

Covariance functions for libgp

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1 Gaussian Process

We are given $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$ and $\mathbf{z} = (z_1, \dots, z_n)$ with $\mathbf{x}_i \in \mathbb{R}^d$ and $z_i \in \mathbb{R}$. The joint distribution of \mathbf{z} is given by,

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z} | 0, \mathbf{C}_n) \quad (1)$$

where \mathbf{C}_n is a matrix with elements $(\mathbf{C}_n)_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j)$ and $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ is the covariance function of the Gaussian process. It should hold that $k(\mathbf{x}, \mathbf{y}) = k(\mathbf{y}, \mathbf{x})$

Given a new point $(\mathbf{x}_{n+1}, z_{n+1})$, the conditional distribution of z_{n+1} on \mathbf{X} and \mathbf{z} is given by,

$$p(z_{n+1} | \mathbf{X}, \mathbf{z}, \mathbf{x}_{n+1}) = \mathcal{N}\left(z_{n+1} | \mu(\mathbf{x}_{n+1}), \sigma^2(\mathbf{x}_{n+1})\right), \quad (2)$$

where

$$\mu(\mathbf{x}_{n+1}) = \mathbf{k}^\top \mathbf{C}_n^{-1} \mathbf{y}, \quad (3)$$

and

$$\sigma^2(\mathbf{x}_{n+1}) = c - \mathbf{k}^\top \mathbf{C}_n^{-1} \mathbf{k}. \quad (4)$$

Here, $(\mathbf{k})_i = k(\mathbf{x}_i, \mathbf{x}_{n+1})$, $i = 1, \dots, n$ and $c = k(\mathbf{x}_{n+1}, \mathbf{x}_{n+1})$ and satisfy,

$$\mathbf{C}_{n+1} = \begin{pmatrix} \mathbf{C}_n & \mathbf{k}^\top \\ \mathbf{k} & c \end{pmatrix}. \quad (5)$$

1.1 Derivatives of the Gaussian process w.r.t. state variables

We are interested in calculating derivatives of $\mu(\mathbf{x})$ w.r.t. the state variable \mathbf{x} . Thus

$$\frac{d\mu(\mathbf{x})}{d\mathbf{x}} = \frac{d\mathbf{k}^\top}{d\mathbf{x}} \mathbf{C}_n^{-1} \mathbf{y}, \quad (6)$$

where the matrix $\frac{d\mathbf{k}^\top}{d\mathbf{x}}$ has elements,

$$\left(\frac{d\mathbf{k}^\top}{d\mathbf{x}}\right)_{i,j} = \frac{dk(\mathbf{x}, \mathbf{x}_i)}{dx_j}, \quad (7)$$

for $i = 1, \dots, n$ and $j = 1, \dots, d$.

2 Covariance Functions

2.1 Linear Covariance

name	cov_linear_one
formula	$k(\mathbf{x}, \mathbf{y}) = \vartheta^2(1 + \mathbf{x} \cdot \mathbf{y})$
parameters	ϑ
log-parameters	$\varphi = -\log \vartheta$
$\frac{dk}{d\varphi}(\vartheta)$	$-2\vartheta^2(1 + \mathbf{x} \cdot \mathbf{y})$
$\frac{dk(\mathbf{x}, \mathbf{x}_i)}{dx_j}$	$x_{i,j}$

2.2 Linear Covariance with Automatic Relevance Determination

name	cov_linear_ard
formula	$k(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^d \frac{x_i y_i}{\lambda_i}$
parameters	$\boldsymbol{\vartheta} = (\lambda_1, \dots, \lambda_d)$
log-parameters	$\varphi = \log \boldsymbol{\vartheta}$
$\frac{dk}{d\varphi_i}(\boldsymbol{\vartheta})$	$-2 \frac{x_i y_i}{\lambda_i}$
$\frac{dk(\mathbf{x}, \mathbf{x}_i)}{dx_j}$	$\frac{x_{i,j}}{\lambda_j}$

2.3 Squared exponential covariance function with isotropic distance measure

name	cov_se_iso
formula	$k(\mathbf{x}, \mathbf{y}) = \alpha^2 \exp\left(-\frac{1}{2\lambda^2} \ \mathbf{x} - \mathbf{y}\ ^2\right),$
parameters	$\boldsymbol{\vartheta} = (\lambda, \alpha)$
log-parameters	$\varphi = \log \boldsymbol{\vartheta}$
$\frac{dk}{d\varphi_1}(\boldsymbol{\vartheta})$	$\frac{1}{\lambda^2} \ \mathbf{x} - \mathbf{y}\ ^2 k(\mathbf{x}, \mathbf{y})$
$\frac{dk}{d\varphi_2}(\boldsymbol{\vartheta})$	$2k(\mathbf{x}, \mathbf{y})$
$\frac{dk(\mathbf{x}, \mathbf{x}_i)}{dx_j}$	$\lambda^{-2} (x_{i,j} - x_j) k(\mathbf{x}, \mathbf{x}_i)$

2.4 Squared exponential covariance function with Automatic Relevance Determination

name	cov_se_ard
formula	$k(\mathbf{x}, \mathbf{y}) = \alpha^2 \exp \left(-\frac{1}{2} \sum_{i=1}^d \frac{(x_i - y_i)^2}{\lambda_i^2} \right),$
parameters	$\boldsymbol{\vartheta} = (\lambda_1, \dots, \lambda_d, \alpha)$
log-parameters	$\boldsymbol{\varphi} = \log \boldsymbol{\vartheta}$
$\frac{dk}{d\varphi_i}(\boldsymbol{\vartheta})$	$\frac{1}{\lambda_i^2} \ \mathbf{x} - \mathbf{y}\ ^2 k(\mathbf{x}, \mathbf{y}), \quad i = 1, \dots, d$
$\frac{dk}{d\varphi_{d+1}}(\boldsymbol{\vartheta})$	$2k(\mathbf{x}, \mathbf{y})$

2.5 Independent covariance function (white noise)

name	cov_noise
formula	$k(\mathbf{x}, \mathbf{y}) = \alpha^2 \delta(\ \mathbf{x} - \mathbf{y}\)$
parameters	$\vartheta = \alpha$
log-parameters	$\varphi = \log \vartheta$
$\frac{dk}{d\varphi}(\vartheta)$	$2\alpha^2 \delta(\ \mathbf{x} - \mathbf{y}\)$

2.6 Periodic covariance function

name	cov_periodic
formula	$k(\mathbf{x}, \mathbf{y}) = \sigma_f^2 \exp \left(-2\lambda^{-2} \sin^2 \frac{\pi \ \mathbf{x} - \mathbf{y}\ }{T} \right)$
parameters	$\boldsymbol{\vartheta} = (\alpha, \sigma_f, T)$
log-parameters	$\boldsymbol{\varphi} = \log \boldsymbol{\vartheta}$
$\frac{dk}{d\varphi_1}(\boldsymbol{\vartheta})$	$4 k(\mathbf{x}, \mathbf{y}) \lambda^{-2} \sin^2 \frac{\pi \ \mathbf{x} - \mathbf{y}\ }{T}$
$\frac{dk}{d\varphi_2}(\boldsymbol{\vartheta})$	$2 k(\mathbf{x}, \mathbf{y})$
$\frac{dk}{d\varphi_3}(\boldsymbol{\vartheta})$	$4 k(\mathbf{x}, \mathbf{y}) \lambda^{-1} \beta \frac{\sin \beta}{\lambda} \cos \beta, \quad \beta = \frac{\pi \ \mathbf{x} - \mathbf{y}\ }{T}$