Vector-valued Gaussian Processes

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I. Overview of Gaussian Processes

Gaussian processes generalize the multivariate Gaussian distribution and can be used to describe a probability distribution over families of functions.

i. Multivariate Gaussian Distribution

The multivariate normal distribution is used to model *random vectors* (vectors of jointly distributed random variables).

$$\begin{aligned} \boldsymbol{x} \in \mathbb{R}^N &\sim \mathcal{N}_N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \\ \boldsymbol{\mu} \in \mathbb{R}^N &= (\mu_1, \mu_2, ..., \mu_N)^\top = (\mathbb{E}(x_1), \mathbb{E}(x_2), ..., \mathbb{E}(x_N))^\top \\ \boldsymbol{\Sigma} \in \mathbb{R}^{N\times N} &= \mathbb{E}\Big((\boldsymbol{x}-\mu)(\boldsymbol{x}-\mu)^\top\Big) = \big[\mathrm{cov}(x_i, x_j)\big]_{i,j}^N \\ x_i &\sim \mathcal{N}(\mu_i, \boldsymbol{\Sigma}_{ii}) \end{aligned} \tag{1}$$

ii. Gaussian Processes (GPs)

- *Gaussian process* (GP): an uncountably infinite collection of random variables; any finite sample is a draw from a MV Gaussian distribution.
- GPs are fully specified by a *mean function* m and *covariance (kernel) function* k.
- The kernel function must produce a positive semi-definite matrix when evaluated on a set of input points (or vectors).

We focus on the *squared exponential kernel* $k : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$, defined as:

$$k(x, x') = \alpha^2 \exp\left(-\frac{1}{2\rho^2}\,\|x - x'\|^2\right). \tag{2}$$

- $\|\cdot\|$ is the Euclidean Norm: $\|\boldsymbol{x}\| = \sqrt{x_1 + x_2 + \cdots + x_N}$
- α and ρ are *hyperparameters* (chosen, or estimated from data)

II. Gaussian Process Regression – Univariate $\mathbf{y}$

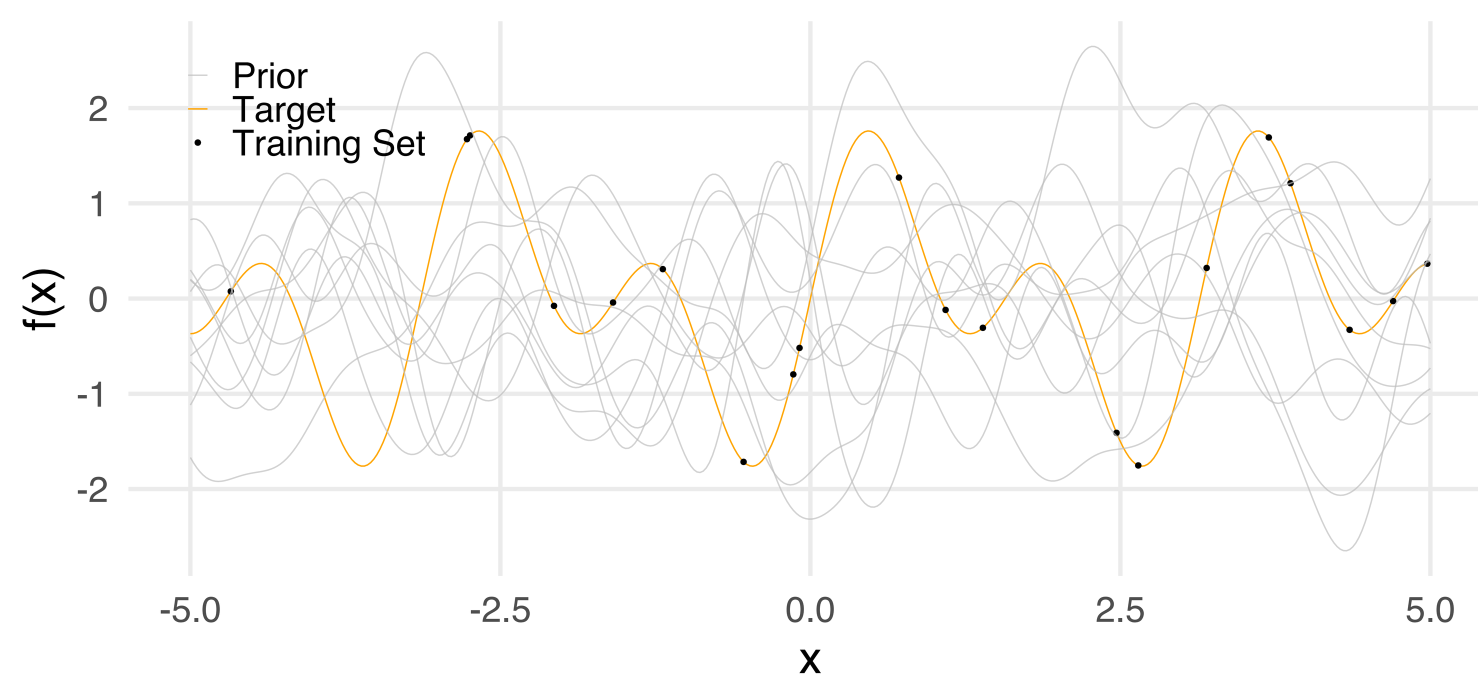
In practice, Gaussian Processes are often brought to bear on *regression problems*, in which an analyst has collected a dataset $S = (\boldsymbol{x}, \boldsymbol{y}) = \{(x_i, y_i) : x_i \in \mathbb{R}^p, y_i \in \mathbb{R}^d, i \in 1, 2, ..., N\}$ with the goal of learning the relationship f between $\boldsymbol{x}$ and $\boldsymbol{y}$.

Let $f(x) = \sin(2x) + \sin(4x)$ be an unknown function that an analyst is attempting to model using sampled data. Let $N = 20$ and $M = 400 - N$. We wish to use our sample S to predict the values $\boldsymbol{y}_* = f(\boldsymbol{x}_*)$ for test data $\boldsymbol{x}_* \in \mathbb{R}^M$.

We can draw samples from the prior distribution:

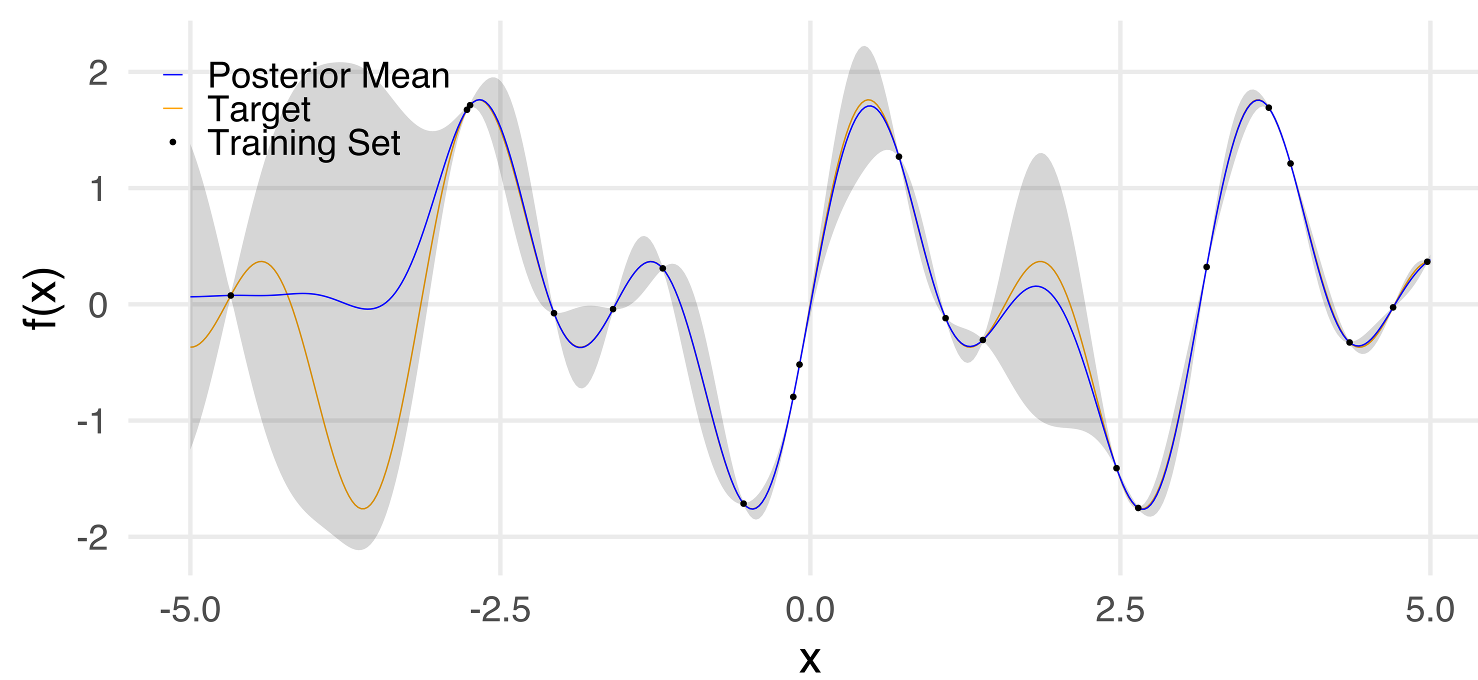
$$\begin{aligned} f &\sim \mathcal{GP}(\boldsymbol{0}, k) \\ \boldsymbol{y}_* &\sim \mathcal{N}_M(\boldsymbol{0}, k(\boldsymbol{x}_*, \boldsymbol{x}_*)) \\ k(\boldsymbol{x}_*, \boldsymbol{x}_*) \in \mathbb{R}^{M\times M} &= \big[k(\boldsymbol{x}_{*i}, \boldsymbol{x}_{*j})\big]_{i,j}^M. \end{aligned} \tag{3}$$

- Draws from the prior distribution (shown in grey) don't necessarily agree with our data points.
- Kernel choice determines properties of f (e.g., smoothness)



Our prior model for f and our observed data S can be combined to form a *posterior* distribution:

$$\begin{aligned} \boldsymbol{y}_* \mid \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{x}_* &\sim \mathcal{N}_M\big(\hat{\mu}, \hat{\Sigma}\big) \\ \hat{\mu} \in \mathbb{R}^M &= k(\boldsymbol{x}_*, \boldsymbol{x})(k(\boldsymbol{x}, \boldsymbol{x}))^{-1}\boldsymbol{y} \\ \hat{\Sigma} \in \mathbb{R}^{M\times M} &= k(\boldsymbol{x}_*, \boldsymbol{x}_*) - k(\boldsymbol{x}_*, \boldsymbol{x})(k(\boldsymbol{x}, \boldsymbol{x}))^{-1}k(\boldsymbol{x}_*, \boldsymbol{x})^\top \\ k(\boldsymbol{x}, \boldsymbol{x}) \in \mathbb{R}^{N\times N} &= \big[k(x_i, x_j)\big]_{i,j}^N \\ k(\boldsymbol{x}_*, \boldsymbol{x}) \in \mathbb{R}^{M\times N} &= \big[k(x_{*i}, x_j)\big]_{i,j}^{M,N}. \end{aligned} \tag{4}$$



III. Multioutput GPR – Vector-valued $\mathbf{y}$

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