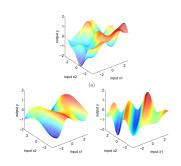
# Introduction to Machine Learning

## **Covariance Functions for GPs**



#### Learning goals

- Covariance functions encode key assumptions about the GP
- Know common covariance functions like squared exponential and Matérn

## COVARIANCE FUNCTION OF A GP

The marginalization property of the Gaussian process implies that for any finite set of input values, the corresponding vector of function values is Gaussian:

$$\textbf{\textit{f}} = \left[ f\left(\textbf{\textit{x}}^{(1)}\right),...,f\left(\textbf{\textit{x}}^{(n)}\right) \right] \sim \mathcal{N}\left(\textbf{\textit{m}},\textbf{\textit{K}}\right),$$

- The covariance matrix K is constructed based on the chosen inputs {x<sup>(1)</sup>, ..., x<sup>(n)</sup>}.
- Entry  $\mathbf{K}_{ij}$  is computed by  $k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$ .
- Technically, for **every** choice of inputs  $\{\mathbf{x}^{(1)}, ..., \mathbf{x}^{(n)}\}$ , K needs to be positive semi-definite in order to be a valid covariance matrix.
- A function k(.,.) satisfying this property is called **positive definite**.

## COVARIANCE FUNCTION OF A GP

 Recall, the purpose of the covariance function is to control to which degree the following is fulfilled:

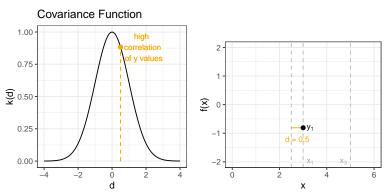
If two points  $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$  are close in  $\mathcal{X}$ -space, their function values  $f(\mathbf{x}^{(i)}), f(\mathbf{x}^{(j)})$  should be close (**correlated**!) in  $\mathcal{Y}$ -space.

• Closeness of two points  $\mathbf{x}^{(i)}$ ,  $\mathbf{x}^{(j)}$  in input space  $\mathcal{X}$  is measured in terms of  $\mathbf{d} = \mathbf{x}^{(i)} - \mathbf{x}^{(j)}$ :

$$k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = k(\mathbf{d})$$

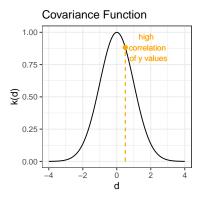
## **COVARIANCE FUNCTION OF A GP: EXAMPLE**

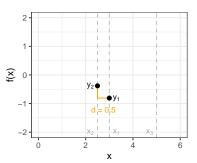
- Let  $f(\mathbf{x})$  be a GP with  $k(\mathbf{x}, \mathbf{x}') = \exp(-\frac{1}{2} ||\mathbf{d}||^2)$  with  $\mathbf{d} = \mathbf{x} \mathbf{x}'$ .
- Consider two points  $\mathbf{x}^{(1)} = 3$  and  $\mathbf{x}^{(2)} = 2.5$ .
- If you want to know how correlated their function values are, compute their correlation!



## **COVARIANCE FUNCTION OF A GP: EXAMPLE**

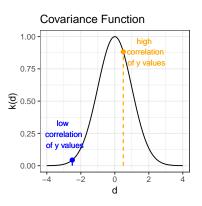
• Assume we observed a value  $y^{(1)} = -0.8$ , the value of  $y^{(2)}$  should be close under the assumption of the above Gaussian process.

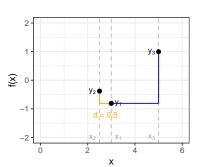




## **COVARIANCE FUNCTION OF A GP: EXAMPLE**

- Let us compare another point  $\mathbf{x}^{(3)}$  to the point  $\mathbf{x}^{(1)}$
- We again compute their correlation
- Their function values are not very much correlated;  $y^{(1)}$  and  $y^{(3)}$  might be far away from each other





## **COVARIANCE FUNCTIONS**

There are three types of commonly used covariance functions:

- k(., .) is called stationary if it is as a function of  $\mathbf{d} = \mathbf{x} \mathbf{x}'$ , we write  $k(\mathbf{d})$ .
  - Stationarity is invariance to translations in the input space:

$$k(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{d})=k(\boldsymbol{0},\boldsymbol{d})$$

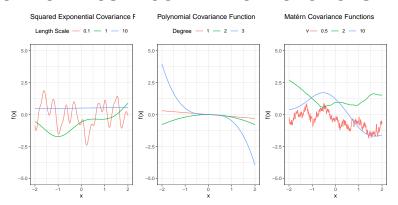
- k(.,.) is called isotropic if it is a function of  $r = ||\mathbf{x} \mathbf{x}'||$ , we write k(r).
  - Isotropy is invariance to rotations of the input space and implies stationarity.
- k(.,.) is a dot product covariance function if k is a function of  $\mathbf{x}^T \mathbf{x}'$

## **COMMONLY USED COVARIANCE FUNCTIONS**

Name	$k(\boldsymbol{x}, \boldsymbol{x}')$ $\sigma_0^2$
constant	$\sigma_0^2$
linear	$\sigma_0^2 + oldsymbol{x}^{ au} oldsymbol{x}'$
polynomial	$(\sigma_0^2 + \boldsymbol{x}^T \boldsymbol{x}')^p$
squared exponential	$\exp(-\frac{\ \mathbf{x}-\mathbf{x}'\ ^2}{2\ell^2})$
Matérn	$ \frac{1}{2^{\nu}\Gamma(\nu)} \left( \frac{\sqrt{2\nu}}{\ell} \ \boldsymbol{x} - \boldsymbol{x}'\  \right)^{\nu} K_{\nu} \left( \frac{\sqrt{2\nu}}{\ell} \ \boldsymbol{x} - \boldsymbol{x}'\  \right) $
exponential	$\exp\left(-\frac{\ \mathbf{x}-\mathbf{x}'\ }{\ell}\right)$

 $K_{\nu}(\cdot)$  is the modified Bessel function of the second kind.

## COMMONLY USED COVARIANCE FUNCTIONS



- Random functions drawn from Gaussian processes with a Squared Exponential Kernel (left), Polynomial Kernel (middle), and a Matérn Kernel (right,  $\ell=1$ ).
- The length-scale hyperparameter determines the "wiggliness" of the function.
- ullet For Matérn, the u parameter determines how differentiable the process is.

## SQUARED EXPONENTIAL COVARIANCE FUNCTION

The squared exponential function is one of the most commonly used covariance functions.

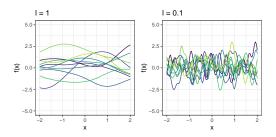
$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\ell^2}\right).$$

#### Properties:

- It depends merely on the distance  $r = \|\mathbf{x} \mathbf{x}'\| \to \text{isotropic}$  and stationary.
- Infinitely differentiable → sometimes deemed unrealistic for modeling most of the physical processes.

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2\ell^2} \|\mathbf{x} - \mathbf{x}'\|^2\right)$$

 $\ell$  is called **characteristic length-scale**. Loosely speaking, the characteristic length-scale describes how far you need to move in input space for the function values to become uncorrelated. Higher  $\ell$  induces smoother functions, lower  $\ell$  induces more wiggly functions.



For  $p \ge 2$  dimensions, the squared exponential can be parameterized:

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2} \left(\mathbf{x} - \mathbf{x}'\right)^{\top} \mathbf{M} \left(\mathbf{x} - \mathbf{x}'\right)\right)$$

Possible choices for the matrix **M** include

$$extbf{\emph{M}}_1 = \ell^{-2} extbf{\emph{I}} \qquad extbf{\emph{M}}_2 = \text{diag}(\ell)^{-2} \qquad extbf{\emph{M}}_3 = \Gamma \Gamma^\top + \text{diag}(\ell)^{-2}$$

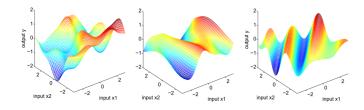
where  $\ell$  is a p-vector of positive values and  $\Gamma$  is a  $p \times k$  matrix.

The 2nd (and most important) case can also be written as

$$k(\mathbf{d}) = \exp\left(-\frac{1}{2}\sum_{i=1}^{p} \frac{d_j^2}{l_j^2}\right)$$

What is the benefit of having an individual hyperparameter  $\ell_i$  for each dimension?

- The  $\ell_1, \ldots, \ell_p$  hyperparameters play the role of **characteristic** length-scales.
- Loosely speaking,  $\ell_i$  describes how far you need to move along axis i in input space for the function values to be uncorrelated.
- Such a covariance function implements **automatic relevance determination** (ARD), since the inverse of the length-scale  $\ell_i$  determines the relevancy of input feature i to the regression.
- If  $\ell_i$  is very large, the covariance will become almost independent of that input, effectively removing it from inference.
- If the features are on different scales, the data can be automatically **rescaled** by estimating  $\ell_1, \ldots, \ell_D$



For the first plot, we have chosen  $\mathbf{M} = \mathbf{I}$ : the function varies the same in all directions. The second plot is for  $\mathbf{M} = \operatorname{diag}(\ell)^{-2}$  and  $\ell = (1,3)$ : The function varies less rapidly as a function of  $x_2$  than  $x_1$  as the length-scale for  $x_1$  is less. In the third plot  $\mathbf{M} = \Gamma\Gamma^T + \operatorname{diag}(\ell)^{-2}$  for  $\Gamma = (1,-1)^T$  and  $\ell = (6,6)^T$ . Here  $\Gamma$  gives the direction of the most rapid variation. (Image from Rasmussen & Williams, 2006)