AutoML: Gaussian Processes

Covariance Functions for GPs

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Covariance function of a GP I

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

$$\boldsymbol{f} = \left[f\left(\mathbf{x}^{(1)}\right), ; f\left(\mathbf{x}^{(n)}\right) \right] \sim \mathcal{N}\left(\boldsymbol{m}, \boldsymbol{K}\right),$$

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