

ML Assignment 1

Oishik Dasgupta

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Theorem: Prove that under gaussian noise assumption linear regression amounts to least squares.

Proof:

Let us assume that the target variables and the inputs are related via the equation

$$y_i = \theta^T x_i + \epsilon_i$$

where ϵ_i is an error term that captures either unmodelled effects or random noise. Let us further assume that the ϵ_i are distributed IID according to a Gaussian distribution with mean zero and some variance σ^2 . We can write this assumption as

$$\epsilon_i \sim N(0, \sigma^2)$$

i.e., the density of ϵ_i is given by

$$p(\epsilon_i) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\epsilon_i)^2}{2\sigma^2}\right)$$

This implies that

$$p(y_i|x_i;\theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - \theta^T x_i)^2}{2\sigma^2}\right)$$

The notation " $p(y_i|x_i;\theta)$ " indicates that this is the distribution of y_i given x_i and parameterized by θ . Note that we should not condition on $\theta(p(y_i|x_i;\theta))$, since θ is not a random variable. We can also write the distribution of y_i as $y_i|x_i;\theta \sim N(\theta^T x_i, \sigma^2)$.

Given X (the design matrix, which contains all the x_i 's) and θ , what is the distribution of the y_i 's? probability of the data is given by $p(\vec{y}|X;\theta)$. This quantity is typically viewed a function of \vec{y} (and perhaps X), for a fixed value

of θ . When we wish to explicitly view this as a function of θ , we will instead call it the likelihood function:

$$L(\theta) = L(\theta; X, \vec{y}) = p(\vec{y}|X; \theta)$$

Note that by the independence assumption on the ϵ_i 's (and hence also the y_i 's given the x_i 's), this can also be written

$$\begin{aligned} L(\theta) &= \prod_{i=1}^m p(y_i|x_i; \theta) \\ &= \prod_{i=1}^m \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - \theta^T x_i)^2}{2\sigma^2}\right) \end{aligned}$$

Now given this probabilistic model relating the y_i 's and the x_i 's, what is a reasonable way of choosing our best guess of the parameters θ ? The principle of maximum likelihood says that we should choose θ so as to make the data as high probability as possible. i.e., we should choose θ to maximize $L(\theta)$. Instead of maximizing $L(\theta)$, we can maximize any strictly increasing function of $L(\theta)$. In particular, the derivations will be a bit simpler if we instead maximize the log likelihood $l(\theta)$:

$$\begin{aligned} l(\theta) &= \log L(\theta) \\ &= \log \prod_{i=1}^m \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - \theta^T x_i)^2}{2\sigma^2}\right) \\ &= \sum_{i=1}^m \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - \theta^T x_i)^2}{2\sigma^2}\right) \\ &= m \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^m (y_i - \theta^T x_i)^2 \end{aligned}$$

Hence, maximizing $l(\theta)$ gives the same answer as minimizing

$$\frac{1}{2} \sum_{i=1}^m (y_i - \theta^T x_i)^2,$$

which we recognize to be $J(\theta)$, our original least-squares cost function.

To summarize: Under the previous probabilistic assumptions on the data, least-squares regression corresponds to finding the maximum likelihood estimate of θ . This is thus one set of assumptions under which least-squares regression can be justified as a very natural method that's just doing MLE.