07-280 Linear Regression

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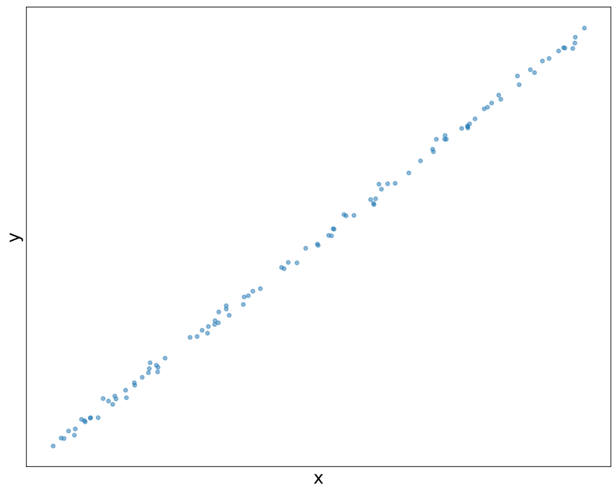
Say you have data: $\mathcal{X} = \mathbb{R}$, $\mathcal{Y} = \mathbb{R}$.



You may want to understand the data or predict y from x. Let's fit a line!

Recall ERM:

$$\arg\min_{h \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - h(x^{(i)}) \right)^2 \qquad \leftarrow \text{squared loss since we have real valued labels}$$

Here, $\mathcal{H}$ = all functions $\mathbb{R} \to \mathbb{R}$ that can be represented as a line.

How do these functions look like? Two parameters $\omega \in \mathbb{R}$, $b \in \mathbb{R}$

$$h_{\omega,b}(x) = x \cdot \omega + b$$

How do we find the best fitting line, i.e., the $\arg\min$ for ERM?

$$\arg\min_{\omega, b \in \mathbb{R}} \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - (x^{(i)} \cdot \omega + b) \right)^2$$

For ease of understanding, suppose we consider $b = 0$. In other words, we want $h(0) = 0$. Then:

$$\arg\min_{\omega \in \mathbb{R}} \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - x^{(i)} \cdot \omega \right)^2$$

$$= \arg\min_{\omega \in \mathbb{R}} \frac{1}{N} \left(\sum_{i=1}^{N} y^{(i)^2} + \omega^2 \sum_{i=1}^{N} x^{(i)^2} - 2\omega \sum_{i=1}^{N} y^{(i)} x^{(i)} \right)$$

(by completing the squares)

$$= \arg\min_{\omega \in \mathbb{R}} \left(\omega \sqrt{\sum_{i=1}^{N} x^{(i)^2}} - \frac{\sum_{i=1}^{N} y^{(i)} x^{(i)}}{\sqrt{\sum_{i=1}^{N} x^{(i)^2}}} \right)^2$$

This is minimized when this term is zero, i.e., $\omega \cdot \sum_{i=1}^{N} x^{(i)^2} - \sum_{i=1}^{N} y^{(i)} x^{(i)} = 0$

$\therefore$ Minimizer is $\omega = \frac{\sum_{i=1}^{N} y^{(i)} x^{(i)}}{\sum_{i=1}^{N} x^{(i)^2}}$. The resulting h is a line $y = \omega x$ with slope ω.

Let us now generalize this idea. Let $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \mathbb{R}$. Given training data $(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})$, we will consider functions $h : \mathbb{R}^d \to \mathbb{R}$ of the form $h(x) = x^T \omega + b$, where $\omega \in \mathbb{R}^d$ and $b \in \mathbb{R}$. Without loss of generality, assume first coordinate of x is fixed at 1. Let $\theta = \begin{bmatrix} b \\ \omega \end{bmatrix}$. Consider $h_\theta(x) = x^T \theta$.

Then ERM: $\arg\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - x^{(i)^T} \theta \right)^2$.

Let $X = \begin{bmatrix} \leftarrow & x^{(1)^T} & \rightarrow \\ \leftarrow & x^{(2)^T} & \rightarrow \\ & \vdots & \\ \leftarrow & x^{(N)^T} & \rightarrow \end{bmatrix}$, $y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)}. \end{bmatrix}$.

Then ERM is $\arg\min_{\theta} \frac{1}{N} \|y - X\theta\|_2^2$. (By the way, can you simply set $\theta = X^{-1} y$? No.)

Expanding the squared term, we get ERM:

$$\arg\min_{\theta} \, (y - X\theta)^T (y - X\theta)$$

$$= \arg\min_{\theta} \, y^T y - \theta^T X^T y - y^T X \theta + \theta^T X^T X \theta$$

$$= \arg\min_{\theta} \, -2\theta^T X^T y + \theta^T X^T X \theta.$$

Let $A = X^T X$, $b = X^T y$ (relating to our previous simpler scalar case, $X^T X$ is like $\sum x_i^2$, $X^T y$ is like $\sum x_i y_i$). Assume A is invertible.

Then ERM: $\arg\min_{\theta} \, -2\theta^T b + \theta^T A \theta + b^T A^{-1} b - b^T A^{-1} b$

$$= \arg\min_{\theta} \, (\theta - A^{-1} b)^T A (\theta - A^{-1} b) - b^T A^{-1} b$$

$$= \arg\min_{\theta} \, \|X(\theta - (X^T X)^{-1} X^T y)\|_2^2$$

Minimized when $\theta = (X^T X)^{-1} X^T y$.