

Deterministic Representation

Model: $f: \mathbf{x} \rightarrow y, f(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$

Training data: $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$, or $\mathbf{X} = \begin{bmatrix} -\mathbf{x}_1^T - \\ \vdots \\ -\mathbf{x}_N^T - \end{bmatrix}$ and $\mathbf{y} = [y_1, \dots, y_N]^T$

Evaluation: $RSS(\mathbf{w}) = \sum_{n=1}^N (y_n - \mathbf{w}^T \mathbf{x}_n)^2 = (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$ (residual sum of squares)

Optimization through analytic solution (ordinary least squares solution):

$$\frac{\partial RSS(\mathbf{w})}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w}^{\text{OLS}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Rule for adding a constant to a Normal random variable

If $X \sim \mathcal{N}(\mu, \tau^2)$, then $X + c \sim \mathcal{N}(\mu + c, \tau^2)$

Noisy observation model (assuming Gaussian noise)

Model: $y = \mathbf{w}^T \mathbf{x} + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2)$

In the above rule for adding a constant to a Normal random variable, if we substitute $\mu := 0$, $\tau^2 := \sigma^2$, and $c := \mathbf{w}^T \mathbf{x}$, we get $y \sim \mathcal{N}(\mathbf{w}^T \mathbf{x}, \sigma^2)$

Data likelihood, assuming training samples are independent and identically distributed (i.i.d):

$$\begin{aligned} \mathcal{L}(\mathcal{D}) &= \prod_{n=1}^N p(y_n | \mathbf{x}_n, \mathbf{w}) \\ &= \prod_{n=1}^N \mathcal{N}(\mathbf{w}^T \mathbf{x}_n, \sigma^2) \\ &= \prod_{n=1}^N \frac{1}{\sigma \sqrt{2\pi}} \exp \left[-\frac{(y_n - \mathbf{w}^T \mathbf{x}_n)^2}{2\sigma^2} \right] \end{aligned}$$

Log-likelihood:

$$\begin{aligned} l(\mathcal{D}) &= \log \mathcal{L}(\mathcal{D}) \\ &= \log \left\{ \prod_{n=1}^N \frac{1}{\sigma \sqrt{2\pi}} \exp \left[-\frac{(y_n - \mathbf{w}^T \mathbf{x}_n)^2}{2\sigma^2} \right] \right\} \\ &= \sum_{n=1}^N \log \left(\frac{1}{\sigma \sqrt{2\pi}} \right) - \sum_{n=1}^N \frac{(y_n - \mathbf{w}^T \mathbf{x}_n)^2}{2\sigma^2} \\ &= -N \log \sigma - N \log(2\pi)^{1/2} - \sum_{n=1}^N \frac{(y_n - \mathbf{w}^T \mathbf{x}_n)^2}{2\sigma^2} \\ &= -\frac{N}{2} \log \sigma^2 - \frac{1}{2\sigma^2} \sum_{n=1}^N (y_n - \mathbf{w}^T \mathbf{x}_n)^2 + \text{const} \\ &= -\frac{1}{2} \left[N \log \sigma^2 + \frac{1}{\sigma^2} \sum_{n=1}^N (y_n - \mathbf{w}^T \mathbf{x}_n)^2 \right] + \text{const} \end{aligned}$$

By substituting $RSS(\mathbf{w}) = \sum_{n=1}^N (y_n - \mathbf{w}^T \mathbf{x}_n)^2$ and $s = \sigma^2$, we get:

$$l(\mathcal{D}) = -\frac{1}{2} \left[N \log s + \frac{1}{s} RSS(\mathbf{w}) \right] + \text{const}$$

Maximum likelihood estimation (MLE) is equivalent to minimizing RSS:

$$\max l(\mathcal{D}) \Leftrightarrow \min RSS(\mathbf{w})$$

Estimation of the noise variance:

We maximize the data log-likelihood with respect to $s = \sigma^2$:

$$\begin{aligned} \frac{\partial l(\mathcal{D})}{\partial s} &= \frac{\partial}{\partial s} \left\{ -\frac{1}{2} \left[N \log s + \frac{1}{s} RSS(\mathbf{w}) \right] \right\} \\ &= -\frac{1}{2} \left[\frac{N}{s} - \frac{1}{s^2} RSS(\mathbf{w}) \right] \\ &= -\frac{1}{2s} \left[N - \frac{1}{s} RSS(\mathbf{w}) \right] \end{aligned}$$

$$\frac{\partial l(\mathcal{D})}{\partial s} = 0 \Leftrightarrow s = \frac{1}{N} RSS(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N (y_n - \mathbf{w}^T \mathbf{x}_n)^2$$

The MLE of noise variance coincides with the average RSS:

$$\sigma_{\text{MLE}}^2 = \frac{1}{N} RSS(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N (y_n - \mathbf{w}^T \mathbf{x}_n)^2$$