Exercise sheet: Gaussian Processes

The following exercises have different levels of difficulty indicated by (*), (**), (***). An exercise with (*) is a simple exercise requiring less time to solve compared to an exercise with (***), which is a more complex exercise. Don't worry if you can't do a (***) exercise, as these are beyond what will be expected in the exam. They are instead intended to encourage further reading and deeper understanding.

1. (*) If someone is using an exponentiated quadratic covariance function, and they increase the lengthscale, what effect will this increase have on the covariance between two points (e.g. at $x_1 = 1$ and $x_2 = 3$)?

2. (*) For an arbitrary choice of covariance function: Does the covariance between points always get smaller as the two points are placed further apart?

3. (*) Are covariances always positive? (do all covariance functions lead to positive covariances?)

4. (*) What is the mean and covariance of $p(y_2)$ if,

$$\begin{bmatrix} \boldsymbol{y_1} \\ \boldsymbol{y_2} \end{bmatrix} \sim N\left(\begin{bmatrix} \boldsymbol{\mu_1} \\ \boldsymbol{\mu_2} \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma_{11}} & \boldsymbol{\Sigma_{12}} \\ \boldsymbol{\Sigma_{12}^\top} & \boldsymbol{\Sigma_{22}} \end{bmatrix}\right)$$

5. (**) We have two observations:

$$X = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

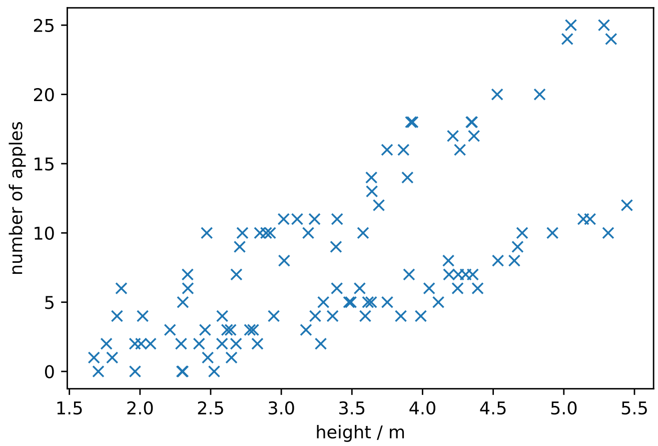
$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ 1 \end{bmatrix}$$

We don't currently know y_1, yet. We will use the exponentiated quadratic with a lengthscale of 2 (and kernel variance of 1) to compute a prediction at $x_* = 3$.

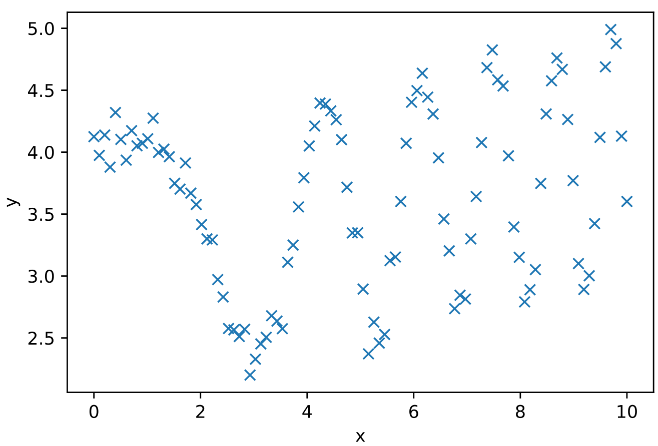
$$k(x_1, x_2) = \exp\left(\frac{-(x_1 - x_2)^2}{2l^2}\right)$$

a. Compute $\boldsymbol{k}_{*f}$ and K_{ff}^{-1}.
b. Compute the product $\boldsymbol{k}_{*f} K_{ff}^{-1}$ and so write down an expression for the posterior mean, in the form of a matrix times $\boldsymbol{y}$. Substitute in the value of y_2 that we know, thereby having a (linear) expression for y_* in terms of y_1.
c. You will find that the prediction, y_* linearly dependent on y_1, in a negative direction: So as y_1 gets larger, y_* gets smaller. Explain why. What is the intuition for this result?

6. (*) In an orchard there are two types of apple tree (you don't know which is which). You measure the number of apples for different trees and plot them against the tree heights. What would be the problem(s) with modelling this with standard Gaussian process regression, with a Gaussian likelihood?



7. (**) You have some data you want to fit with a Gaussian process. What would be the problem with using a standard exponentiated quadratic kernel?



8. (***) What makes a valid kernel? The definition is that it must be positive semidefinite. Specifically, a kernel is said to be positive semidefinite if[1],

$$\int k(\boldsymbol{x}_1, \boldsymbol{x}_2) f(\boldsymbol{x}_1) f(\boldsymbol{x}_2) d\boldsymbol{x}_1 d\boldsymbol{x}_2 \geq 0$$

this is sort of the infinite version of the finite version for a matrix, $\boldsymbol{x}^\top K_{xx} \boldsymbol{x} \geq 0 \; \forall \; \boldsymbol{x} \in \mathcal{R}^D$. Where K_{xx} is the covariance matrix between our points in $\boldsymbol{x}$. We'll use this finite version as it's easier to work with. The linear kernel (for one dimensional x) is $k(x_1, x_2) = x_1 x_2$. Show that this is a valid kernel. Hint: Write out the covariance matrix between an arbitrary pair of points, $[x_1, x_2]$ and compute $\boldsymbol{x}^\top K_{xx} \boldsymbol{x}$, expanding out the expression so it is the simple sum of terms with various combinations of x_1 and x_2. Think about if any of the terms can be negative?

[1] I've been a bit loose with the notation here, see p80 of C. E. Rasmussen & C. K. I. Williams, Gaussian Processes for Machine Learning, for more precise notation and further discussion.