

## Linear Regression

Given a data set  $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ , where  $\mathbf{x}_i \in \mathbb{R}^{d+1}$  and  $y_i \in \mathbb{R}$ .

### Linear Regression by Least Squares

$$y_i = \mathbf{w}^T \mathbf{x}_i,$$

where  $\mathbf{x}_i = (1, x_{i1}, x_{i2}, \dots, x_{id})^T$  and  $\mathbf{w} = (w_0, w_1, \dots, w_d)^T$ .

Average Fitting error is

$$\begin{aligned} L &= \frac{1}{n} \sum_i^n (y_i - \mathbf{w}^T \mathbf{x}_i)^2 \\ &= \frac{1}{n} \|\mathbf{y} - \bar{\mathbf{X}} \mathbf{w}\|^2 \end{aligned}$$

where  $\mathbf{y} = (y_1, \dots, y_n)$  and  $\bar{\mathbf{X}} \in \mathbb{R}^{n \times (d+1)}$ .

$$0 = \left. \frac{\partial L}{\partial \mathbf{w}} \right|_{\mathbf{w}=\hat{\mathbf{w}}} = -\frac{2}{n} \bar{\mathbf{X}}^T (\mathbf{y} - \bar{\mathbf{X}} \hat{\mathbf{w}}) \Rightarrow \hat{\mathbf{w}} = (\bar{\mathbf{X}}^T \bar{\mathbf{X}})^{-1} \bar{\mathbf{X}}^T \mathbf{y}$$

$$\hat{\mathbf{y}} = \bar{\mathbf{X}} (\bar{\mathbf{X}}^T \bar{\mathbf{X}})^{-1} \bar{\mathbf{X}}^T \mathbf{y}$$

Projection matrix  $P = \bar{\mathbf{X}} (\bar{\mathbf{X}}^T \bar{\mathbf{X}})^{-1} \bar{\mathbf{X}}^T$  projects an arbitrary vector to the column space of  $\bar{\mathbf{X}}$ .

### Linear Regression by Maximum Likelihood

$$y_i = \mathbf{w}^T \mathbf{x}_i + \epsilon_i,$$

假设  $\mathbf{w}$  与  $\mathbf{x}_i$  给定。

**Assumption 1:**  $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ ,  $y_i | \mathbf{x}_i, \mathbf{w}, \sigma \sim \mathcal{N}(\mathbf{w}^T \mathbf{x}_i, \sigma^2)$ .

**Assumption 2:** IID.  $P((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)) = \prod_i P((\mathbf{x}_i, y_i))$ .

$$\begin{aligned} L &= P(y_1, \dots, y_n | \mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{w}, \sigma) \\ &= \frac{P((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n) | \mathbf{w}, \sigma)}{P(\mathbf{x}_1, \dots, \mathbf{x}_n | \mathbf{w}, \sigma)} \\ &= \frac{\prod_{i=1}^n P(\mathbf{x}_i, y_i | \mathbf{w}, \sigma)}{\prod_{i=1}^n P(\mathbf{x}_i | \mathbf{w}, \sigma)} \\ &= \prod_{i=1}^n P(y_i | \mathbf{x}_i, \mathbf{w}, \sigma) \end{aligned}$$

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$$\begin{aligned} &\begin{aligned} \log L &= \sum_{i=1}^n \log \left( \frac{1}{\sqrt{2\pi} \sigma} \exp \left\{ -\frac{1}{2\sigma^2} (y_i - \mathbf{w}^T \mathbf{x}_i)^2 \right\} \right) \\ &= -\frac{n}{2} \log 2\pi - n \log \sigma - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mathbf{w}^T \mathbf{x}_i)^2 \end{aligned} \\ &\end{aligned}$$

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$$\begin{aligned}
\log L &= \sum_i^n \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{\frac{1}{2\sigma^2}(y_i - \mathbf{w}^T \mathbf{x}_i)^2\right\}\right) \\
&= -\frac{n}{2} \log 2\pi - n \log \sigma - \frac{1}{2\sigma^2} \sum_i^n (y_i - \mathbf{w}^T \mathbf{x}_i)^2 \\
\log L &= \sum_i^n \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{\frac{1}{2\sigma^2}(y_i - \mathbf{w}^T \mathbf{x}_i)^2\right\}\right) \\
&= -\frac{n}{2} \log 2\pi - n \log \sigma + \frac{1}{2\sigma^2} \sum_i^n (y_i - \mathbf{w}^T \mathbf{x}_i)^2
\end{aligned}$$

$$\begin{aligned}
0 &= \left. \frac{\partial \log L}{\partial \mathbf{w}} \right|_{\mathbf{w}=\hat{\mathbf{w}}} \\
&= \frac{1}{\sigma^2} \sum_{i=1}^n \mathbf{x}_i y_i - \mathbf{x}_i \mathbf{x}_i^T \hat{\mathbf{w}} \\
&= \frac{1}{\sigma^2} (\bar{\mathbf{X}}^T \mathbf{y} - \bar{\mathbf{X}}^T \bar{\mathbf{X}} \hat{\mathbf{w}}) \\
\Rightarrow \hat{\mathbf{w}} &= (\bar{\mathbf{X}}^T \bar{\mathbf{X}})^{-1} \bar{\mathbf{X}}^T \mathbf{y}
\end{aligned}$$