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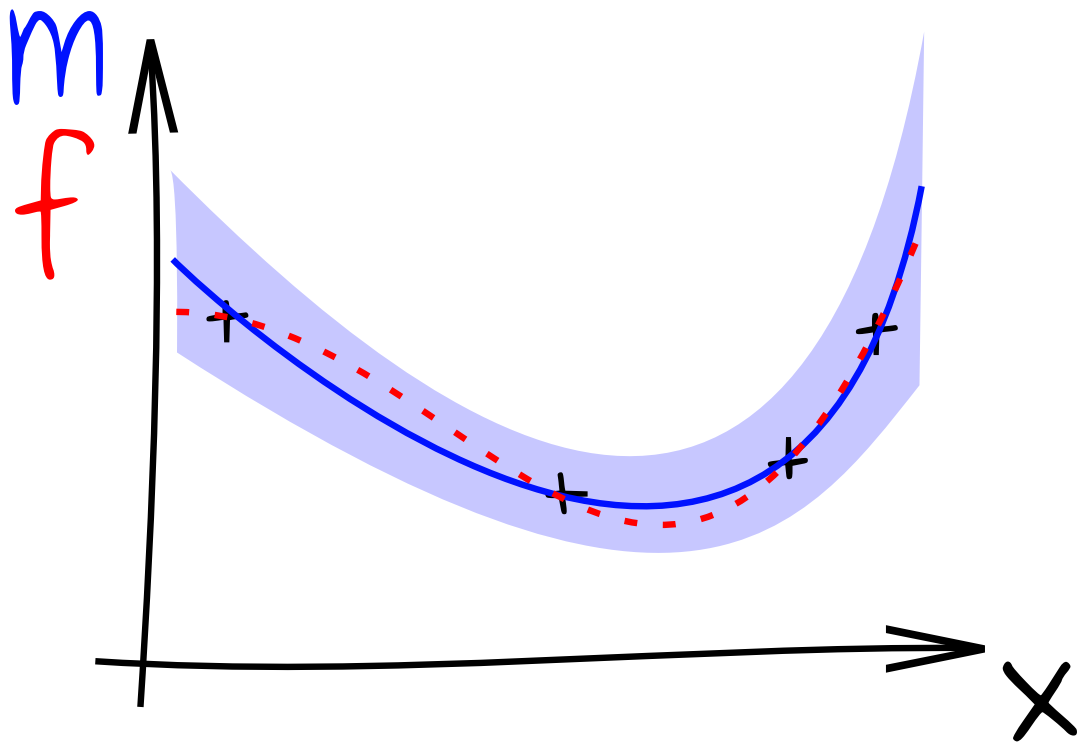
Introduction to statistical modelling

Nicolas Durrande, nicolas@prowler.io

PROWLER.io, Cambridge (UK) – Mines St-Étienne (France)

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 $F = f(X)$).

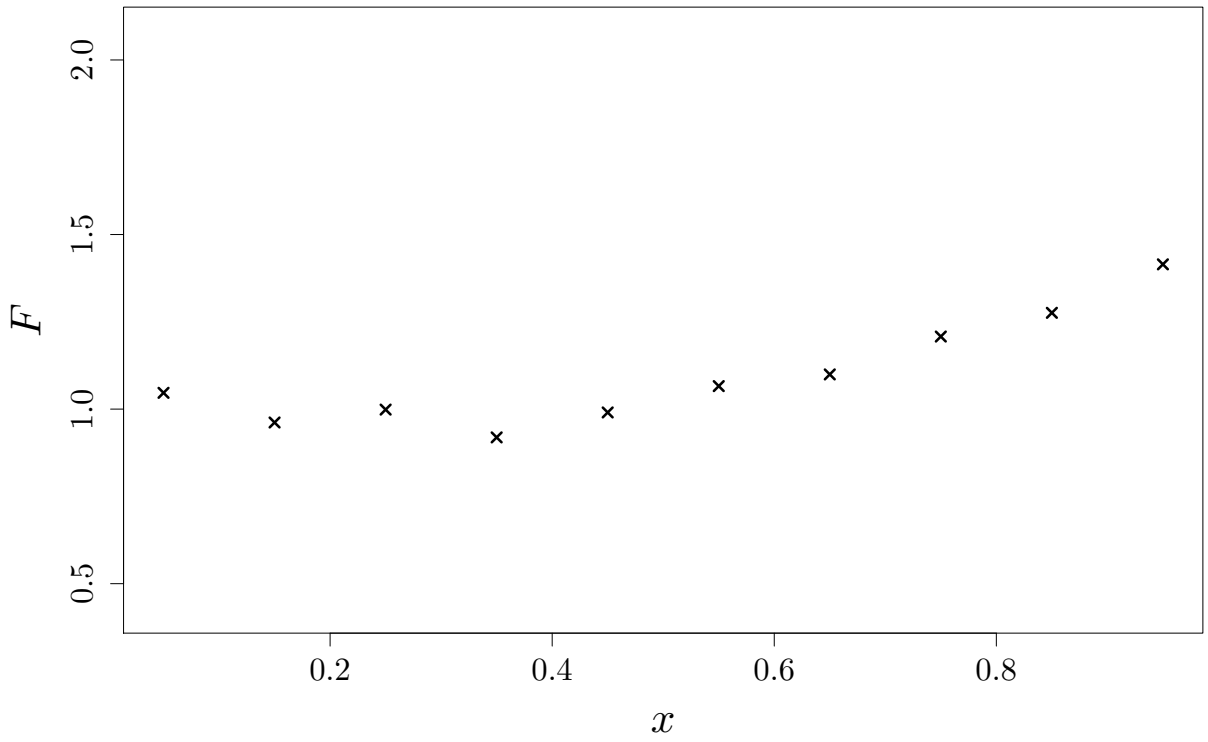
We will now discuss two types of statistical models:

- Linear regression
- Gaussian process regression

Linear Regression

Example

If we consider the following observations:

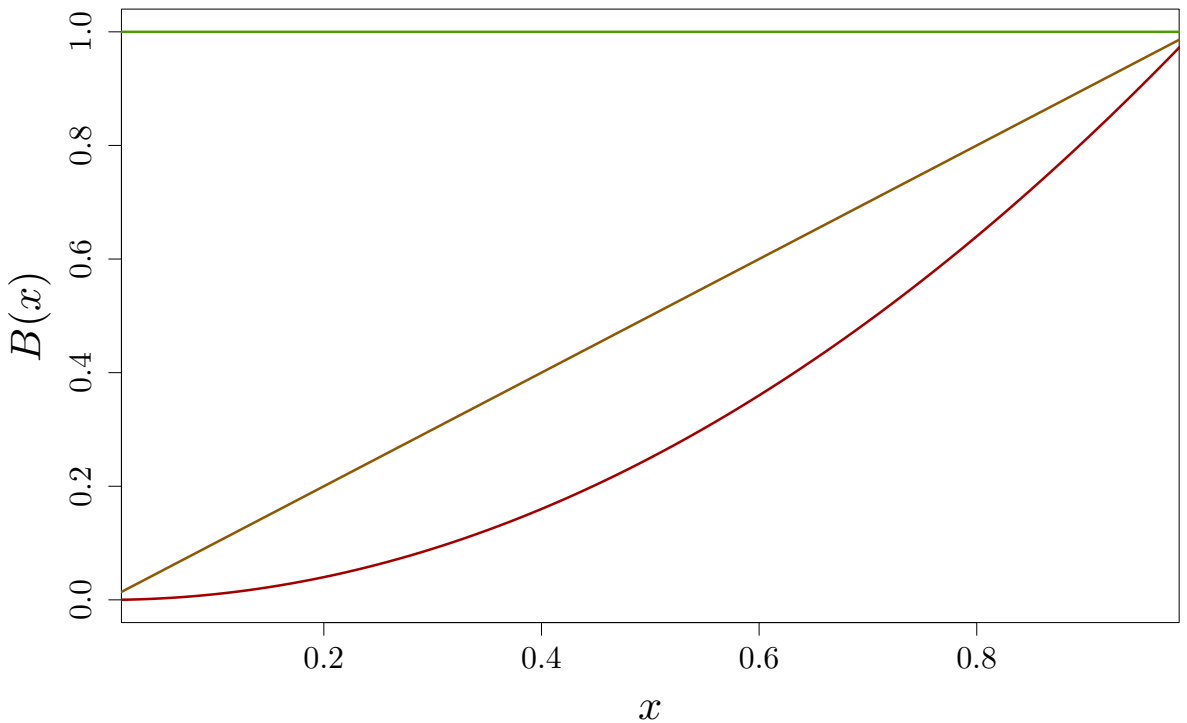


Example

We assume the observations are drawn from

$$F_i = \sum_{k=0}^{2} \beta_k b_k(X_i) + \varepsilon_i \qquad (= B(X_i)\beta + \varepsilon_i)$$

with $b_0(x) = 1,\ b_1(x) = x,\ b_2(x) = x^2$, unknown β_i and i.i.d ε_i.

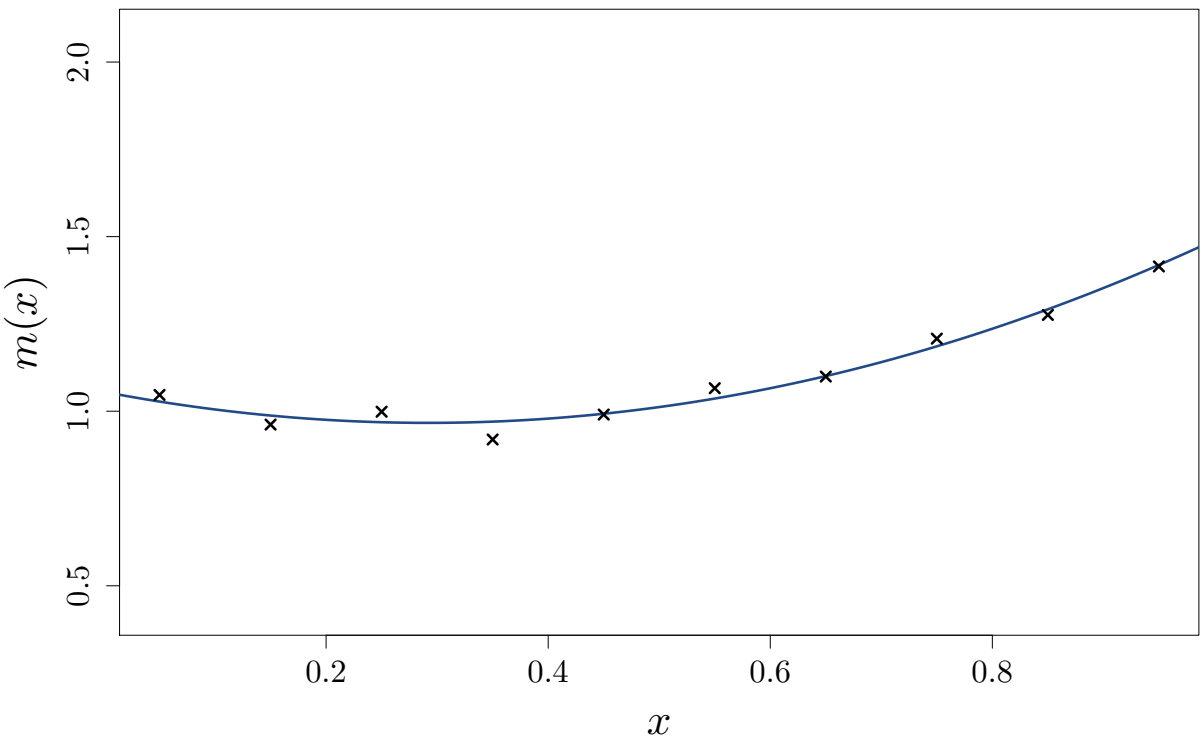


Example

The best linear unbiased estimator of β is

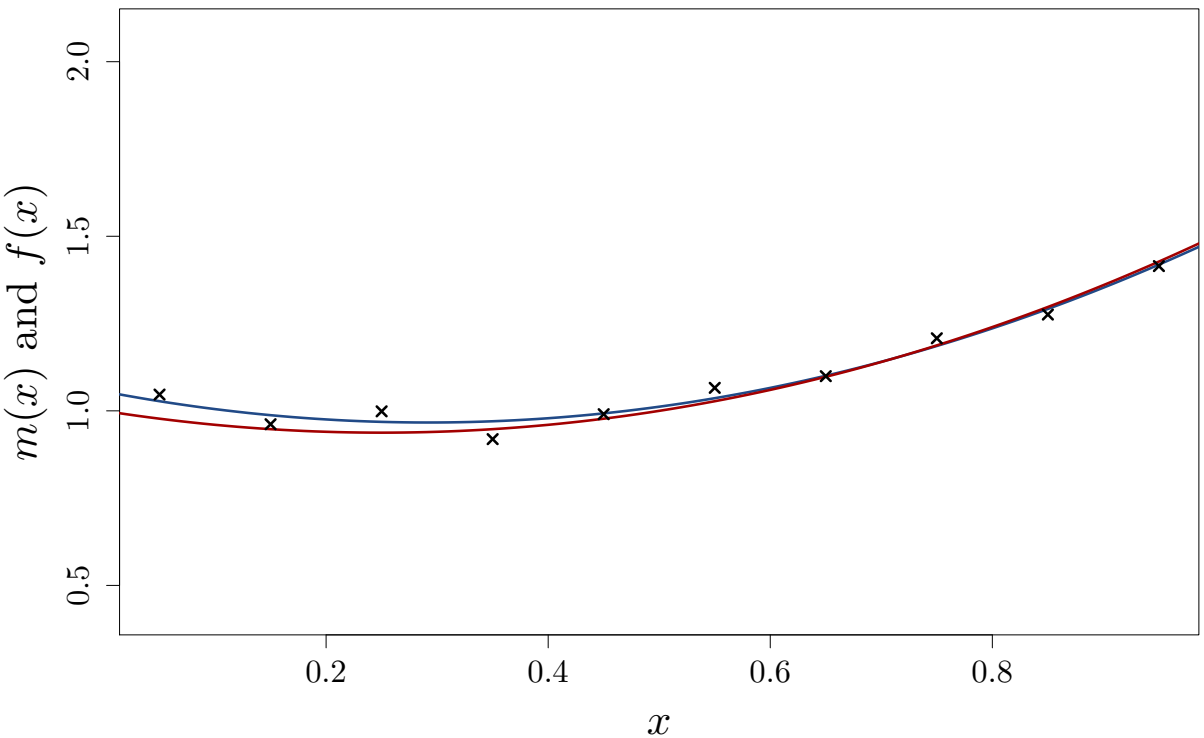
$$\hat{\beta} = (B(X)^t B(X))^{-1} B(X)^t F.$$

We obtain $\hat{\beta} = (1.06, -0.61, 1.04)^T$ and the model is:



Example

There is of course an error between the true generative function and the model



Can this error be quantified?

The initial assumption is $F = B(X)\beta + \varepsilon$ and we have computed an estimator of β:

$$\hat{\beta} = (B(X)^t B(X))^{-1} B(X)^t F.$$

$\hat{\beta}$ can thus be seen as a sample from the random variable:

$$\hat{\beta} = (B(X)^t B(X))^{-1} B(X)^t (B(X)\beta + \varepsilon).$$

What about the distribution of $\hat{\beta}$?

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What about the distribution of $\hat{\beta}$?

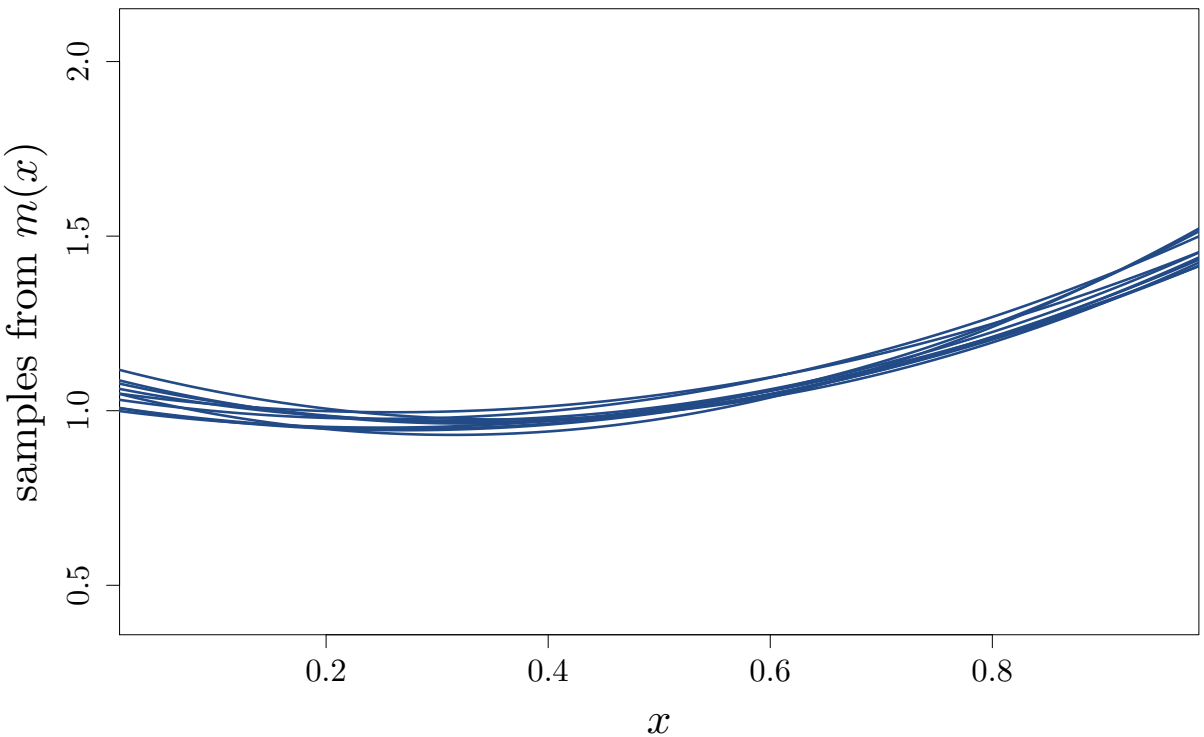
- Its expectation is $\beta \Rightarrow$ The estimator is unbiased
- Its covariance matrix is

$$(B(X)^t B(X))^{-1} B(X)^t \operatorname{cov}[\varepsilon, \varepsilon^t] B(X) (B(X)^t B(X))^{-1}$$

- If ε is multivariate normal, then $\hat{\beta}$ is also multivariate normal.

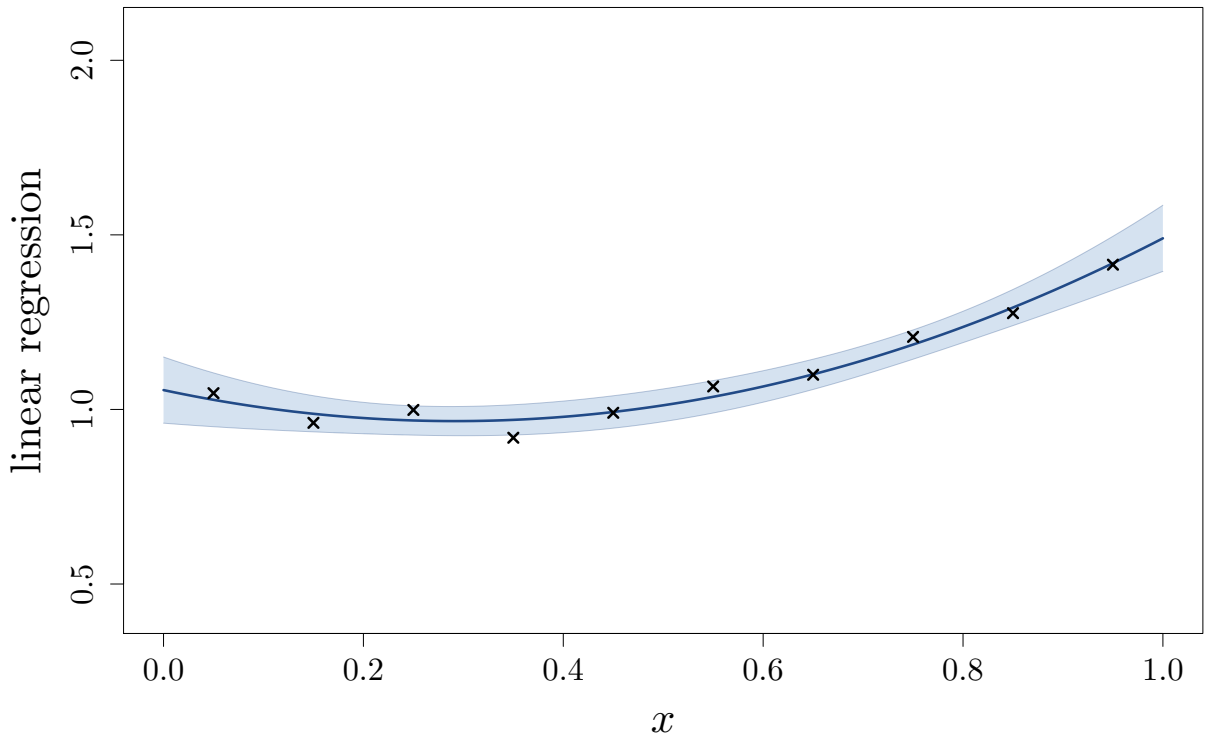
Sampling in the distribution of $\hat{\beta}$ gives us a large variety of models which represent the uncertainty about our estimation:

Back to the example



Back to the example

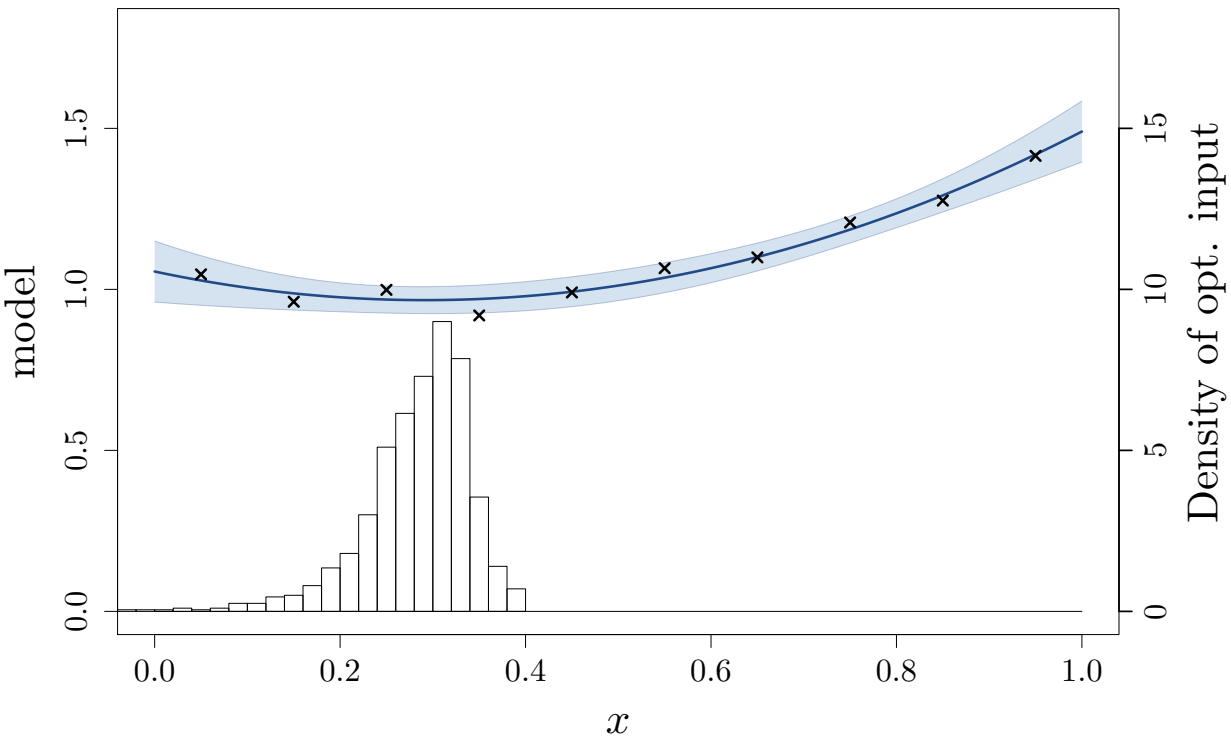
The previous picture can be summarized by showing the mean of m and 95% confidence intervals



This statistical model can be used for **uncertainty quantification**:

Back to the example

If we are interested in the value $x^\star$ minimizing $f(x)$:



we obtain a distribution for $x^\star$.

We could dedicate the entire course to linear regression models...

- model validation
- choice of basis functions
- influence of input locations
- ...

We will just stress a few **pros and cons of these models**:

+ provide a good noise filtering
+ are easy to interpret
− are not flexible (need to choose the basis functions)
− do not interpolate
− may explode when using high order polynomials (over-fitting)

Gaussian Process Regression

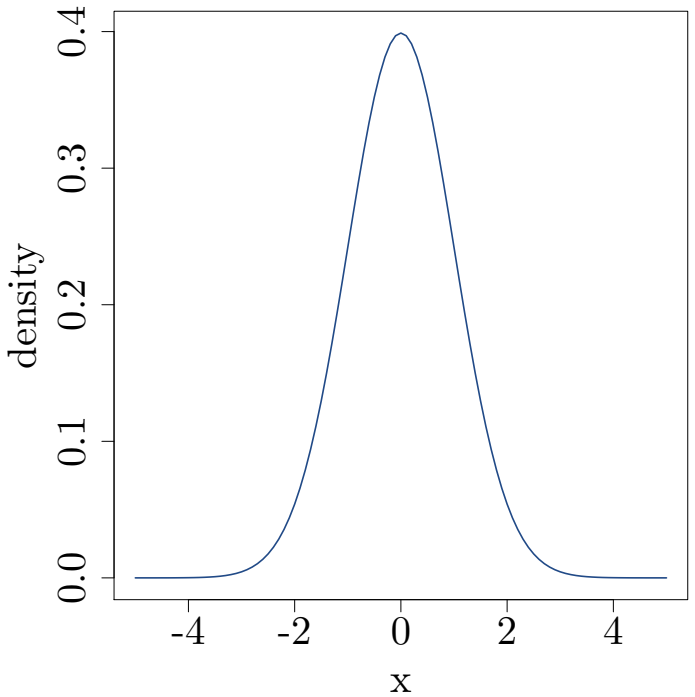
This section is organised in 3 subsections:

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** $\Sigma = \mathrm{E}[YY^t] - \mathrm{E}[Y]\,\mathrm{E}[Y]^t$

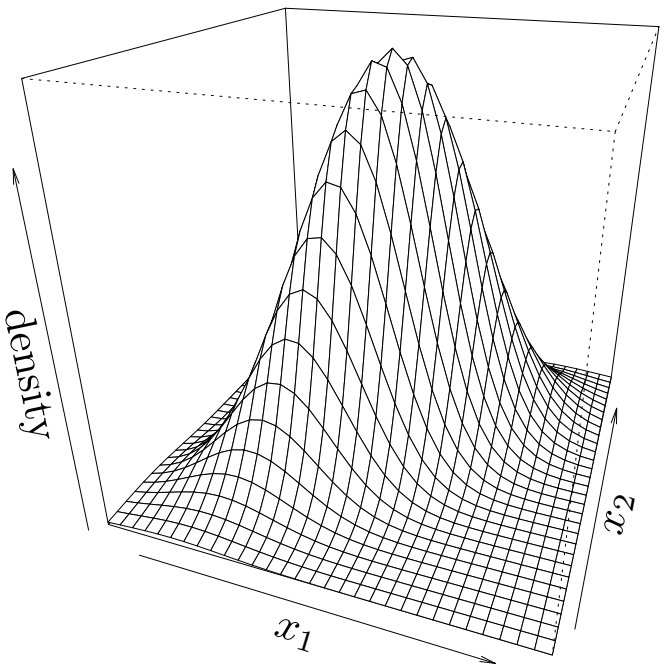
Property:

A covariance matrix is

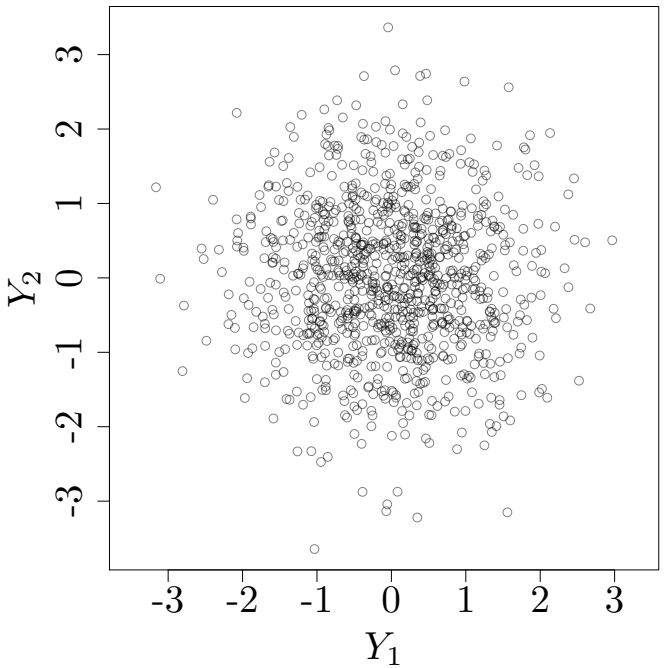
- symmetric $K_{i,j} = K_{j,i}$
- positive semi-definite $\forall \alpha \in \mathbb{R}^n, \alpha^t K \alpha \geq 0$.

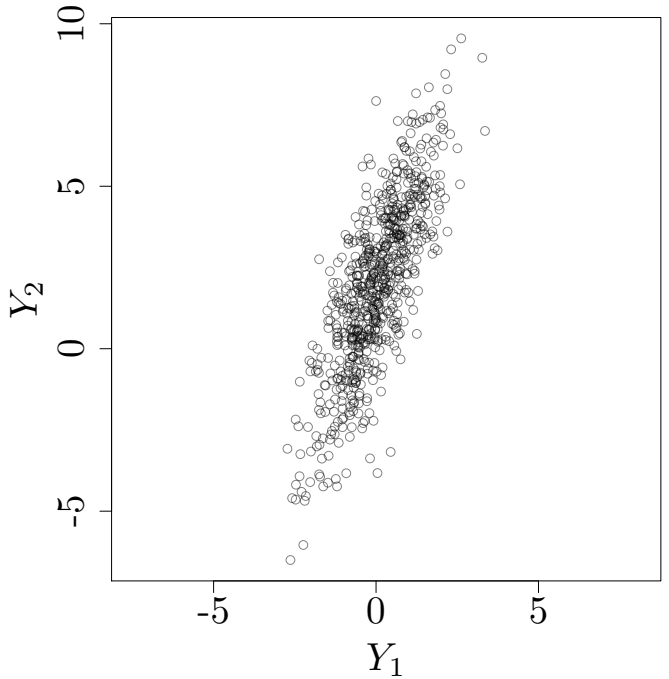
The density of a multivariate Gaussian is:

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



Samples from a multivariate normal



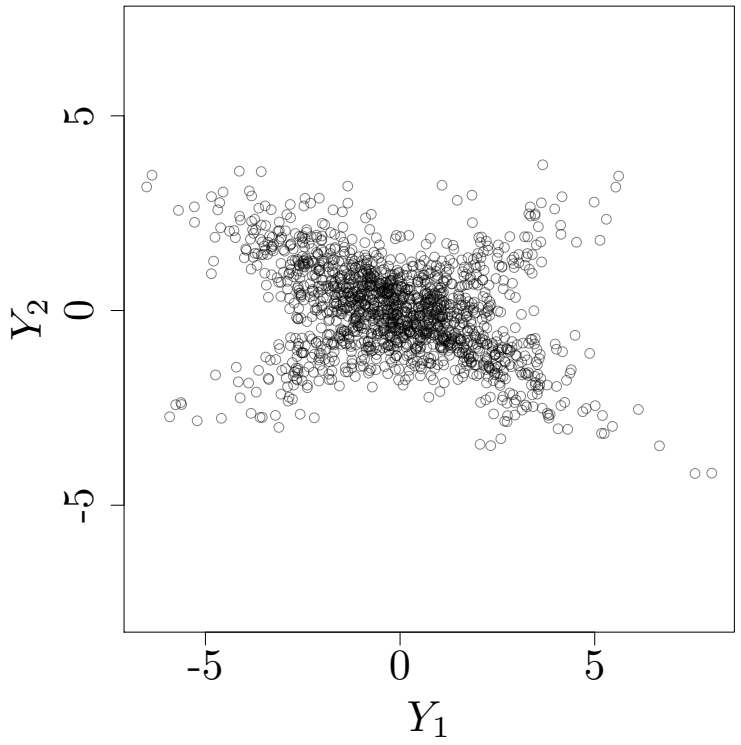


Exercise

- 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

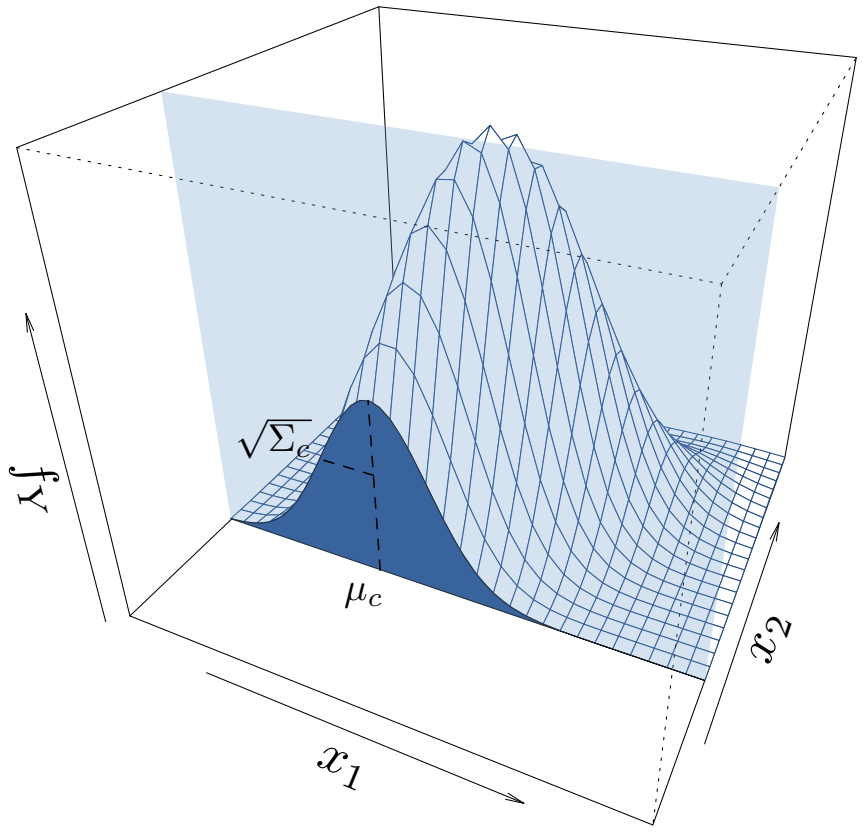
Counter example



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

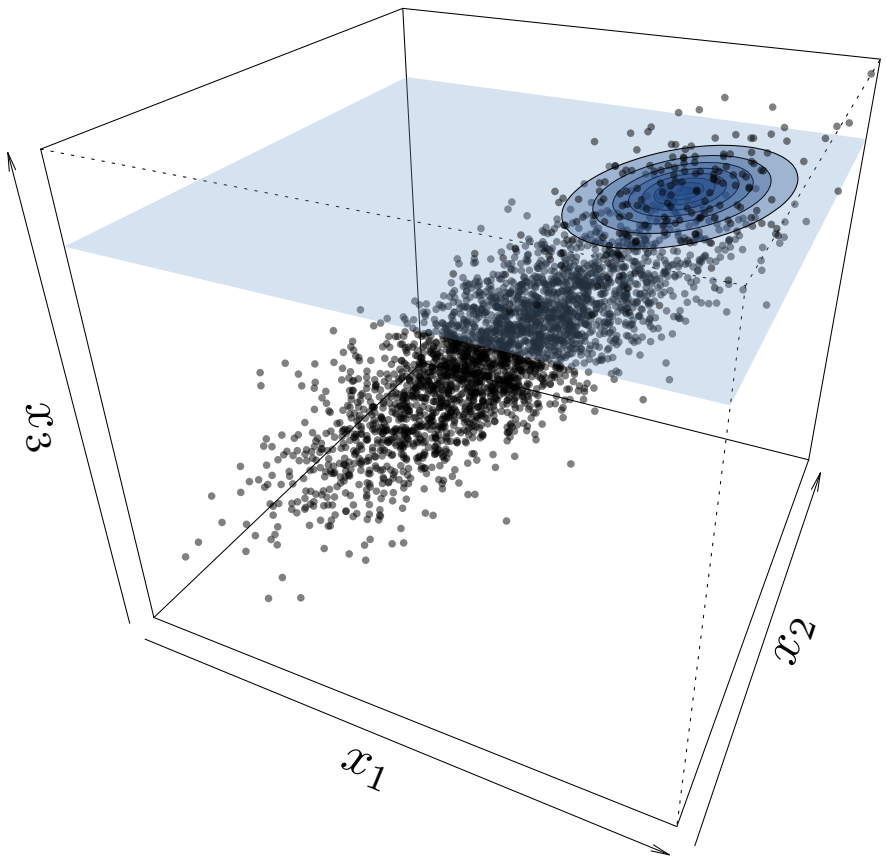
$$\begin{pmatrix} \text{cov}(Y,Y) & \text{cov}(Y,Z) \\ \text{cov}(Z,Y) & \text{cov}(Z,Z) \end{pmatrix}.$$

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!

⇒ 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	$k(x,y) = \sigma^2 \exp\left(-\frac{1}{2}\|\|x-y\|\|_\theta^2\right)$

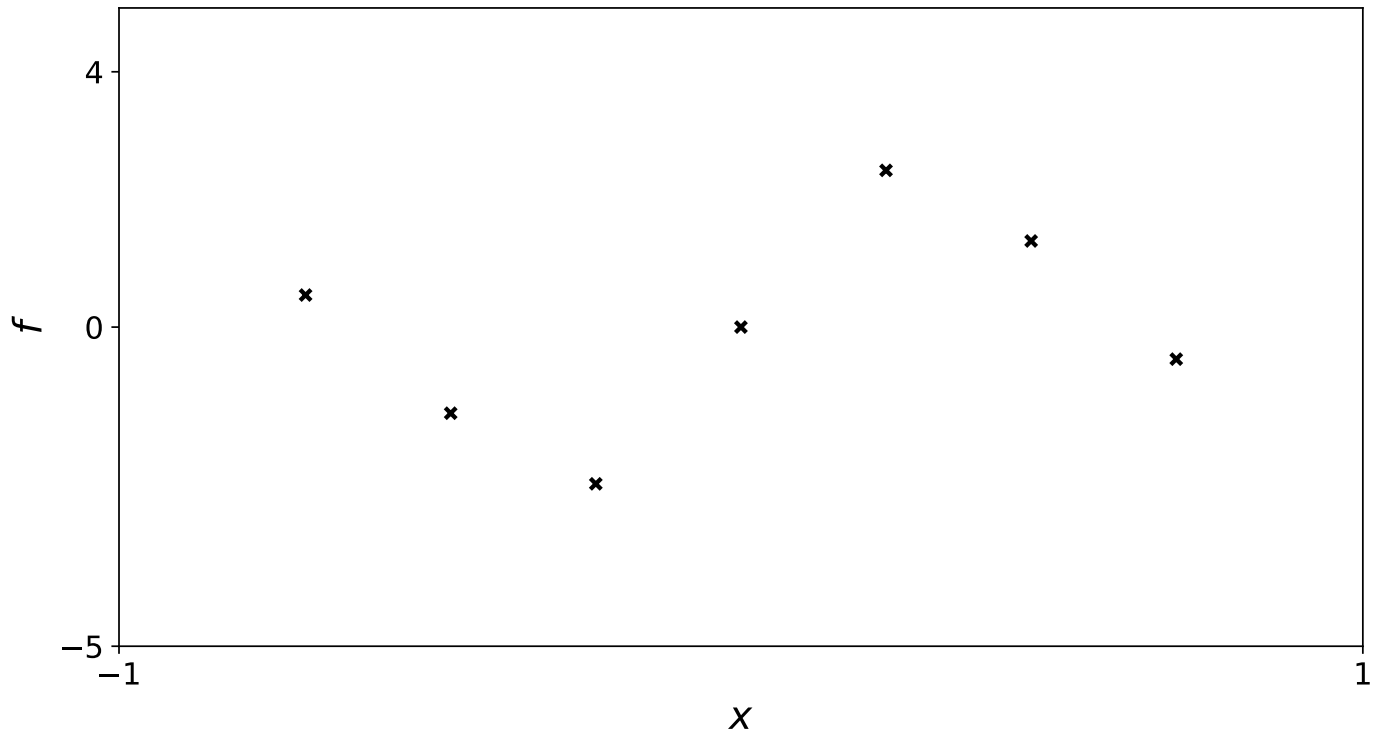
where

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

$\Rightarrow$ R demo

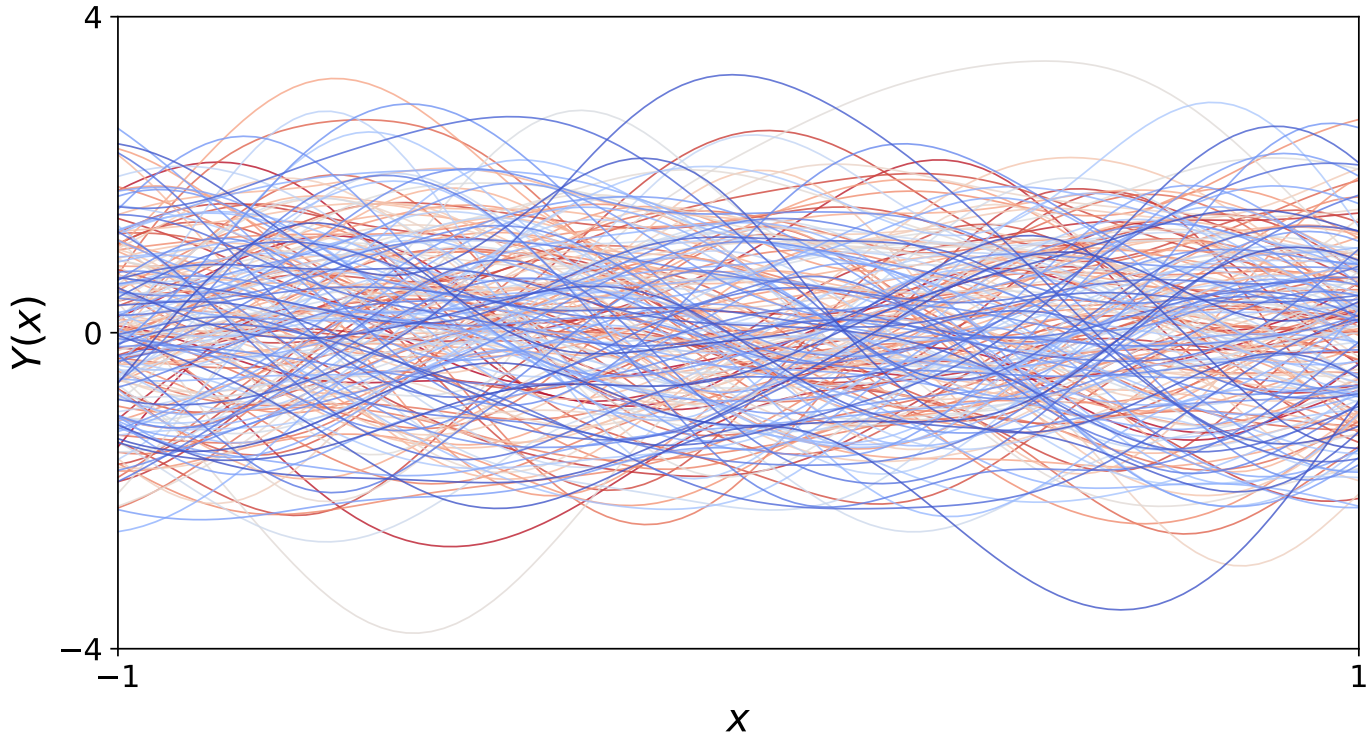
Gaussian process regression

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 $Z \sim \mathcal{N}(0, k)$:



The posterior distribution $Y(\cdot)|Y(X) = F$:

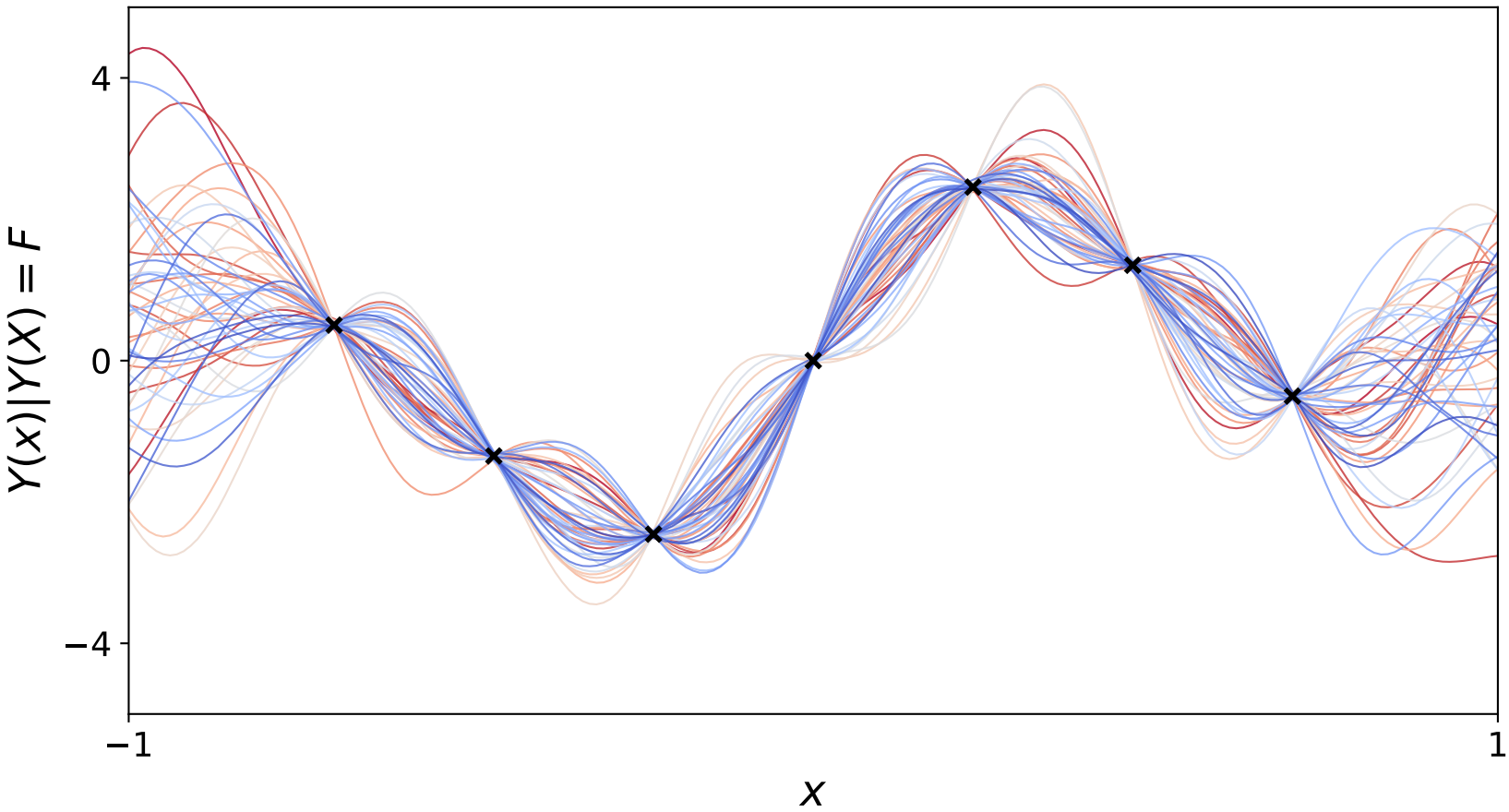
- Is still Gaussian
- Can be computed analytically

It is $\mathcal{N}(m(\cdot), c(\cdot,\cdot))$ with:

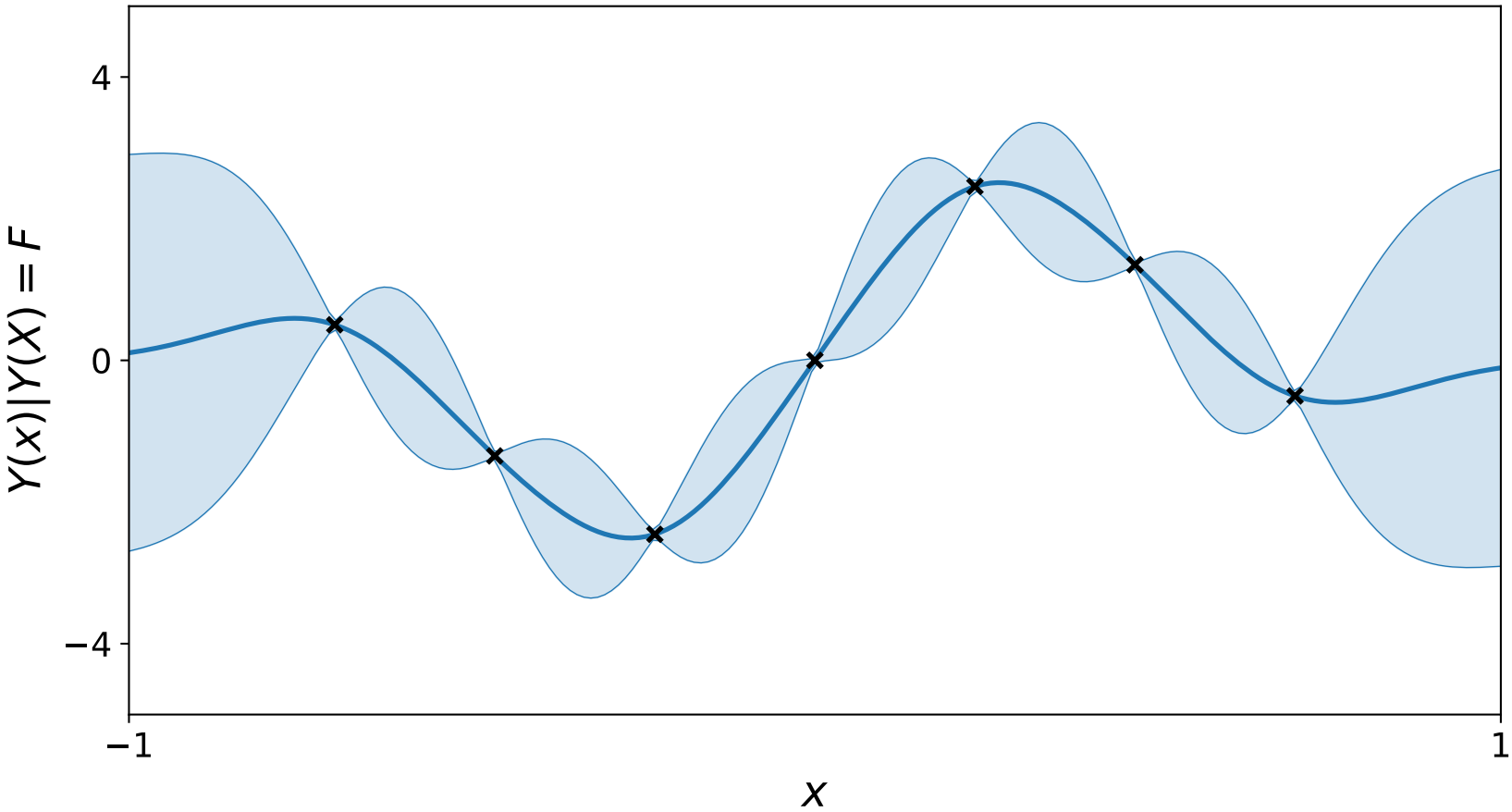
$$\begin{aligned} m(x) &= \mathrm{E}[Y(x)|Y(X)=F] \\ &= k(x,X)k(X,X)^{-1}F \end{aligned}$$

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

Samples from the posterior distribution



It can be 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:

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

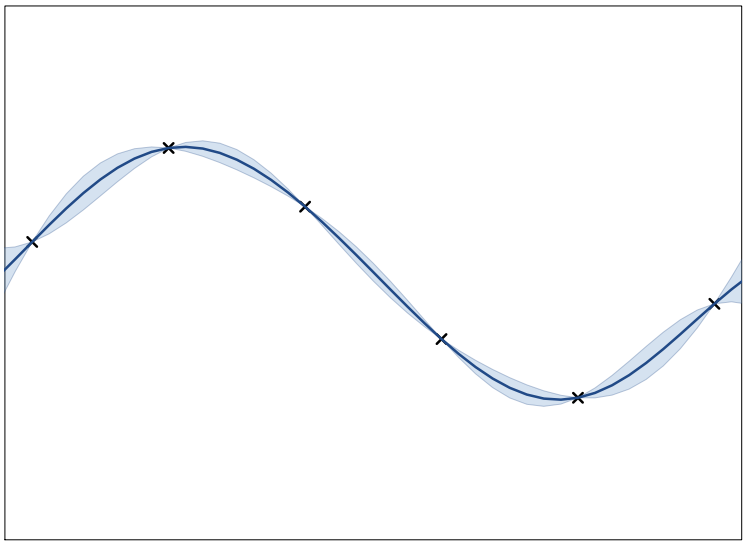
A few remarkable properties of GPR models

- 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.

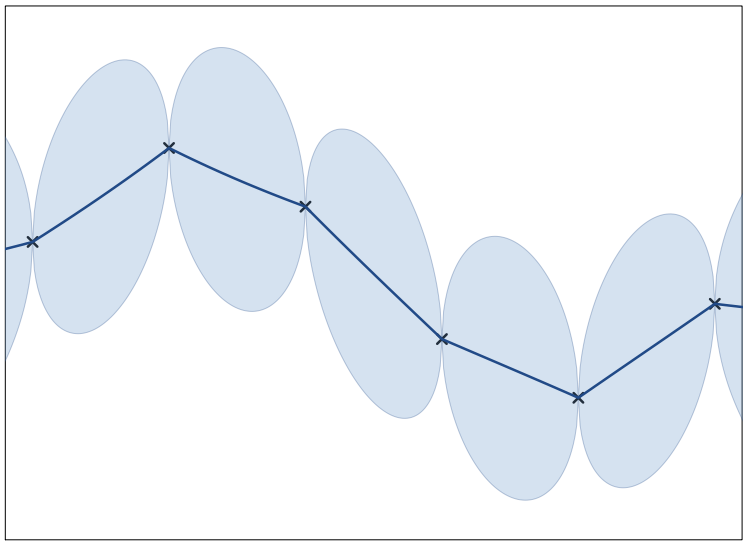
Can we prove them?

Changing the kernel has a huge impact on the model:

Gaussian kernel:

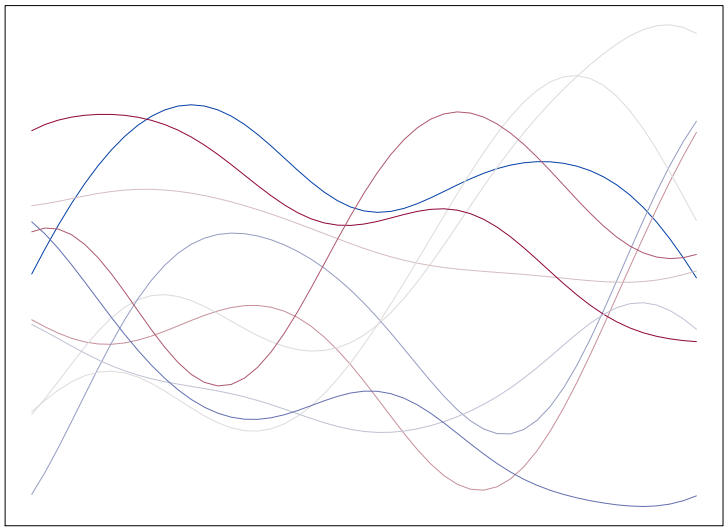


Exponential kernel:

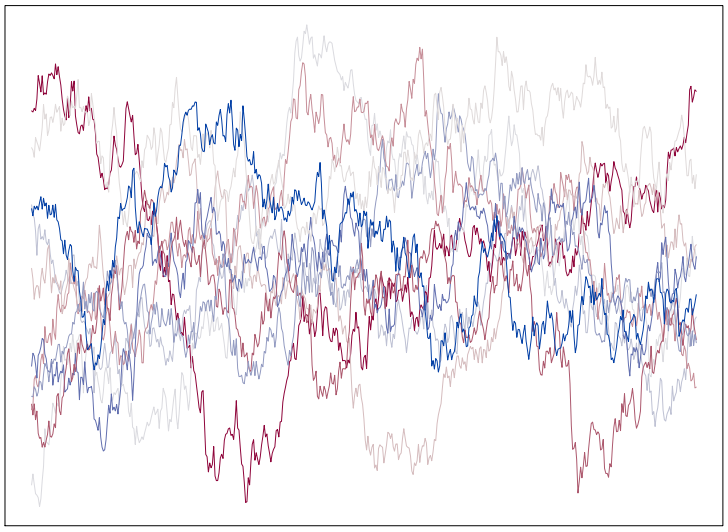


This is because changing the kernel means changing the prior on f

Gaussian kernel:

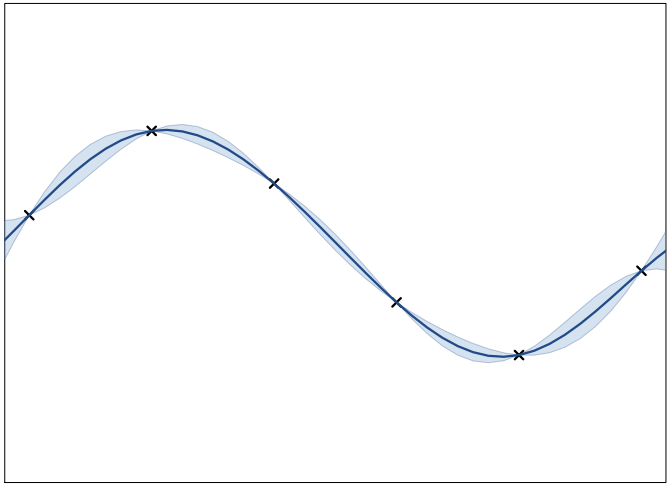


Exponential kernel:

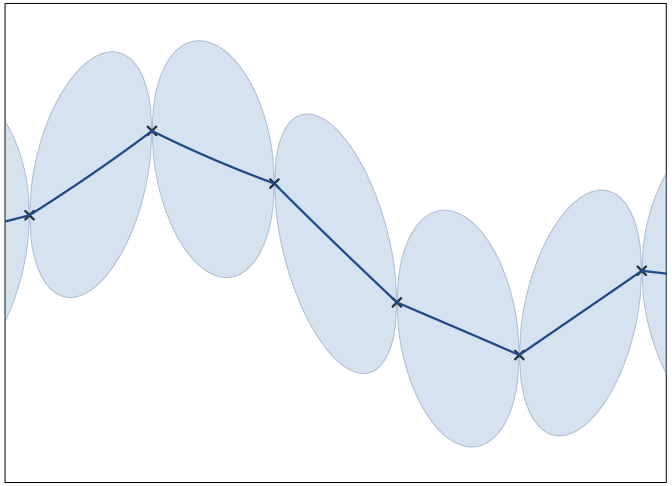


There is no kernel that is intrinsically better... it depends on data!

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 ?
- ...

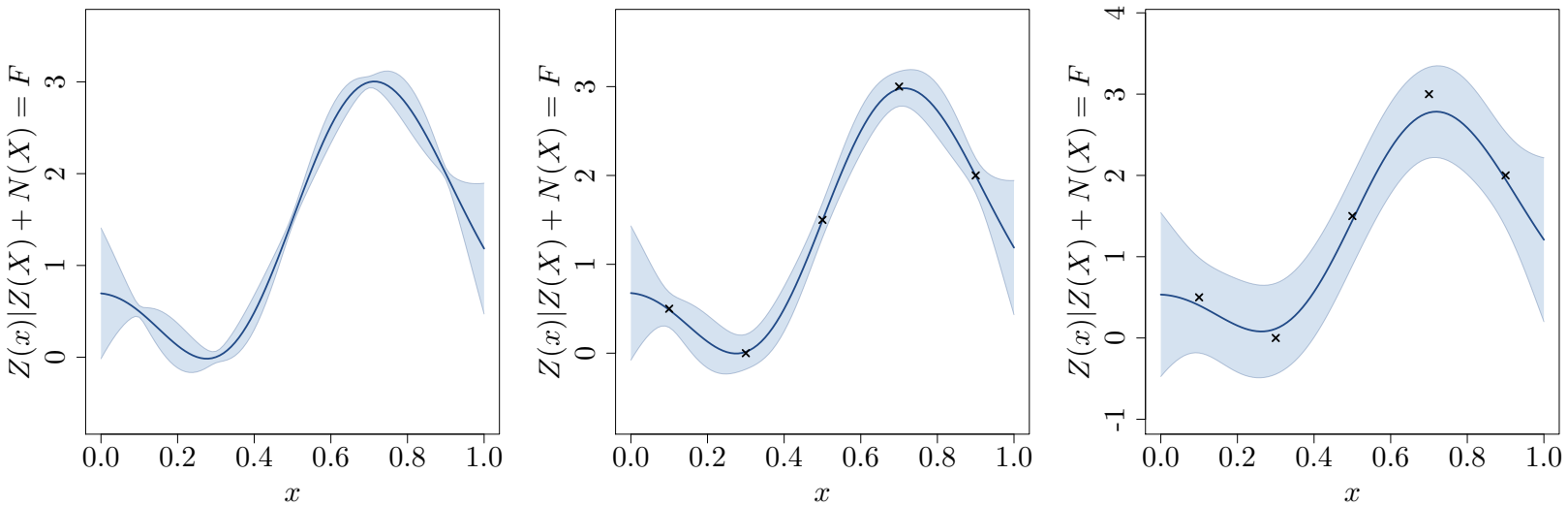
We are not always interested in models that interpolate the data.
For example, if there is some observation noise: $F = f(X) + \varepsilon$. Let

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

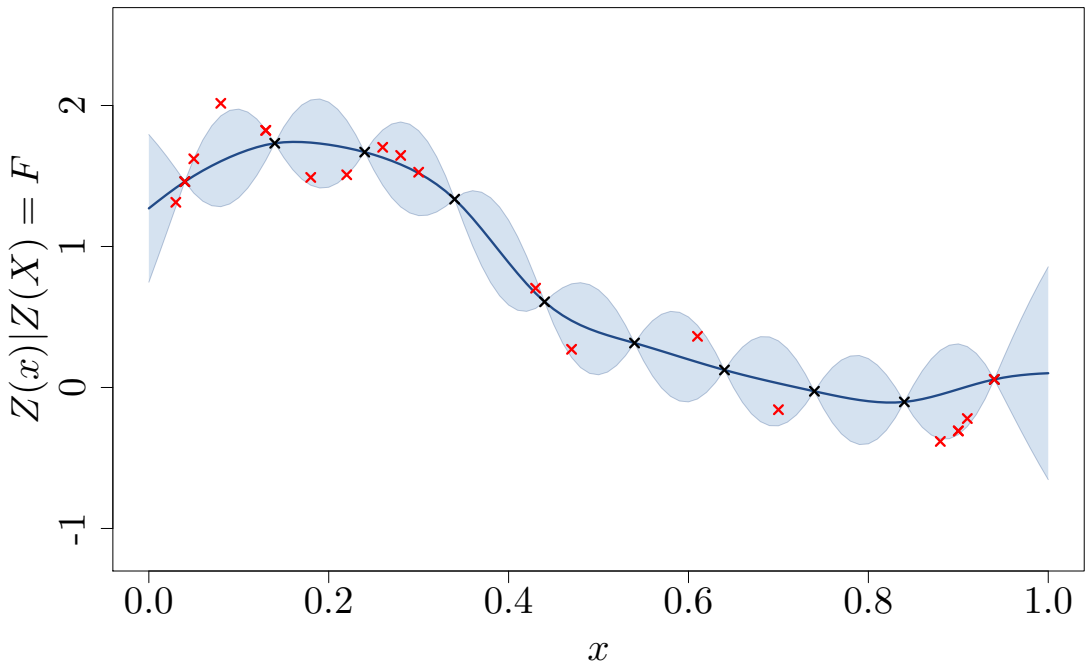
Model validation

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:

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

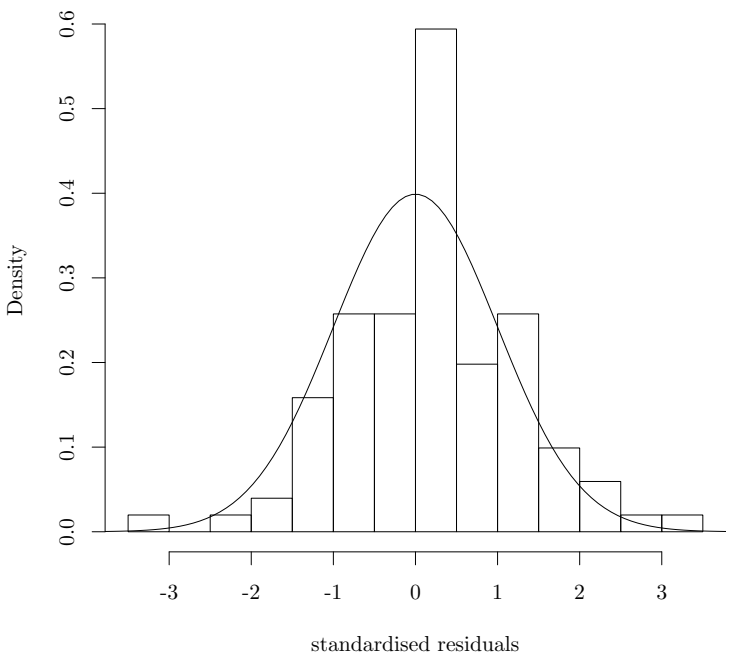
$$\text{A "normalised" criterion} \qquad Q_2 = 1 - \frac{\sum (F_t - m(X_t))^2}{\sum (F_t - \text{mean}(F_t))^2}$$

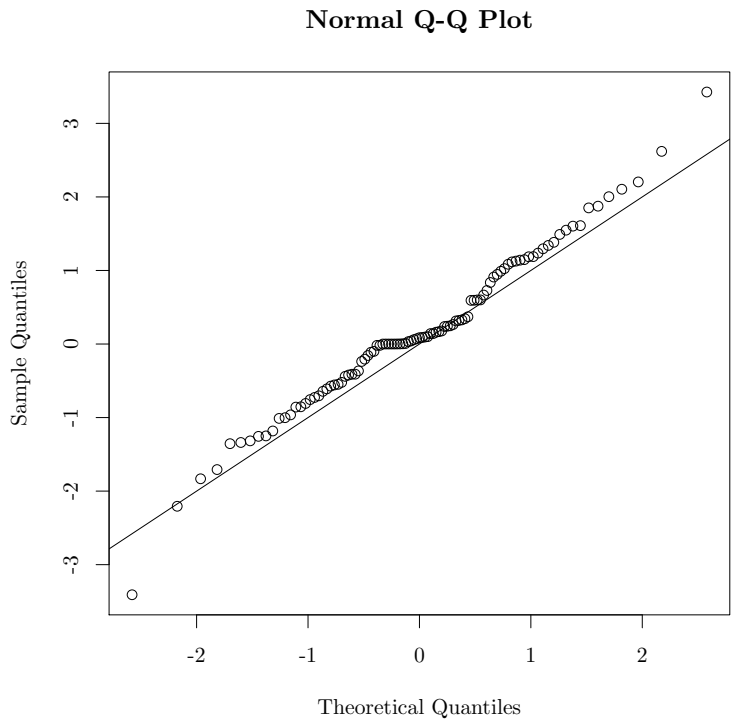
On the above example we get $MSE = 0.038$ and $Q_2 = 0.95$.

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 $\mathcal{N}(0, 1)$:





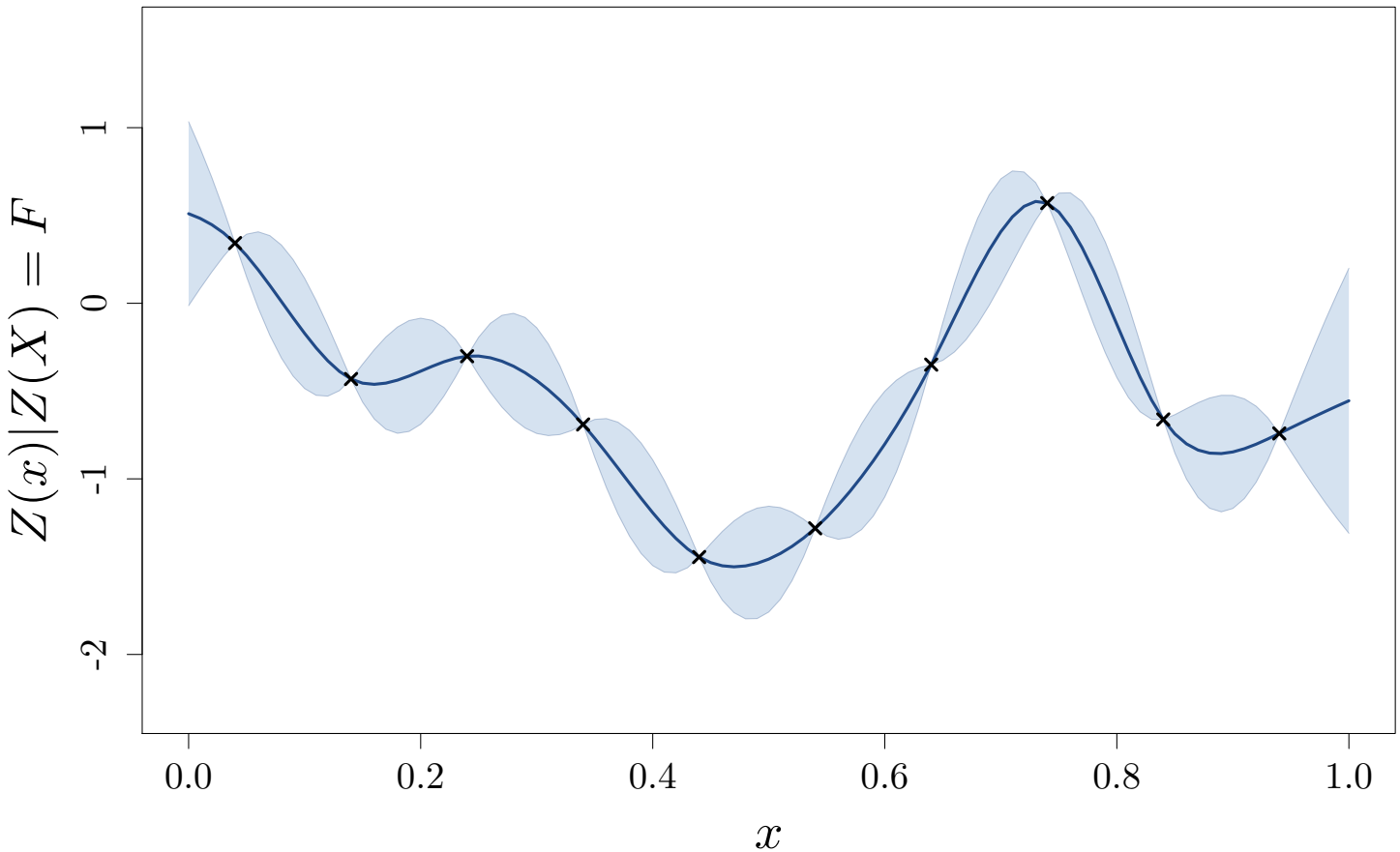
When no test set is available, another option is to consider cross validation methods such as leave-one-out.

The steps are:

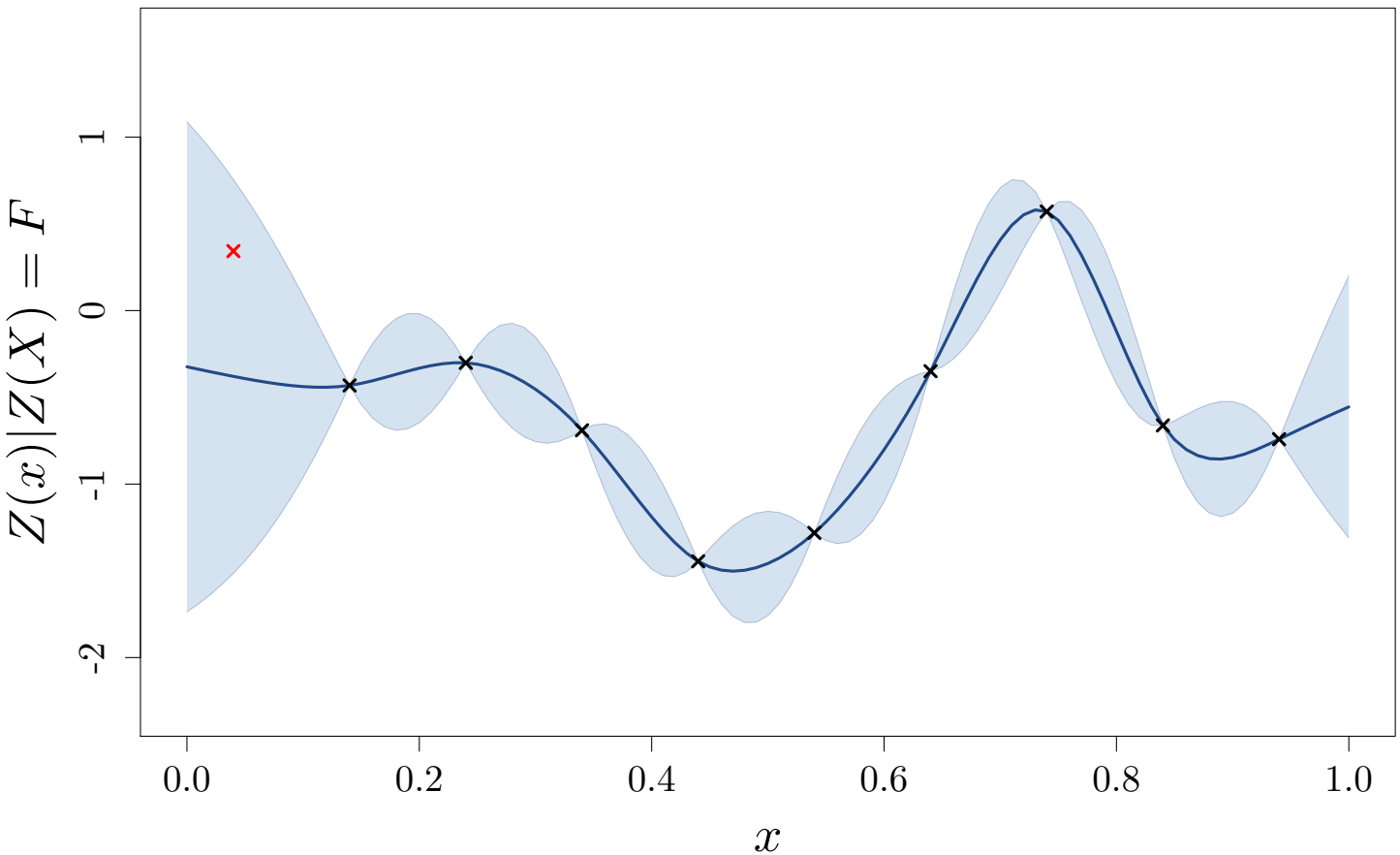
1. build a model based on all observations except one
2. compute the model error at this point

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

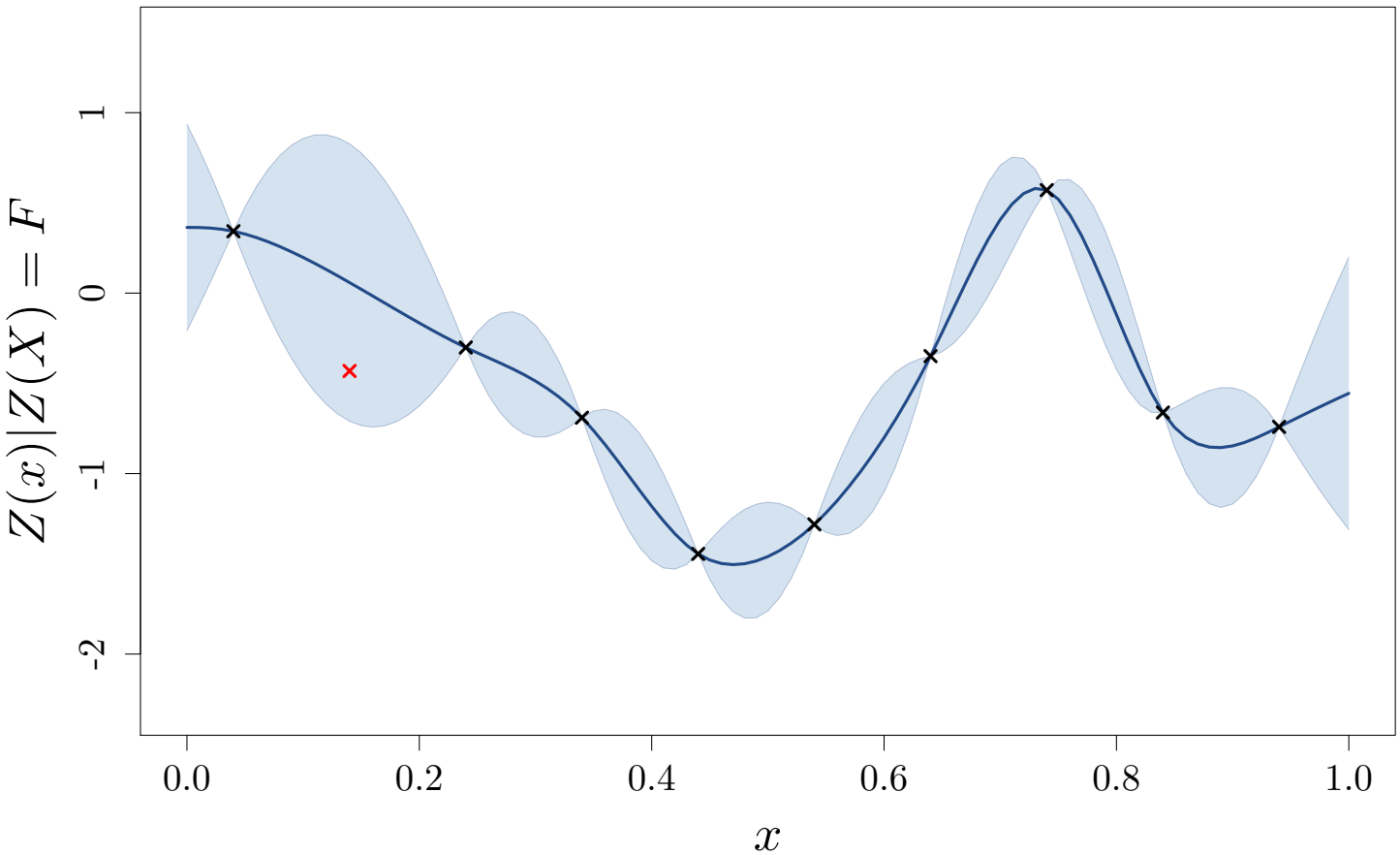
Model to be tested:



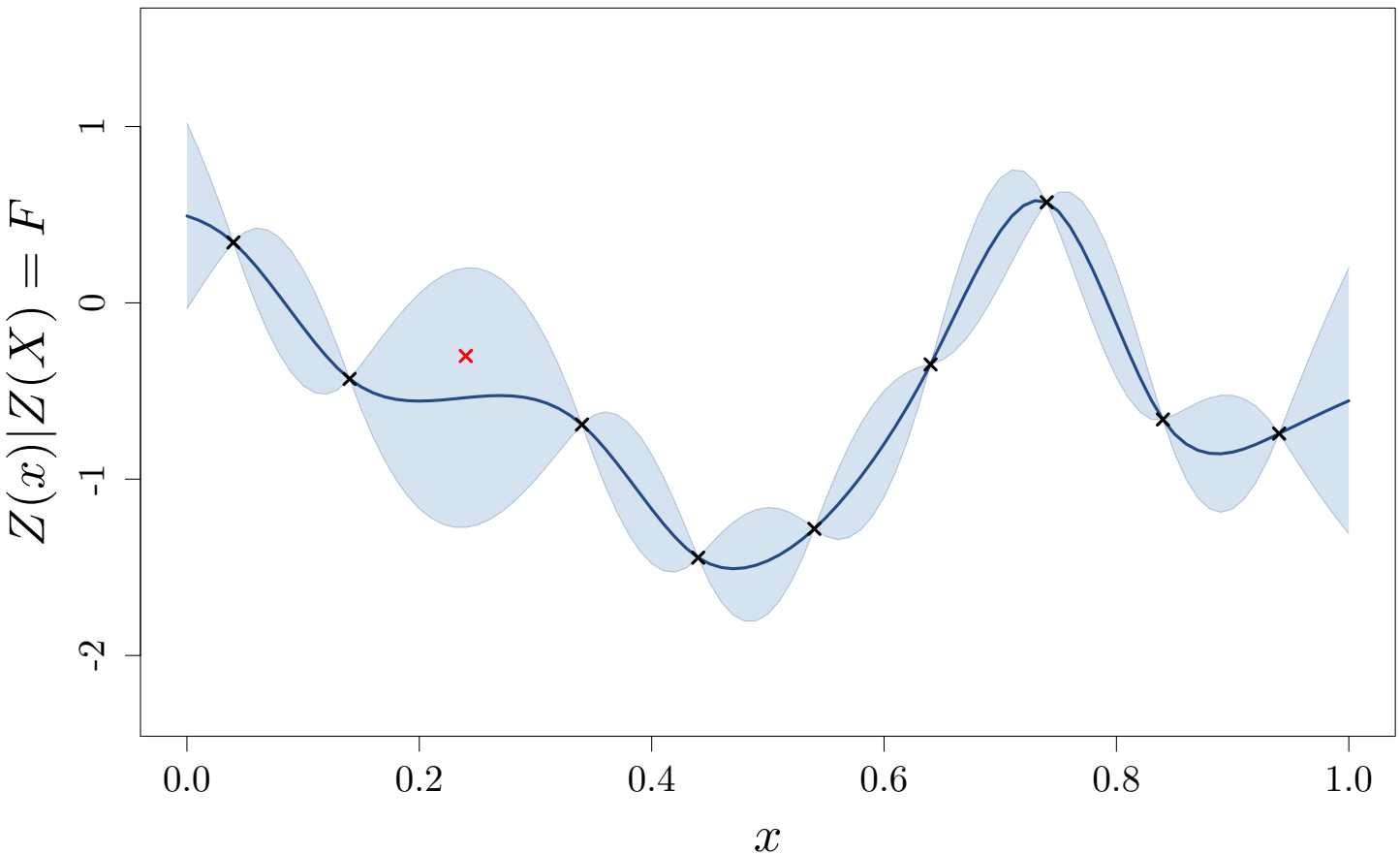
Step 1:



Step 2:



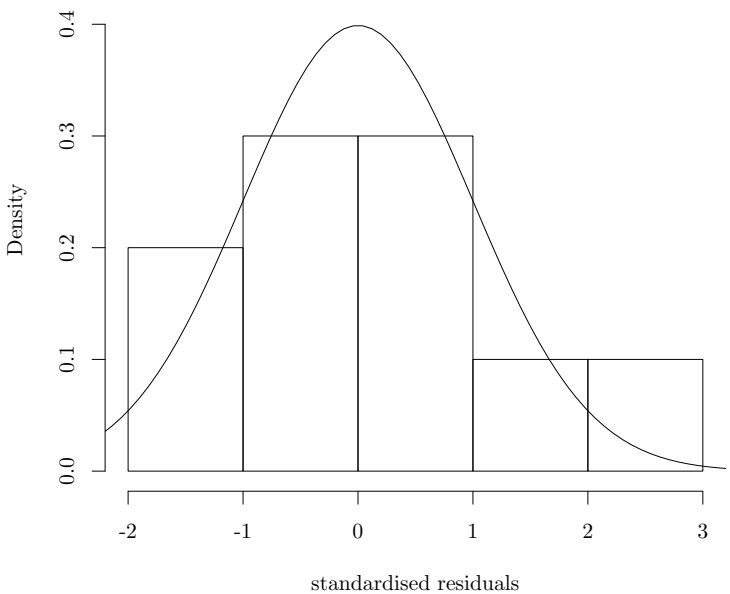
Step 3:

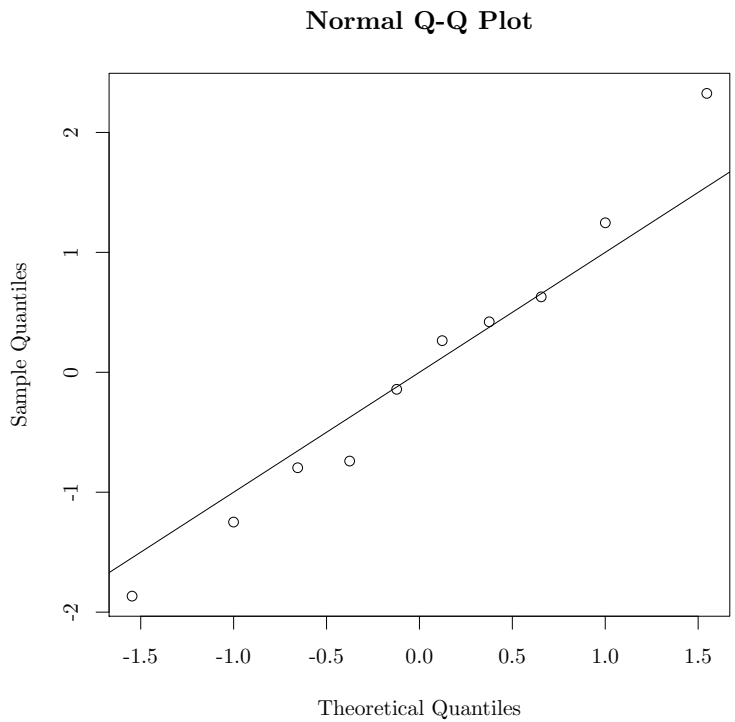


We finally obtain:

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

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.





Conclusion

Important points:

- Statistical models are useful when little data is available. they allow to
  - interpolate or approximate functions
  - Compute quantities of interests (such as mean value, optimum, ...)
  - Get an error measure
- GPR is similar to linear regression but the assumption is much weaker (not a finite dimensional space)

Reference

Carl Edward Rasmussen and Chris Williams, *Gaussian processes for machine learning*, MIT Press, 2006. (free version online).