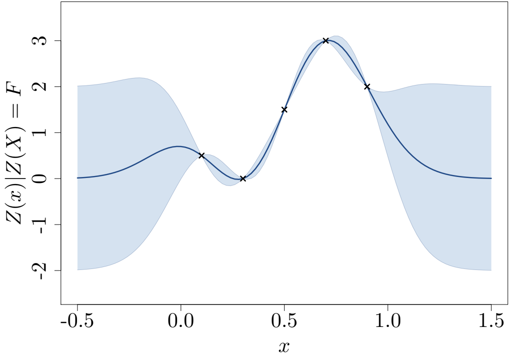
Short course on Statistical Modelling for Optimization – lecture 3/4

Gaussian Process regression

February 2015, Universidad Tecnológica de Pereira (Columbia)

Nicolas Durrande (durrande@emse.fr) – Mines St-Étienne (France)

We have seen on day 1 how to build Gaussian process regression models:



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

We will discuss these models in more details today.

Outline of todays lecture

- Parameters estimation
- Model validation
- Kernel designs
- “Exotic” informations

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.

Example

We consider 100 sample from a Matern 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.

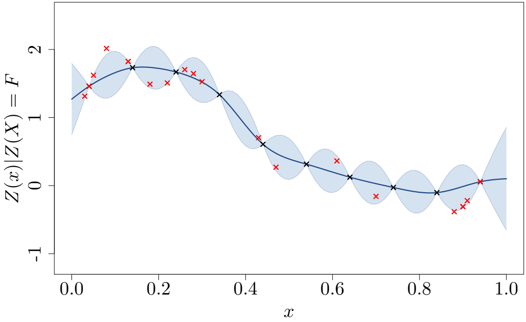
Model validation

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 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:

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

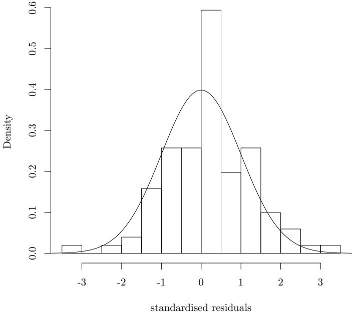
$$\text{A ``normalised'' criterion} \qquad Q_2 = 1 - \frac{\sum (F_t - m(X_t))^2}{\sum (F_t - \mathrm{mean}(F_t))^2}$$

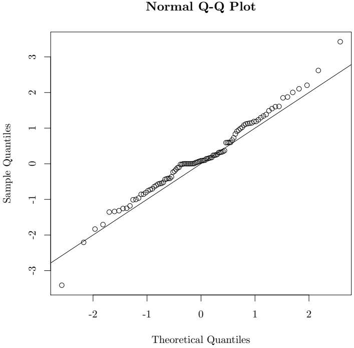
On the above example we get $MSE = 0.038$ and $Q_2 = 0.95$.

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:

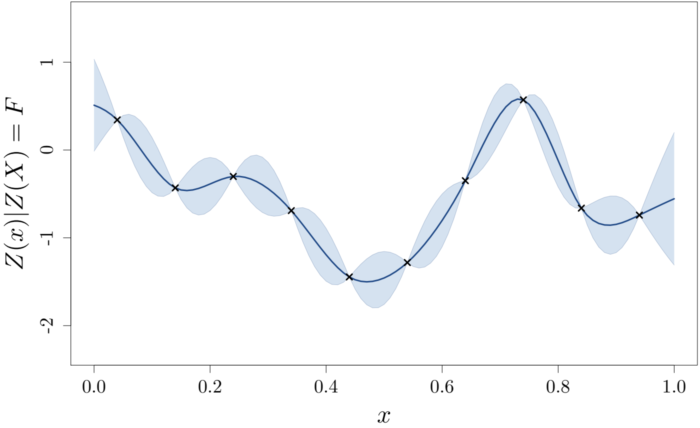
1. build a model based on all observations except one
2. compute the model error at this point

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

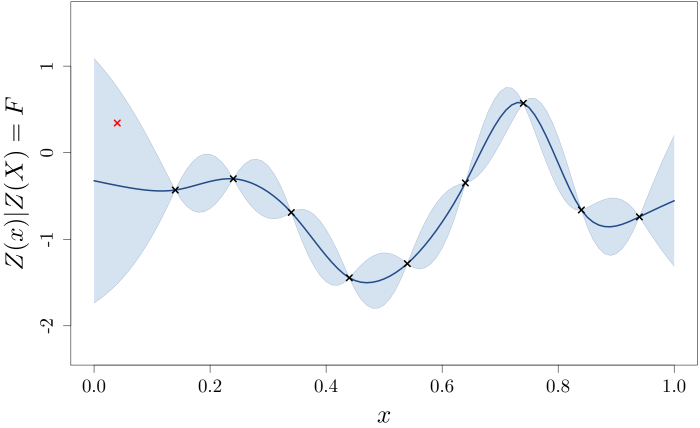
On the previous example we obtain $MSE = 0.24$ and $Q_2 = 0.34$.

Why doesn't the model perform as good previously?

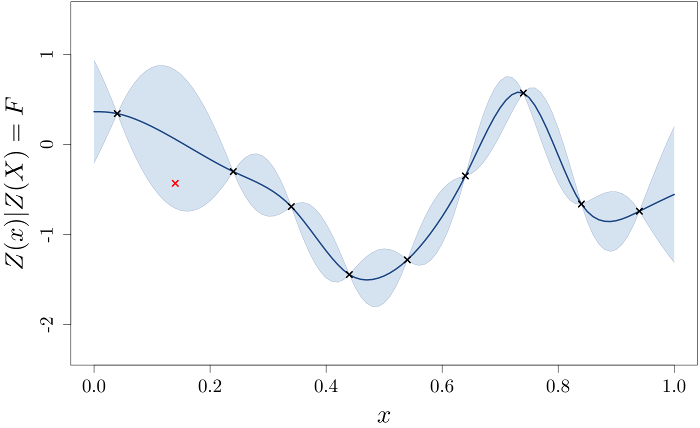
Model to be tested:



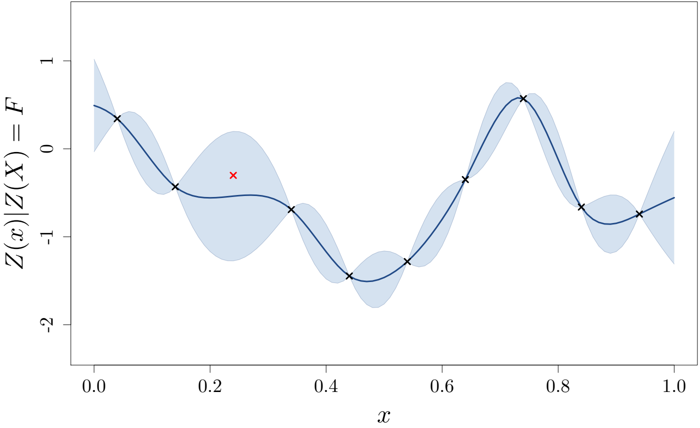
Step 1:



Step 2:

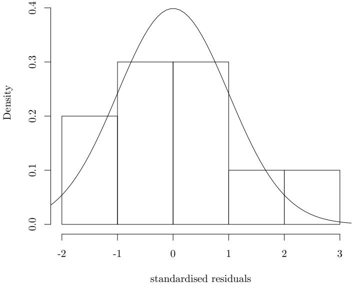


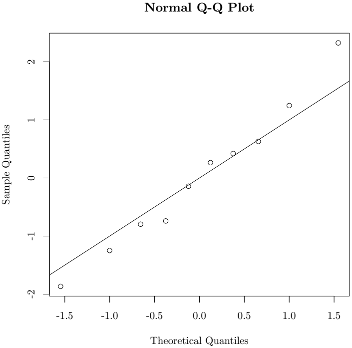
Step 3:



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:





Making new from old

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

Kernels can be:

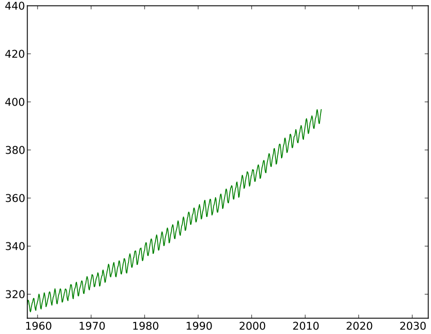
- Summed together
  - On the same space $k(x, y) = k_1(x, y) + k_2(x, y)$
  - On the tensor space $k(x, y) = k_1(x_1, y_1) + k_2(x_2, y_2)$
- Multiplied together
  - On the same space $k(x, y) = k_1(x, y) \times k_2(x, y)$
  - On the tensor space $k(x, y) = k_1(x_1, y_1) \times k_2(x_2, y_2)$
- Composed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

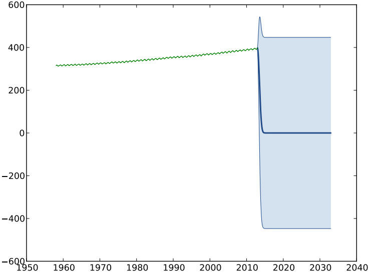


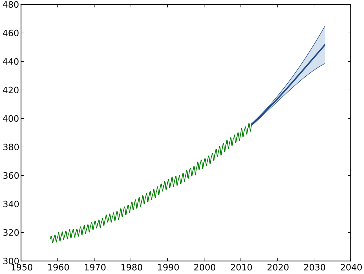
Let's try to predict the concentration for the next 20 years.

Sum of kernels over the same space

We first consider a squared-exponential kernel:

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





The results are terrible!

Sum of kernels over the same space

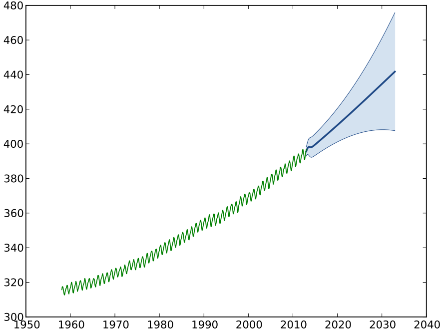
What happen if we sum both kernels?

$$k(x, y) = k_{rbf1}(x, y) + k_{rbf2}(x, y)$$

Sum of kernels over the same space

What happen if we sum both kernels?

$$k(x,y) = k_{rbf1}(x,y) + k_{rbf2}(x,y)$$



The model is drastically improved!

Sum of kernels over the same space

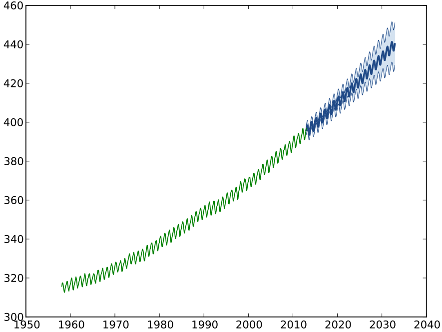
We can try the following kernel:

$$k(x, y) = \sigma_0^2 x^2 y^2 + k_{rbf1}(x, y) + k_{rbf2}(x, y) + k_{per}(x, y)$$

Sum of kernels over the same space

We can try the following kernel:

$$k(x,y) = \sigma_0^2 x^2 y^2 + k_{rbf1}(x,y) + k_{rbf2}(x,y) + k_{per}(x,y)$$



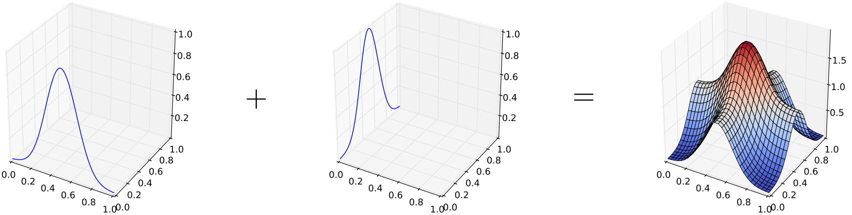
Once again, the model is significantly improved.

Sum of kernels over tensor space

Property

$$k(x, y) = k_1(x_1, y_1) + k_2(x_2, y_2) \tag{1}$$

is valid covariance structure.

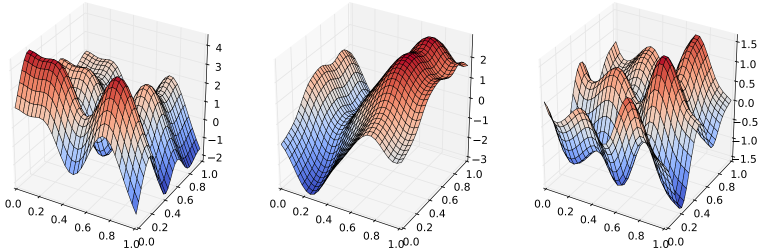


Remark:

- 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)

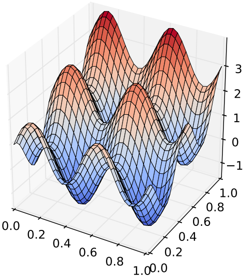
Tensor Additive kernels are very useful for

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

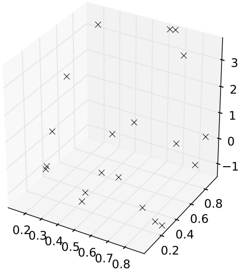
Sum of kernels over tensor space

We consider the test function $f(x) = \sin(4\pi x_1) + \cos(4\pi x_2) + 2x_2$ and a set of 20 observation in $[0,1]^2$

Test function



Observations

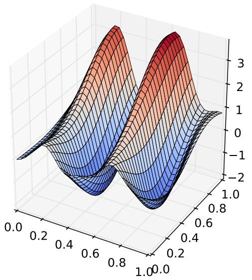


Sum of kernels over tensor space

We obtain the following models:

Gaussian kernel

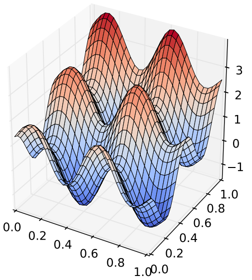
Mean predictor



RMSE is 1.06

Additive Gaussian kernel

Mean predictor



RMSE is 0.12

Sum of kernels over tensor space

Remark

- It is straightforward to show that the mean predictor is additive

$$\begin{aligned} m(x) &= (k_1(x_1, X_1) + k_2(x_2, X_2))k(X,X)^{-1}F \\ &= \underbrace{k_1(x_1, X_1)k(X,X)^{-1}F}_{m_1(x_1)} + \underbrace{k_1(x_1, X_1)k(X,X)^{-1}F}_{m_2(x_2)} \end{aligned}$$

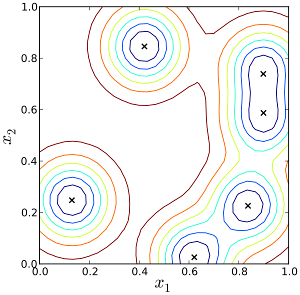
$\Rightarrow$ The mean predictor shares the prior behaviour.

Sum of kernels over tensor space

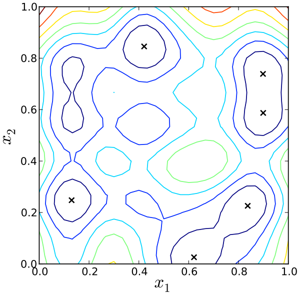
Remark

- The prediction variance has interesting features

pred. var. with kernel product

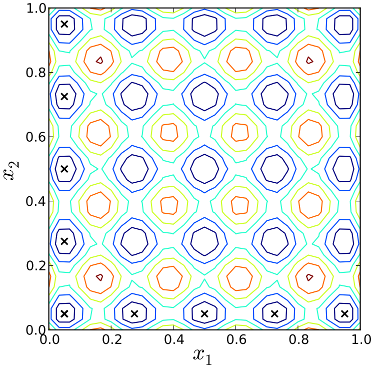


pred. var. with kernel sum



Sum of kernels over tensor space

This property can be used to construct a design of experiment that covers the space with only $cst \times d$ points.



Prediction variance

Product over the same space

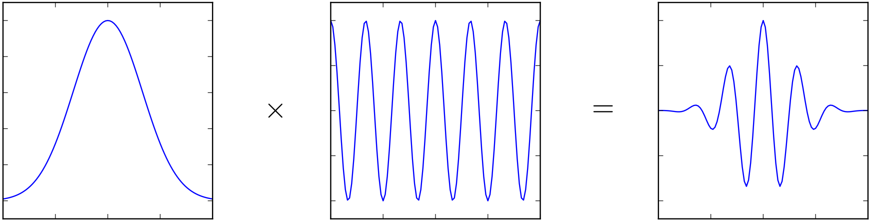
Property

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

is valid covariance structure.

Example

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



Product over the tensor space

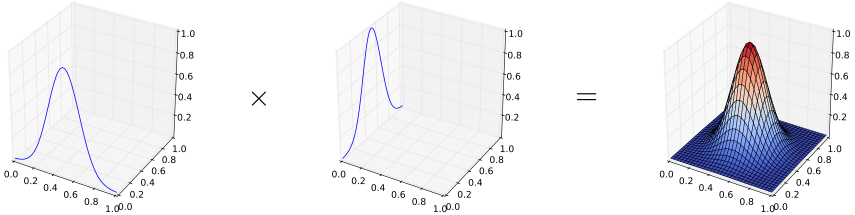
Property

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

is valid covariance structure.

Example

We multiply 2 squared exponential kernel



Calculation shows we obtain 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

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

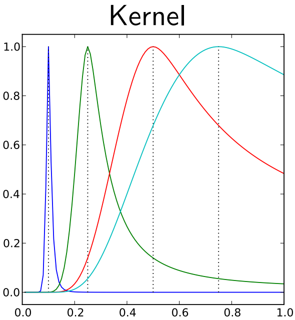
Remarks:

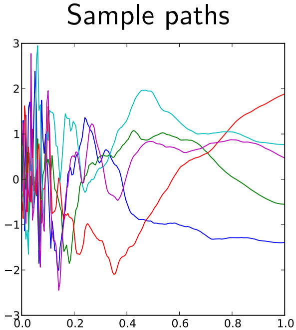
- k corresponds to the covariance of $Z(x) = Z_1(f(x))$
- This can be seen as a (non-linear) rescaling of the input space

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:



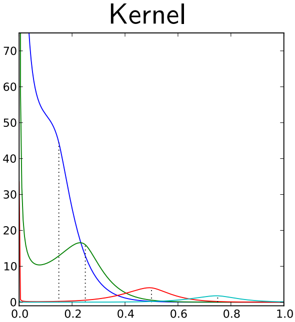


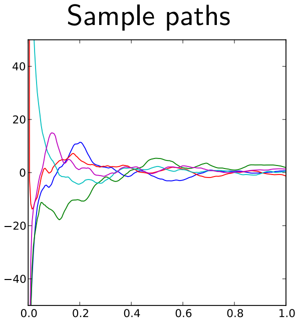
All these transformations can be combined!

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 $k_1(x,y) = (1 + |x-y|)e^{-|x-y|}$:





Bochner's theorem

Theorem (Bochner)

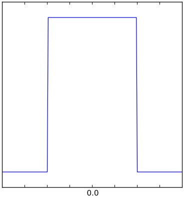
A continuous stationary function $k(x, y) = \tilde{k}(x - y)$ is positive definite if and only if $\tilde{k}$ is the Fourier transform of a finite positive measure:

$$\tilde{k}(t) = \int_{\mathbb{R}} e^{-i\omega t} \mathrm{d}\mu(\omega)$$

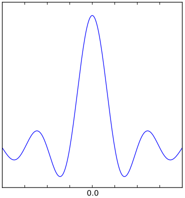
This result is very useful to prove the positive definiteness of stationary functions.

Example

We consider the following measure:



Its Fourier transform gives $\tilde{k}(t) = \dfrac{\sin(t)}{t}$:



As a consequence, $k(x, y) = \dfrac{\sin(x-y)}{x-y}$ is a valid covariance function.

Bochner theorem can be used to prove the positive definiteness of many usual stationary kernels

- The Gaussian is the Fourier transform of itself
  $\Rightarrow$ it is psd.
- Matern kernels are the Fourier transforms of $\frac{1}{(1+\omega^2)^p}$
  $\Rightarrow$ they are psd.
- the constant function is the Fourier transform of $\delta_{x,y}$
  $\Rightarrow$ it is psd.

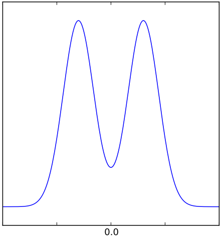
It can also be generalised to distributions:

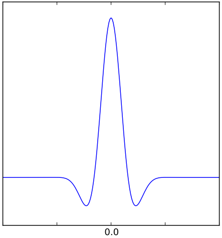
- $\delta_{x,y}$ is the Fourier transform of the constant function
  $\Rightarrow$ it is psd.

Spectral approximation with a mixture of Gaussian (A. Wilson, ICML 2013)

The inverse Fourier transform of a (symmetrised) non centred Gaussian is:

$$\mu(\omega) \quad \overrightarrow{\mathcal{F}} \quad \tilde{k}(t)$$



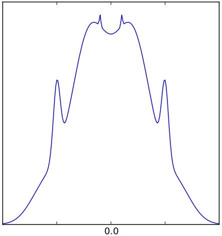


This can be generalised to a measure based on the sum of Gaussians.

Spectral approximation with a mixture of Gaussian (A. Wilson, ICML 2013)

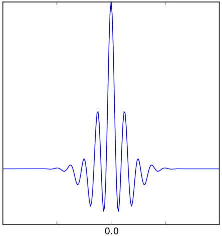
We obtain a kernel that is parametrised by the means and the bandwidths of Gaussian bells in the measure space:

$\mu(\omega)$



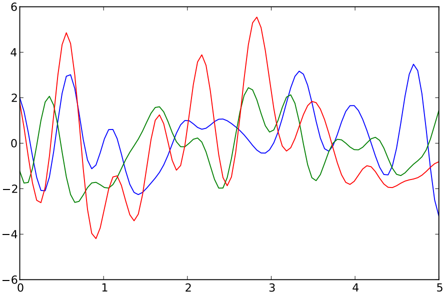
$$\xrightarrow{\mathcal{F}}$$

$\tilde{k}(t)$



Spectral approximation with a mixture of Gaussian (A. Wilson, ICML 2013)

The sample paths have the following aspect:



Effect of a linear operator

Effect of a linear operator

Property

Let L be a linear operator that commutes with the covariance, then $k(x,y) = L_x(L_y(k_1(x,y)))$ is a kernel.

Example

We want to approximate a function $[0,1] \to \mathbb{R}$ that is symmetric with respect to 0.5. We will consider 2 linear operators:

$$L_1 : f(x) \to \begin{cases} f(x) & x < 0.5 \\ f(1-x) & x \geq 0.5 \end{cases}$$

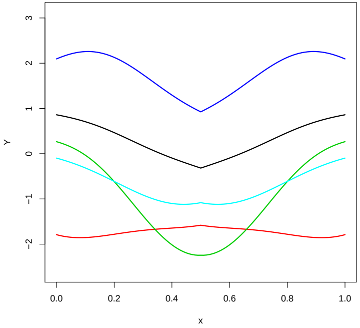
$$L_2 : f(x) \to \frac{f(x) + f(1-x)}{2}.$$

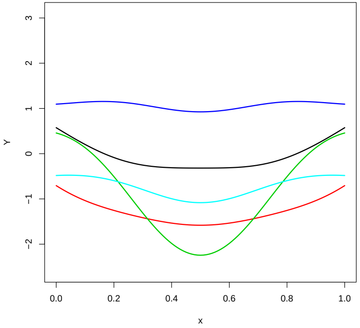
Exercice: Compute the kernel associated to the second operator.

Effect of a linear operator: example [Ginsbourger 2013]

Examples of associated sample paths are

$k_1 = L_1(L_1(k))$ $\qquad\qquad$ $k_2 = L_2(L_2(k))$

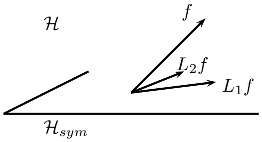




The differentiability is not always respected!

Effect of a linear operator

These linear operator are projections onto a space of symmetric functions:



Is there an optimal projection?

$\Rightarrow$ This can be difficult... but it raises interesting questions!

Effect of a linear operator

Can we construct a GP such that the integrals of the paths are null?

We can think of the following application:

$$L : f(x) \to f(x) - \int f(s)\,\mathrm{d}s.$$

More generally, for all $g : [0,1] \to \mathbb{R}$, the application

$$L_g : f(x) \to f(x) - \frac{g(x)}{\int g(s)\,\mathrm{d}s} \int f(s)\,\mathrm{d}s$$

will center f. It turns out that the optimal g is $g(x) = \int k(x,s)\,\mathrm{d}s$

Exercice

1. Compute the associated kernel.
2. What is the distribution of $Z | \int Z = 0$?

Adding "exotic" observations

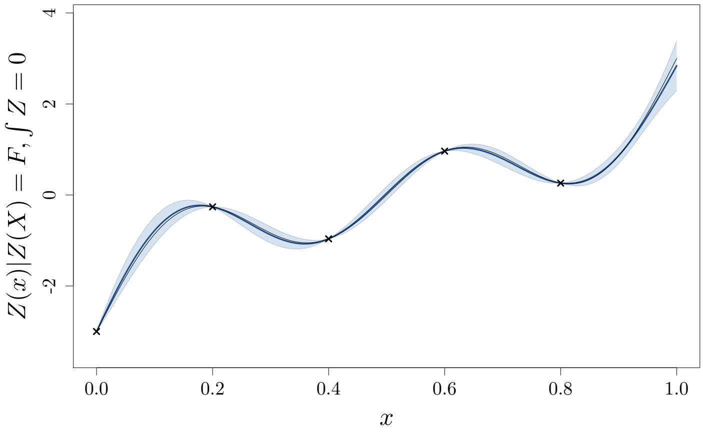
Up to now, we have only considered regular observation of the kind $f(X)$.

According to what we have just seen, the conditioning can also include observation of the integral. This can be generalised to other linear operators such as the derivative:

$$Z \;\Big|\; Z(X) = F, \int Z = a, \frac{\mathrm{d}Z}{\mathrm{d}x}(X') = F'$$

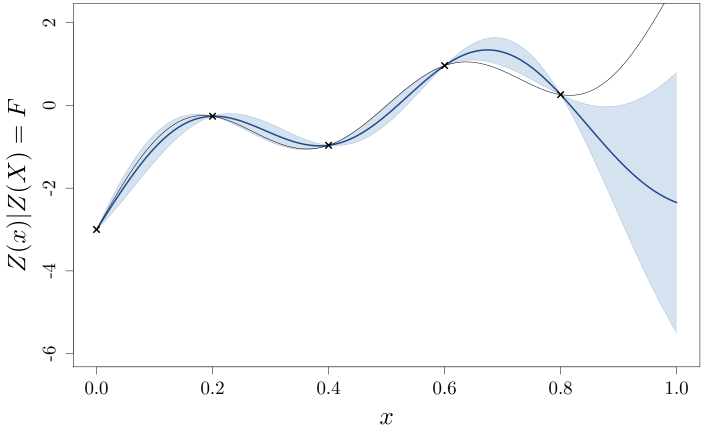
Example

If we take into account that the function is centred, we obtain:

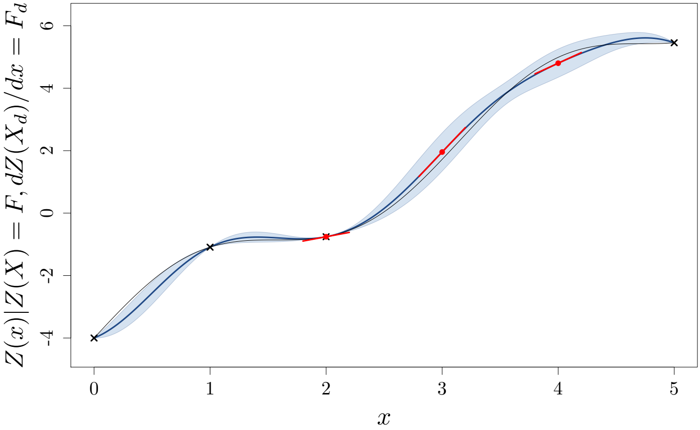


Example

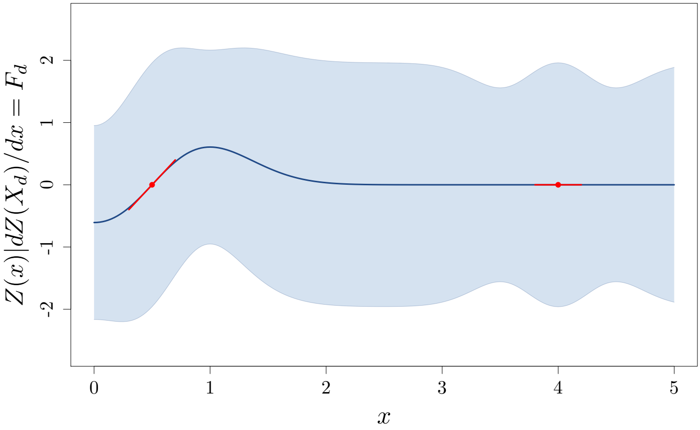
Whereas if we ignore it:



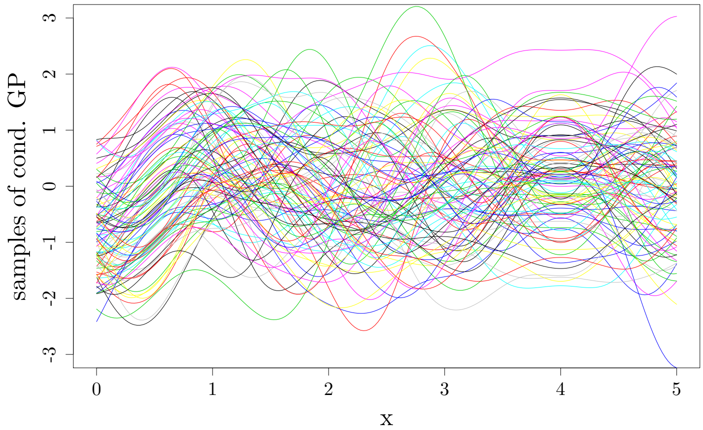
Similarly, we can include in the model some derivatives observations:



We can see interesting behaviour if we look at a model with only derivatives.



As always, we can simulate conditional paths:



Conclusion

Small Recap We have seen that

- It is possible to build as many kernels as you want
  - Given some data, there is not one GP model but an infinity...
- Kernels encode the prior belief on the function to approximate.
  - They can (and should) be tailored to the problem at hand.
- It is possible to include more than regular function observations.
- If you want the decisions based on your model to be reliable, model validation is of the utmost importance.

3 tools for designing new kernels:

Making new from old

Various operations can be applied to kernels while keeping the psd :

- sum
- product
- composition with a function

Bochner Theorem

is very useful to prove a stationary kernel is psd.

Linear operators

If we have a linear application that transforms any function into a function satisfying the desired property, it is possible to build a GP fulfilling the requirements.