ENBIS pre-conference workshop

Introduction to Kriging using R and JMP

Nicolas Durrande – Mines Saint-Étienne

durrande@emse.fr

We have seen this morning how to build Kriging models and what are the assumptions they rely on. We get into more details:

1. it is straightforward to change the prior belief
2. parameters can be included in models to get a better fit between prior belief and data
3. one must **validate** a model before using it!

Kernels

For a given set of observations, the model is fully determined by the prior covariance function $k(x, y) = \text{cov}[Z(x), Z(y)]$:

$$m(x) = k(x, X)k(X, X)^{-1}F$$
$$v(x) = k(x, x) - k(x, X)k(X, X)^{-1}k(X, x)$$

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.

Proving that a function is psd is often intractable. However there are a lot of functions that have already been proven to be psd:

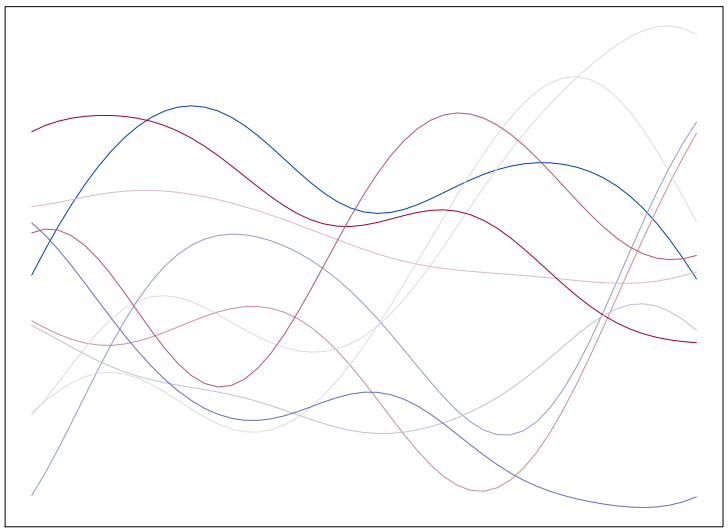
squared exp.	$k(x,y) = \sigma^2 \exp\left(-\frac{(x-y)^2}{2\theta^2}\right)$
Matern 5/2	$k(x,y) = \sigma^2 \left(1 + \frac{\sqrt{5}\lvert x-y\rvert}{\theta} + \frac{5\lvert x-y\rvert^2}{3\theta^2}\right) \exp\left(-\frac{\sqrt{5}\lvert x-y\rvert}{\theta}\right)$
Matern 3/2	$k(x,y) = \sigma^2 \left(1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

When k is a function of $x - y$, the kernel is called **stationary**.

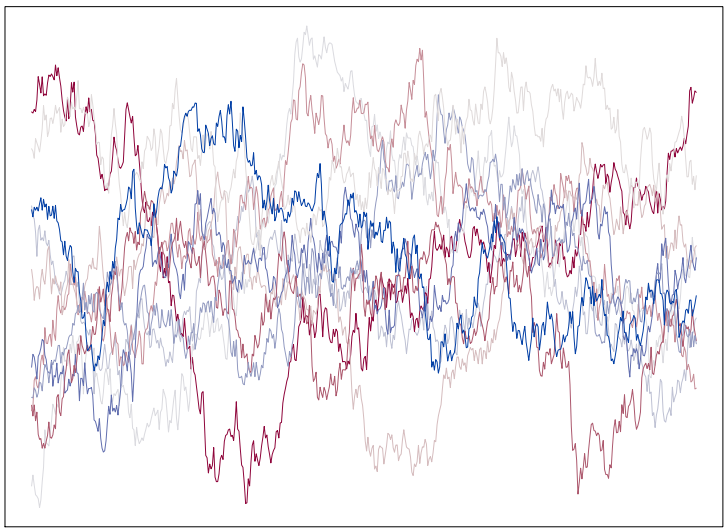
σ^2 is called the **variance** and θ the **lengthscale**.

Changing kernel means changing the prior belief on f

Gaussian kernel:

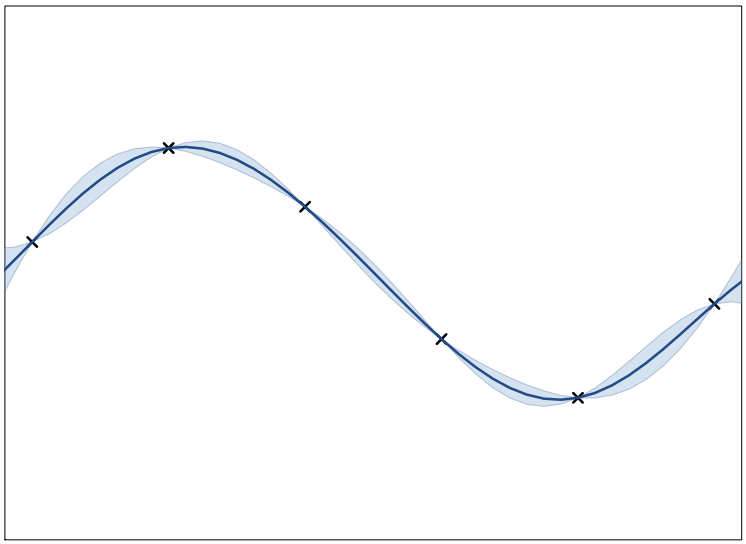


Exponential kernel:

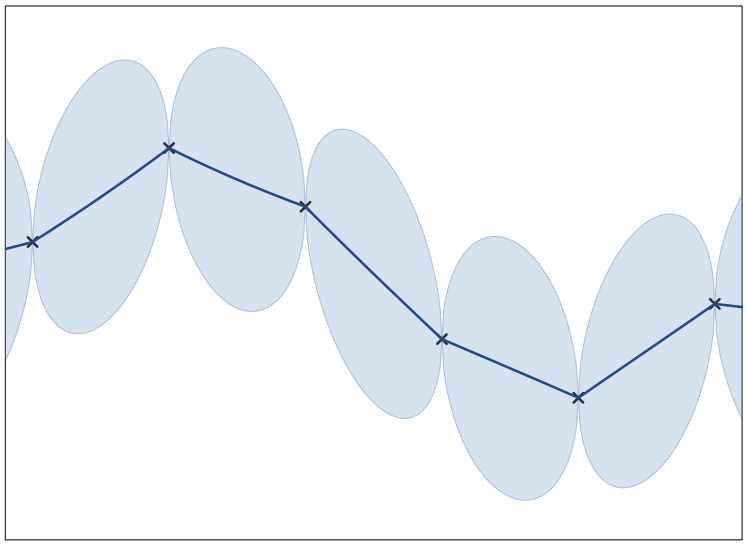


It thus has a huge impact on the model:

Gaussian kernel:



Exponential kernel:



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

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 ?
- ...

Furthermore, it is possible to introduce rescaling parameters to adjust the prior distribution to our belief.

For $d \geq 2$, there can be one rescaling parameter per dimension:

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

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

If all θ_i are equal, we say that the kernel/process is **isotropic**.

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.

The likelihood quantifies the adequacy between a distribution and some observations.

Definition

Let f_Y be a pdf depending on some parameters p and let $y_1, \ldots, y_n$ be independent observations. The **likelihood** is defined as

$$L(p) = \prod_{i=1}^{n} f_Y(y_i; p).$$

A high value of $L(p)$ indicates the observations are likely to be drawn from $f_Y(.; p)$.

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

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

It is thus possible to maximise L with respect to the kernel's parameters in order to find a well suited prior.

In practice, the value of σ^2 can be obtained analytically. Others, such as θ, need numerical optimization.

Example

We consider 100 sample from a Matérn $5/2$ process with parameters $\sigma^2 = 1$ and $\theta = 0.2$, and n observation points. We then try to recover the kernel parameters using MLE.

n	5	10	15	20
σ^2	1.0 (0.7)	1.11 (0.71)	1.03 (0.73)	0.88 (0.60)
θ	0.20 (0.13)	0.21 (0.07)	0.20 (0.04)	0.19 (0.03)

MLE can be applied regardless to the dimension of the input space.

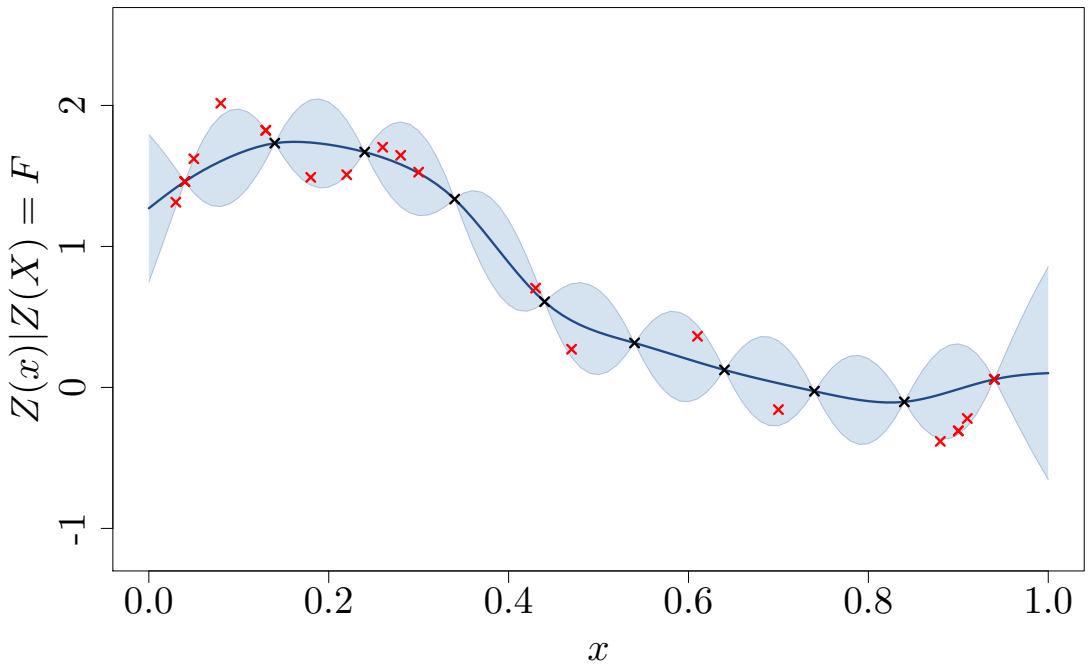
Model validation

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 is how to get a good model:

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

The idea is to compare the model predictions with real values on new data.



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:

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

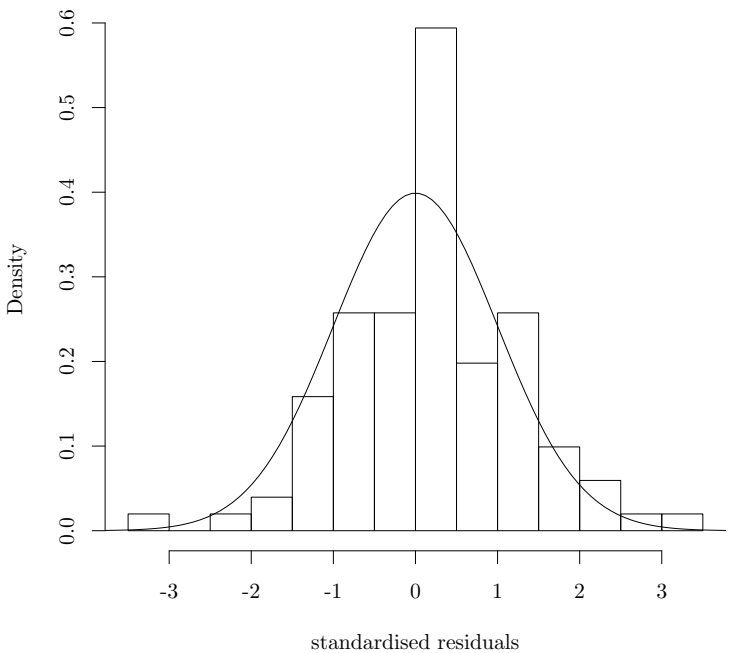
$$\text{A "normalised" criterion} \qquad Q_2 = 1 - \frac{\sum (F_t - m(X_t))^2}{\sum (F_t - \text{mean}(F_t))^2}$$

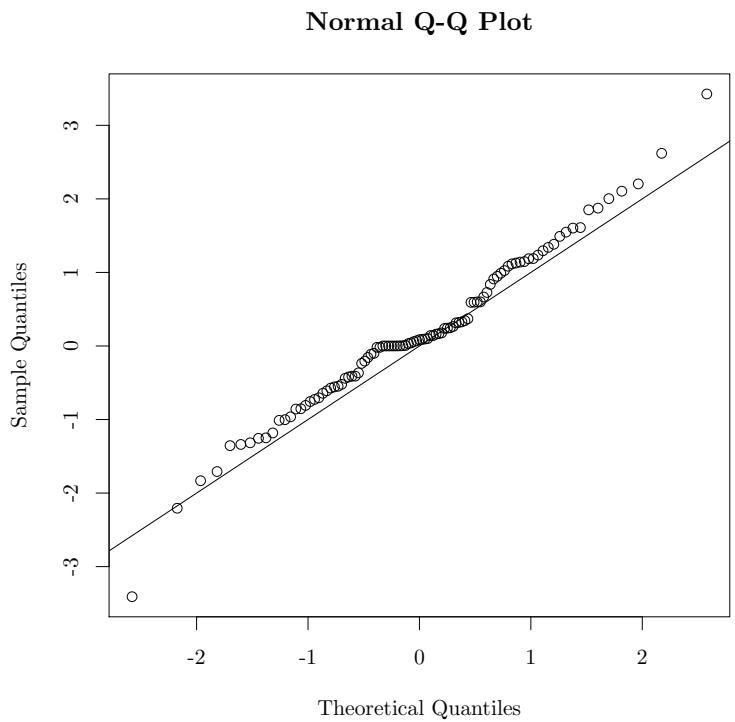
On the above example we get $MSE = 0.038$ and $Q_2 = 0.95$.

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





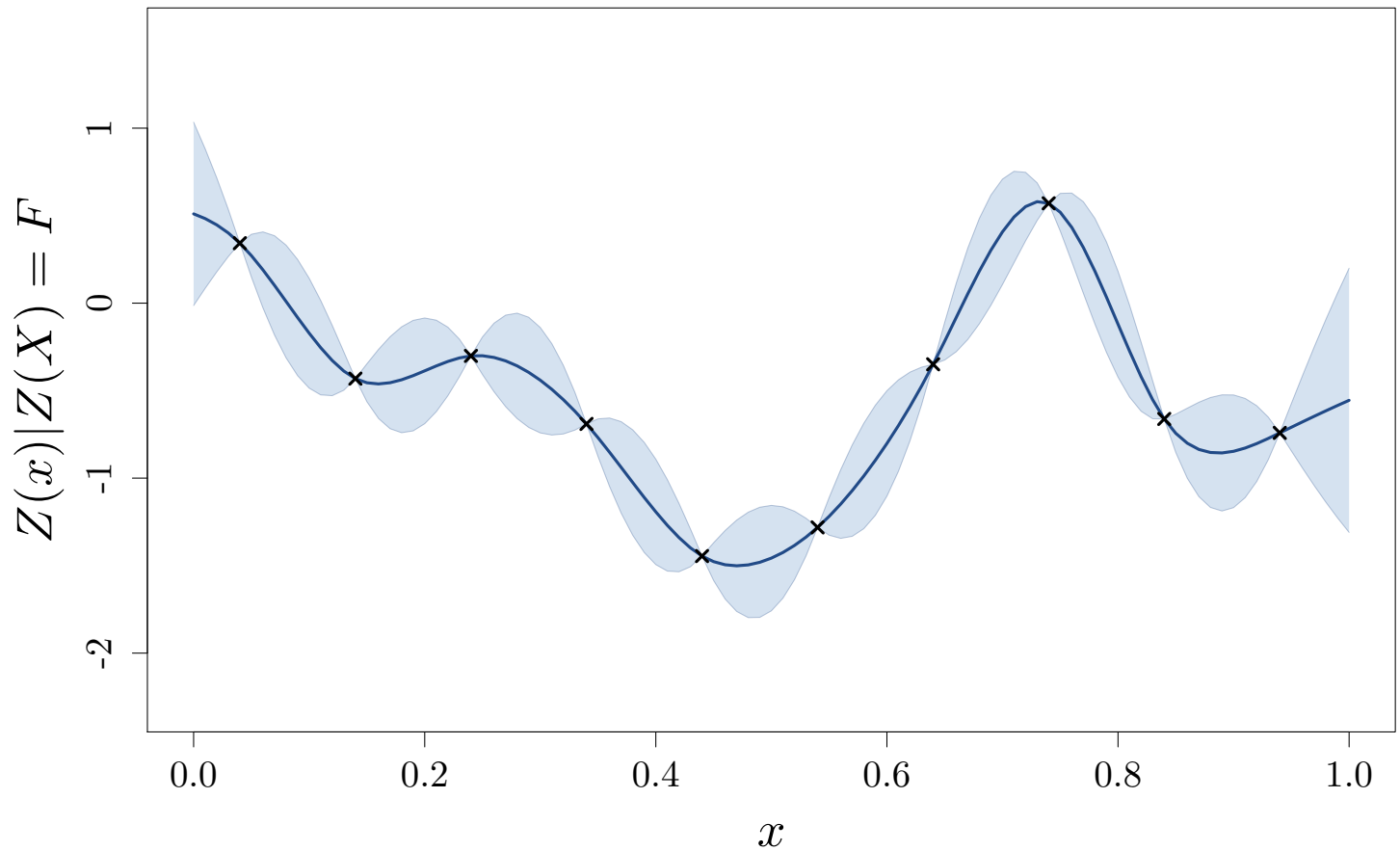
When no test set is available, another option is to consider cross validation methods such as leave-one-out.

The steps are:

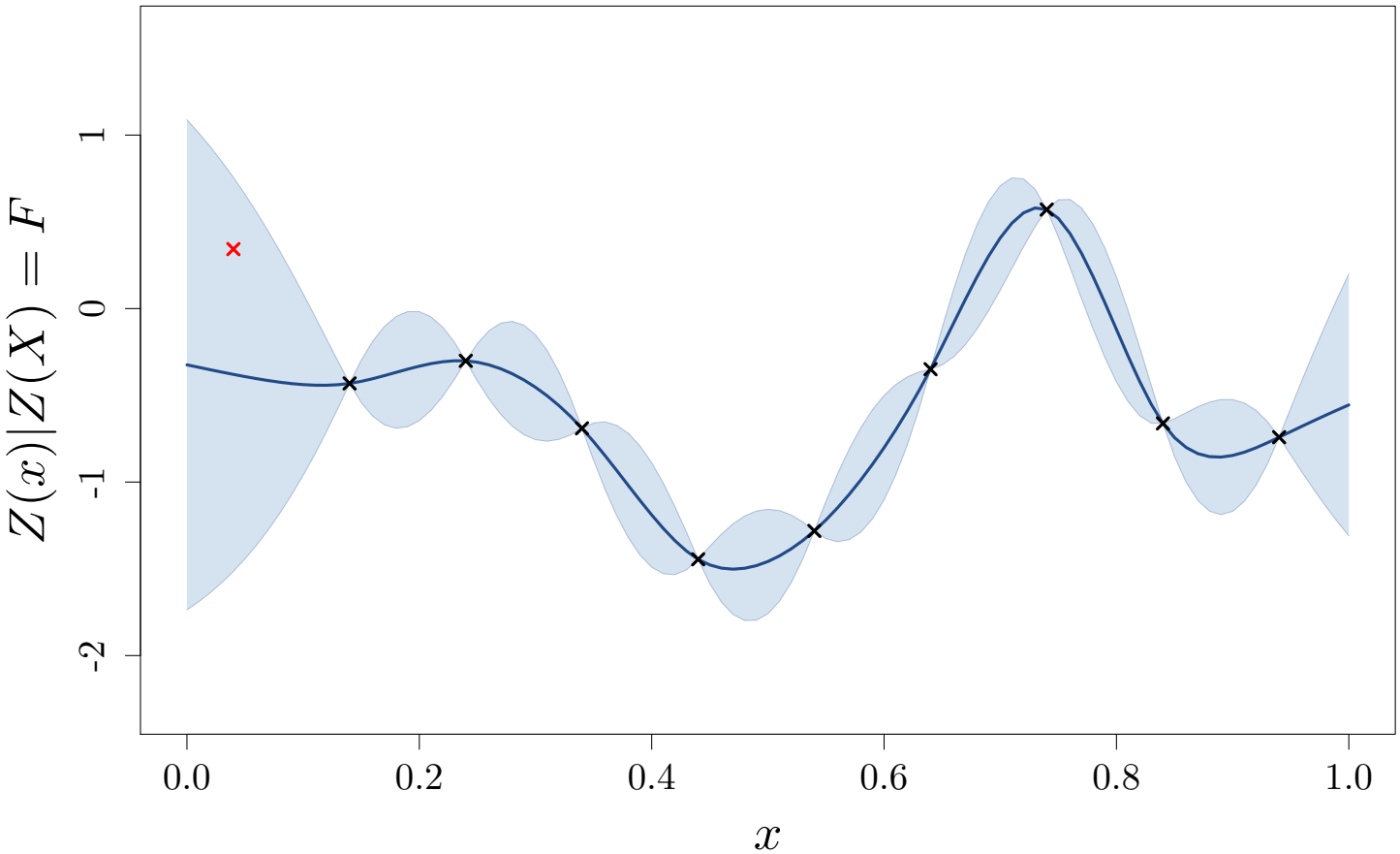
1. build a model based on all observations except one
2. compute the model error at this point

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

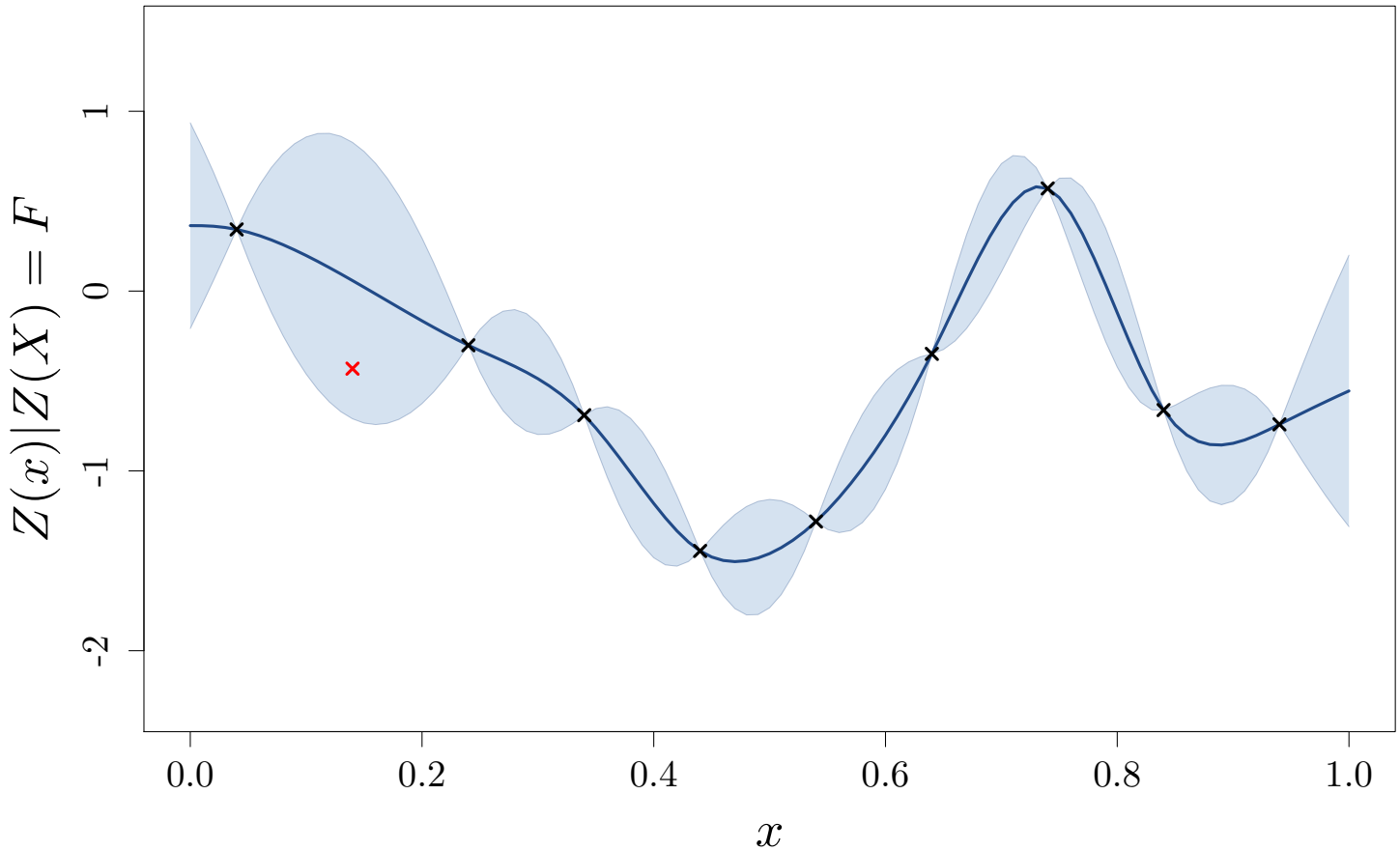
Model to be tested:



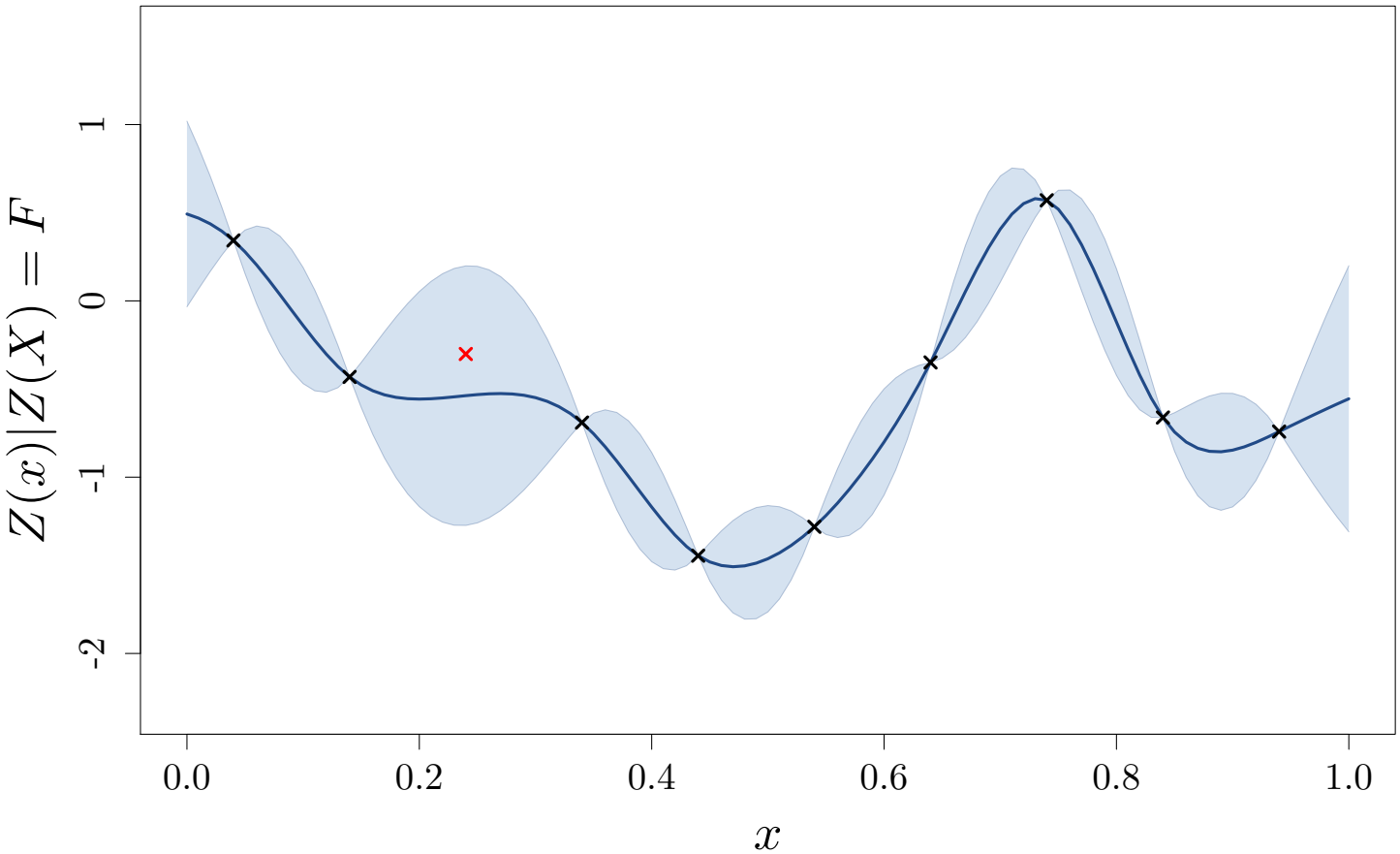
Step 1:



Step 2:



Step 3:



On this example, we obtain $MSE = 0.24$ and $Q_2 = 0.34$.

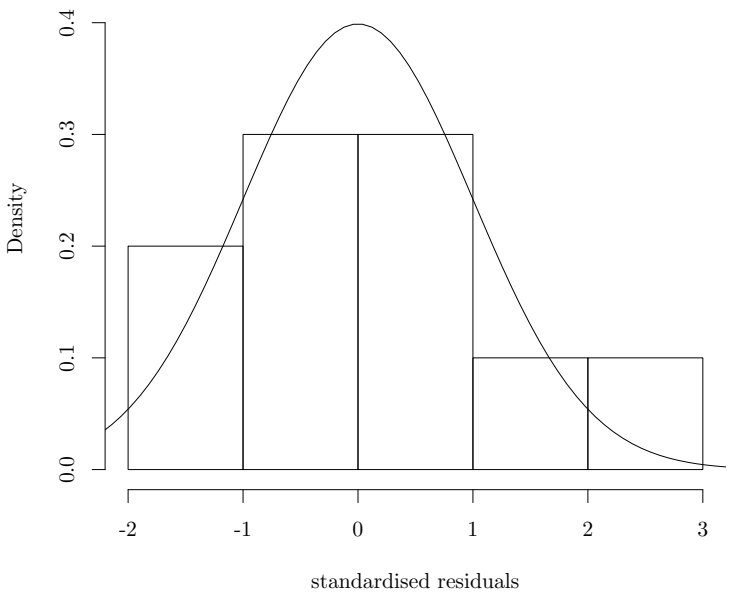
Why doesn't the model perform as good previously?

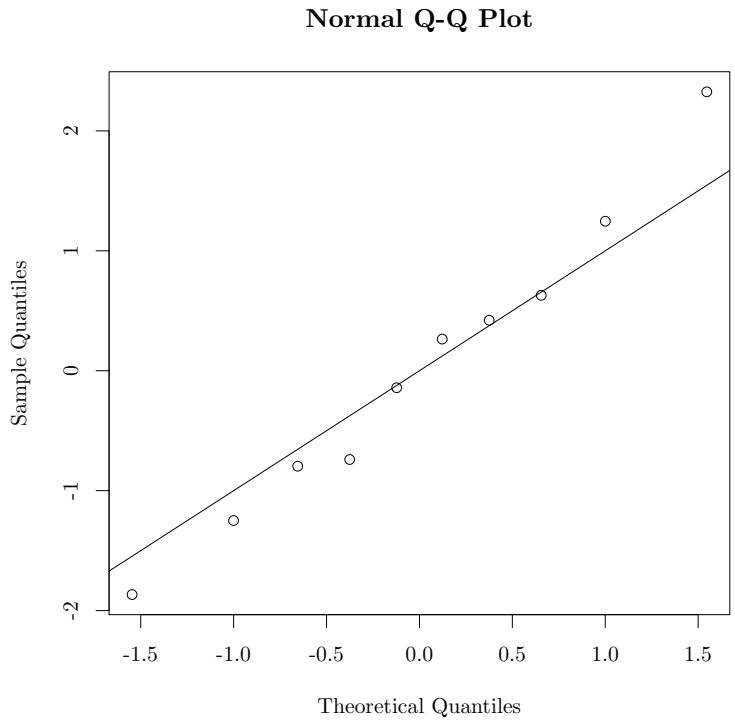
On this example, we obtain $MSE = 0.24$ and $Q_2 = 0.34$.

Why doesn't the model perform as good previously?

It turns out that the error is always computed at the 'worst' location!

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. We obtain:

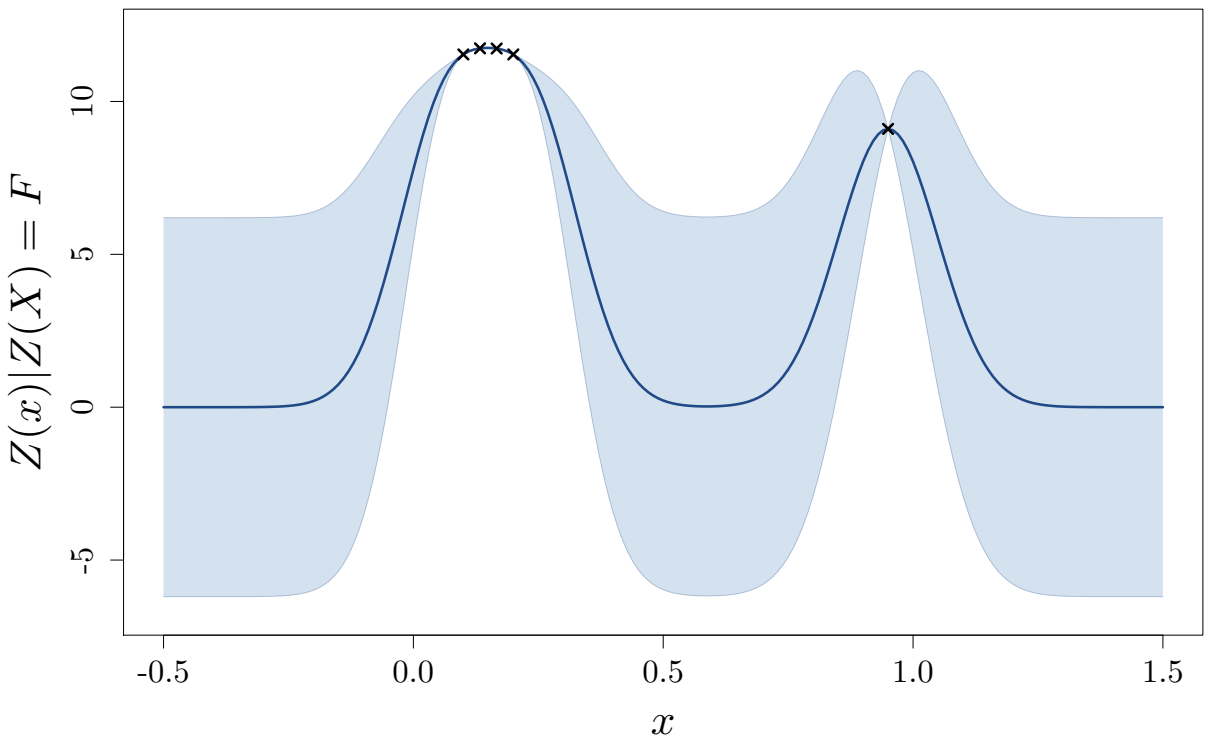




Trends

We have seen that GPR models go back to zero if we consider a centred prior.

This behaviour is not always wanted



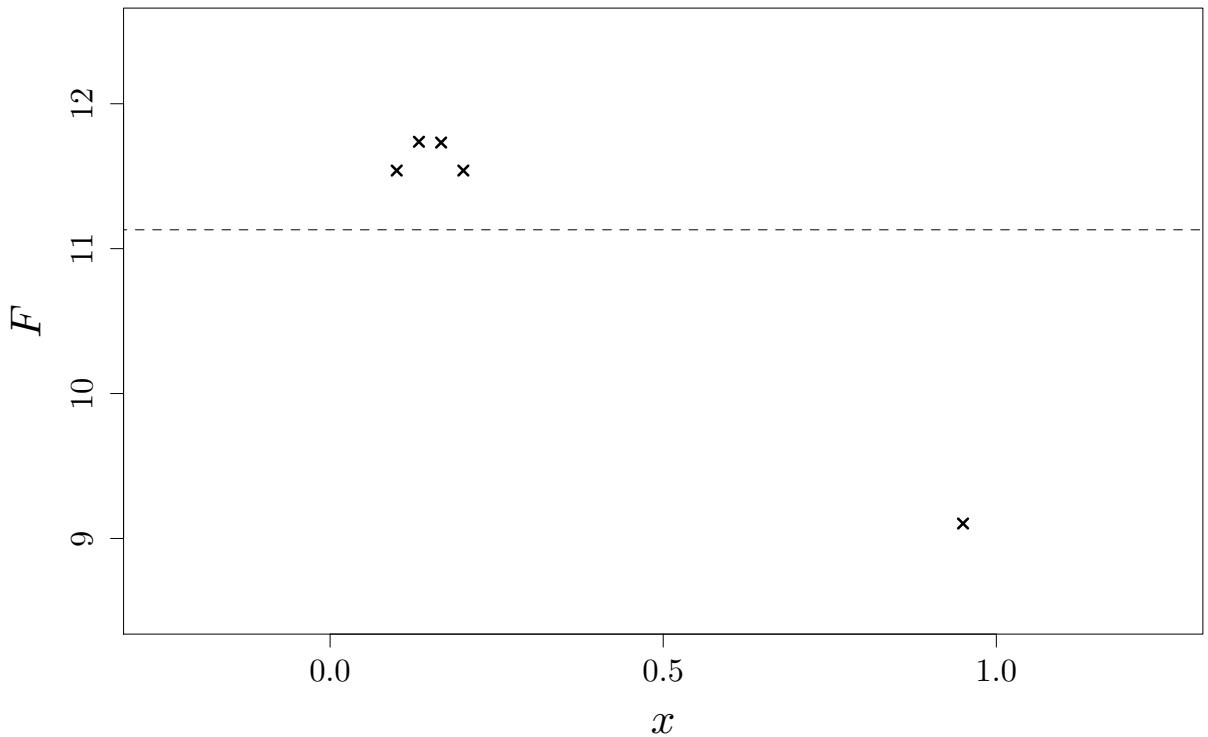
We may want to introduce some trend in models... One can distinguish:

- **simple kriging**: there is no trend or it is known
- **ordinary kriging**: the trend is a constant
- **universal kriging**: the trend is given by basis functions

The question is how to estimate the trend coefficients. Hereafter, we will focus on ordinary kriging and write t the mean value.

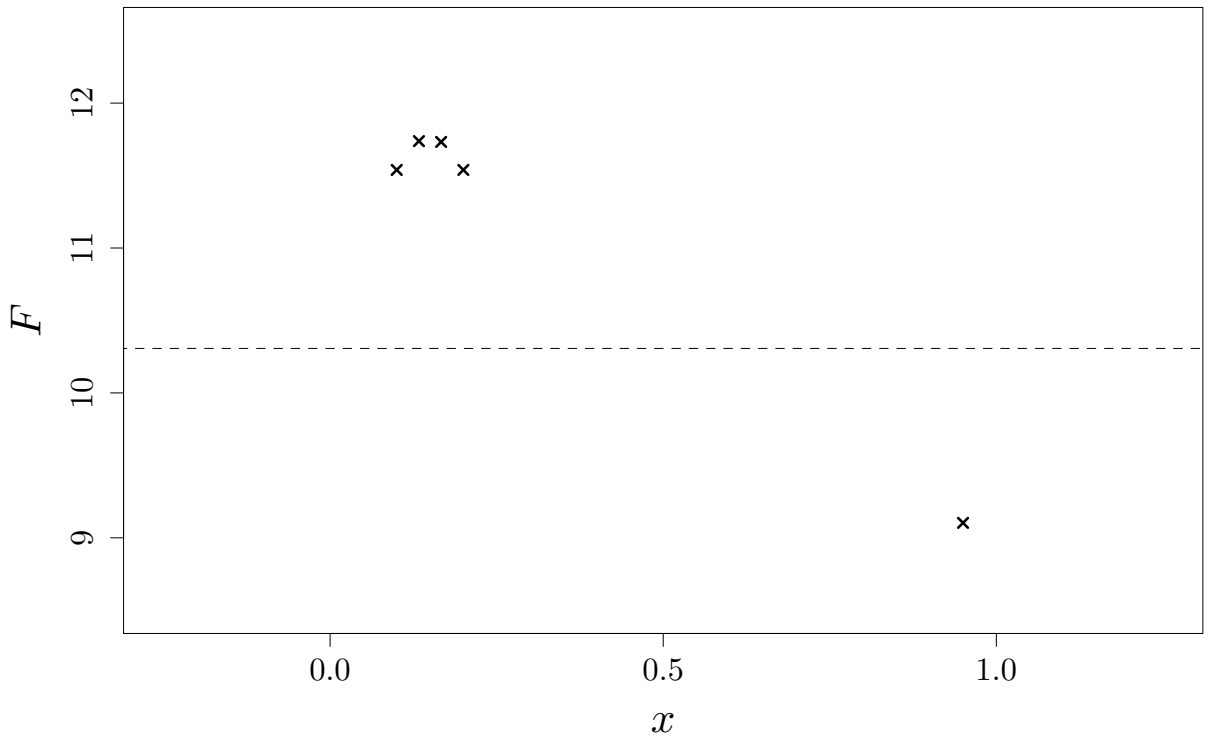
Basic least squares minimization gives

$$\hat{t} = \frac{1}{n}\sum_{i=1}^{n} F_i = \frac{\mathbf{1}^t F}{\mathbf{1}^t \mathbf{1}}$$



Generalised least squares is more appropriate

$$\hat{t} = \frac{\mathbf{1}^t k(X,X)^{-1} F}{\mathbf{1}^t k(X,X)^{-1} \mathbf{1}}$$



This can be seen as maximum likelihood estimation.

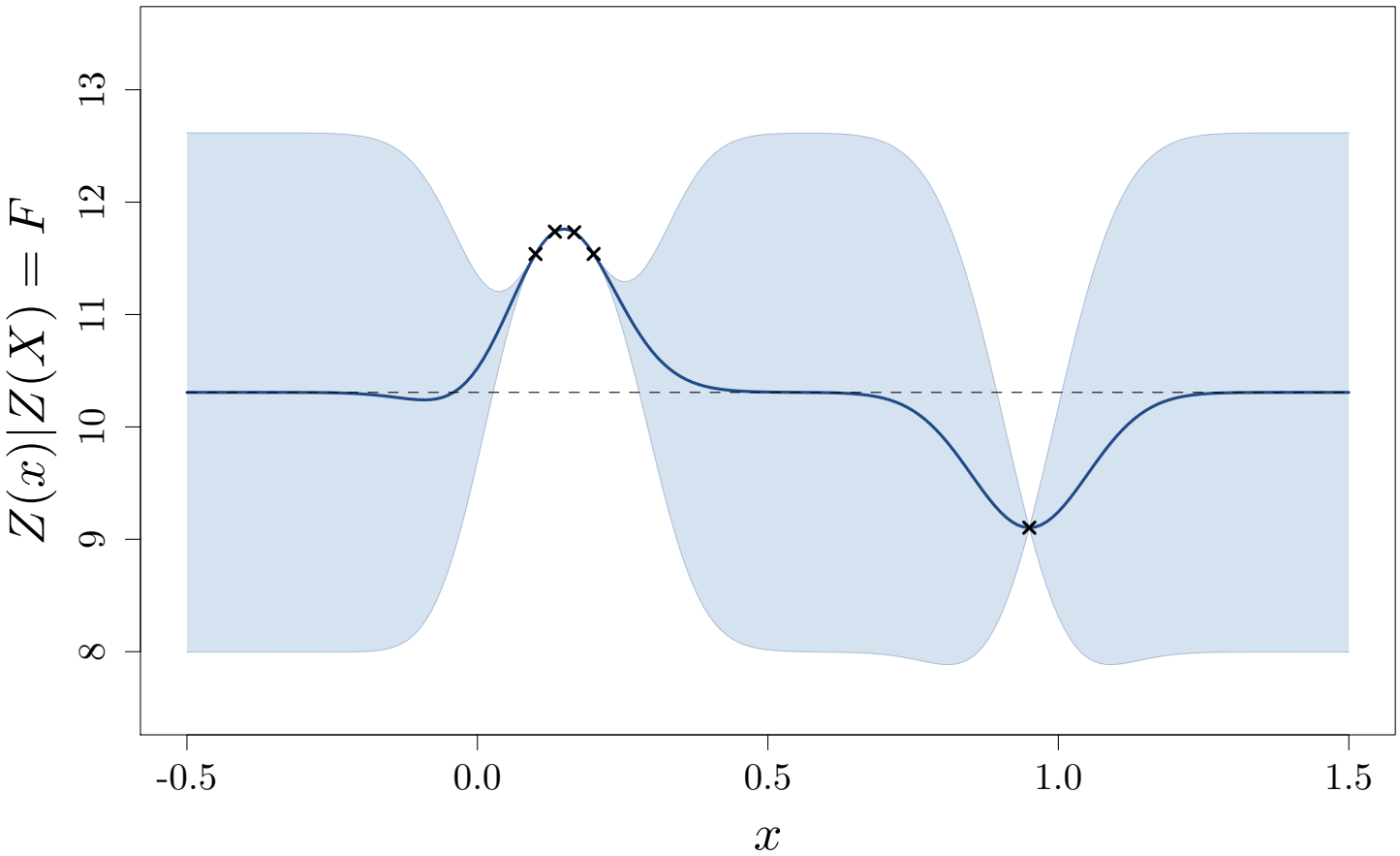
The expression of the **best predictor** is given by the usual conditioning of a GP:

$$m(x) = \mathrm{E}[Z(x)|Z(X) = F] = \hat{t} - k(x, X)k(X, X)^{-1}(F - \hat{t})$$

Regarding the **model variance**, it must account for the estimator's variance.

$$\mathrm{var}[Z(x)|Z(X)] = k(x, x) - k(x, X)k(X, X)^{-1}k(X, x) + \frac{(\mathbf{1} + k(x, X)k(X, X)^{-1}\mathbf{1})^t(\mathbf{1} + k(x, X)k(X, X)^{-1}\mathbf{1})}{\mathbf{1}^t k(X, X)^{-1}\mathbf{1}}$$

On the previous example we obtain:



Lab session (20 min)

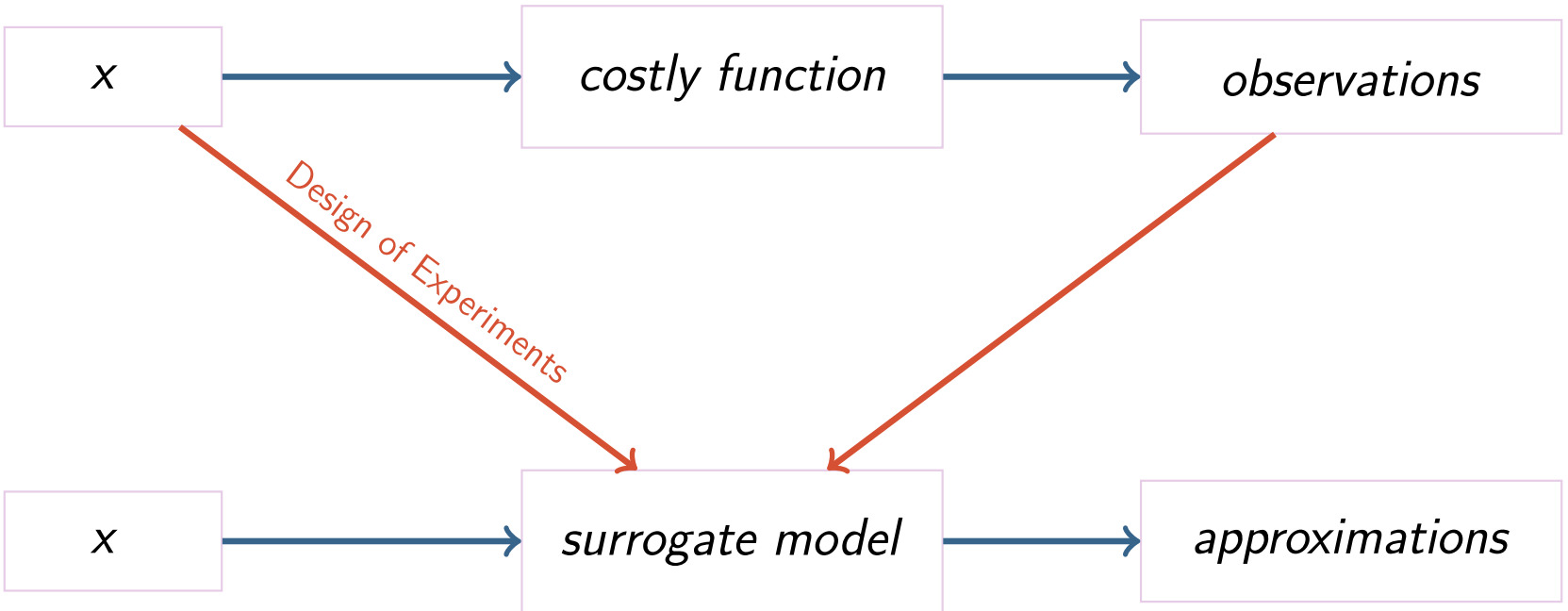
1. reload the kriging model you obtained this morning on the catapult data. (you can also use the provided one if you wish).
2. Apply the `print()` function to your model, can you understand the output?
3. Apply the `plot()` function to your model to get some cross validation diagnostics.
4. Try changing the trend and kernel to improve the model.
5. What location can you suggest for the optimum?

$$x_1 = \quad , \; x_2 = \quad , \; x_3 = \quad , \; x_4 = \quad .$$

Run the simulator at that location, is there an improvement?

Application to optimization

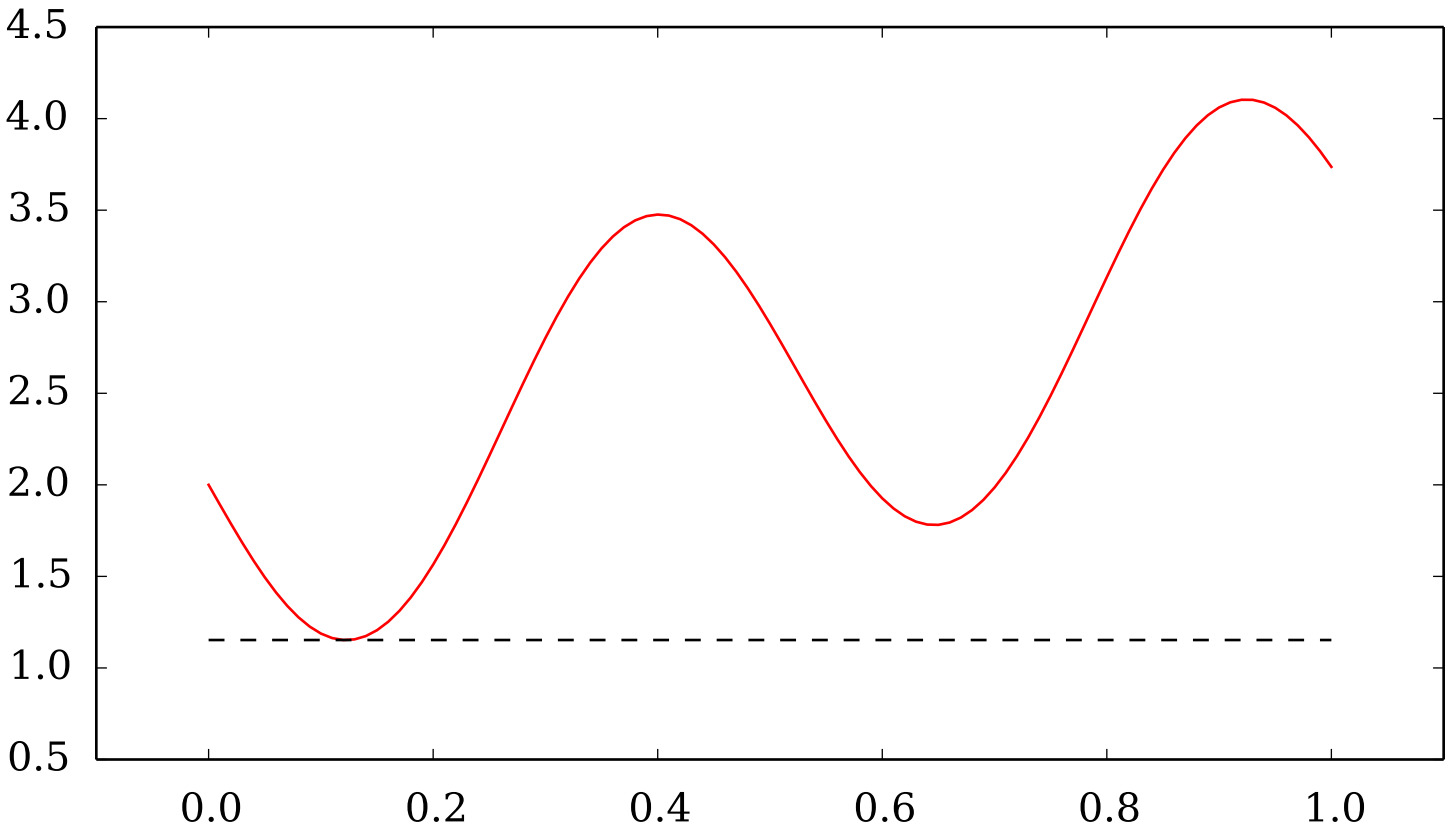
Framework


x
costly function
observations
Design of Experiments
x
surrogate model
approximations

Example : optimization

Case study

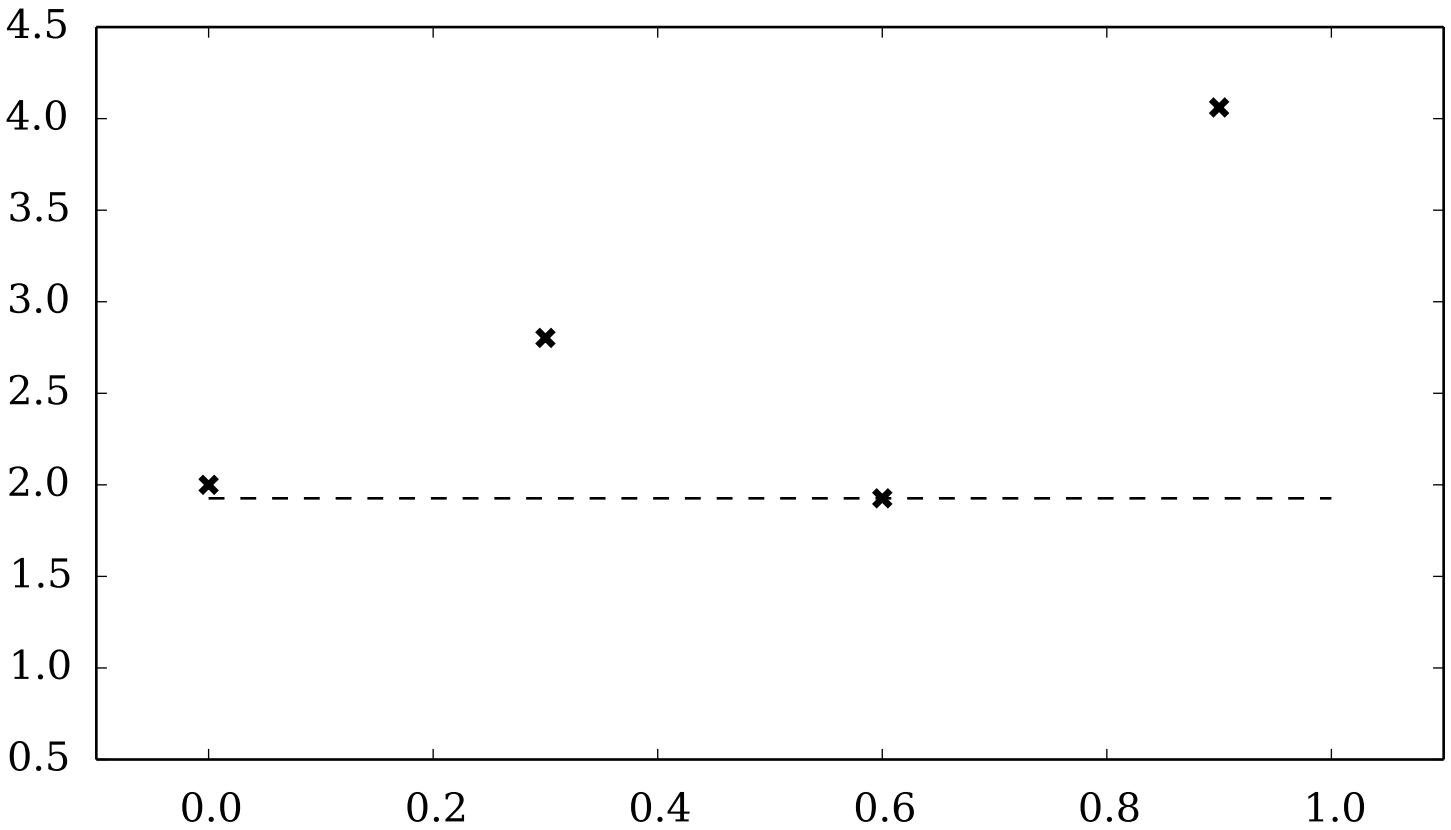
We want to minimize the following function...



Example : optimization

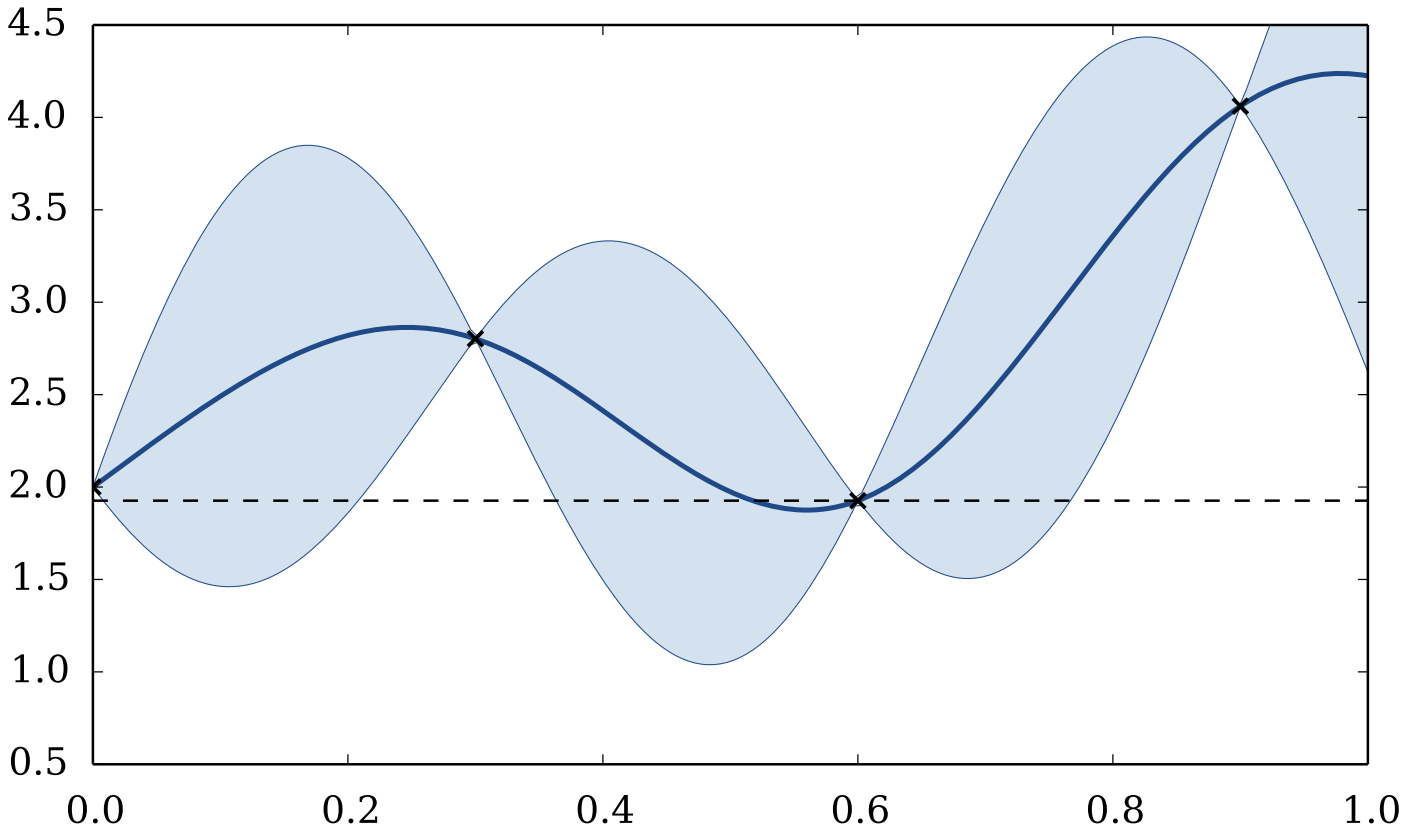
Case study

... which is costly.



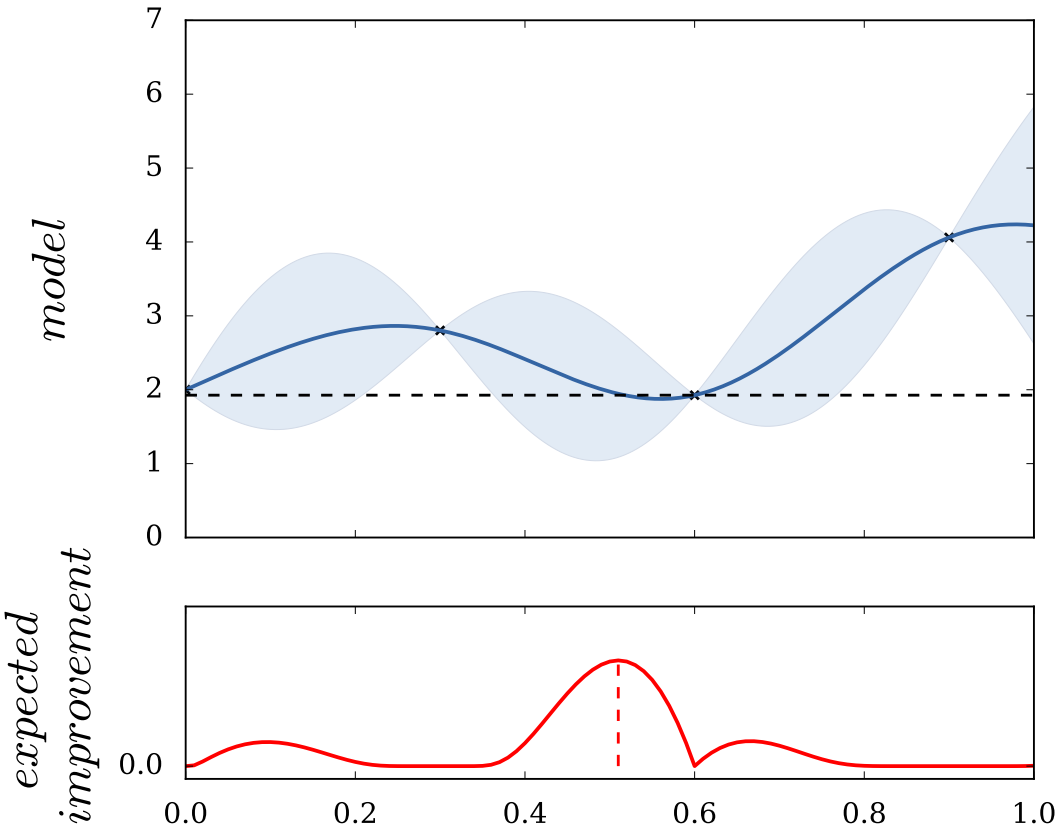
Example : optimization

We build a kriging model



Example : optimization

A common criterion is the **expected improvement**

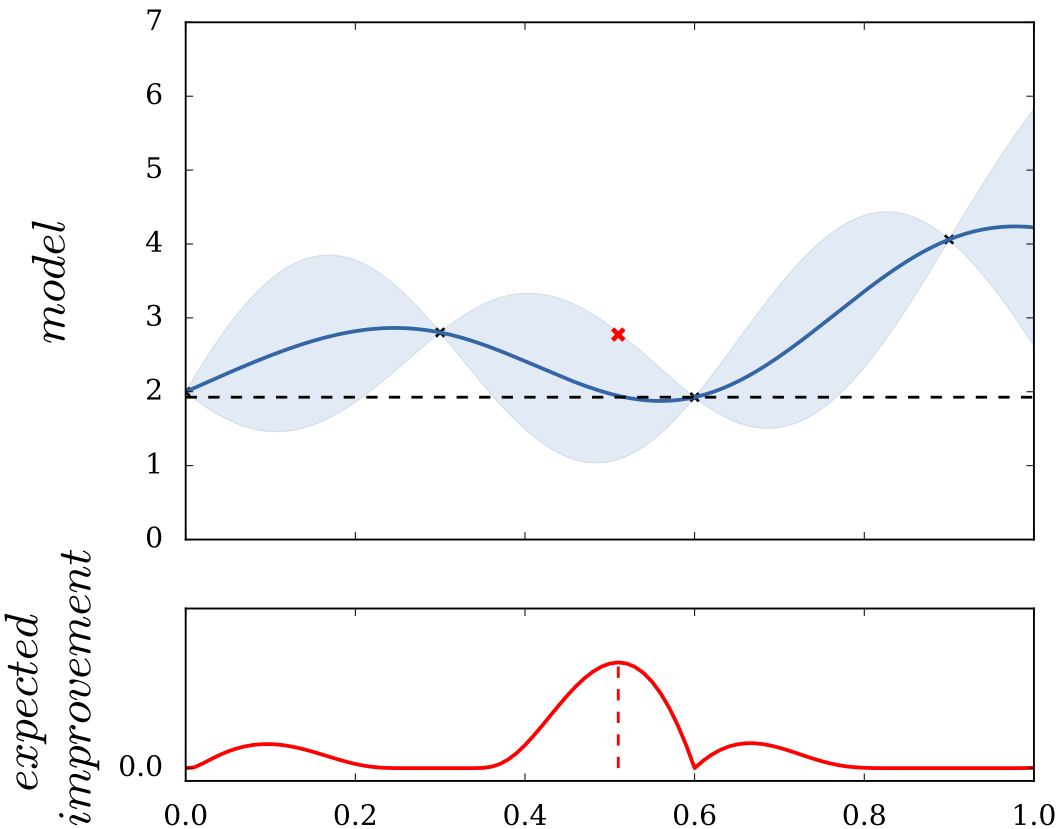


$$EI(x) = \sqrt{v(x)}(u(x)cdf(u(x)) + pdf(u(x)))$$

$$\text{with } u(x) = \frac{\min(F) - m(x)}{\sqrt{v(x)}}$$

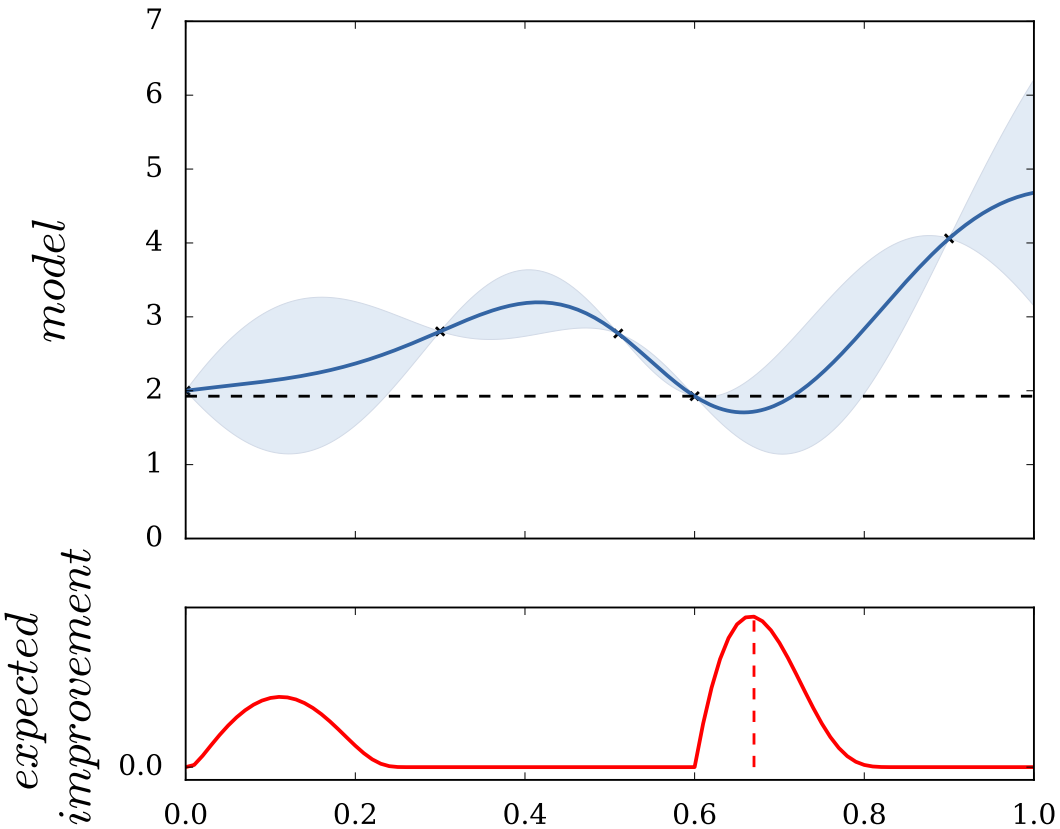
Example : optimization

We run another experiment where this criterion is maximum



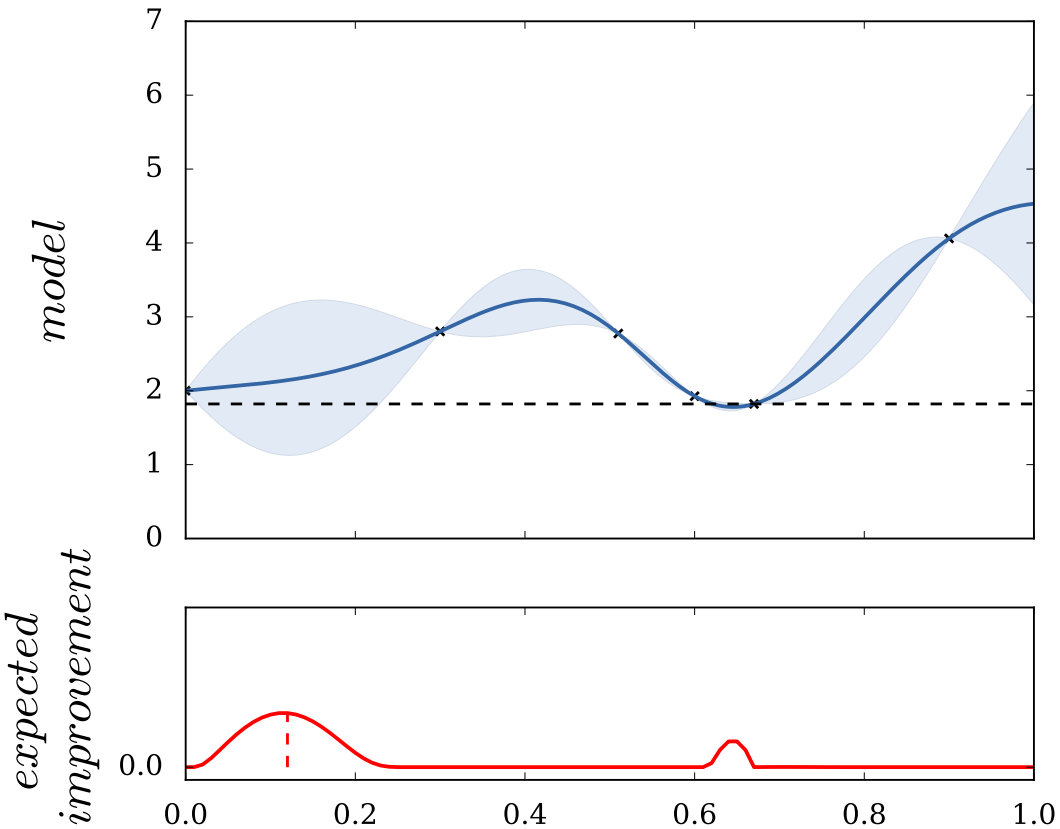
Example : optimization

Iteration 2 :



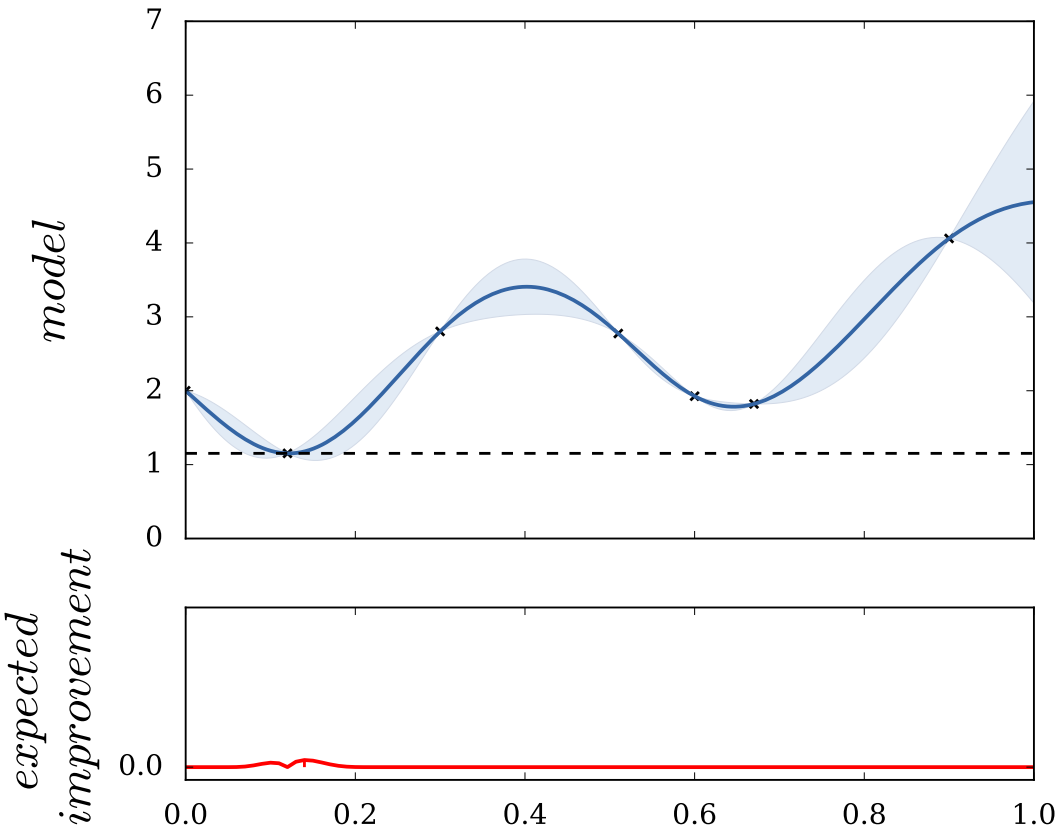
Exemple d'application : optimisation

Iteration 3 :



Exemple d'application : optimisation

Iteration 4 :



Lab session (20 min)

1. We are interested here in a maximization problem... update `Y` and the kriging model to make them suitable for usual minimization algorithms.
2. Get the new location of the point maximising the EI (see function `max_EI` from package `DiceOptim`)
3. Run the experiment at this location and update the model. Has the minimum been improved ?
4. Make 20 iterations using `EGO.nsteps`. You can look at the results using the function `visualizeEGO`.
5. What is the optimal value you obtain ?

$$x_1 = \quad , \; x_2 = \quad , \; x_3 = \quad , \; x_4 = \quad , \; Y_{min} = \quad .$$

Conclusion

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 some uncertainty measure

Small Recap We have seen that

- Many kernels can be used to build models.
  - Given some data, there is not one GP model but an infinity...
- Kernels encode the prior belief on the function to approximate.
  - They should be chosen accordingly
- Model/kernel parameters can tuned to the problem at hand
- GPR models do not necessarily interpolate.
- Model validation is of the utmost importance
  - mean **and** predicted (co-)variance

Limitations

The complexity of using kriging models is in building the model

- $\mathcal{O}(n^2)$ for the storage footprint
  - storage of the covariance matrix $k(X, X)$
- $\mathcal{O}(n^3)$ for the number of operations
  - inversion of the covariance matrix $k(X, X)$

In practice, the maximum number of observation for classical models lies in the range [1000, 10000].

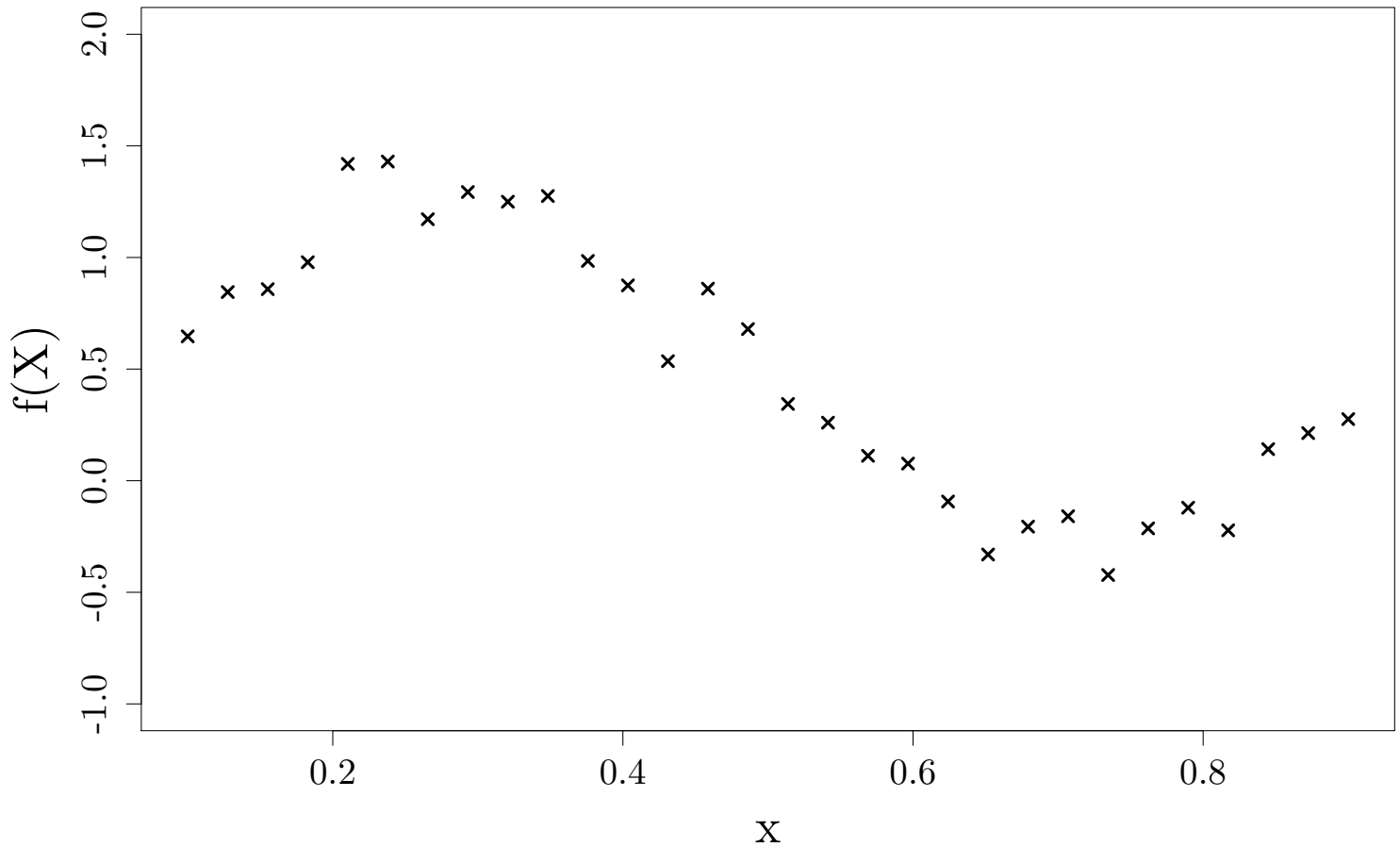
Another common issue is the numerical stability of the matrix inversion

- pseudo-inverse
- nugget (or jitter)

Appendix

Approximation

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



Approximation

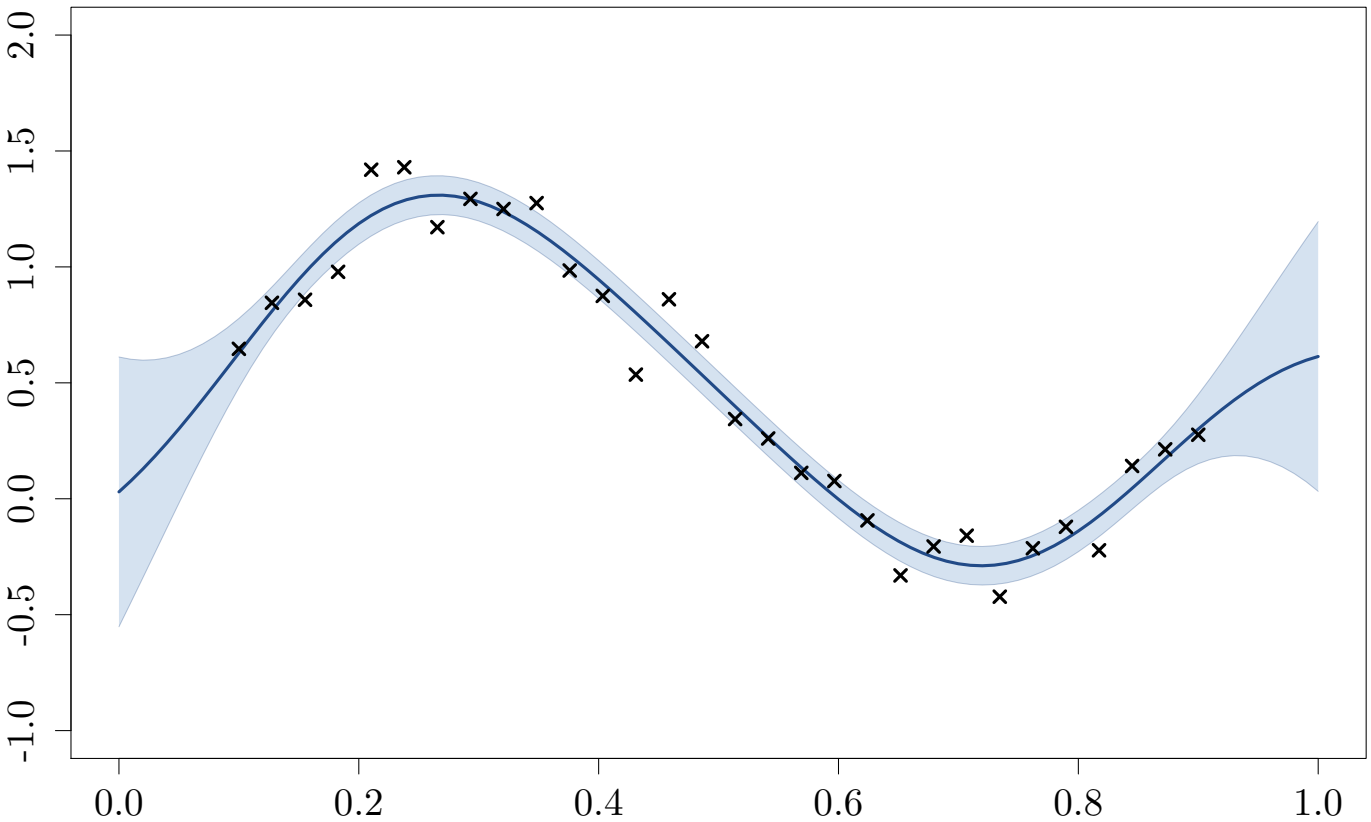
Let N be a process $\mathcal{N}(0, n)$ that represent the observation noise. The expressions of GPR with noise are

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

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

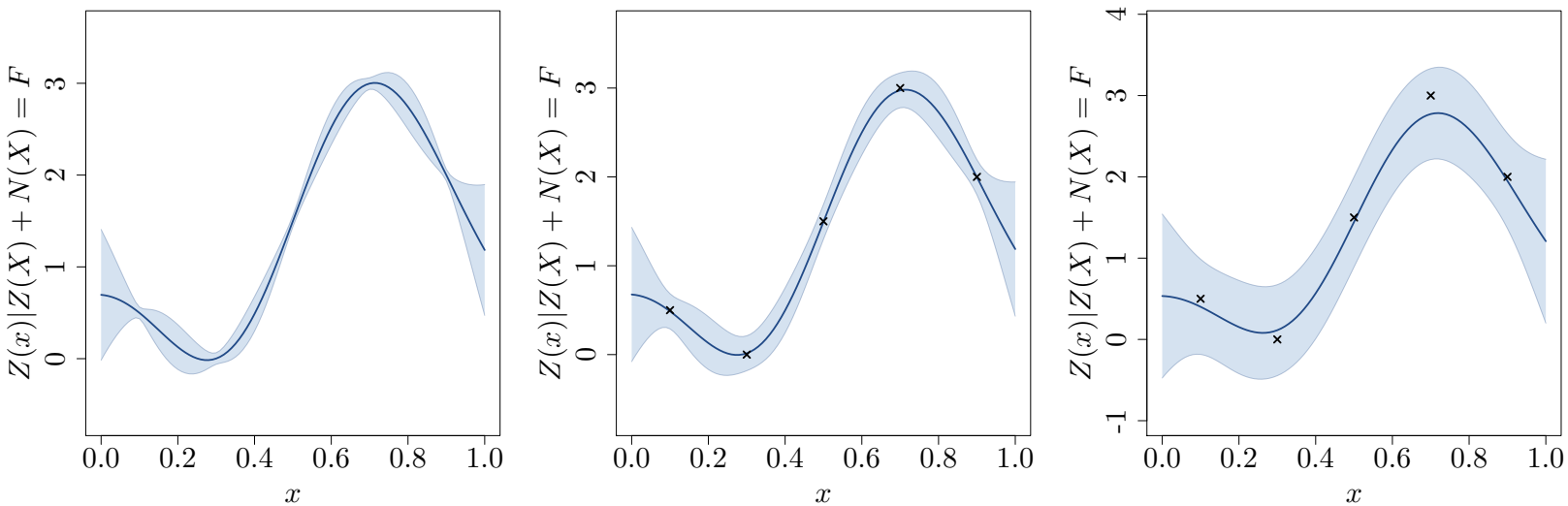
Approximation

We obtain the following model



Approximation

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



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

In practice, τ^2 can be estimated with Maximum Likelihood.