Loss functions

Introduction

In this article, we will focus on the selection of loss functions for regression and classifications tasks. First, we justify minimizing the mean square error (MSE) as loss function for linear regression. We will proceed from the statement of the regression as a task with an infinite number of outcomes, thereby naturally assuming that the loss function in this case will be continuous. In contrast, the task of classification has a discrete number of outcomes, and its loss function does not have the same nature as for regression. We will introduce a metric on the distribution space approximating the classification values, and show that although the introduced value may not have all the properties of the metric, it can nevertheless serve to determine the “distance” between distributions, that is, it can be successfully used as loss function. The considered quantity called *cross entropy*, and it is widely used in commercial libraries (TensorFlow, PyTorch) when constructing classification models.

1. Maximum likelihood estimation (MLE) and KL Divergence

There are many ways to introduce a metric on a distribution space. Some metrics were borrowed from functional analysis, while others, due to their special properties, were introduced for special cases. Such cases include pre-metrics that satisfy only part of the axiomatics of metrics, but however, they are often used to specify the topology of the distribution space, and to some extent play the role of the distance on it. Such is the pre-metric that is known from information theory: the Kullback-Leibler divergence. For discrete distributions, it is defined as

$$D_{KL}(P||Q) = \sum_{x \in X} P(x)\log(\frac{P(x)}{Q(x)}) \quad (1)$$

And for continuous distributions:

$$D_{KL}(P||Q) = \int_{\infty}^{-\infty} p(x)\log(\frac{p(x)}{q(x)})dx$$

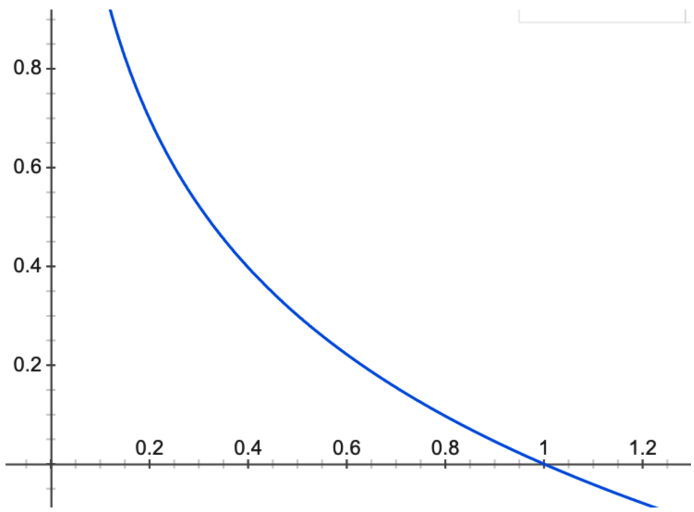
This divergence is not symmetrical and does not satisfy the triangle inequality:

$$D_{KL}(P||Q) \neq D_{KL}(Q||P)$$

The only fact that the Kullback-Leibler divergence is related to the metric is that it is not negative and is equal to zero only for $P = Q$ almost everywhere.

In order to explain the meaning of the introduced quantity, let us step back a step and try to formalise the intuitive idea that the amount of information that an event carries is the greater the less this event, i.e. the less likely the event, the more informative it is.

This is expressed well by the function on the graph below:



The probability of the event is plotted on the x axis, its “amount of information" on the y axis. You can notice that this function on the segment $[0 \leq x \leq 1]$ fits perfectly to the given intuitive expression.

1. It takes 0 on a value of 1 - the maximum allowable probability value, i.e. the information contained in the event that is certain to happen (with probability 1) is zero.
2. The lower the probability of an event, the greater its information: $\lim\limits_{x \to +0} = \infty$
3. $\forall x \in [0 \geq x \geq 1] : I(x) \geq 0$

The considered value was introduced by C. Shannon in the epoch-making work [4], and received the name of the event’s *self information*:

$$I(x) = -\,logp(x)$$

It is easily generalised from a single event to the entire (discrete) distribution:

$$H(X) = -\sum_{i=1}^{m} p(x) \times \log p(x)$$

In this case, it is called the *entropy* (*information entropy*) of a random variable.

Considering entropy as a measure of chaos or distribution uncertainty, we now note its features for known distributions.

1. In general, an non-uniform distribution has less entropy than a uniform

2. The uniform distribution has the largest entropy of all possible:
$H(P) = -\sum_{i=1}^{n} \frac{1}{n} \log \frac{1}{n} = -\frac{n}{n}(-\log n) = \log n$, where n is the number of tests.

3. The entropy of Gaussian:
$H(P) = \ln(\sigma\sqrt{2\pi e})$ independent of the mean. (This is calculated using the discrete Abel transform or integration by parts for the continuous case).

4. The Laplace distribution (double exponential), which is often used as the limit distribution in schemes of summing a random number of random variables, has entropy:
$H(X) = -\int_{-\infty}^{+\infty} \frac{2}{\lambda} e^{-\lambda|x-a|} \log \frac{2}{\lambda} e^{-\lambda|x-a|} dx = \log \frac{2}{\lambda}$ also independent of the mean.
(Calculated by the same way)

5. Finally, the entropy of the binomial distribution:

$$H(X) = \sum_{m=0}^{n} C_n^m p^m q^{n-m} \log(C_n^m p^m q^{n-m})^{-1} = -\sum_{m=0}^{n} C_n^m p^m q^{n-m} \left[\log C_n^m + m \log p + (n-m)\log q\right] =$$

$$= -\sum_{m=1}^{n} C_n^m p^m q^{n-m} \log C_n^m - n(p \log p + q \log q)\,.$$

Generally speaking, informational entropy is deeply related to physical entropy. Nature seems to us not to be orderly, i.e. any manifestations of the organized structure of physical space can be considered as manifestations of a temporary anomaly. The uniform distribution of properties with its maximum entropy is, in fact, the essence of the second law of thermodynamics.

When comparing the two distributions, it makes sense to consider the *cross entropy*, which is defined as:

$$H(P,Q) = -\sum_{x \in X} p(x_i) \log q(x_i)$$

There are no problems with generalising the introduced values to continuous distributions. In this case, the quantity under consideration is called *differential entropy* and is derived as the first term of the asymptotic expansion of entropy [5].

Here, we are primarily interested in the discrete case, so let us return to the Kullback-Leibler divergence and write out its discrete form in more detail:

$$D_{KL}(P||Q) = \sum_{x \in X} P(x) \log(\frac{P(x)}{Q(x)}) = -\sum_{x \in X} p(x) \log q(x) + \sum_{x \in X} p(x) \log p(x) = H(P,Q) - H(P)$$

where $H(P,Q)$ - cross entropy between P and Q, $H(P)$ - entropy of P.

For now, as an important milestone, we have:

$$D_{KL}(P||Q) = H(P,Q) - H(P) \quad (2)$$

Kullback-Leibler divergence also applies to continuous distributions. For example, we find a Kullback-Leibler divergence between two normal distributions $p(x) = \mathbb{N}(x | \mu_1, \sigma_1)$ and $q(x) = \mathbb{N}(x | \mu_2, \sigma_2)$ (PRML, Bishop ex. 1.30, p.64)

$$D_{KL}(p||q) = -\int p(x) \log q(x) dx + \int p(x) \log p(x) dx =$$

$$= \frac{1}{2} \log(2\pi\sigma_2^2) + \frac{\sigma_1^2 + (\mu_1 - \mu_2)^2}{2\sigma_2^2} - \frac{1}{2}(1 + \log 2\pi\sigma_1^2) =$$

$$= \log \frac{\sigma_2}{\sigma_1} + \frac{\sigma_1^2 + (\mu_1 - \mu_2)^2}{2\sigma_2^2} - \frac{1}{2}$$

The last expression gives 0 when $\mu_1 = \mu_2$ and $\sigma_1 = \sigma_2$.

For further discussion, recall the definition of the likelihood function. It is a function of the distribution parameter $f_x(x | \theta) : \Theta \to R$ and defined as:

$$\Theta_{ML} = \prod_{i=1}^{\infty} p(x_i | \theta)$$

Here $p(x_i)$ it can be chosen either as a CDF (Cumulative Distribution Function, or **as a PDF (Probability DensityFunction)**

Its argmax will not change during logarithm, so:

$$\Theta_{ML} = \arg\max_{\Theta} \prod_{i=1}^{m} p_{model}(x_i, \Theta) = \arg\max_{\Theta} \sum_{i \div 1}^{m} \log p_{model}(x_i, \Theta)$$

Argmax will not change also when divided by m, therefore:

$$\Theta_{ML} = arg \max_{\Theta} \mathbb{E} \log p_{model}(x, \Theta)$$ **(3)**

Now, recalling **(1)**, we can write:

$$D_{KL}(P_{data} || P_{model}) = \mathbb{E}_{data}[\log p_{data}(x) - \log p_{model}(x)]$$

but since the left term of the resulting expression does not depend on P_{model}, in minimising the divergence, we actually only have to minimise

$$-\mathbb{E}[\log p_{model}(x)]$$

which coincides with **(3)**

Thus, **maximising the likelihood is equivalent to minimising the Kullback-Leibler divergence.**

2. Maximum likelihood estimation (MLE) and linear regression2. Maximum likelihood estimation (MLE) and linear regression

2.1 Linear regression with normal noise

If we consider linear regression in the form:

$Y = w^T X + \epsilon$ **(4)**

where ϵ - normally distributed random variable (noise) with expected value μ and dispersion σ, i.e. $\epsilon \sim N(\mu, \sigma^2)$, then the values of Y are also distributed normally with a probability density corresponding to a multidimensional normal distribution. The likelihood function of such a distribution, in which the probability density is used, takes the form

$$L(\Theta) = \prod_{i=1}^{m} p(y_i | x_i; w, \sigma) = \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} \times e^{-\frac{(y_i - w_i x_i)^2}{2\sigma^2}},$$

where Θ - vector(w, σ).

After logarithm (because $\log(\prod_{i=1}^{m} a_i b_i) = \sum_{i=1}^{m} \log a_i b_i$) this gives:

$$\ln \prod_{i=1}^{m} p(y_i | x_i; w, \sigma) = \sum_{i=1}^{m} \ln p(y_i | x_i; w, \sigma) = \sum_{i=1}^{m} \ln[\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(\frac{y_i - \hat{y}_i}{\sigma})^2}] =$$
$$= \sum_{i=1}^{m} [\ln(2\pi\sigma^2)^{-\frac{1}{2}} + \ln e^{-\frac{1}{2}(\frac{y_i - \hat{y}_i}{\sigma})^2}] = \sum_{i=1}^{m} [-\frac{1}{2} \ln(2\pi) - \log \sigma - \frac{1}{2\sigma^2}(y_i - \hat{y}_i)^2] =$$
$$= -\frac{m}{2} \log(2\pi) - m \ln \sigma - \frac{1}{2\sigma^2} \sum_{i=1}^{m} (y_i - \hat{y}_i)^2$$

where $\hat{y}_i$ - model calculation result for an element x_i, a m - number of sample items. But since the first two members of the right-hand side of the last expression are independent of the model parameters (σ - constant), then you can write

$$\Theta_{ML} = \arg\max_{\Theta} - \sum_{i=1}^{m} \frac{1}{2} | y_i - \hat{y}_i |^2 = \min \sum_{i=1}^{m} | y_i - \hat{y} |^2$$

Comparing this expression with the definition of the mean square error:

$$MSE = \frac{1}{m} \sum_{i=1}^{m} | \hat{y}_i - y_i |^2$$

you can easily see that the likelihood maximisation relative to the desired vector Θ is, in fact, minimization of the mean square error for the same parameters.
Which, in fact, shows that MSE is the optimal function of the linear regression error.

2.2 Linear regression with Laplace noise

If the noise in linear regression has a Laplace distribution:

$$p(x) = \frac{\alpha}{2} e^{-\alpha|x-\beta|}$$

with zero mean ($\beta = 0$), then the logarithmic maximum likelihood estimation gives:

$$Q_{ML} = \arg\min_q \frac{1}{m} \sum_{i=1}^{m} |a(x_i) - y_i|$$

i.e.. Mean Absolute Error (MAE).

2.3 Recapitulation

Thus, linear regression can be defined without assuming a normal noise distribution. Its parameters can be calculated according to standard deviation (MSE), however, this method will be optimal only in the case of a normal distribution.

Literature

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