

$$MSE_f = E[(f(x) - y)^2] \quad \begin{matrix} f: \text{estimator} \\ x \in \mathbb{R}^d \\ y \in \mathbb{R} \end{matrix} \quad \begin{matrix} \text{nonlinear} \\ \text{linear} \end{matrix}$$

$$\boxed{f \in C^\infty(\mathbb{R}^d)} \quad \begin{matrix} f \in C(\mathbb{R}) \\ |f| \in C^1(\mathbb{R}) \end{matrix}$$

Taylor expansion

$$\underset{\substack{\uparrow \\ x \in \mathbb{R}^d}}{f(x)} = f(x_0) + \underbrace{\nabla f(x_0)(x - x_0)}_{\substack{\lim_{x \rightarrow x_0} \frac{o(x - x_0)}{x - x_0} = 0}} + o(x - x_0)$$

$$f \in \mathcal{F} \xrightarrow{\text{model class}} \mathcal{F} = \{f; f = ax^2 + bx + c, a, b, c \in \mathbb{R}\}$$

$$\text{linear model} \rightarrow \mathcal{F} = \{f; f = a^T x + b, a \in \mathbb{R}^d, x \in \mathbb{R}^d, b \in \mathbb{R}\}$$

$$\boxed{f^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} E[(f(x) - y)^2]}$$

Known x distribution and y

What if we don't know the distribution?

If we observe (x_i, y_i) from $P(x, y)$
 $i = 1, 2, \dots, n$

$$\boxed{\frac{1}{n} \sum_{i=1}^n (f(x_i) - y_i)^2} \rightarrow \text{Empirical MSE}$$

in probability

$$E[(f(x) - y)^2]$$

* Law of large numbers

and continuous mapping

$$f \in C(\mathbb{R}^d), \quad \begin{matrix} p.d \\ x_n \xrightarrow{f} x \\ f(x_n) \xrightarrow{f} f(x) \end{matrix}$$

$$\frac{1}{n} \sum_{i=1}^n (f(x_i)^2 - 2f(x_i)y_i + y_i^2)$$

$$= \frac{1}{n} \sum_{i=1}^n f(x_i)^2 - \frac{1}{n} \sum_{i=1}^n 2f(x_i)y_i + \frac{1}{n} \sum_{i=1}^n y_i^2$$

$$= E[f(x)^2] - 2E[f(x)y] + E[y^2]$$

$$= E[(f(x) - y)^2]$$

$$\left. \begin{aligned} \underline{f^*} &= \underset{f \in \mathcal{F}}{\operatorname{argmin}} E[(f(x) - y)^2] \\ \underline{\hat{f}} &= \underset{f \in \mathcal{F}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^n (f(x_i) - y_i)^2 \end{aligned} \right\} \begin{matrix} \text{best predictor} \\ \text{in } \mathcal{F} \end{matrix}$$

$$E[(f^*(x) - \hat{f}(x))^2] \rightarrow 0 \quad ? \quad \Rightarrow \quad \hat{f} \rightarrow f^*$$

Least squared error $\rightarrow$ minimize MSE

$$L(f, (x, y)) = \underbrace{g(f(x), y)}_{\substack{\text{prediction} \\ \text{response}}} \quad \begin{matrix} g(x, y) = (x - y)^2 \\ \text{loss function} \end{matrix}$$

$$= f(x)$$

$$MLE: \quad g(f(x), y) = \exp\{-\dots\}$$

log-loss

$$\text{Example: } \mathcal{F} = \{f; f(x) = \alpha + x^T \beta, \alpha \in \mathbb{R}, \beta \in \mathbb{R}^d\} \quad \text{parametric method}$$

$$MSE_f = R(\alpha, \beta) = E[(\alpha + x^T \beta - y)^2] \\ = E[\alpha^2 + \underbrace{(x^T \beta)^2}_{(E[x^T] \beta)^2} + y^2 + \underbrace{2\alpha x^T \beta}_{2\alpha y - 2x^T \beta y}]$$

$$\begin{cases} \frac{\partial R(\alpha, \beta)}{\partial \alpha} = 2E[\alpha] + 2E[x^T \beta] - 2E[y] = 0 \\ \frac{\partial R(\alpha, \beta)}{\partial \beta} = 2E[x^T \beta \cdot x] + E[2\alpha x] - E[2y x] = 0 \end{cases}$$

1+d " = "

1+d param.

solve the linear system

$$\Rightarrow \underline{\gamma} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in \mathbb{R}^{1+d}, \quad \underline{\beta} \in \mathbb{R}^d \quad \beta = \begin{pmatrix} 1 \\ x \end{pmatrix}$$

Gamma

$$\underline{z} = \begin{pmatrix} 1 \\ x \end{pmatrix} \in \mathbb{R}^{1+d} \quad \begin{matrix} \boxed{\alpha + \beta^T x} \\ \boxed{\gamma^T z} \end{matrix}$$

differentiating

$$\Rightarrow \underline{E[z z^T]} \gamma = E[z y]$$

invertible

$$z z^T \in \mathbb{R}^{(1+d) \times (1+d)}$$

$$z y \in \mathbb{R}^{1+d}$$

$$\Rightarrow \underline{\gamma} = E[z z^T]^{-1} E[z y]$$

$$\frac{\sum_{i=1}^n (z_i^T \gamma - y_i)^2}{\sum_{i=1}^n (z_i^T \gamma - y_i)^2} = \underline{\|z \gamma - y\|_2^2}$$

$$\begin{matrix} z = \begin{pmatrix} z_1^T \\ z_2^T \\ \vdots \\ z_n^T \end{pmatrix} \in \mathbb{R}^{n \times (1+d)} \\ y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \in \mathbb{R}^n \end{matrix}$$

$$\|y\|_2 = \sqrt{y_1^2 + \dots + y_n^2}$$

$$\frac{\partial \|z \gamma - y\|_2^2}{\partial \gamma} = 2 \cdot (z \gamma - y) \cdot z$$

$$\frac{(z \gamma - y)^T (z \gamma - y)}{\mathbb{R}^n}$$

$$= \boxed{(z \gamma)^T \cdot (z \gamma)} - 2(z \gamma)^T \cdot y + y^T y$$

$$2 z^T z \gamma - 2 z^T y$$

$$= 2 z^T (z \gamma - y) = 0$$

$$\underline{z^T z} \gamma = \underline{z^T y}$$

$$N_d(0, I_d) \quad x = \begin{pmatrix} x_1 \\ \vdots \\ x_d \end{pmatrix} \quad \begin{matrix} x_i \text{ is a R.V. } \sim N(0, 1) \\ x_i \text{ i.i.d.} \end{matrix}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & \ddots & 1 \end{pmatrix}$$

$$x \sim N_d(0, I_d) \quad \frac{1}{\sqrt{2\pi}} \exp\{-\frac{1}{2} x_i^2\}$$

$$\text{pdf } f(x) = \left(\frac{1}{2\pi}\right)^{\frac{d}{2}} \cdot \exp\{-\frac{1}{2} \sum_{i=1}^d x_i^2\}$$

$$x \in \mathbb{R}^d \quad -\frac{1}{2} x^T I_d x = -\frac{1}{2} x^T x \quad \text{Cov}(x_1, x_1)$$

$$\Sigma = \text{Cov}(x, x) = \begin{bmatrix} \square & \square \\ (1, 2) & \square \\ \vdots & \vdots \end{bmatrix}_{d \times d}$$

$$\text{Cov}(x_i, x_j)$$

$$N_d(0, \Sigma) \quad \text{pdf } f(x) = \left(\frac{1}{2\pi \det(\Sigma)}\right)^{\frac{d}{2}} \exp\left\{-\frac{1}{2 \det(\Sigma)} x^T \Sigma x\right\}$$

zero mean and Σ exists.

$$\underline{z} = \begin{pmatrix} 1 \\ x \end{pmatrix} \in \mathbb{R}^{1+d}$$

$$E[z z^T]$$

$$\text{Cov}(z, z) = \begin{matrix} \begin{matrix} 1 & 0 \\ 0 & \Sigma \end{matrix} \\ \begin{matrix} \uparrow \\ \downarrow \end{matrix} \end{matrix} \quad \begin{matrix} \text{Cov}(1, x_i) \text{ } i=1, \dots, d \\ 0 \\ \text{Cov}(1, 1) \end{matrix}$$

$$\text{Cov}(x, x)$$

$$\text{Cov}(z, z) = \begin{bmatrix} 1 & 0 \\ 0 & \Sigma \end{bmatrix}$$

$$E[z z^T] = \text{Cov}(z, z) + E[z] E[z^T]$$

zero-mean

$$\det(\text{Cov}(z, z)) = |\underline{\Sigma}|$$