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Introduction to Gaussian Processes

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Outline

Gaussian Processes

Gaussian processes, the definition...

- An equivalent way is considering the inference directly in **function-space**. We use a **Gaussian process** (GP) to describe a distribution over functions.

Definition

A **Gaussian process** is a collection of random variables, any finite number of which have a joint Gaussian distribution.

- A Gaussian process is completely specified by its **mean function** and **covariance function** of a real process $f(x)$, defined as

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})], \quad k\left(\mathbf{x}, \mathbf{x}'\right) = \mathbb{E}\left[(f(\mathbf{x}) - m(\mathbf{x}))\left(f\left(\mathbf{x}'\right) - m\left(\mathbf{x}'\right)\right)\right]$$

- Finally we obtain

$$f(\mathbf{x}) \sim \mathcal{GP}\left(m(\mathbf{x}), k\left(\mathbf{x}, \mathbf{x}'\right)\right)$$

Definition

A function $k : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ is a **Mercer kernel**, if for any finite collection $X = [x_1, \ldots, x_N]$, the matrix $k_{XX} \in \mathbb{R}^{N \times N}$ with elements $k_{XX,(i,j)} = k\left(x_i, x_j\right)$ is positive semidefinite.

Lemma

Any kernel that can be written as

$$(T_k f)(\mathbf{x}) = \int_{\mathbb{X}} k\left(\mathbf{x}, \mathbf{x}'\right) f\left(\mathbf{x}'\right) d\mu\left(\mathbf{x}'\right)$$

is a Mercer kernel.

Definition

Let $\mu : \mathbb{X} \to \mathbb{R}$ be any function, $k : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ be a Mercer kernel. A **Gaussian process** $p(f) = \mathcal{GP}(f; \mu, k)$ is a probability over the function $f : \mathbb{X} \to \mathbb{R}$, such that every finite restriction to function values $f_X := \left[f_{x_1}, \ldots, f_{x_N}\right]$ is a Gaussian distribution $p\left(f_X\right) = \mathcal{N}\left(f_X; \mu_X, k_{XX}\right)$.

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