

Gaussian Processes

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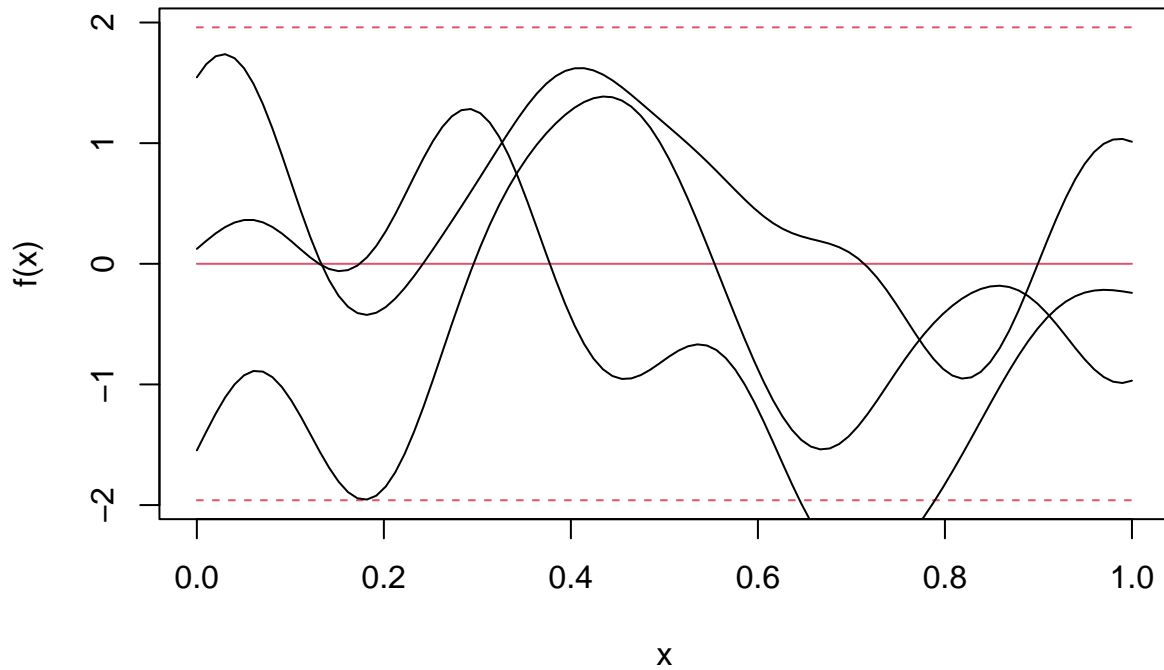
A Gaussian process (GP) is stochastic process (a distribution over functions) such that for any finite set of input values the function values have a multivariate Gaussian distribution, e.g. for $\mathbf{x} \in \mathbb{R}^d$,

$$f(\mathbf{x}) \sim N(\mu(\mathbf{x}) = \mathbf{0}, \Sigma = K(\mathbf{x}, \mathbf{x})),$$
$$K(\mathbf{x}, \mathbf{x}')_{i,j} = \sigma_f^2 \exp\left(\frac{(x_i - x'_j)^2}{2l^2}\right).$$

```
# Functions to sample from and predict values of a Gaussian process.
source("GP_funcs.R")

# Plot samples from a GP
plot_GP_samps(
  l = 0.1, # Length scale
  sigma_f = 1, # Function standard deviation
  n_samps = 3 # Number of samples
)
```

Samples from a Gaussian process



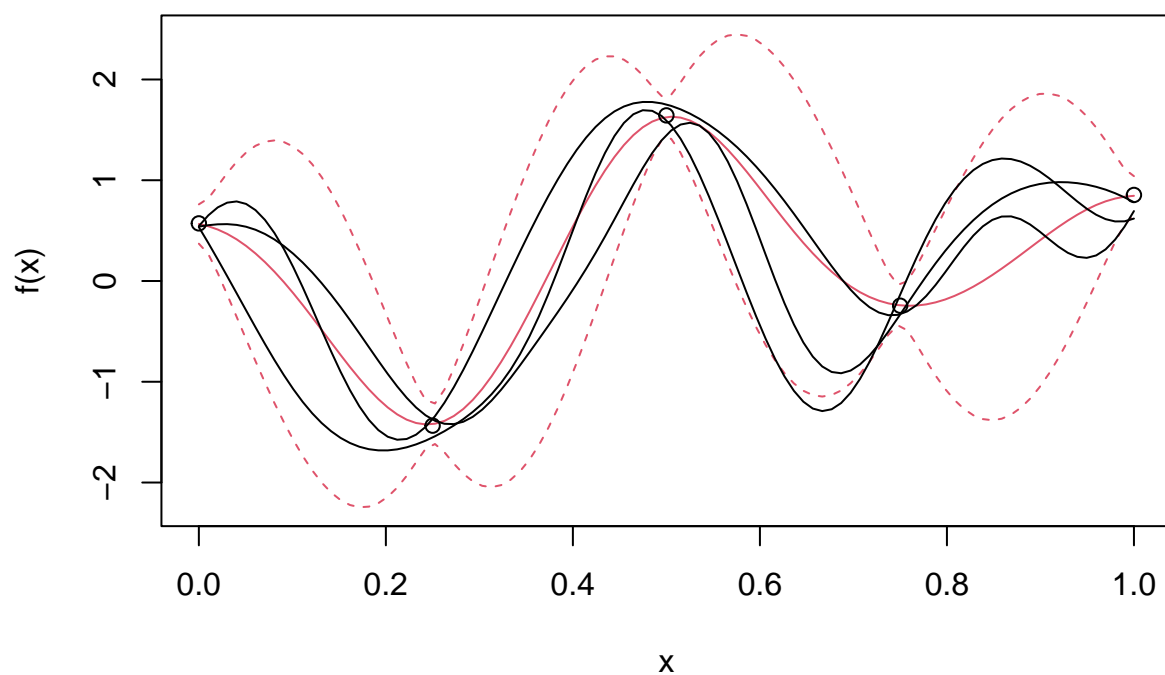
Gaussian process regression

A GP can be used as a functional prior. The posterior is then the conditional distribution of functions given observations at a set of input values. If the observations are assumed to include some Gaussian noise this is another GP, e.g.

$$\begin{aligned} \mathbf{y} &= f(\mathbf{x}) + \epsilon, \\ f(\mathbf{x}) &\sim N(\mu(\mathbf{x}) = \mathbf{0}, \Sigma = K(\mathbf{x}, \mathbf{x})), \\ \epsilon &\sim N(0, \sigma_n^2 I_d), \\ \implies f(\mathbf{x}') | \mathbf{y}(\mathbf{x}) &\sim N(\mu(\mathbf{x}'), \Sigma), \\ \mu(\mathbf{x}') &= K(\mathbf{x}', \mathbf{x}) [K(\mathbf{x}, \mathbf{x}) + \sigma_n^2 I_d]^{-1} \mathbf{y}(\mathbf{x}), \\ \Sigma &= K(\mathbf{x}', \mathbf{x}') - K(\mathbf{x}', \mathbf{x}) [K(\mathbf{x}, \mathbf{x}) + \sigma_n^2 I_d]^{-1} K(\mathbf{x}, \mathbf{x}'). \end{aligned}$$

```
plot_GP_regression(  
    n_obs = 5, # Number of points to observe  
    l = 0.1, # Length scale  
    sigma_f = 1, # Function standard deviation  
    sigma_n = 0.1 # Noise standard deviation  
)
```

Gaussian process regression

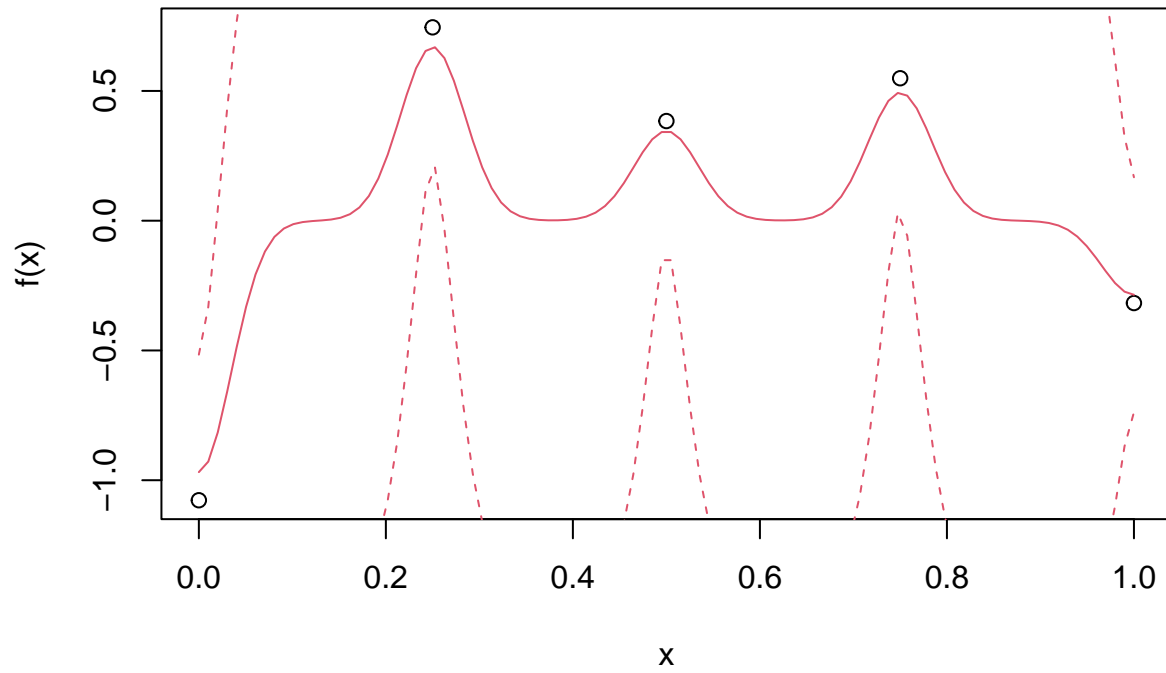


There are various methods of model selection and hyper-parameter tuning.

```
plot_GP_fit(  
  n_obs = 5, # Number of points to observe  
  l = 0.1, # Length scale  
  sigma_f = 1, # Function standard deviation  
  sigma_n = 0.1 # Noise standard deviation  
)
```

```
## [1] "Optimiser converged"
```

Gaussian process fit



These notes were taken mainly from C. E. Rasmussen & C. K. I. Williams, Gaussian Processes for Machine Learning, the MIT Press, 2006.