

→ Linear Regression :- $D: \{(x_1, y_1), \dots, (x_N, y_N)\}$
 $n = 1, 2, \dots, N$

For likelihood function,

$$P(y|x) = N(y | f(x), \sigma^2)$$

where, $x_n \in \mathbb{R}^D$ are inputs

$y_n \in \mathbb{R}$ are noisy function values.

$$y = f(x) + \epsilon, \quad \text{where } \epsilon \sim N(0, \sigma^2)$$

i.i.d. gaussian noise.

Now, consider the parameters are linear in model.

$$P(y|x, \theta) = N(y | x^T \theta, \sigma^2)$$

$$\Leftrightarrow y = x^T \theta + \epsilon$$

$\theta \in \mathbb{R}^D \leftarrow$ parameters.

Using Probabilistic graphical model,

$$P(y|x, \theta) = P(y_1, \dots, y_N | x_1, \dots, x_N, \theta)$$

$$= \prod_{n=1}^N P(y_n | x_n, \theta)$$

$$= \prod_{n=1}^N N(y_n | x_n^T \theta, \sigma^2)$$

where $x = \{x_1, \dots, x_N\}$

$y = \{y_1, \dots, y_N\}$

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For maximum likelihood of parameters,

$$\theta_{ML} = \arg \max_{\theta} p(Y/X, \theta)$$

take negative log-likelihood,

$$\begin{aligned} L(\theta) &:= -\log p(Y/X, \theta) = -\log \prod_{n=1}^N p(y_n | x_n, \theta) \\ &= -\sum_{n=1}^N \log p(y_n | x_n, \theta) \end{aligned}$$

we know that $y = x^T \theta + \epsilon$, $\epsilon \sim N(0, \sigma^2)$

$$\begin{aligned} L(\theta) &= -\sum_{n=1}^N \log \left(\frac{1}{\sqrt{2\pi}\sigma^2} e^{-\frac{(y_n - x_n^T \theta)^2}{2\sigma^2}} \right) \\ &= \frac{1}{2\sigma^2} \sum_{n=1}^N (y_n - x_n^T \theta)^2 \\ &= \frac{1}{2\sigma^2} (Y - X\theta)^T (Y - X\theta) \quad \left| \begin{array}{l} x_i := [x_{i1}, \dots, x_{iN}]^T \in \mathbb{R}^{N \times D} \\ Y := [y_1, \dots, y_N]^T \in \mathbb{R}^N \end{array} \right. \\ &= \frac{1}{2\sigma^2} \|Y - X\theta\|^2 \end{aligned}$$

differentiate w.r.t. θ ,

$$\begin{aligned} \frac{dL}{d\theta} &= \frac{d}{d\theta} \left(\frac{1}{2\sigma^2} (Y - X\theta)^T (Y - X\theta) \right) \\ &= \frac{1}{2\sigma^2} \frac{d}{d\theta} (Y^T Y - 2Y^T X\theta + \theta^T X^T X \theta) \\ &= \frac{d}{d\theta} \left(\frac{1}{2\sigma^2} (Y^T - \theta^T X^T) (Y - X\theta) \right) \end{aligned}$$

$$\frac{dL}{d\theta} = \frac{1}{2\sigma^2} \frac{d}{d\theta} (y^T y - y^T x \theta - \theta^T x^T y + \theta^T x^T x \theta)$$

$$\frac{dL}{d\theta} = \frac{1}{2\sigma^2} \frac{d}{d\theta} (y^T y - 2y^T x \theta + \theta^T x^T x \theta)$$

$$(\because (\theta^T x^T y)^T = y^T x \theta)$$

$$\frac{dL}{d\theta} = \frac{1}{2\sigma^2} (-2y^T x + 2\theta^T x^T x)$$

$$\frac{dL}{d\theta} = \frac{1}{\sigma^2} (-y^T x + \theta^T x^T x) = 0^T$$

$$-y^T x + \theta_{ML}^T x^T x = 0^T$$

$$\theta_{ML}^T x^T x = (y^T x)$$

$$\theta_{ML}^T = y^T x (x^T x)^{-1}$$

$$\theta_{ML} = (y^T x (x^T x)^{-1})^T$$

$$\theta_{ML} = (x^T x)^{-1} x^T y$$

Now, if inputs are m non-linear transformation,

$$P(y|x, \theta) = \mathcal{N}(y | \phi^T(x) \theta, \sigma^2)$$

$$\Leftrightarrow y = \phi^T(x) \theta + \epsilon$$

$$= \sum_{k=0}^{K-1} \theta_k \phi_k(x) + \epsilon$$

where $\phi: \mathbb{R}^D \rightarrow \mathbb{R}^K$ non linear transformation of input x .

$\phi_k: \mathbb{R}^D \rightarrow \mathbb{R}$ k^{th} component of feature vector ϕ .

$$\Phi = \begin{bmatrix} \phi^T(x_1) \\ \vdots \\ \phi^T(x_N) \end{bmatrix} = \begin{bmatrix} \phi_0(x_1) & \dots & \phi_{K-1}(x_1) \\ \vdots & & \vdots \\ \phi_0(x_N) & \dots & \phi_{K-1}(x_N) \end{bmatrix}_{N \times K}$$

Taking negative -log likelihood

$$-\log p(Y|x, \theta) = \frac{1}{2\sigma^2} (y - \Phi\theta)^T (y - \Phi\theta) + c$$

maximum likelihood estimation for parameter,

$$\theta_{ML} = (\Phi^T \Phi)^{-1} \Phi^T y$$