高斯回归

① (贝叶斯)线性回归

$$y = X^T w \qquad (n \geq N)$$

$$\min \|Y - X^T w\|_2$$

似然函数

$$p(Y \mid X, w) = \prod p(y_i \mid x_i, w)$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} \prod_i e^{-\frac{1}{2\sigma^2}(y_i - x_i^T w)^2}$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(y - X^T w)^T \frac{1}{\sigma^2 I}(y - X^T w)}$$

先验分布 $w \sim \frac{1}{\sqrt{|2\pi\Sigma_0|}} e^{-\frac{1}{2} w^T \Sigma_0^{-1} w}$

后验分布

$$p(w \mid X, y) \propto e^{-\frac{1}{2\sigma^2}(y - X^T w)^T(y - X^T w)} e^{-\frac{1}{2} w^T \Sigma_0^{-1} w}$$

$$-\frac{1}{2\sigma^2}(y^T y - w^T X y - y^T X^T w + w^T X X^T w) - \frac{1}{2} w^T \Sigma_0^{-1} w$$

二次式 $-\frac{1}{2} w^T\left(\frac{XX^T}{\sigma^2} + \Sigma_0^{-1}\right) w + \underline{\frac{1}{2\sigma^2}(w^T X y + y^T X^T w)}$

$$-\frac{1}{2}(w - \hat{w})^T\left(\frac{XX^T}{\sigma^2} + \Sigma_0^{-1}\right)(w - \hat{w})$$

$$\left(\frac{XX^T}{\sigma^2} + \Sigma_0^{-1}\right)\hat{w} = \frac{1}{\sigma^2} X y$$

$$\Rightarrow \quad (XX^T + \sigma^2 \Sigma_0^{-1})\hat{w} = X y$$

ridge
山脊回归
损失函数加了山脊一样的

正则项

$$f(x) = \psi(x)^T w \qquad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} \psi(x_1)^T \\ \psi(x_2)^T \\ \vdots \\ \psi(x_n)^T \end{pmatrix} w = X^T w$$

$$f_* = p(f_* \mid x_*, X, y)$$
$$= N\Big(\psi(x_*)^T (XX^T + \sigma^2 \Sigma_0^{-1})^{-1} X y,$$
$$\psi(x_*)^T \big(\tfrac{1}{\sigma^2} XX^T + \Sigma_0^{-1} \big)^{-1} \psi(x_*) \Big)$$

$$\psi(x_*)^T \sigma^{-2} (\Sigma_0 - \Sigma_0 X (X^T \Sigma_0 X + \sigma^2 I)^{-1} X^T \Sigma_0) X y$$
$(X^T\Sigma_0 X + \sigma^2 I - \sigma^2 I)$
$$= \psi(x_*)^T \sigma^{-2} (\Sigma_0 X y - \Sigma_0 X (X^T \Sigma_0 X + \sigma^2 I)^{-1} \underline{X^T \Sigma_0 X} y)$$
$$= \psi(x_*)^T \sigma^{-2} (\Sigma_0 X y - \Sigma_0 X (y - (X^T \Sigma_0 X + \sigma^2 I)^{-1} \sigma^2 I y))$$
$$= \psi(x_*)^T \sigma^{-2} \quad \Sigma_0 X (X^T \Sigma_0 X + \sigma^2 I)^{-1} \sigma^2 I y$$
$$= \psi(x_*)^T \Sigma_0 X (X^T \Sigma_0 X + \sigma^2 I)^{-1} y$$

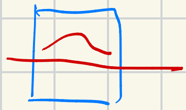
$$\psi(x_*)^T \sigma^2 (XX^T + \sigma^2 \Sigma_0^{-1})^{-1} \psi(x_*)$$
$$= \psi(x_*)^T (\Sigma_0 - \Sigma_0 X (X^T \Sigma_0 X + \sigma^2 I)^{-1} X^T \Sigma_0) \psi(x_*)$$

$$f_* \sim N\Big(\underbrace{\psi(x_*)^T \Sigma_0 X}_{K_*^T} (\underbrace{X^T \Sigma_0 X}_{K} + \sigma^2 I)^{-1} y,$$
$$\underbrace{\psi(x_*)^T \Sigma_0 \psi(x_*)}_{k(x_*, x_*)} - \underbrace{\psi(x_*)^T \Sigma_0 X}_{K_*^T} (\underbrace{X^T \Sigma_0 X}_{K} + \sigma^2 I)^{-1} \underbrace{X^T \Sigma_0 \psi(x_*)}_{K_*} \Big)$$

② 高斯过程

$$\begin{pmatrix} f \\ f^* \end{pmatrix} = N\left(0,\ \begin{bmatrix} K(X,X) & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{bmatrix}\right)$$

$$e^{-\frac{1}{2}\underbrace{[f^T\ f_*^T]}_{=y} \begin{bmatrix} K(X,X) & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{bmatrix}^{-1} \begin{bmatrix} f \\ f_* \end{bmatrix}} \to y$$



$$\overset{L}{\begin{bmatrix} I & 0 \\ -K(X_*,X)K^{-1}(X,X) & I \end{bmatrix}} \overset{K}{\begin{bmatrix} K(X,X) & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{bmatrix}} \overset{L^T}{\begin{bmatrix} I & -K^{-1}(X,X)K(X,X^*) \\ 0 & I \end{bmatrix}}$$

$$= \overset{D}{\begin{bmatrix} K(X,X) & 0 \\ 0 & \underbrace{K(X_*,X_*) - K(X_*,X)K(X,X)^{-1}K(X,X_*)}_{S} \end{bmatrix}}$$

$$K^{-1} = L^T D^{-1} L$$

$$\exp\left(-\frac{1}{2}\left[f^T,\ f_*^T - f^T K^{-1}(X,X)K(X,X^*)\right] \begin{bmatrix} K(X,X)^{-1} & \\ & S^{-1} \end{bmatrix} \begin{bmatrix} f \\ f_* - \underbrace{K(X_*,X)K^{-1}(X,X)f}_{m_*} \end{bmatrix}\right)$$

$$\propto \exp\left(-\frac{1}{2}(f_* - m_*)^T S^{-1}(f_* - m_*)\right)$$

期望不为0的高斯过程

$$g(x) \sim GP\left(h(x)^T b,\ K(x,x') + h(x)^T B\, h(x')\right)$$

定义 $H = [h(x_1)\ h(x_2) \cdots h(x_n)]$

$H_* = [h(x_{1*})\ h(x_{2*}) \cdots h(x_{n*})]$

$K = k(X, X) \qquad K_* = k(X_*\ X)$

$$Eg(X_*) = H_*^T b + (K_* + H_*^T B H)\underbrace{(K + H^T B H)^{-1}}_{K^{-1} - K^{-1}H^T \underbrace{(HK^{-1}H^T + B^{-1})^{-1}}_{S^{-1}} H K^{-1}}(y - H^T b)$$

$$= H_*^T(b + BH(K + H^TBH)^{-1}(y - H^Tb))$$
$$+ K_*(K + H^TBH)^{-1}(y - H^Tb)$$
$$= H_*^T(b + S^{-1}HK^{-1}(y - H^Tb))$$
$$+ K_*K^{-1}(I - H^TS^{-1}HK^{-1})(y - H^Tb)$$
$$= H_*^T S^{-1}((HK^{-1}H^T + B^{-1})b + HK^{-1}y - HK^{-1}H^Tb)$$
$$+ K_*K^{-1}(y - H^T(\underbrace{b}_{S^{-1}Sb} + S^{-1}HK^{-1}y - S^{-1}HK^{-1}H^Tb))$$
$$= H_*^T S^{-1}(B^{-1}b + HK^{-1}y)$$
$$+ K_*K^{-1}(y - H^T S^{-1}(B^{-1}b + HK^{-1}y))$$
$$= H_*^T \underline{S^{-1}(B^{-1}b + HK^{-1}y)}$$
$$+ K_*K^{-1}(y - H^T \underbrace{S^{-1}(B^{-1}b + HK^{-1}y)}_{\bar\beta})$$

$$= H_*^T\bar\beta + K_*K^{-1}(y - H^T\bar\beta)$$
$$= K_*K^{-1}y + (H_*^T - K_*K^{-1}H^T)\bar\beta$$

$$\mathrm{Cov}\, g(x_*) = k(x_*, x_*) + H_*^T B H_* - (k_* + H_*^T B H)[K^{-1} - K^{-1} H^T S^{-1} H K^{-1}](k_*^T + H^T B H_*)$$

$$= k(x_*, x_*) - k_* K^{-1} k_*^T + H_*^T B H_*$$
$$+ k_* K^{-1} H^T S^{-1} H K^{-1} k_*^T$$
$$- k_* (K^{-1} - K^{-1} H^T S^{-1} H K^{-1}) H^T B H_* \Rightarrow -k_* K^{-1} H^T S^{-1} H_*$$
$$- H_*^T B H (K^{-1} - K^{-1} H^T S^{-1} H K^{-1}) k_*^T \Rightarrow -H_*^T S^{-1} H K^{-1} k_*^T$$
$$- H_*^T B H (K^{-1} - K^{-1} H^T S^{-1} H K^{-1})(H^T B H_*)$$
$$\Rightarrow H_*^T S^{-1} H_* - H_*^T B H_*$$

$$= k(x_*, x_*) - k_* K^{-1} k_*^T$$
$$+ k_* K^{-1} H^T S^{-1} H K^{-1} k_*^T$$
$$- k_* K^{-1} H^T S^{-1} H_*$$
$$- H_*^T S^{-1} H K^{-1} k_*^T$$
$$+ H_*^T S^{-1} H_*$$

$$= \mathrm{cov}(f_*) + (H_*^T - k_* K^{-1} H^T) S^{-1} (H_* - H K^{-1} k_*^T)$$