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 $\mathbf{x} \in \mathbb{R}^d$,

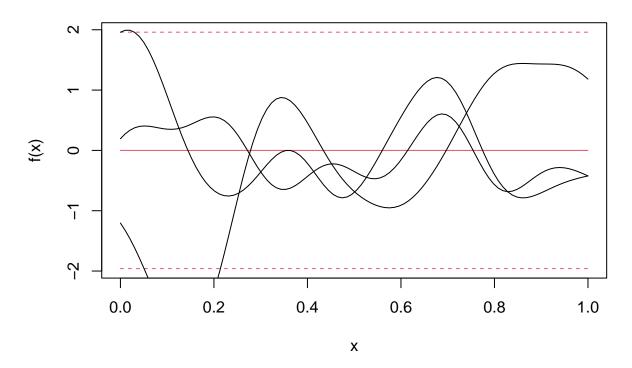
$$f(\mathbf{x}) \sim N(\mu(\mathbf{x}) = \mathbf{0}, \Sigma = K(\mathbf{x}, \mathbf{x})),$$

 $K(\mathbf{x}, \mathbf{x}')_{i,j} = \sigma_f^2 \exp\left(\frac{(x_i - x_j')^2}{2l^2}\right).$

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

# Plot samples from a GP
plot_GP_samps(
    1 = 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.

$$\mathbf{y} = f(\mathbf{x}) + \epsilon,$$

$$f(\mathbf{x}) \sim N(\mu(\mathbf{x}) = \mathbf{0}, \Sigma = K(\mathbf{x}, \mathbf{x})),$$

$$\epsilon \sim N(0, \sigma_n^2 I_d),$$

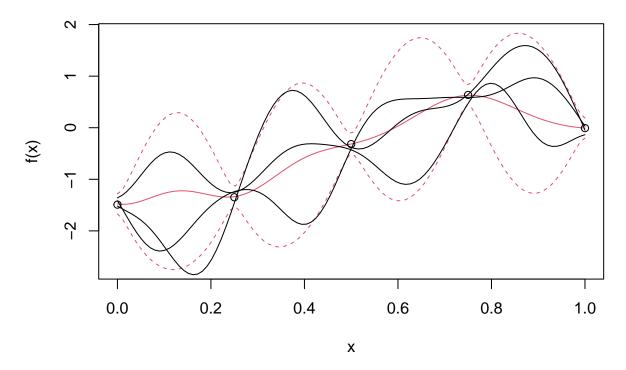
$$\implies f(\mathbf{x}') | \mathbf{y}(\mathbf{x}) \sim N(\mu(\mathbf{x}'), \Sigma),$$

$$\mu(\mathbf{x}') = K(\mathbf{x}', \mathbf{x}) [K(\mathbf{x}, \mathbf{x}) + \sigma_n^2 I_d]^{-1} \mathbf{y}(\mathbf{x}),$$

$$\Sigma = K(\mathbf{x}', \mathbf{x}') - K(\mathbf{x}', \mathbf{x}) [K(\mathbf{x}, \mathbf{x}) + \sigma_n^2 I_d]^{-1} K(\mathbf{x}, \mathbf{x}').$$

```
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.

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