协方差函数

① 线性回归

$$y = x^T w + y_0 \qquad w_i \sim N(0,1) \qquad y_0 \sim N(0, \sigma_0^2)$$

$$E\,(x^T w + y_0)(x'^T w + y_0) = E\, x^T (w w^T) x' + \sigma_0^2$$
$$= x^T x' + \sigma_0^2$$

② 平稳的核函数

均方连续 $E(f(x_k) - f(x_*))^2$

$$= k(x_k, x_k) - 2k(x_k, x_*) + k(x_*, x_*)$$
$$= 2k(0) - 2k(x_k - x_*)$$

$\Leftrightarrow$ continuity of k at $k(0)$

均方可微

$$\underset{h\to 0}{E} \left\| \frac{f(x + he_i) - f(x)}{h} - \frac{\partial f(x)}{\partial x_i} \right\|^2 \to 0$$

$$\operatorname{cov}\left(\frac{\partial f(x)}{\partial x_i}, \frac{\partial f(x)}{\partial x_i'}\right) = \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_i'} k(x, x') = \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_i'} k(x - x')$$
$$= -\frac{\partial^2}{\partial r_i^2} k(0)\Big|_{r = x - x'}$$

$$\frac{k(x+he_i, x+he_i) + k(x, x) - k(x+he_i, x) - k(x, x+he_i)}{h^2}$$

$$+ \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_i'} k(x, x') - \frac{\partial k(x+he_i, x')}{\partial x_i'} + \frac{\partial}{\partial x_i'} k(x, x') - \frac{\partial}{\partial x_i} k(x, x+he_i)$$

$$+ \frac{\partial}{\partial x_i} k(x, x') \Rightarrow 0$$

$$k(\tau) = \int_{R^N} e^{2\pi i s\cdot\tau} \rho(s)\, ds$$

$$k(x, x') = \int_{R^N} e^{2\pi i s(x-x')} \rho(s)\, ds$$

$$= E_s\, \overline{e^{-2\pi i s\cdot x}} \cdot e^{-2\pi i s\cdot x'}$$

特征 $s \sim \rho(s)$ $\quad e^{2\pi i s\cdot x}$ $\Rightarrow$ Fourier 特征

③ 例子

i) 平方指数 $k(r) = \exp\left(-\frac{r^2}{2l^2}\right)$

$$\rho(s) = \int \exp\left(-\frac{r^2}{2l^2}\right) e^{2\pi i s r}\, dr$$

$$= \int \exp\left(-\frac{1}{2l^2}(r - 2\pi i s l^2)^2 - 2\pi^2 s^2 l^2\right) dr$$

$$\propto \exp(-2\pi^2 s^2 l^2)$$

$$k(x, x') \simeq \sigma^2 \sum \phi_c(x)\, \phi_c(x')$$

$$\simeq \sigma^2 \int_{-\infty}^{\infty} \phi_c(x)\, \phi_c(x')\, dc$$

$$= \sigma^2 \int_{-\infty}^{\infty} e^{-\frac{1}{2l^2}(x-c)^2} e^{-\frac{1}{2l^2}(x'-c)^2} dc$$

$$= \sigma^2 \int_{-\infty}^{\infty} e^{-\frac{1}{l^2}\left[\left(c - \frac{x+x'}{2}\right)^2 + \left(\frac{x-x'}{2}\right)^2\right]} dc$$

$$= \sigma^2 \sqrt{2\pi}\, \frac{l}{\sqrt{2}}\, e^{-\frac{1}{4l^2}(x-x')^2}$$

ii) Matern 函数

当 $\nu \to \infty$

$$\lim_{\alpha\to\infty} \left(1 + \frac{x^2}{2\alpha}\right)^{-\alpha} = \exp\left(-\frac{x^2}{2}\right) \qquad \Gamma(n) = (n-1)!$$

$$p(s) \sim \frac{\nu^{\frac{d}{2}}(2\nu)^{\nu}}{l^{2\nu}}\left(\frac{2\nu}{l^2}+4\pi^2 s^2\right)^{-(\nu+\frac{d}{2})}$$

$$\sim \left(\frac{2\nu}{l^2}\right)^{\nu+\frac{d}{2}}\left(\frac{2\nu}{l^2}+4\pi^2 s^2\right)^{-(\nu+\frac{d}{2})}$$

$$\sim \left(1+\frac{4\pi^2 s^2}{2\nu/l^2}\right)^{-(\nu+\frac{d}{2})}$$

$$\sim \exp\left(-2\pi^2 s^2 l^2\right)$$

当 $\nu=\frac{1}{2}$

$k(r;\frac{1}{2}) = \exp(-\frac{r}{l}) \qquad r=\|x\|$

在 $r=0$ 非二次可微

$\frac{\partial k}{\partial x_i} = \frac{\partial k}{\partial r}\cdot\frac{x_i}{\|x\|}$ 不连续

当 $\nu=\frac{3}{2}$

$$\frac{\partial k}{\partial x_i} = k\left(-\frac{\sqrt{3}}{l}\right)\frac{x_i}{\|x\|} + \exp\left(\frac{-\sqrt{3}r}{l}\right)\frac{\sqrt{3}}{l}\frac{x_i}{\|x\|}$$

$$= \exp\left(\frac{-\sqrt{3}r}{l}\right)\frac{x_i}{\|x\|}\left(\frac{\sqrt{3}r}{l}\right)$$

$$= \exp\left(-\frac{\sqrt{3}}{l}r\right)\frac{x_i\sqrt{3}}{l}$$

$$\frac{\partial^2 k}{\partial x_i \partial x_j} = \frac{\sqrt{3}}{l}\exp\left(\frac{-\sqrt{3}}{l}r\right)\left[\underbrace{\frac{x_j}{\|x\|}\left(\frac{-\sqrt{3}}{l}\right)x_i}_{\to 0} + \delta_{ij}\right]$$

OU 过程

$dX_t = -X_t dt + dW_t$

iii) 混合核函数

和 $f(x)=f_1(x)+f_2(x)$

$$cov[f(x)\ f(x')]=cov[f_1(x)+f_2(x),\ f_1(x')+f_2(x')]$$

$$=k_1(x,x')+k_2(x\ x')$$
$$+cov[f_1(x)\ f_2(x')]+cov[f_2(x)\ f_1(x')]$$

假设 $f_1(x)$ $f_2(x)$ 独立

积 $f(x)=f_1(x)f_2(x)$

$$cov[f_1(x)\ f_2(x)\ f_1(x')\ f_2(x')]$$
$$=cov[f_1(x)\ f_1(x')]\ cov[f_2(x)\ f_2(x')]$$
$$=k_1(x\ x')\ k_2(x,x')$$

归一化 $k(x,x)=1$

④ 核函数的特征函数分析

Mercer 定理 $\Longleftrightarrow$ Hermitian 矩阵可对角化

无限维推广

有限测度空间 $\int d\mu(x)<+\infty$

$$\int\sum\lambda_i\phi_i(x)\phi_i^*(x')\phi_j(x')\,d\mu(x')=\sum_i\lambda_i\phi_i(x)\int\phi_i^*(x')\phi_j(x')\,d\mu(x')$$
$$=\lambda_j\phi_j(x)$$

$\phi_1\rightarrow\phi_\infty$ 低频到高频

$\lambda_i \sim i^{-\alpha}$ 衰减率对应了 k 的光滑程度

$$\int k(x,x')\,\phi_k(x')\,\rho(x')\,dx' = \lambda_k\,\phi_k(x)$$

选点 $x_1\ x_2 \cdots x_n \sim \rho(x)$

$$\sum_i \frac{1}{n} k(x, x_i)\,\phi_k(x_i) = \lambda_k\,\phi_k(x)$$

$$K\,u_k = (n\lambda_k)\,u_k \qquad u_k^T u_k = 1$$

$$\int \phi_k\,\phi_k\,\rho\,dx = 1 \iff \frac{1}{n}\phi_k^T\phi_k = 1$$

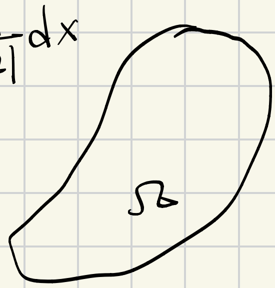
$$\phi_k = \sqrt{n}\,u_k \qquad \lambda_k = \frac{\lambda_{k,mat}}{n}$$

计算新的点

$$\phi_k(x) = \sum \frac{1}{n\lambda_k} k(x, x_i)\,\phi_k(x_i)$$
$$= \sum \frac{\sqrt{n}}{\lambda_{k,mat}} k(x, x_i)\,u_k$$

有限空间上的核函数

$\mu(x) = \frac{1}{|\Omega|}dx$



$$f(x) = \sum_{i=1}^{\infty} w_i \sqrt{\lambda_i}\,\phi_i \qquad w_i \sim N(0, 1)$$

$$\int \phi_i(x)\,\phi_j(x)\,d\Omega = \delta_{ij}$$

$$\Rightarrow k(x, x') = \sum_i \lambda_i\,\phi_i(x)\,\phi_i(x')$$

$$\mathrm{cov}[f(x), f(x')] = \mathrm{cov}\left[\sum w_i \sqrt{\lambda_i}\, \phi_i(x) \sum w_j \sqrt{\lambda_j}\, \phi_j(x')\right]$$

$$= \sum_{i,j} \mathrm{cov}[w_i, w_j] \sqrt{\lambda_i} \sqrt{\lambda_j}\, \phi_i(x)\, \phi_j(x')$$

$$= \sum_i \lambda_i\, \phi_i(x)\, \phi_i(x')$$

$\lambda_i \sim i^{-\alpha}$ 比如 $\lambda_i = \dfrac{\delta^2}{i^\alpha + \tau^2}$

$$T_k = \delta^2(-\Delta + \tau^2)^{-\alpha/2} : L_2(\Omega) \to L_2(\Omega)$$

$$\delta^2(-\Delta + \tau^2)^{-\alpha/2} \phi_k = \lambda_k \phi_k$$

$$\phi_i = \frac{\lambda}{\delta^2} (-\Delta + \tau^2)^{\alpha/2} \phi$$

当 $\Omega = [0, 1]$, Dirichlet 边界条件

$$\phi = \sin(i\pi x)$$

$$(-\Delta + \tau^2)^{\alpha/2} \phi = ((i\pi)^2 + \tau^2)^{\alpha/2} \sin(i\pi x)$$

$$\lambda = \frac{\delta^2}{((i\pi)^2 + \tau^2)^{\alpha/2}} \sim O(i^{\alpha})$$