Machine Learning Course - CS-433

Maximum Likelihood

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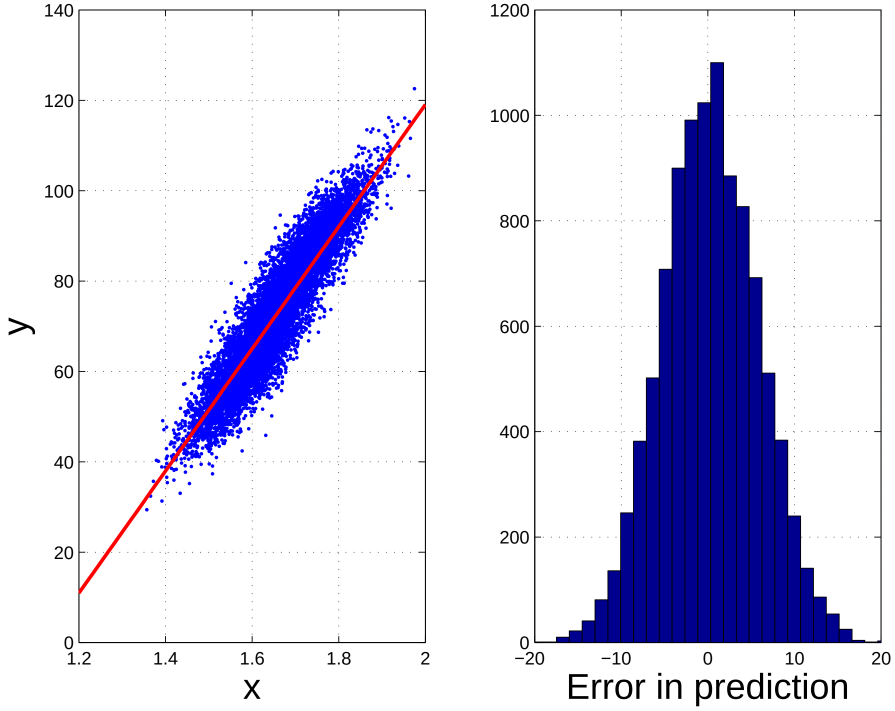
Motivation

In the previous lecture we arrived at the least-squares (LS) problem in the following way: we postulated a particular cost function (square loss) and then, given data, found that model that minimizes this cost function. In the current lecture we will take an alternative route. The final answer will be the same, but our starting point will be probabilistic. In this way we find a second interpretation of the LS problem.



Gaussian distribution and independence

Recall the definition of a Gaussian random variable in $\mathbb{R}$ with mean μ and variance σ^2. It has a density of

$$p(y \,|\, \mu, \sigma^2) = \mathcal{N}(y \,|\, \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y-\mu)^2}{2\sigma^2}\right].$$

In a similar manner, the density of a Gaussian random vector with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$ (which must be a positive semi-definite matrix) is

$$\mathcal{N}(\mathbf{y} \,|\, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^D \, det(\boldsymbol{\Sigma})}} \exp\left[-\tfrac{1}{2}(\mathbf{y}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{y}-\boldsymbol{\mu})\right].$$

Also recall that two random variables X and Y are called independent when their densities factor, $p(x, y) = p(x)p(y)$.

A probabilistic model for least-squares

We assume that our data is generated by the model,

$$y_n = \mathbf{x}_n^\top \mathbf{w} + \epsilon_n,$$

where the ϵ_n (the noise) is a zero-mean Gaussian random variable with variance σ^2 and the noise that is added to the various samples is independent of each other, and independent of the input. Note that the model $\mathbf{w}$ is unknown. Therefore, given N samples, the likelihood of the data vector $\mathbf{y} = (y_1, \cdots, y_N)$ given the input $\mathbf{x} = (x_1, \cdots, x_N)$ and the model $\mathbf{w}$ is equal to

$$p(\mathbf{y} \,|\, \mathbf{x}, \mathbf{w}) = \prod_{n=1}^{N} p(y_n \,|\, \mathbf{x}_n, \mathbf{w}) = \prod_{n=1}^{N} \mathcal{N}(y_n \,|\, \mathbf{x}_n^\top \mathbf{w}, \sigma^2).$$

The probabilistic view point is that we should maximize this likelihood over the choice of model $\mathbf{w}$. I.e., the “best” model is the one that maximizes this likelihood.

Defining cost with log-likelihood

Instead of maximizing the likelihood, we can take the logarithm of the likelihood and maximize it instead. Not surprisingly the resulting expression is called the log-likelihood (LL). As mentioned, we take this as our cost function that should be maximized. We get

$$\mathcal{L}_{LL}(\mathbf{w}) := \log\, p(\mathbf{y} \,|\, \mathbf{X}, \mathbf{w}) = -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \text{cnst}.$$

Compare the LL to the MSE (mean squared error) that we discussed in our last lecture:

$$\begin{aligned} \mathcal{L}_{LL}(\mathbf{w}) &= -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \text{cnst} \\ \mathcal{L}_{MSE}(\mathbf{w}) &= \frac{1}{2N} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 \end{aligned}$$

It is clear that maximizing the LL is equivalent to minimizing the MSE. Since we maximize the likelihood (log-likelihood), the model that we get when peforming this maximization, is called the *maximum-likelihood estimage* (MLE). We will therefore write in the sequel the acronym MLE instead of LL. So we have

$$\arg\min_{\mathbf{w}} \mathcal{L}_{MSE}(\mathbf{w}) = \arg\max_{\mathbf{w}} \mathcal{L}_{MLE}(\mathbf{w}).$$

This gives us an alternative interpretation of the LS problem. This interpretation has some advantages that we discuss now.

Properties of MLE

Let us just mention, the following basic fundamental properties of ML estimators. The proofs of these properties is

beyond the scope of this course but these statements show why it might be a good idea to use this criterion in the first place.
Note that the MLE cost function is a *sample* approximation to the *expected log-likelihood*:

$$\mathcal{L}_{LL}(\mathbf{w}) \approx \mathbb{E}_{p(y,\mathbf{x})}\big[\log p(y \,|\, \mathbf{x}, \mathbf{w})\big]$$

Because of the above, one can show that under some conditions the MLE estimate is consistent, i.e., it will give us the correct model assuming that we have a sufficient amount of data.

$$\mathbf{w}_{MLE} \;\longrightarrow^{p}\; \mathbf{w}_{TRUE} \quad \text{in probability}$$

Why should this be true? Note that for every parameter $\mathbf{w}$ the empirical log-likelihood converges (in probability) to the true log-likelihood (the expected value). Assume that the true log-likelihood has a unique maximizer, that it is smooth, and that the convergence is uniform over all parameters. It is then intuitive that the maximum of the empirical log-lilihood converges to the maximum of the true loglikelihood as the number of samples tends to infinity.
Much more is true under suitable conditions. The MLE is asymptotically normal, i.e.,

$$(\mathbf{w}_{MLE} - \mathbf{w}_{TRUE}) \;\longrightarrow^{d}\; \frac{1}{\sqrt{N}}\mathcal{N}(\mathbf{w}_{MLE} \,|\, \mathbf{0}, \mathbf{F}^{-1}(\mathbf{w}_{TRUE}))$$

where $\mathbf{F}(\mathbf{w}) = -\mathbb{E}_{p(\mathbf{y})}\left[\frac{\partial^2 \mathcal{L}}{\partial \mathbf{w} \partial \mathbf{w}^\top}\right]$ is the Fisher information.
MLE is efficient, i.e. it achieves the Cramer-Rao lower bound.

$$\text{Covariance}(\mathbf{w}_{MLE}) = \mathbf{F}^{-1}(\mathbf{w}_{TRUE})$$

Another example

In the above derivation we assumed that the noise is Gaussian. But this is not the only possible choice. It is instructive to rederive the expression assuming instead a Lapace distribution:

$$p(y_n \mid \mathbf{x}_n, \mathbf{w}) = \frac{1}{2b} e^{-\frac{1}{b}|y_n - \mathbf{x}_n^\top \mathbf{w}|}$$