

Linear Regression - 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 through residual sum of squares (no regularization):

$$J(\mathbf{w}) = RSS(\mathbf{w}) = \sum_{n=1}^N (y_n - \mathbf{w}^T \mathbf{x}_n)^2 = (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

Evaluation through residual sum of squares (l2-norm regularization):

$$\begin{aligned} J(\mathbf{w}) &= RSS(\mathbf{w}) + \lambda \sum_{d=1}^D w_d^2 \\ &= RSS(\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2 \\ &= (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2 \\ &= \mathbf{y}^T \mathbf{y} - 2\mathbf{w}^T (\mathbf{X}^T \mathbf{y}) + \mathbf{w}^T (\mathbf{X}^T \mathbf{X}) \mathbf{w} + \lambda \mathbf{w}^T \mathbf{w} \\ &= \mathbf{y}^T \mathbf{y} - 2\mathbf{w}^T (\mathbf{X}^T \mathbf{y}) + \mathbf{w}^T (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{D \times D}) \mathbf{w} \end{aligned}$$

Optimization (analytical/closed-form solution):

$$\nabla J(\mathbf{w}) = 0 \Rightarrow -2\mathbf{X}^T \mathbf{y} + 2(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{D \times D}) \mathbf{w} = 0 \Rightarrow \mathbf{w}^* = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{D \times D})^{-1} \mathbf{X}^T \mathbf{y}$$

Linear Regression - Noisy observation model

Assuming Gaussian noise and Gaussian prior on the weights

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

Model Posterior (given the observed data and the prior belief):

$$\begin{aligned} p(\mathbf{w}|\mathcal{D}) &= p(\mathcal{D}|\mathbf{w})p(\mathbf{w}) \\ &= \prod_{n=1}^N p(y_n|\mathbf{x}_n, \mathbf{w}) \prod_{d=1}^D p(w_d) \\ &= \prod_{n=1}^N \mathcal{N}(\mathbf{w}^T \mathbf{x}_n, \sigma^2) \prod_{d=1}^D \mathcal{N}(0, \tau^2) \\ &= \prod_{n=1}^N \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(y_n - \mathbf{w}^T \mathbf{x}_n)^2}{2\sigma^2}\right] \cdot \prod_{d=1}^D \frac{1}{\tau\sqrt{2\pi}} \exp\left(-\frac{w_d^2}{2\tau^2}\right) \end{aligned}$$

Performing logarithmic transformation

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

Optimization (analytical/closed-form solution):

$$\nabla_{\mathbf{w}}(\log p(\mathbf{w}|\mathcal{D})) = 0 \Rightarrow$$

$$-2\frac{1}{\sigma^2} \mathbf{X}^T \mathbf{y} + 2\frac{1}{\sigma^2} (\mathbf{X}^T \mathbf{X}) \mathbf{w} + 2\frac{1}{\tau^2} \mathbf{w} = 0 \Rightarrow$$

$$\left(\frac{1}{\sigma^2} \mathbf{X}^T \mathbf{X} + \frac{1}{\tau^2} \mathbf{I}_{D \times D} \right) \mathbf{w} - \frac{1}{\sigma^2} \mathbf{X}^T \mathbf{y} = 0$$

$$\left(\mathbf{X}^T \mathbf{X} + \frac{\sigma^2}{\tau^2} \mathbf{I}_{D \times D} \right) \mathbf{w} - \mathbf{X}^T \mathbf{y} = 0$$

$$\mathbf{w}^* = (\mathbf{X}^T \mathbf{X} + \frac{\sigma^2}{\tau^2} \mathbf{I}_{D \times D})^{-1} \mathbf{X}^T \mathbf{y}$$