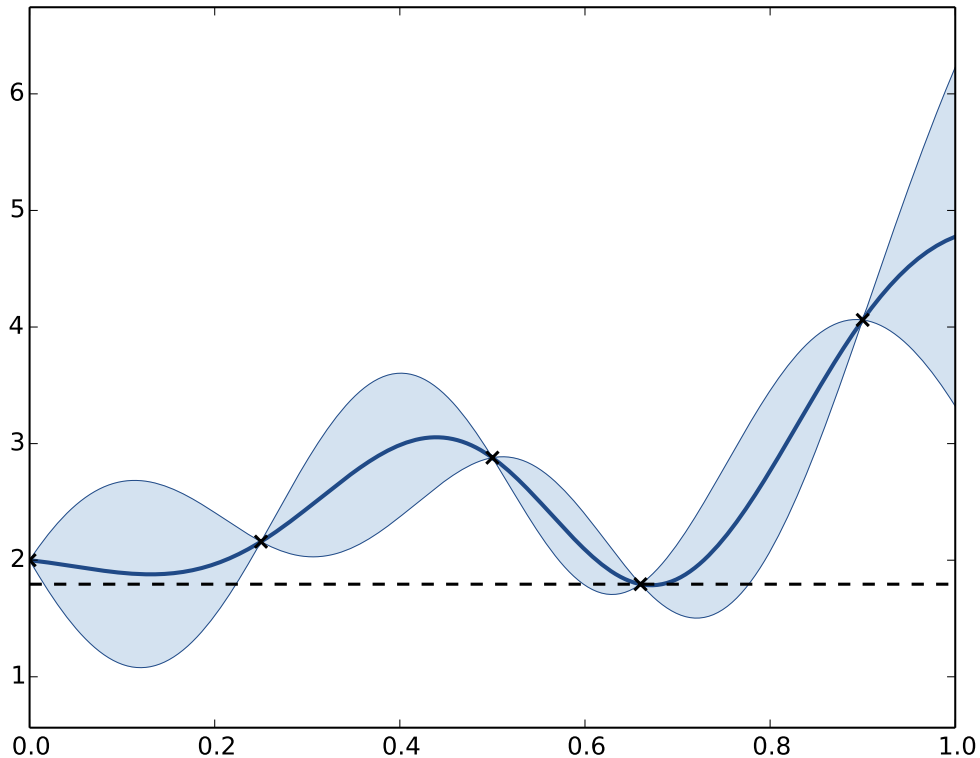
Global optimization methods are a trade-off between

- Exploitation of past good results
- Exploration of the space

How can GPR models be helpful?



In our example, the best observed value is 1.79

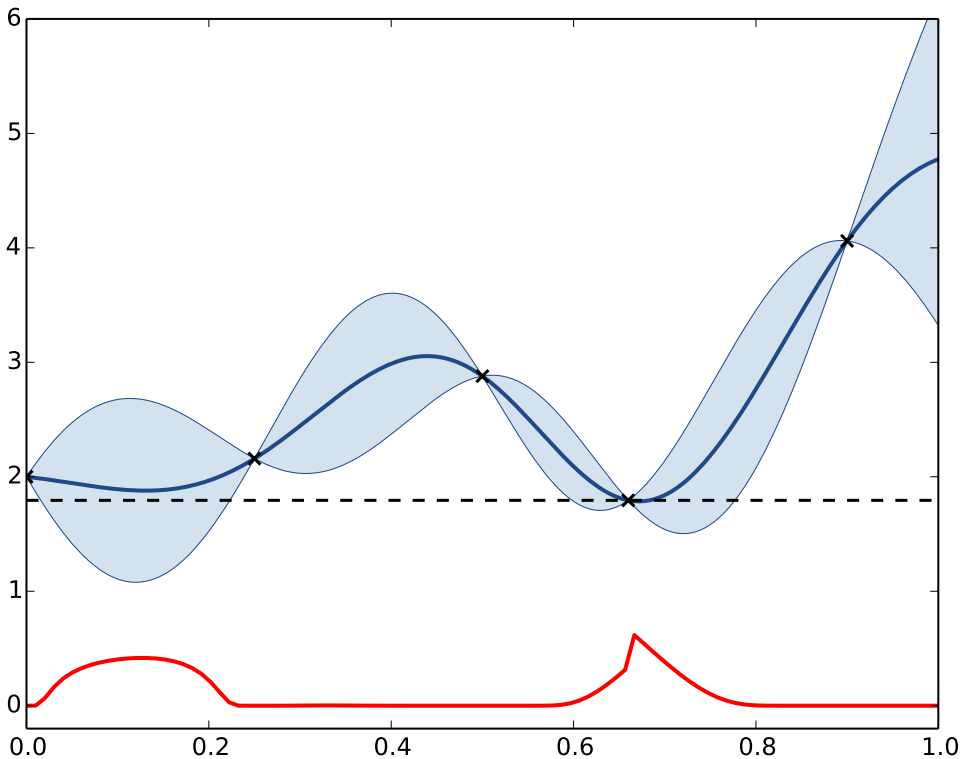


Various criteria can be studied

- probability of improvement
- Expected improvement

Probability of Improvement:

$$PI(x) = cdf\left(\frac{\min(F) - m(x)}{\sqrt{(c(x,x))}}\right)$$



The point with the highest PI is often very close to the best observed value. We can show that there is a x in the neighbourhood of x^* such that $PI(x) \geq 0.5$.

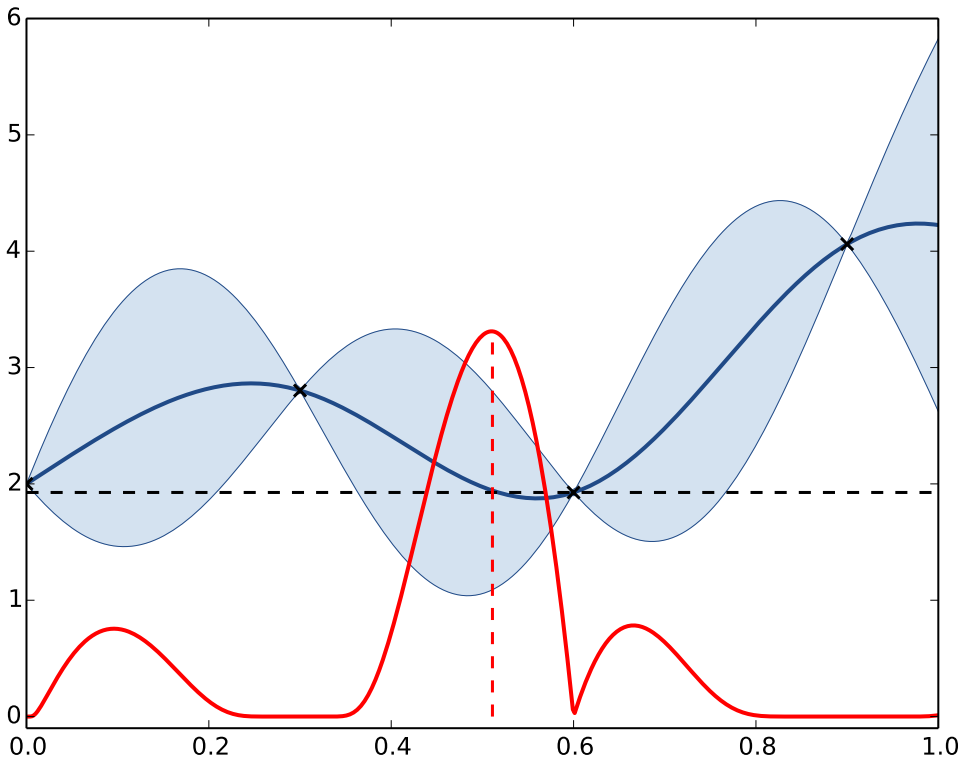
For such points, the improvement cannot be large...

Can we find another criterion?

Expected Improvement:

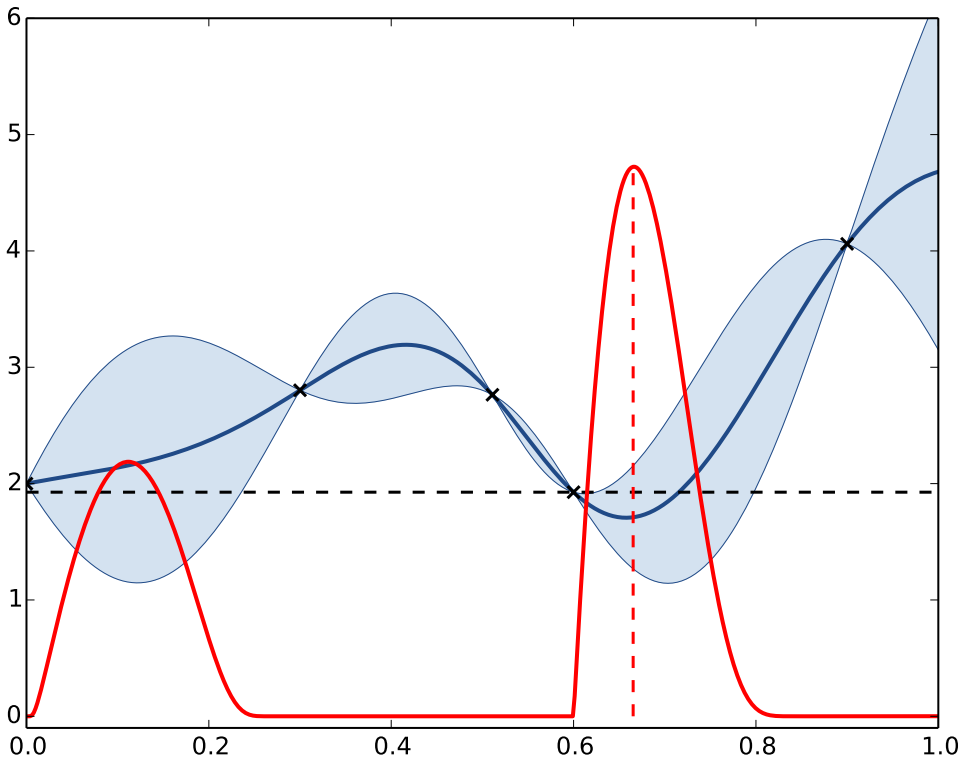
$$EI(x) = \int_{-\infty}^{\min(F)} \max(0, Y(x)) \; dy(x) = \cdots =$$

$$\sqrt{c(x,x)}(u(x)cdf(u(x)) + pdf(u(x))) \quad \text{with } u(x) = \frac{\min(F) - m(x)}{\sqrt{(c(x,x))}}$$



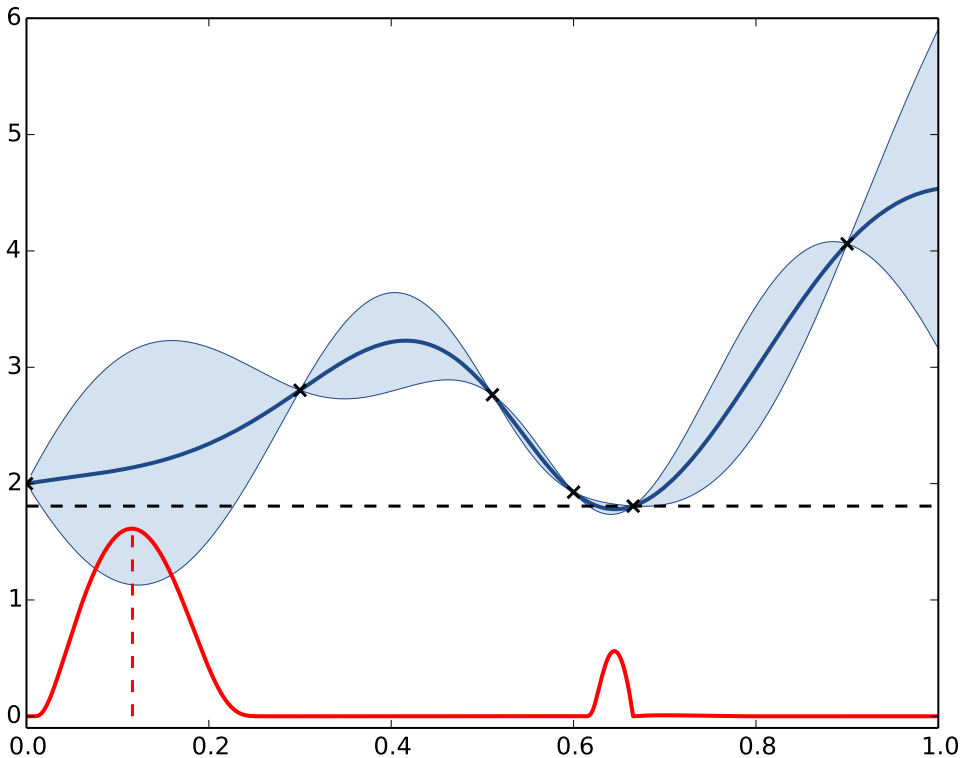
Expected Improvement

Let's see how it works... iteration 1



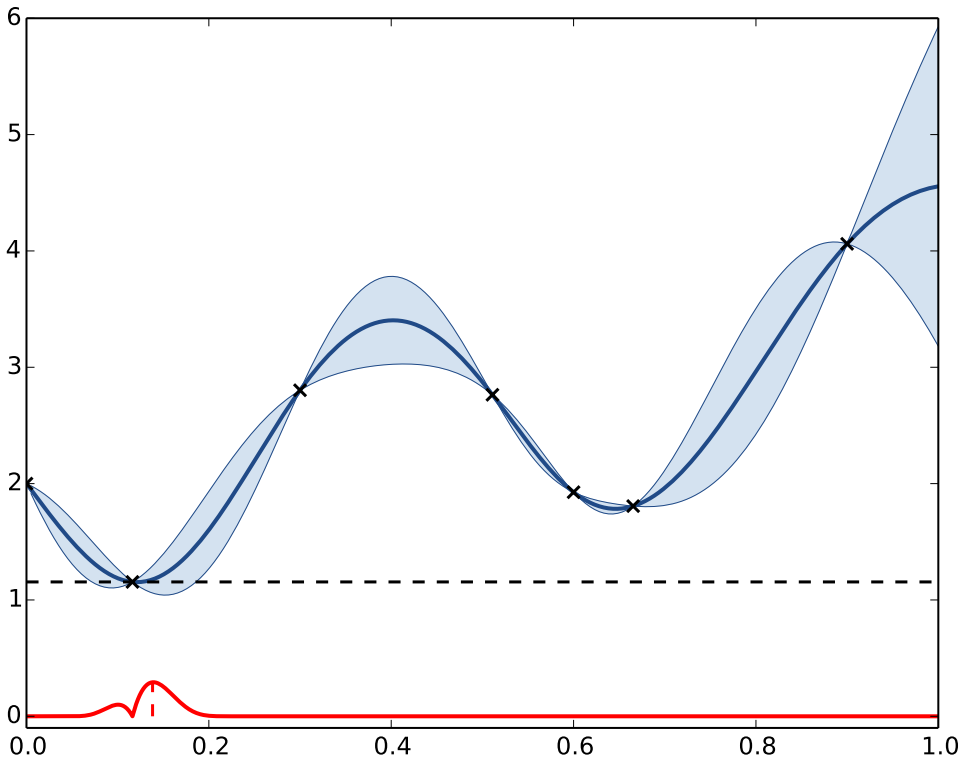
Expected Improvement

Let's see how it works... iteration 2



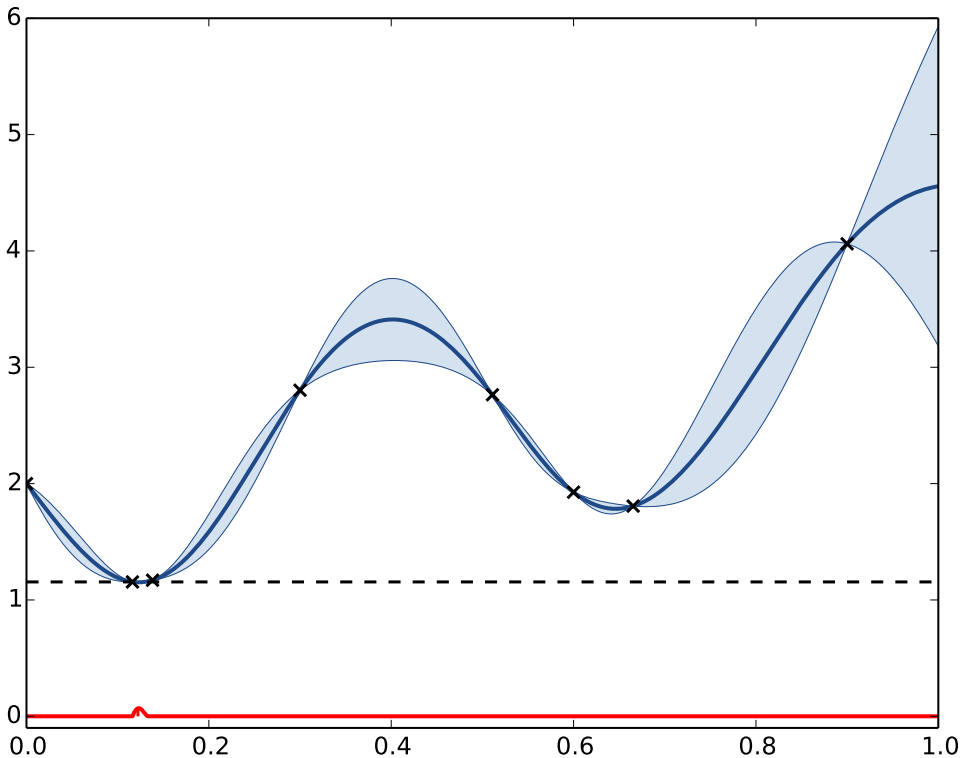
Expected Improvement

Let's see how it works... iteration 3



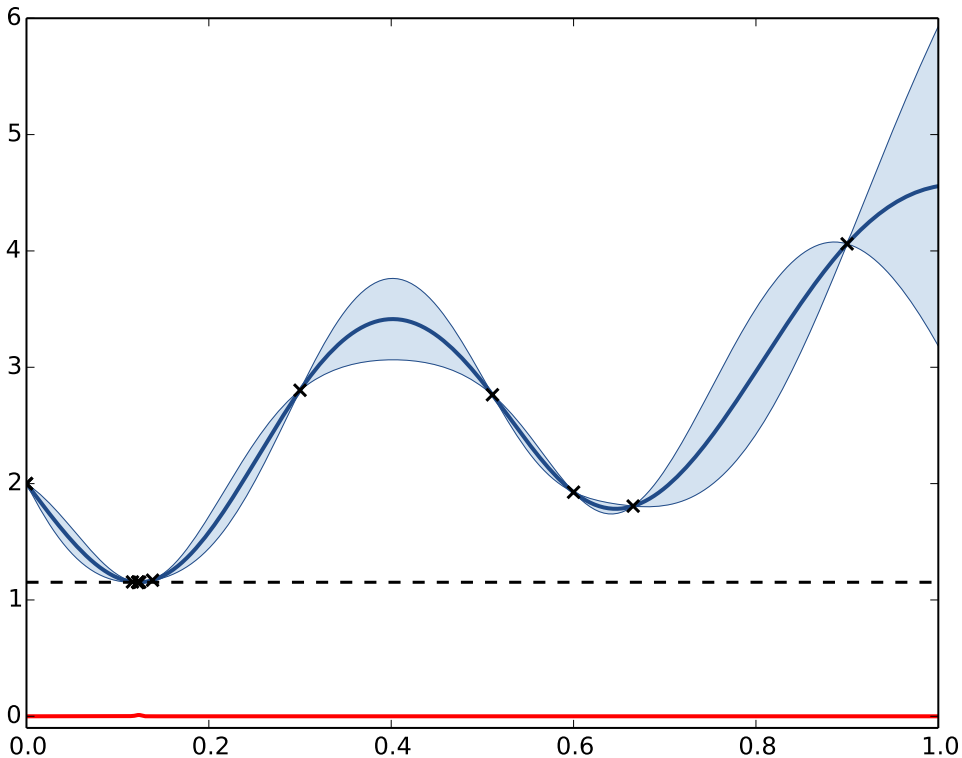
Expected Improvement

Let's see how it works... iteration 4



Expected Improvement

Let's see how it works... iteration 5



Expected Improvement

This algorithm is called **Efficient Global Optimization** (EGO, Jones et al., 1998):

1. make an initial design of experiments X and calculate the associated F, $t = \texttt{length}(F)$
2. built a GP from (X, F) (max. log-likelihood on σ and θ_i's)
3. $X_{t+1} = \arg\max_x EI(x)$
4. calculate $F_{t+1} = f(X_{t+1})$, increment t
5. stop ($t > t^{\max}$) or go to 2.

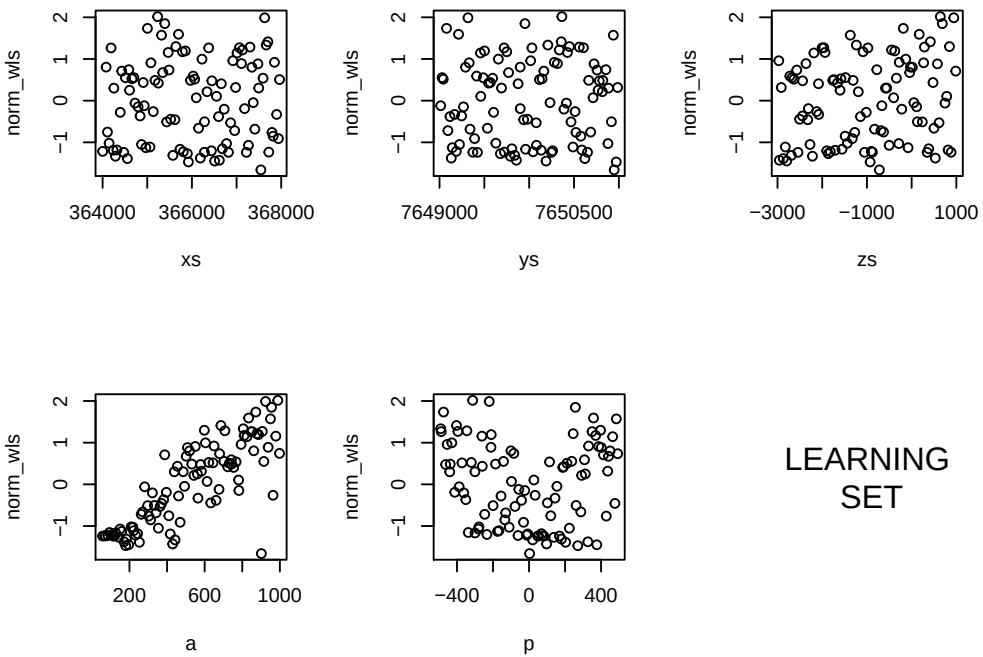
\+ EGO provides a good trade-off between exploitation and exploration without arbitrary parameters.

\+ It requires few function observations (10 in the example) to get close to optimal regions.

Example in 5d: surface displacements misfit minimization

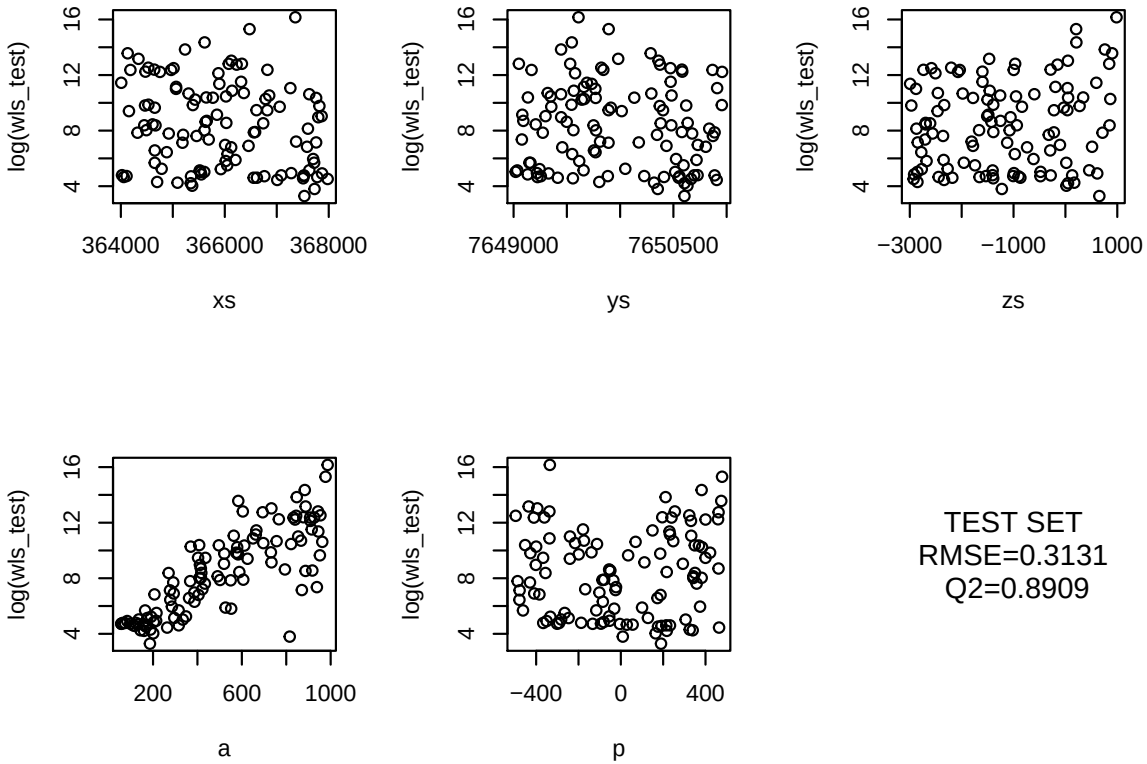
$\Rightarrow$ demo with `mainInversionPunctualDisplSource.R`

!!! normalize the data: WLS has a few very large values, it is always > 0: make it more gaussian, `wls_`$norm = \log(1 + \texttt{wls})$ and all x's and `wls_`$norm$ between 0 and 1.



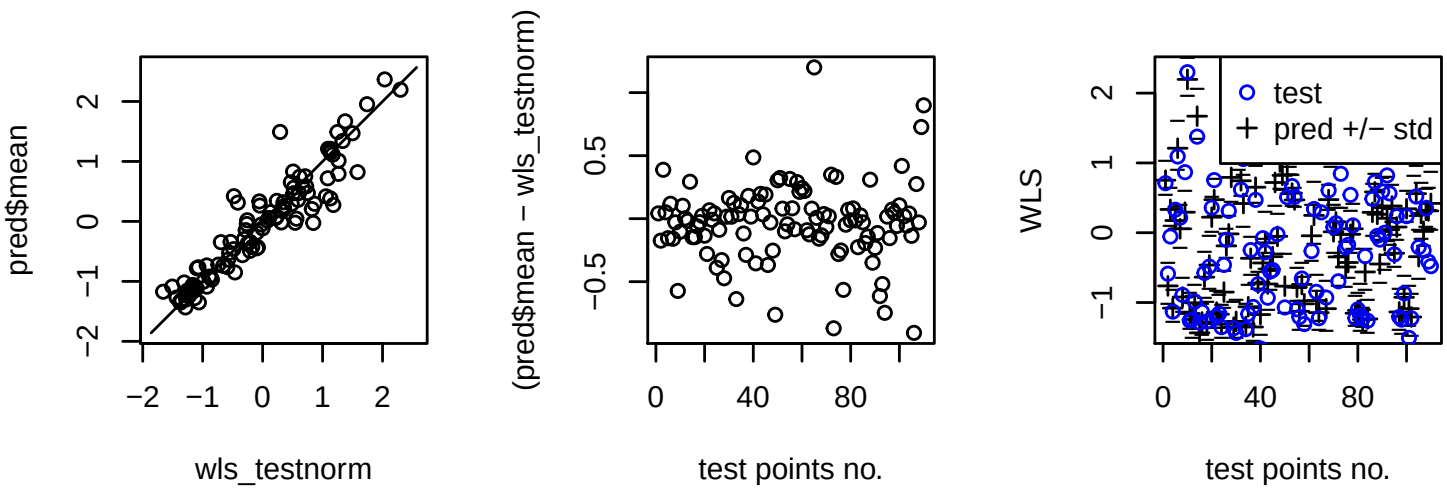
100 $\{xs, ys, zs, a, p\}$ points chosen through an optimized Latin Hypercube Sampling (`R` libraries `DiceDesign` or `lhs`).

(demo with `mainInversionPunctualDisplSource.R`, cont.)



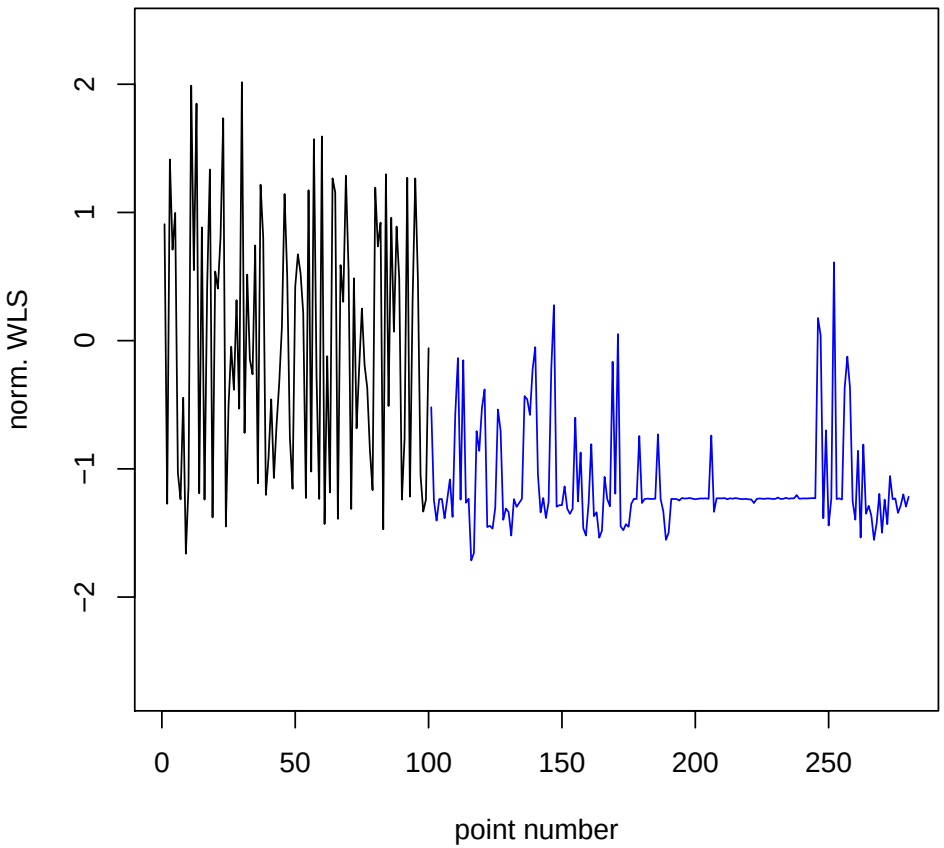
110 random $\{xs, ys, zs, a, p\}$ test points.

(demo with `mainInversionPunctualDisplSource.R`, cont.)



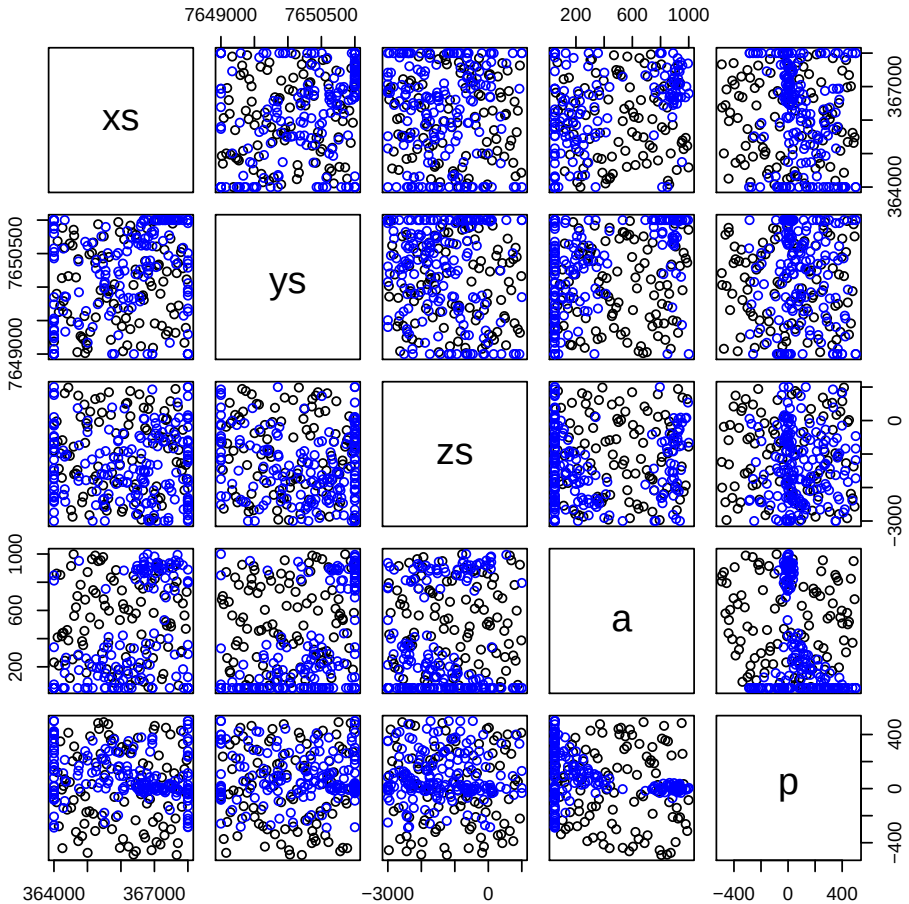
110 test points.

(demo with `mainInversionPunctualDisplSource.R`, cont.)
EGO parameters: anisotropic Matèrn 5/2 kernel, GP updated (log-likelihood maximized) every 5 added points, BFGS with bounded variables (from `optim()` function) restarted from random initial points for maximizing log-likelihood and EI.



Preferential sampling of good regions of S, but global therefore sometimes increasing WLS. Lower bound on θ_i's increased from 0.08 to 0.1 at $t = 250$ (x_i's and θ_i's normed between 0 and 1).

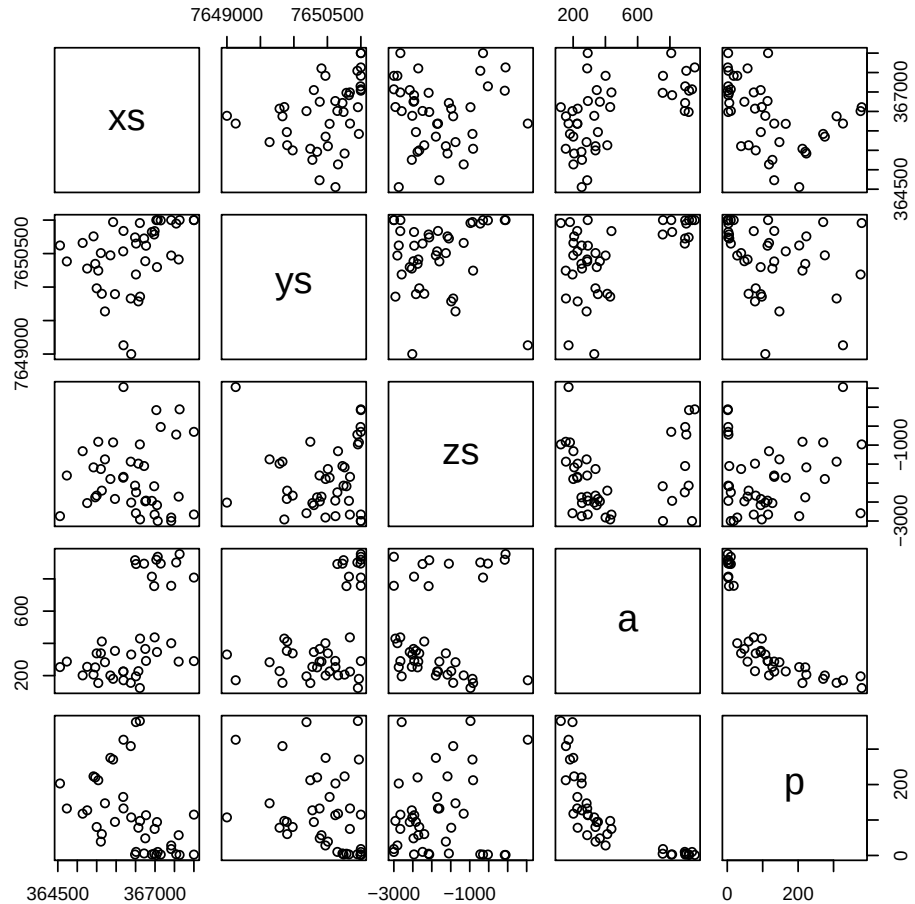
(demo with `mainInversionPunctualDisplSource.R`, cont.)



Black: LHS initial points.
Blue: EGO points.

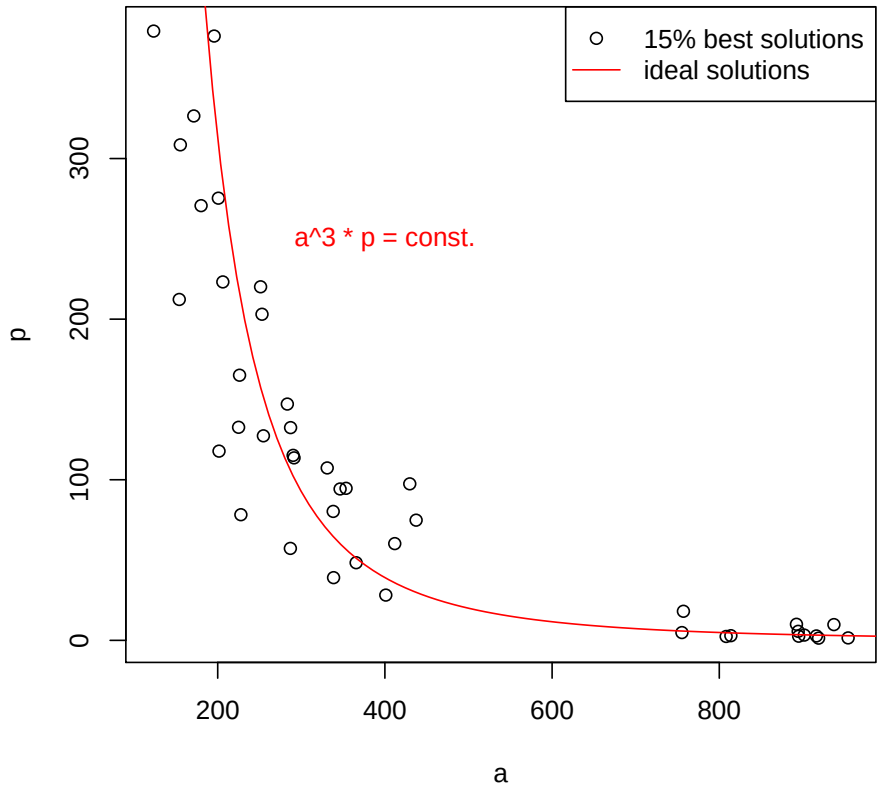
Note the patterns in new points. Accumulation at lower bound of a and mid interval of p before $t = 250$.

(demo with `mainInversionPunctualDisplSource.R`, cont.)



15% best sampled points. Note the "function" for the (a, p) pair, i.e., $a^\star(p^\star)$.

(demo with `mainInversionPunctualDisplSource.R`, cont.)



Mogi model only dependency in a and p is through $a^3 \times p$: it is not identifiable.

EGO tells it by preferential sampling in the valley

$$a^3 \times p = \text{const.} = a^{\star 3} \times p^{\star}$$

Other EGO output: a statistical model of WLS.
The last length scales are an indication of the sensitivity of WLS to each variable: a, p and zs are very sensitive (θ_i's small, in $[0.08, 0.1]$), xs a little sensitive (θ in $[0.1, 2.5]$) and ys insensitive ($\theta \approx 3$).

Difficulties and challenges with EGO

- Standard GPs are limited to $n \approx 1000$ points (covariance matrix inversion).
- EGO clusters points in good regions, the covariance matrix may become ill-conditionned if length scales θ_i are too large w.r.t. X.
- Although the method perfectly applies to large dimensional spaces ($d > 100$), larger d may require larger n, back 2 lines above.
- EGO does not converge in the traditional sense: it creates dense samples in the volume of S. The efficiency comes from the order in which points are sampled.

$\Rightarrow$ these are the topics of current research. Let's mention a few extensions next.

EGO continuations

- Parallelized EGO: estimate the *EI* of groups of points, cf. Ginsbourger et al.
- Finite budget: *EI* of a single x is only optimal at the last iteration. Theory of dynamic *EI*, cf. Ginsbourger et al.
- EGO and bad covariance matrix conditioning: replace points that are close-by by one point and the associated derivatives (cf. M. Osborn, L. Laurent), regularizations (cf. Le Riche et al.)
- SUR strategies: (Step-wise Uncertainty Reduction), reduce the entropy of the optimum (cf. Vasquez et al.), or the average probability of incursions below $min(F)$ (cf. Picheny).

Related problems addressed with GPs

- EGO with constraints: $\min_x f(x)$ s.t. $g(x) \leq 0$, multiply the EI by the probability of constraints satisfaction.
- GP for target attainment: find the set of x s.t. $f(x) = T$, change the EI into $c(x,x) \times \text{pdf}\left((T - m(x))/sqrt(c(x,x))\right)$, cf. Picheny et al.
- GP for probability estimation: find $\mathbb{P}(f(x,U) \leq T)$ where U is a random vector.
- GP for multi-objective optimization: $\min_x\{f_1(x), \ldots f_m(x)\}$, cf. Binois et al.

Robust optimization

Can EGO be adapted when observations are noisy?

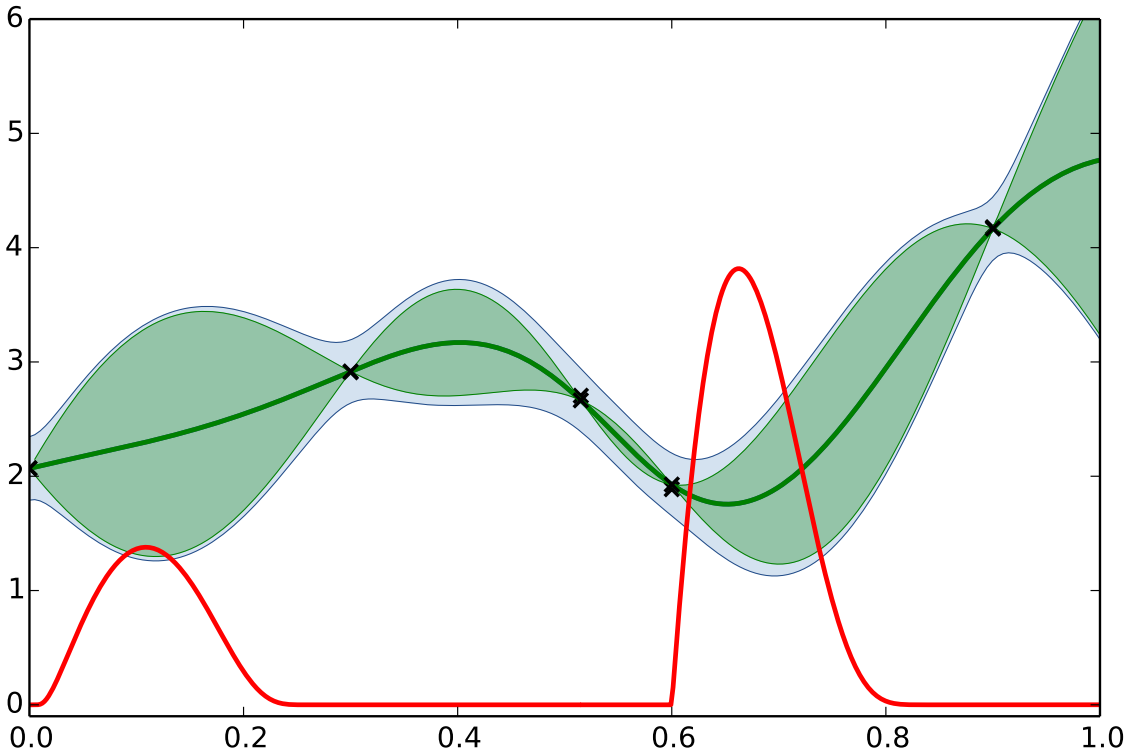
First of all, using the current best observation as a minimum does not make much sense...

Some solutions are

- S1 Build a new model that interpolates $m(X)$ at X where $m(X)$ accounts for the noise (non interpolating GP, e.g. with a white noise part in the kernel).
- S2 Include observation noise and replace $\min(F)$ by $\min(m(X))$ in the EI expression
- S3 Similar to 2 but consider an Expected Mean Improvement (V. Picheny).

Solution 1

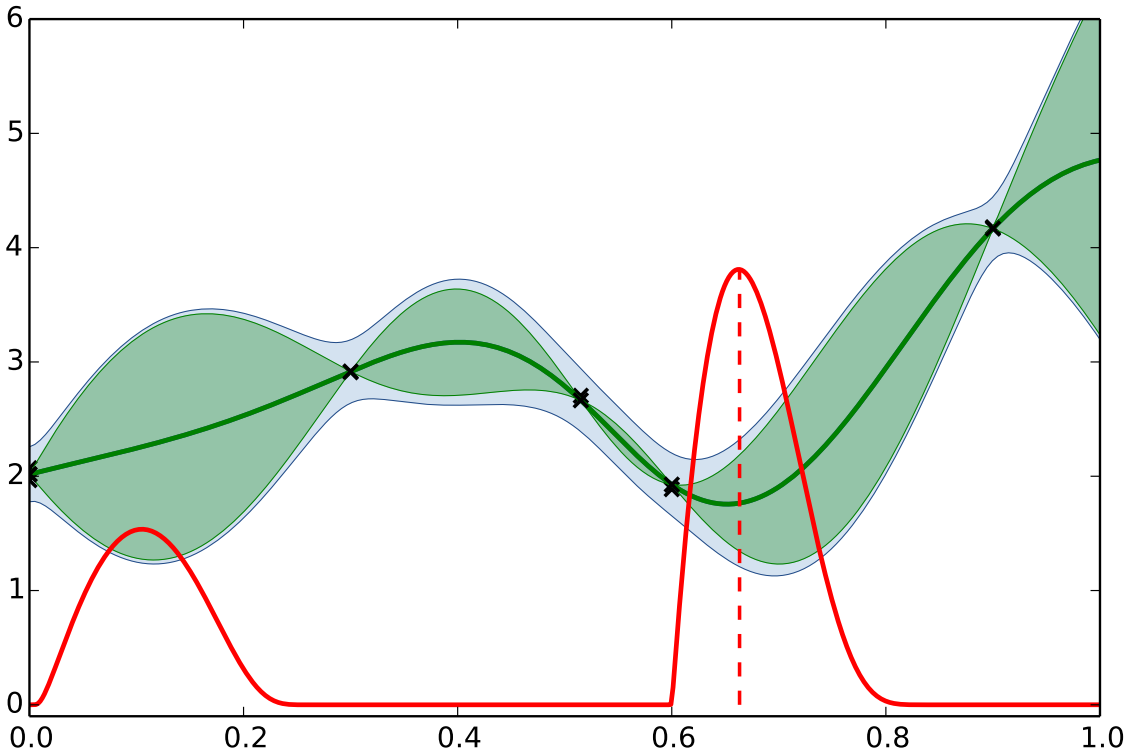
iteration 0



(noisy observations and their denoised versions are both shown as black crosses)

Solution 1

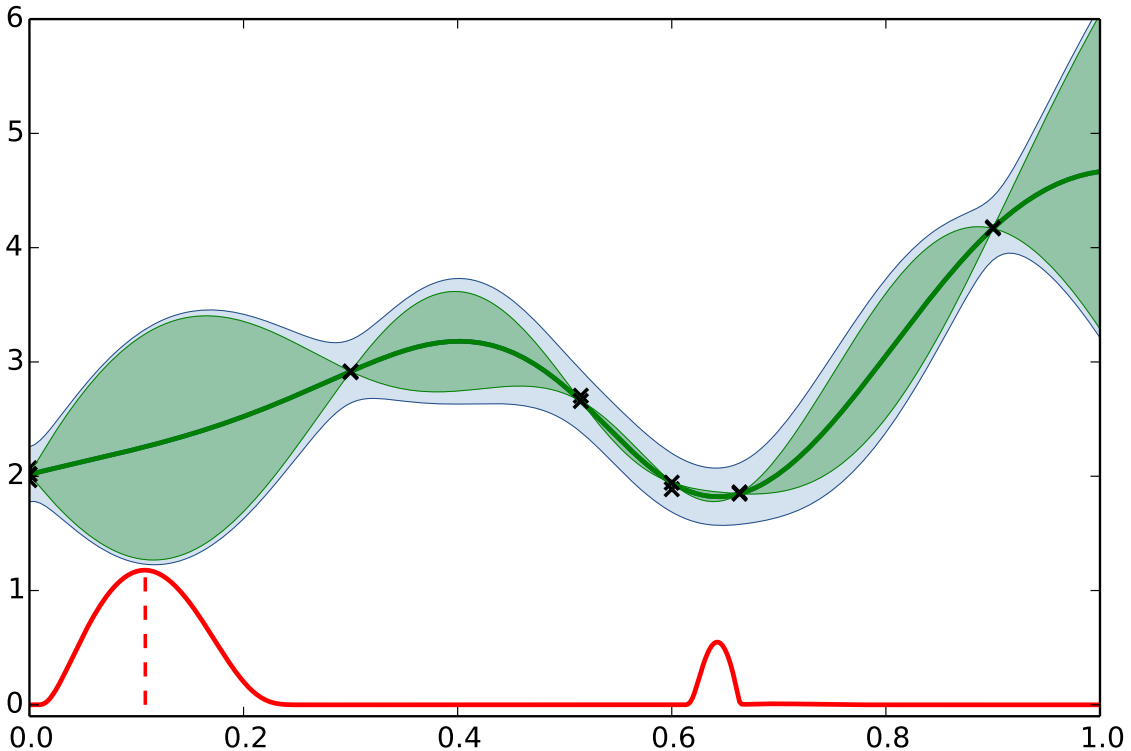
iteration 1



(noisy observations and their denoised versions are both shown as black crosses)

Solution 1

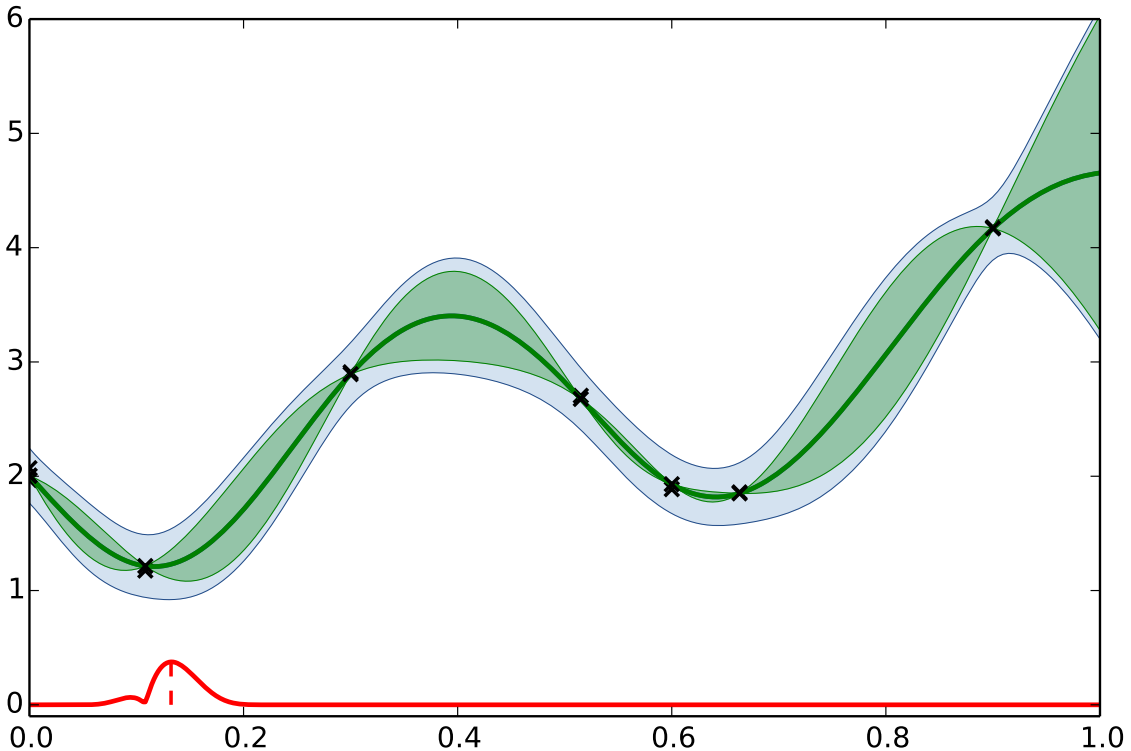
iteration 2



(noisy observations and their denoised versions are both shown as black crosses)

Solution 1

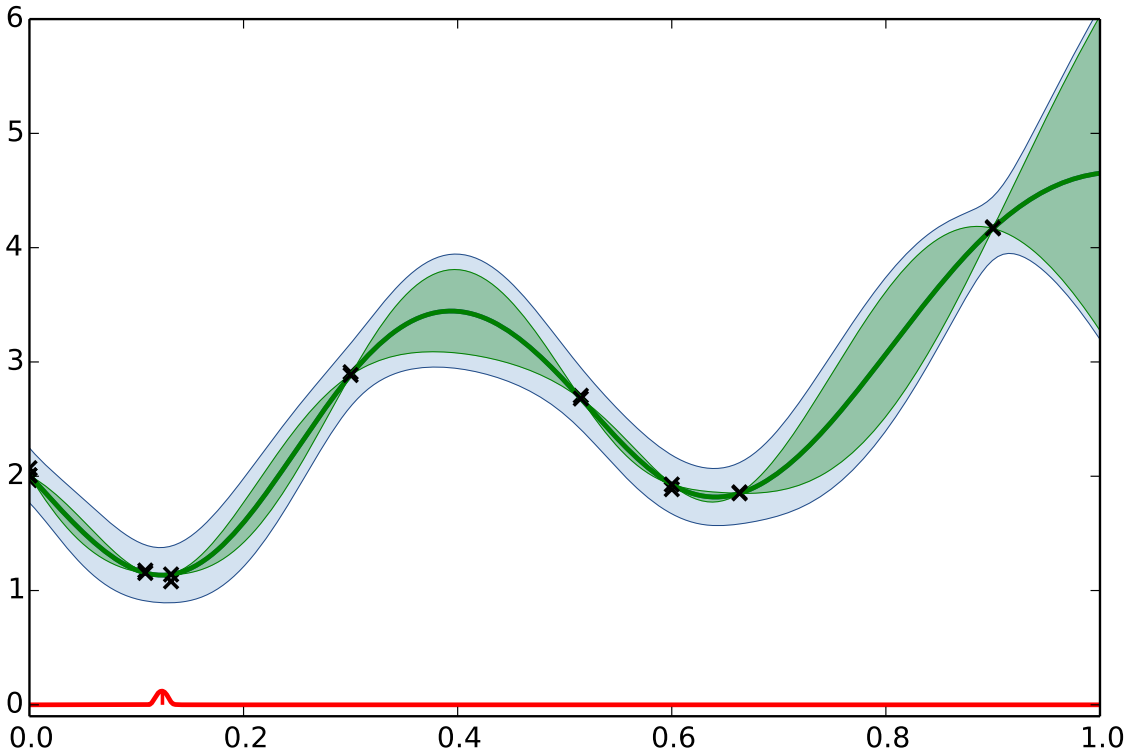
iteration 3



(noisy observations and their denoised versions are both shown as black crosses)

Solution 1

iteration 4



(noisy observations and their denoised versions are both shown as black crosses)

Concluding remarks

Conclusions

- Gaussian Processes offer a mathematically funded and versatile framework for building statistical models.
- The main assumptions are: the phenomenon output is Gaussian, functional choice of covariance function (kernel).
- The statistical model needs physical knowledge: through data + expertise guiding the choice of kernel (which may come from the physical model).
- The statistical model is in essence complementary to the physical model and typically useful for decision making (optimization, uncertainty propagation, ...).