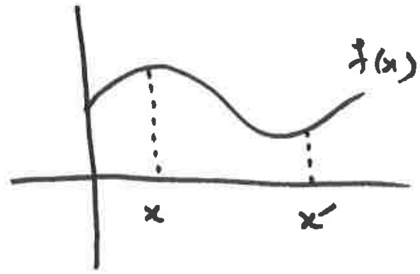
Tutorial on Gaussian Processes

Prior

$$u(x) \sim \mathcal{GP}(0, k(x, x'; \theta))$$

$$\begin{bmatrix} u(x) \\ u(x') \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} k(x, x; \theta) & k(x, x'; \theta) \\ & k(x', x'; \theta) \end{bmatrix}\right)$$

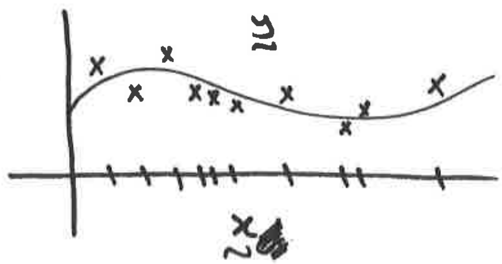


$$k(x, x'; \theta) = \sigma_u^2 \exp\left(-\frac{1}{2} \sum_{d=1}^{D} \frac{(x_d - x_d')^2}{\theta_d^2}\right)$$

Here, $\theta = (\sigma_u^2, \{\theta_d^2\}_{d=1}^{D})$.

Training

$\{\underset{\sim}{x}, \underset{\sim}{y}\}$
$N \times D \quad N \times 1$



$$\underset{\sim}{y} \sim \mathcal{N}(\underset{\sim}{0}, \underbrace{k(\underset{\sim}{x}, \underset{\sim}{x}; \theta) + \sigma^2 I}_{K})$$

$$\underset{\uparrow}{NLML(\theta)} = \frac{1}{2} \underset{\sim}{y}^T K^{-1} \underset{\sim}{y} + \frac{1}{2} \log|K| + \frac{N}{2} \log(2\pi)$$

negative log marginal likelihood

K is $N \times N$ and full. Thus, $O(N^3)$.

Prediction / Posterior

$$\begin{bmatrix} f(x^*) \\ \underset{\sim}{y} \end{bmatrix} \sim \mathcal{N}\left(\underset{\sim}{0}, \begin{bmatrix} k(x^*, x^*; \theta) & k(x^*, \underset{\sim}{x}, \underset{\sim}{\theta}) \\ & \underbrace{k(\underset{\sim}{x}, \underset{\sim}{x}; \theta) + \sigma^2 I}_{K} \end{bmatrix}\right)$$

$$f(x^*) \mid \underset{\sim}{y} \sim \mathcal{N}(\underbrace{k(x^*, \underset{\sim}{x}) \mathbf{K}^{-1} \underset{\sim}{y}}_{\mu(x^*)}, \underbrace{k(x^*, x^*) - k(x^*, \underset{\sim}{x}) \mathbf{K}^{-1} k(\underset{\sim}{x}, x^*)}_{\Sigma(x^*, x^*)})$$ (2)

Tutorial on Multifidelity

Prior

$u_1(x) \sim \mathcal{GP}(0, k_1(x, x'; \theta_1))$

$u_2(x) \sim \mathcal{GP}(0, k_2(x, x'; \theta_2))$ independent

$$\begin{aligned} f_L(x) &= u_1(x) \\ f_H(x) &= \rho u_1(x) + u_2(x) \end{aligned} \Rightarrow \begin{cases} k_{LL}(x, x') = k_1(x, x'; \theta_1) \\ k_{LH}(x, x') = \rho k_1(x, x'; \theta_1) \\ k_{HH}(x, x') = \rho^2 k_1(x, x'; \theta_1) + k_2(x, x'; \theta_2) \end{cases}$$

$$\begin{bmatrix} f_L(x) \\ f_H(x) \end{bmatrix} \sim \mathcal{GP}\left(0, \begin{bmatrix} k_{LL}(x, x') & k_{LH}(x, x') \\ & k_{HH}(x, x') \end{bmatrix}\right)$$

Training

$\{\underset{\sim}{x}_L, \underset{\sim}{y}_L\}$, $\{\underset{\sim}{x}_H, \underset{\sim}{y}_H\}$, $N_L >> N_H$

$N_L \times D$ $\quad N_L \times 1$ $\quad N_H \times D$ $\quad N_H \times 1$

$$\underbrace{\begin{bmatrix} \underset{\sim}{y}_L \\ \underset{\sim}{y}_H \end{bmatrix}}_{\underset{\sim}{y}} \sim \mathcal{N}\left(0, \underbrace{\begin{bmatrix} k_{LL}(\underset{\sim}{x}_L, \underset{\sim}{x}_L) + \sigma_L^2 I & k_{LH}(\underset{\sim}{x}_L, \underset{\sim}{x}_H) \\ & k_{HH}(\underset{\sim}{x}_H, \underset{\sim}{x}_H) + \sigma_H^2 I \end{bmatrix}}_{\mathbf{K}}\right)$$

$$\mathcal{NML}(\theta_1, \theta_2, \rho) = \frac{1}{2} \underset{\sim}{y}^T \mathbf{K}^{-1} \underset{\sim}{y} + \frac{1}{2} \log|\mathbf{K}| + \frac{N_L + N_H}{2} \log(2\pi)$$

Prediction

$f_H(x^*) \mid \underset{\sim}{y} \sim \ldots$

$$f_H(x^*) \mid \underset{\sim}{y} \sim \mathcal{N}\Big(\underbrace{[K_{HL}(x^*, \underset{\sim}{x}_L) \quad K_{HH}(x^*, \underset{\sim}{x}_H)]}_{K(x^*, \underset{\sim}{x})} \mathbf{K}^{-1} \underset{\sim}{y},$$

$$K_{HH}(x^*, x^*) - K(x^*, \underset{\sim}{x}) \mathbf{K}^{-1} K(\underset{\sim}{x}, x^*) \Big)$$

Tutorial on Gaussian Processes for Differential Equations

$\mathcal{L}_x^{\phi} u(x) = f(x)$ for example $\frac{d}{dx} u(x) + \alpha u(x) + \beta \int_0^x u(\xi) d\xi = f(x)$

Prior

$$u(x) \sim \mathcal{GP}(0, K_{uu}(x, x'; \theta))$$

$$\Rightarrow \begin{bmatrix} u(x) \\ f(x) \end{bmatrix} \sim \mathcal{GP}\left(0, \begin{bmatrix} K_{uu}(x, x'; \theta) & K_{uf}(x, x'; \theta, \phi) \\ & K_{ff}(x, x'; \theta, \phi) \end{bmatrix}\right)$$

$$K_{uf}(x, x'; \theta, \phi) = \mathcal{L}_{x'}^{\phi} K_{uu}(x, x'; \theta)$$

$$K_{ff}(x, x'; \theta, \phi) = \mathcal{L}_x^{\phi} \mathcal{L}_{x'}^{\phi} K_{uu}(x, x'; \theta)$$

Training

$\{\underset{\sim}{x}_u, \underset{\sim}{y}_u\}$
$N_u \times D \quad N_u \times 1$

$\{\underset{\sim}{x}_f, \underset{\sim}{y}_f\}$
$N_f \times D \quad N_f \times 1$

$$\underbrace{\begin{bmatrix} \underset{\sim}{y}_u \\ \underset{\sim}{y}_f \end{bmatrix}}_{\underset{\sim}{y}} \sim \mathcal{N}\left(0, \underbrace{\begin{bmatrix} K_{uu}(\underset{\sim}{x}_u, \underset{\sim}{x}_u) + \sigma_u^2 I & K_{uf}(\underset{\sim}{x}_u, \underset{\sim}{x}_f) \\ & K_{ff}(\underset{\sim}{x}_f, \underset{\sim}{x}_f) + \sigma_f^2 I \end{bmatrix}}_{\mathbf{K}}\right)$$

$$NLML(\theta, \phi) = \frac{1}{2} \underset{\sim}{y}^T \mathbf{K}^{-1} \underset{\sim}{y} + \frac{1}{2} \log |\mathbf{K}| + \frac{N_u + N_f}{2} \log(2\pi)$$

Prediction

$$u(x^*) \mid \begin{bmatrix} \underset{\sim}{y}_u \\ \underset{\sim}{y}_f \end{bmatrix} \sim \mathcal{N}\Big(\overbrace{[K_{uu}(x^*, \underset{\sim}{x}_u) \quad K_{uf}(x^*, \underset{\sim}{x}_f)]}^{K(x^*, \underset{\sim}{x})} \mathbf{K}^{-1} \underset{\sim}{y},$$

$$K_{uu}(x^*, x^*) - K(x^*, \underset{\sim}{x}) \mathbf{K}^{-1} K(\underset{\sim}{x}, x^*) \Big)$$