高斯过程求解偏微分方程

① 求解偏微分方程

简单想法 $u(x) = \sum_{i=1}^{n} \alpha_i k(x, x_i)$

$$A\alpha = b \qquad \alpha = A^{-1} b$$

考虑带导数的基底（平稳的核函数）

$$\nabla_x k(x, x_i) = \left[\lim_{\varepsilon \to 0} \frac{k(x+\varepsilon e_j, x_i) - k(x, x_i)}{\varepsilon} \right]_j$$

定义 $\dfrac{k(x+\varepsilon e_j, x_i) - k(x, x_i)}{\varepsilon} = f_\varepsilon$

$$\langle f_\varepsilon - f_{\varepsilon'}, f_\varepsilon - f_{\varepsilon'} \rangle$$

$$= \left\| \frac{k(x+\varepsilon e_j, x_i) - k(x, x_i)}{\varepsilon} - \frac{k(x+\varepsilon' e_j, x_i) - k(x, x_i)}{\varepsilon'} \right\|_{\mathcal{H}}^2$$

$$= \frac{1}{\varepsilon^2} 2k(x_i, x_i) - \frac{k(x_i+\varepsilon e_j, x_i)}{\varepsilon^2} - \frac{k(x_i-\varepsilon e_j, x_i)}{\varepsilon^2}$$

$$\frac{1}{\varepsilon'^2} 2k(x_i, x_i) - \frac{k(x_i+\varepsilon' e_j, x_i)}{\varepsilon'^2} - \frac{k(x_i-\varepsilon' e_j, x_i)}{\varepsilon'^2}$$

$$\frac{1}{\varepsilon\varepsilon'} \Big(k(x_i+\varepsilon e_j, x_i) + k(x_i-\varepsilon e_j, x_i) - k(x_i+(\varepsilon-\varepsilon')e_j, x_i) - k(x_i, x_i) \Big)$$

$= O(\varepsilon') + O(\varepsilon)$ 当 $k \in C^2$ Taylor expansion

$$\Rightarrow \quad \nabla_x k(x, x_i) \in \mathcal{H}_k$$

当 k 足够光滑 $\nabla_x k(x, x_i)$ $\Delta_{xx} k(x, x_i) \cdots\cdots$

都属于 H_k

$$\langle \nabla_x k(x,x_i), f(x)\rangle_j$$

$$= \lim_{\varepsilon\to 0} \left\langle \frac{k(x+\varepsilon e_j, x_i) - k(x, x_i)}{\varepsilon}, f(x) \right\rangle_j$$

$$= \lim_{\varepsilon\to 0} \frac{f(x_i - \varepsilon e_j) - f(x_i)}{\varepsilon}$$

$$= (-1)\ [\nabla_x f](x_i)$$

Laplace 方程求解

$$-\Delta u = f \qquad u = \bar{u} \text{ on } \partial\Omega$$

空间 $S = \text{span}\{ k(x, x_i)\ x_i \in X^{bd},\ \Delta k(x, x_i)\ x_i \in X^{int} \}$

$$u = u_s + u_\perp$$

$$u(x_i) = \langle k(x,x_i), u(x)\rangle_H = \langle k(x, x_i), u_s(x)\rangle_H = u_s(x_i)$$

$$\Delta u(x_i) = \langle \Delta k(x,x_i), u(x)\rangle_H = \langle \Delta k(x,x_i), u_s(x)\rangle_H = \Delta u_s(x_i)$$

$$u = \sum \alpha_i k(x,x_i) + \sum \alpha_i'' \Delta_x k(x, x_i)$$

$$\|u\|_{H_k}^2 = \left\| \sum \alpha_i k(x,x_i) + \sum \alpha_i'' \Delta_x k(x,x_i) \right\|_{H_k}^2$$

$$\langle k(x,x_i), k(x,x_j)\rangle_H = k(x_i, x_j)$$

$$\langle k(x,x_i)\ \Delta_x k(x,x_j)\rangle_H = \Delta_x k(x_i\ x_j)$$

$$\langle \Delta_x k(x,x_i), \Delta_x k(x,x_j) \rangle_{\mathcal{H}} = \Delta_x \Delta_y k(x_i, x_j)$$

$$= [\alpha^T \ \alpha''^T] \underbrace{\begin{bmatrix} k(X^{bd}, X^{bd}), & \Delta_y k(X^{bd}, X^{int}) \\ \Delta_x k(X^{int}, X^{bd}) & \Delta_x \Delta_y k(X^{int}, X^{int}) \end{bmatrix}}_{K_{XX}} \begin{bmatrix} \alpha \\ \alpha'' \end{bmatrix}$$

$$\langle u, k(x,x_i) \rangle = \bar{u}(x_i)$$

$$\langle u, \Delta_x k(x,x_i) \rangle = -f(x_i)$$

$$\Rightarrow K_{XX} \begin{bmatrix} \alpha \\ \alpha'' \end{bmatrix} = f$$

$\Rightarrow$

$$u(x) = k_x X \begin{bmatrix} \alpha \\ \alpha'' \end{bmatrix} = k_x X \, K_{XX}^{-1} f$$

$$\|u(x)\|_{\mathcal{H}_k}^2 = [\alpha \ \alpha'']^T K_{XX} \begin{bmatrix} \alpha \\ \alpha'' \end{bmatrix} = f^T K_{XX}^{-1} f$$

② 算子学习

$f: R^N \to R$

$k: R^N \times R^N \to R$

$\mathcal{H}_k$:

$$f = \sum c_i k(\cdot, x_i)$$

$$f \to \langle k(\cdot, x), f \rangle_{\mathcal{H}_k} = f(x)$$

是有界线性映射

$$|f(x)| = |\langle k(\cdot, x), f \rangle_{\mathcal{H}_k}| \le \underbrace{\|k(\cdot, x)\|_{\mathcal{H}_k}}_{C} \|f\|_{\mathcal{H}_k}$$

当 $f: R^N \to \mathcal{U}$

$\langle k(\ ,x), f \rangle_{H_k} \in R$ $\quad f(x) \in \mathcal{U}$

算子值核函数

$f: A \to \mathcal{U}$

$k: A \times A \to L(\mathcal{U})$

对称性: $k(x, x') = k(x', x)$

正定性: $\sum_{i,j} \langle u_i, k(a_i, a_j) u_j \rangle_{\mathcal{U}} \geq 0$

可再生性:

$k(\cdot, a) u : A \to \mathcal{U}$

$\forall u, a$

$\langle u, f(a) \rangle_{\mathcal{U}} = \langle k(\cdot, a) u, f \rangle_{\mathcal{H}}$

引入了 $\mathcal{U}$

表示定理:

$$\hat{f} = \sum_{i=1}^{n} k(\cdot, a_i) u_i : A \to \mathcal{U}$$

例子:

Brownian bridge

$B(t) = W(t) - tW(1) \qquad t \in (0,1)$

$E\, B(t) = 0$

$E\, B(t) B(s) \qquad t \leq s$

$= E\,[W(t) - tW(1)][W(s) - sW(1)]$

$$= E\left[W(t)W(s) - t\,W(1)W(s) - s\,W(1)W(t) + ts\,W(1)^2\right]$$

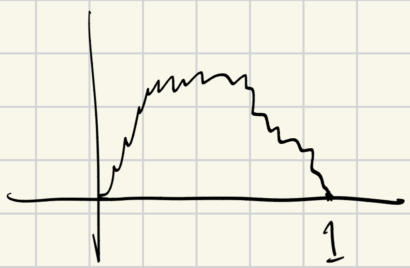
$$= E\left[W(t)^2 - t\,W(s)^2 - s\,W(t)^2 + ts\,W(1)^2\right]$$

$$= t - ts - ts + ts$$

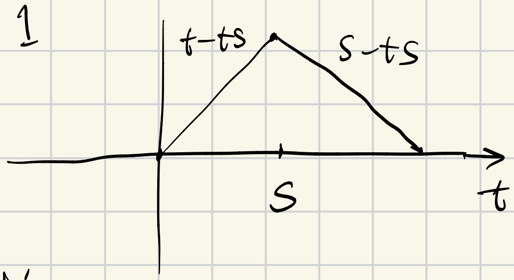
$$= t - ts$$

$$k(t,s) = \min\{t,s\} - ts$$

$$GP(0, k)$$



$k(t,s)$



分片线性函数

$$\mathcal{H}_k = H_0^1((0,1),\mathbb{R}) = \{f \in L_2,\ f' \in L_2,\ f(0) = f(1) = 0\}$$

$$\langle f, g\rangle_{\mathcal{H}} = \langle f', g'\rangle_2$$

$$\langle k(t,s), f(t)\rangle_{\mathcal{H}} = \int k'(t,s) f'(t)\,dt$$

$$= \int_0^s (1-s) f'(t) + \int_s^1 (-s) f'(t)$$

$$= f(x)$$

对算子 $A = (0,1)$ $\quad \mathcal{U} = R^p$

$$K(a, a') = k(a, a') I_{p\times p} \in \mathcal{L}(R^p)$$

$$\sum \langle u_i, K(a_i, a_j) u_j \rangle_{\mathcal{U}} = \sum_{(k)} \sum_{ij} u_i^{(k)} k(a_i, a_j) u_j^{(k)}$$

$$\geq 0$$

$$\mathbf{H}_0^1 = \{ f \in L_2(A, R^p), f' \in L_2(A, R^p)$$

$$f(0) = f(1) = 0 \}$$

$$\langle f, g \rangle_{\mathbf{H}_0^1} = \sum \langle f_i, g_i \rangle_{\mathcal{H}_0^1}$$

$$K(\cdot, a) u = k(\cdot, a) u \in \mathbf{H}_0^1$$

$$\langle u, f(a) \rangle_{\mathcal{U}} = \sum_i u_i f_i(a)$$

$$= \sum_i u_i \langle k(\cdot, a), f_i \rangle_{\mathcal{H}_0^1}$$

$$= \langle K(\cdot, a) u, f \rangle_{\mathbf{H}_0^1}$$

随机特征方法

$$k(a,a') = \int \varphi(a,w) \otimes \varphi(a',w)\, \rho(w)\, dw$$

再生性

$$\begin{aligned}
\langle G(a), u\rangle_{\mathcal{U}} &= \langle G(\cdot), k(\cdot, a)u\rangle_{\mathcal{H}_k} \\
&= \left\langle G(\cdot), \int \varphi(\cdot,w)\langle \varphi(a,w), u\rangle_{\mathcal{U}}\, \rho(w)\, dw\right\rangle \\
&= \int \rho(w)\, \underbrace{\langle G(\cdot), \varphi(\cdot,w)\rangle_{\mathcal{H}_k}}_{c(w)} \langle \varphi(a,w), u\rangle_{\mathcal{U}}\, dw \\
&= \Big\langle \underbrace{\int \rho(w)\, c(w)\, \varphi(a,w)\, dw}_{G(a)}, u\Big\rangle_{\mathcal{U}}
\end{aligned}$$

$$\begin{aligned}
\|G\|_{\mathcal{H}_k}^2 &= \left\langle G, \frac{1}{D}\sum c_i \varphi(\cdot, w_i)\right\rangle_{\mathcal{H}_k} \\
&= \sum \frac{1}{D} c_i \langle G(\cdot), \varphi(\cdot, w_i)\rangle_{\mathcal{H}_k} \\
&= \frac{1}{D}\sum c_i^2
\end{aligned}$$

高斯回归方法

$f(x) = k'_{xX} K'^{-1}_{XX} \vec{\Phi}$ 先预测 $\{u(x_i)\}$

$u(x) = k_{xX} K_{XX}^{-1} \vec{u}$ 再预测 $\}$