Gaussian Process Summer School

Kernel Design

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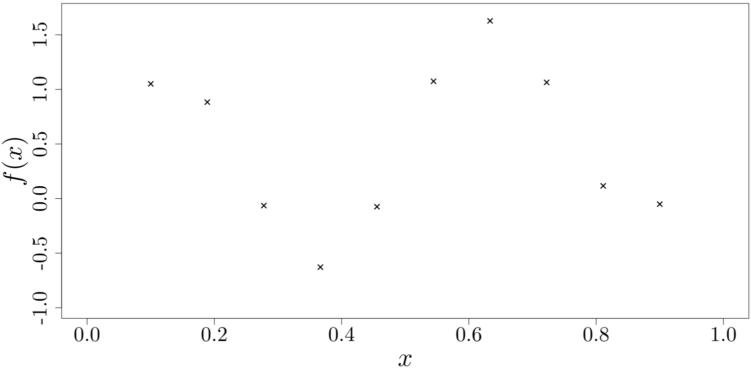
We have seen during the introduction lectures that the distribution of a GP Z depends on two functions :

- the mean $m(x) = \mathrm{E}\left(Z(x)\right)$
- the covariance $k(x, x') = \mathrm{cov}\left(Z(x), Z(x')\right)$

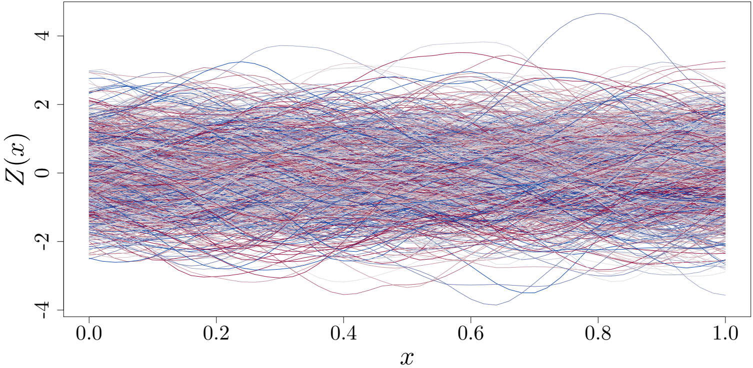
In this talk, we will focus on the **covariance function**, which is often call the **kernel**.

We assume we have observed a function f for a limited number of time points $x_1, \dots, x_n$:

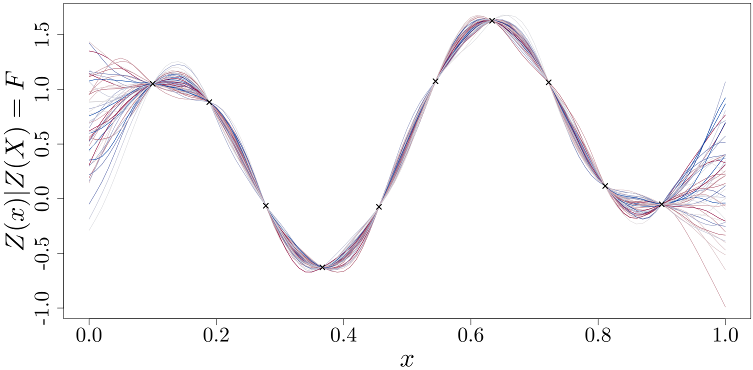


The observations are denoted by $f_i = f(x_i)$ (or $F = f(X)$).

Since f in unknown, we make the general assumption that it is a sample path of a Gaussian process Z :



Combining these two informations means keeping the samples interpolating the data points :

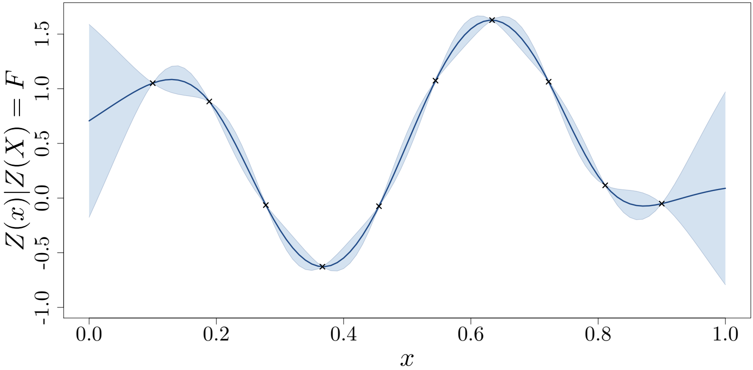


The conditional distribution is still Gaussian with moments :

$$m(x) = \mathrm{E}\left(Z(x)|Z(X)\text{=}F\right) = k(x, X)k(X, X)^{-1}F$$

$$c(x, x') = \mathrm{cov}\left(Z(x), Z(x')|Z(X)\text{=}F\right) = k(x, x') - k(x, X)k(X, X)^{-1}k(X, x')$$

It can be represented as a mean function with confidence intervals.



Let Z be a random process with kernel k. Some properties of kernels can be obtained directly from their definition.

Example

$$k(x,x) = \mathrm{cov}\left(Z(x), Z(x)\right) = \mathrm{var}\left(Z(x)\right) \geq 0$$
$$\Rightarrow k(x,x) \text{ is } \textbf{positive}.$$

$$k(x,y) = \mathrm{cov}\left(Z(x), Z(y)\right) = \mathrm{cov}\left(Z(y), Z(x)\right) = k(y,x)$$
$$\Rightarrow k(x,y) \text{ is } \textbf{symmetric}.$$

We can obtain a thinner result...

We introduce the random variable $T = \sum_{i=1}^{n} a_i Z(x_i)$ where n, a_i and x_i are arbitrary. Computing the variance of T gives :

$$\begin{aligned} \mathrm{var}(T) &= \mathrm{cov}\left(\sum_i a_i Z(x_i), \sum_j a_j Z(x_j)\right) = \sum_i \sum_j a_i a_j \mathrm{cov}\left(Z(x_i), Z(x_j)\right) \\ &= \sum \sum a_i a_j k(x_i, x_j) \end{aligned}$$

Since a variance is positive, we have

$$\sum_i \sum_j a_i a_j k(x_i, x_j) \geq 0$$

for any arbitrary n, a_i and x_i.

Definition

The functions satisfying the above inequality **for all** $n \in \mathbb{N}$, **for all** $x_i \in D$, **for all** $a_i \in \mathbb{R}$ are called positive semi-definite functions.

We have just seen :

$$k \text{ is a covariance} \Rightarrow k \text{ is a positive semi-definite function}$$

The reverse is also true :

Theorem (Loeve)

k corresponds to the covariance of a GP

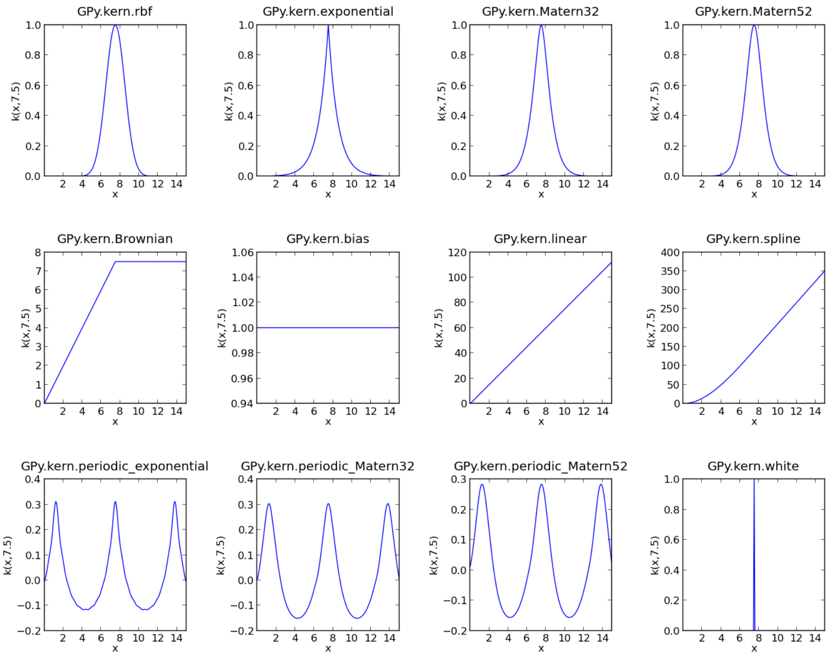
$$\Updownarrow$$

k is a symmetric positive semi-definite function

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

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

When k is a function of $x - y$, the kernel is called **stationary**.
σ^2 is called the **variance** and θ the **lengthscale**.


GPy.kern.rbf
GPy.kern.exponential
GPy.kern.Matern32
GPy.kern.Matern52
GPy.kern.Brownian
GPy.kern.bias
GPy.kern.linear
GPy.kern.spline
GPy.kern.periodic_exponential
GPy.kern.periodic_Matern32
GPy.kern.periodic_Matern52
GPy.kern.white
k(x,7.5)
x

For a few kernels, it is possible to prove they are psd directly from the definition.

- $k(x, y) = \delta_{x,y}$
- $k(x, y) = 1$

For most of them a direct proof from the definition is not possible. The following theorem is helpful for stationary kernels :

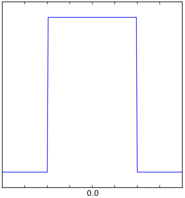
Theorem (Bochner)

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 :

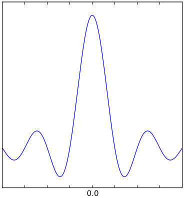
$$\tilde{k}(t) = \int_{\mathbb{R}} e^{-i\omega t} \mathrm{d}\mu(\omega)$$

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.

Usual kernels

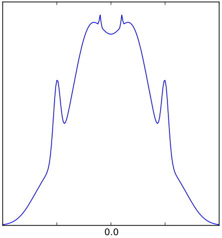
Bochner theorem can be used to prove the positive definiteness of many usual stationary kernels

- The Gaussian is the Fourier transform of itself
  $\Rightarrow$ it is psd.
- Matérn kernels are the Fourier transforms of $\frac{1}{(1+\omega^2)^p}$
  $\Rightarrow$ they are psd.

Unusual kernels

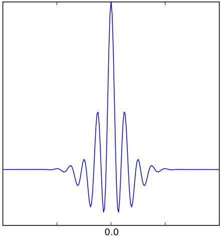
Inverse Fourier transform of a (symmetrised) sum of Gaussian gives (A. Wilson, ICML 2013) :

$\mu(\omega)$



$$\overrightarrow{\mathcal{F}}$$

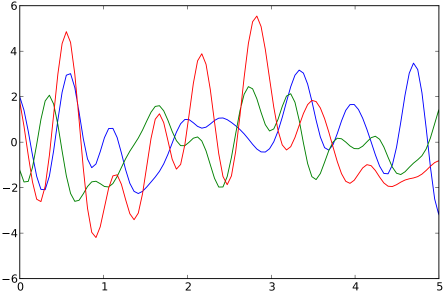
$\tilde{k}(t)$



The obtained kernel is parametrised by its spectrum.

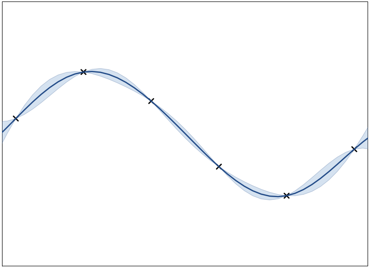
Unusual kernels

The sample paths have the following shape :

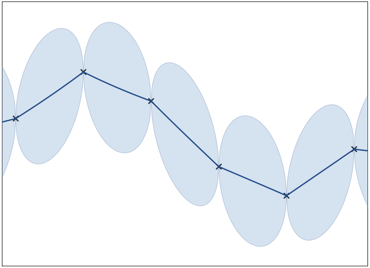


Changing the kernel has a huge impact on the model :

Gaussian kernel:

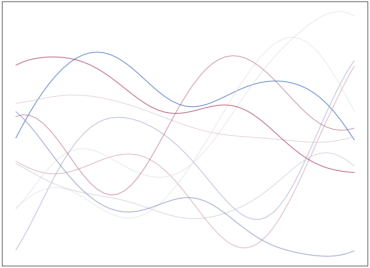


Exponential kernel:

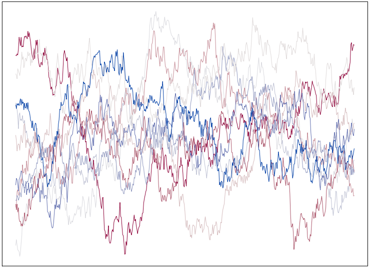


This is because changing the kernel implies changing the prior

Gaussian kernel:



Exponential kernel:



In order to choose a kernel, one should gather all possible informations about the function to approximate...

- Is it stationary ?
- Is it differentiable, what's its regularity ?
- Do we expect particular trends ?
- Do we expect particular patterns (periodicity, cycles, additivity) ?

Kernels often include rescaling parameters : θ for the x axis (length-scale) and σ for the y (σ^2 often corresponds to the GP variance). They can be tuned by

- maximizing the likelihood
- minimizing the prediction error

It is common to try various kernels and to asses the model accuracy. The idea is to compare some model predictions against actual values :

- On a test set
- Using leave-one-out

Two (ideally three) things should be checked :

- Is the mean accurate (MSE, Q^2) ?
- Do the confidence intervals make sense ?
- Are the predicted covariances right ?

Furthermore, it is often interesting to try some input remapping such as $x \to \log(x)$, $x \to \exp(x)$, ...

Making new from old :

Kernels can be :

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

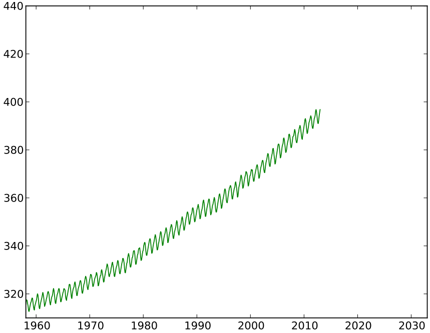
All these operations will preserve the positive definiteness.

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.

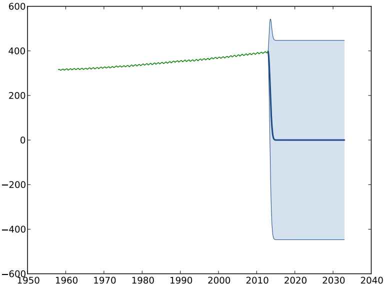


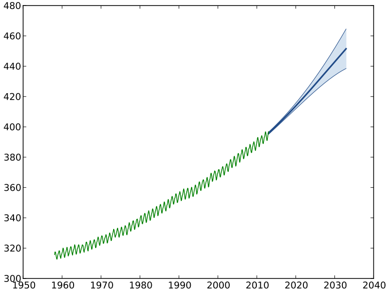
Let's try to predict the concentration for the next 20 years.

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

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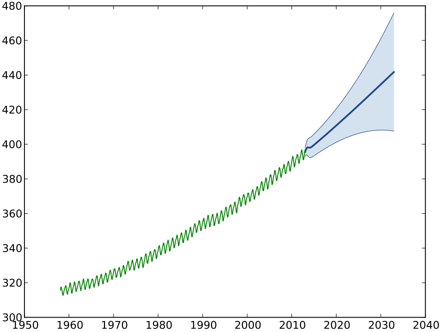


The model is drastically improved !

Sum of kernels over the same space

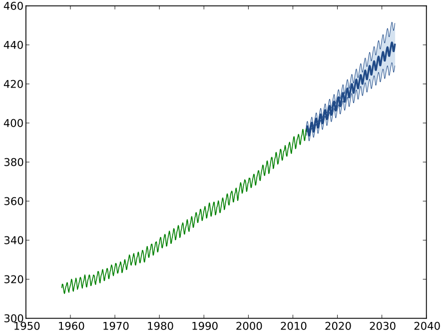
We can try the following kernel :

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

Sum of kernels over the same space

We can try the following kernel :

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



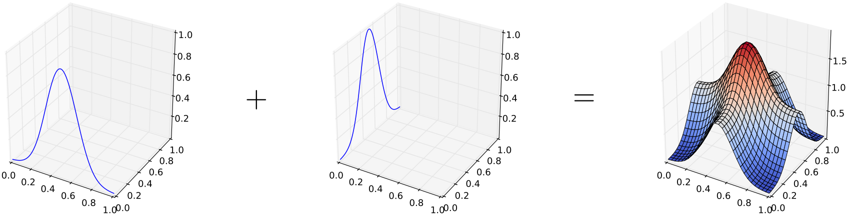
Once again, the model is significantly improved.

Sum of kernels over tensor space

Property

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

is a valid covariance structure.

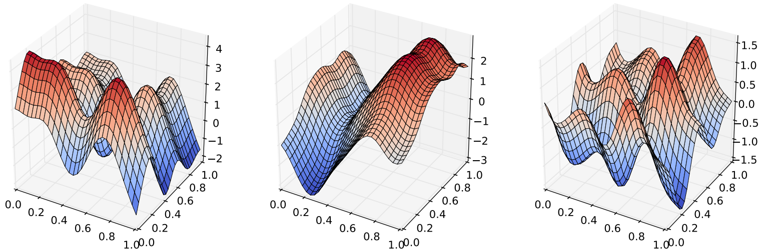


Remark :

- From a GP point of view, k is the kernel of $Z(\mathbf{x}) = Z_1(x_1) + Z_2(x_2)$

Sum of kernels over tensor space

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



⇒ They are additive (up to a modification)

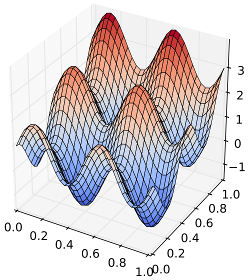
Tensor Additive kernels are very useful for

- Approximating additive functions
- Building models over high dimensional input space

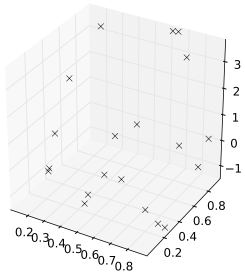
Sum of kernels over tensor space

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

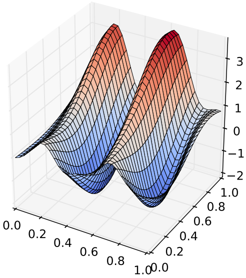


Sum of kernels over tensor space

We obtain the following models :

Gaussian kernel

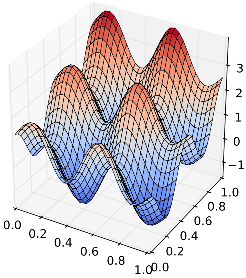
Mean predictor



RMSE is 1.06

Additive Gaussian kernel

Mean predictor



RMSE is 0.12

Sum of kernels over tensor space

Remarks

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

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

$\Rightarrow$ The model shares the prior behaviour.

- The sub-models can be interpreted as GP regression models with observation noise :

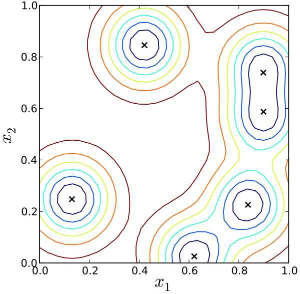
$$m_1(x_1) = \mathrm{E}\left(\ Z_1(x_1) \mid Z_1(X_1) + Z_2(X_2)\text{=}F\ \right)$$

Sum of kernels over tensor space

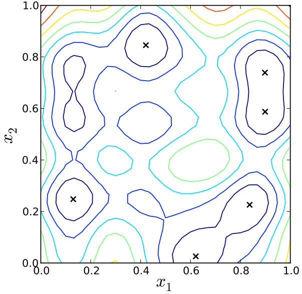
Remark

- The prediction variance has interesting features

pred. var. with kernel product

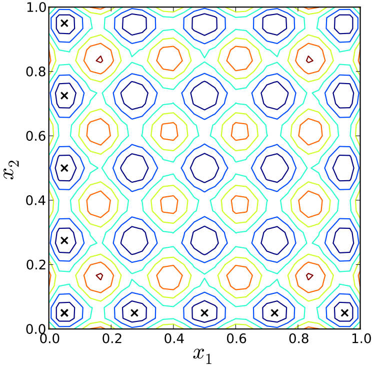


pred. var. with kernel sum



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

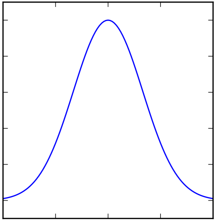
Property

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

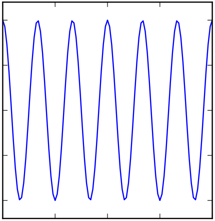
is valid covariance structure.

Example

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



$\times$



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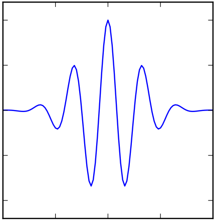


Product over the tensor space

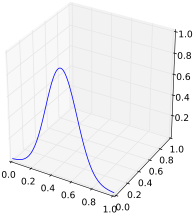
Property

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

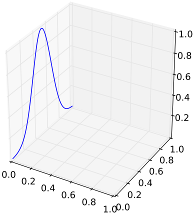
is valid covariance structure.

Example

We multiply two squared exponential kernels



$\times$



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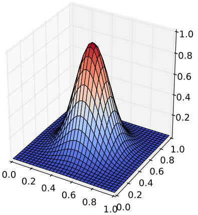


Calculation shows we obtain the usual 2D squared exponential kernels.

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

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

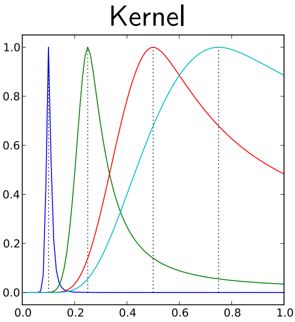
Remarks :

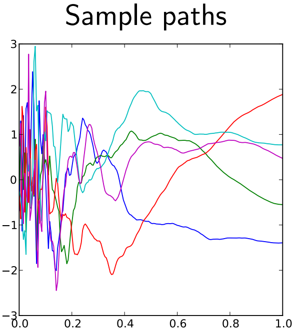
- k corresponds to the covariance of $Z(x) = Z_1(f(x))$
- This can be seen as a (nonlinear) rescaling of the input space

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 :



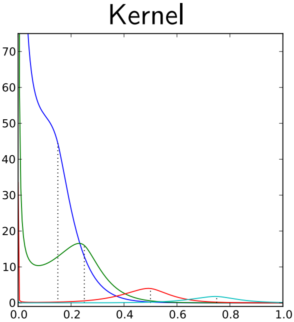


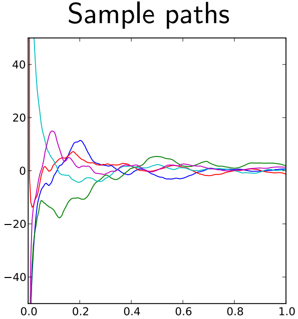
All these transformations can be combined !

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





Effect of a linear operator

Property (Ginsbourger 2013)

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 :

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

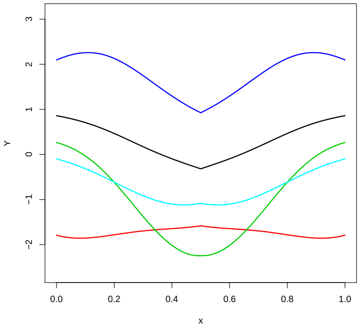
$$L_2 : f(x) \to \frac{f(x) + f(1-x)}{2}.$$

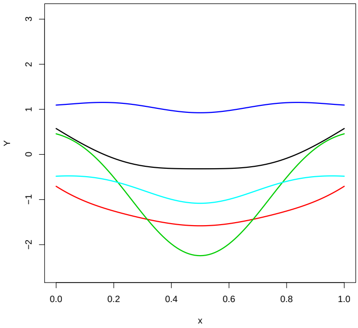
Effect of a linear operator

Example

Associated sample paths are

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

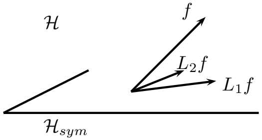




The differentiability is not always respected !

Effect of a linear operator

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



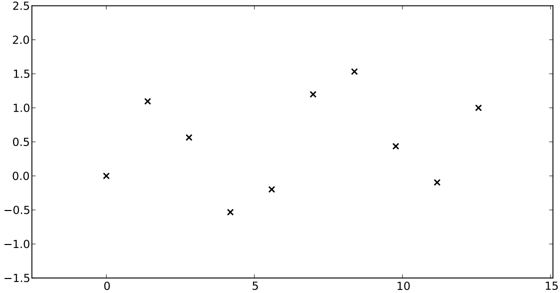
What about the optimal projection ?

⇒ This can be difficult... but it raises interesting questions !

Periodicity detection

We will now discuss the detection of periodicity

Given a few observations can we extract the periodic part of a signal ?



As previously we will build a decomposition of the process in two independent GPs :

$$Z = Z_p + Z_a$$

where Z_p is a GP in the span of the Fourier basis $B(t) = (\sin(t), \cos(t), \dots, \sin(nt), cos(nt))^t$.

Property

It can be proved that the kernel of Z_p and Z_a are

$$k_p(x, y) = B(x)^t G^{-1} B(y)$$
$$k_a(x, y) = k(x, y) - k_p(x, y)$$

where G is the Gram matrix associated to B in the RKHS.

As previously, a decomposition of the model comes with a decomposition of the kernel

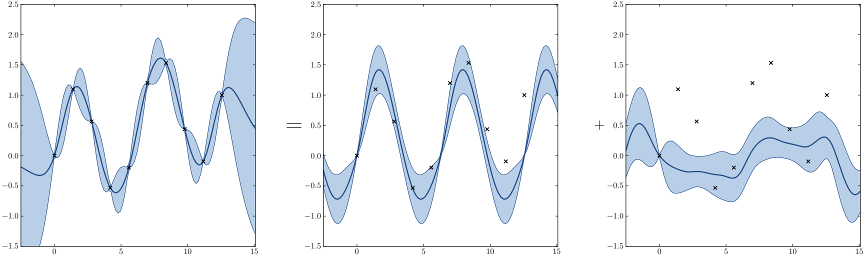
$$\begin{aligned} m(t) &= (k_p(x,X) + k_a(x,X))k(X,X)^{-1}F \\ &= \underbrace{k_p(x,X)k(X,X)^{-1}F}_{\text{periodic sub-model } m_p} + \underbrace{k_a(x,X)k(X,X)^{-1}F}_{\text{aperiodic sub-model } m_a} \end{aligned}$$

and we can associate a prediction variance to the sub-models :

$$\begin{aligned} v_p(t) &= k_p(x,x) - k_p(x,X)^t k(X,X)^{-1} k_p(t) \\ v_a(t) &= k_a(x,x) - k_a(x,X)^t k(X,X)^{-1} k_a(t) \end{aligned}$$

Example

For the observations shown previously we obtain :



Can we can do any better ?

Initially, the kernels are parametrised by 2 variables :

$$k(x, y, \sigma^2, \theta)$$

but writing k as a sum allows to tune independently the parameters of the sub-kernels.

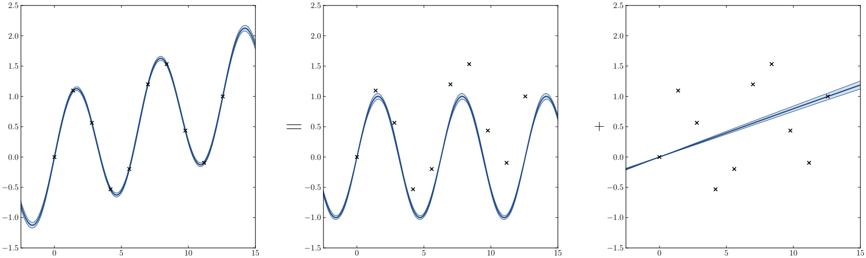
Let k^* be defined as

$$k^*(x, y, \sigma_p^2, \sigma_a^2, \theta_p, \theta_a) = k_p(x, y, \sigma_p^2, \theta_p) + k_a(x, y, \sigma_a^2, \theta_a)$$

Furthermore, we include a 5^{th} parameter in k^* accounting for the period by changing the Fourier basis :

$$B_\omega(t) = (\sin(\omega t), \cos(\omega t), \ldots, \sin(n\omega t), cos(n\omega t))^t$$

MLE of the 5 parameters of k^* gives :



We will now illustrate the use of these kernels for gene expression analysis.

We can apply this method to study the circadian rythm in organisms. We used *arabidopsis* data from Edward 2006.

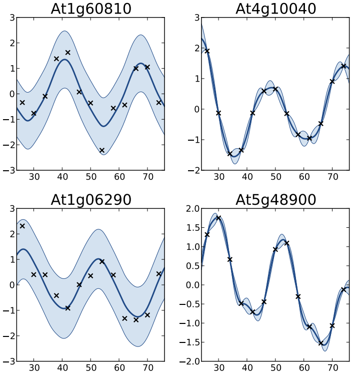
The dimension of the data is :

- 22810 genes
- 13 time points

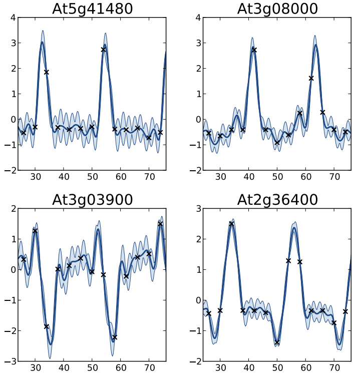
Edward 2006 gives a list of the 3504 most periodically expressed genes. The comparison with our approach gives :

- 21767 genes with the same label (2461 per. and 19306 non-per.)
- 1043 genes with different labels

Let's look at genes with different labels :



periodic for Edward



periodic for our approach

Small recap

We have seen that

- Kernels have a huge impact on the model
- They have to reflect the prior belief on the function to approximate.
- Kernels can (and should) be tailored to the problem at hand.

Although a direct proof of the positive definiteness of a function is often intractable, Bochner theorem allows to build kernels from their power spectrum.

Various operations can be applied to kernels while keeping p.s.d.ness :

Making new from old

- sum
- product
- composition with a function
- these can be combined

Linear operator

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.

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