

A Tiny Lecture. Where Do Loss Functions Come From?

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Given a dataset $\{x_i, y_i\}$, i = 1, 2, ..., N. Consider a model \mathbf{f} which maps each i^{th} sample $x_i \in \mathbb{R}$ into the hypothesis (prediction) $h_i \in (0, 1)$ which in turn should be close to the label $y_i \in \{0, 1\}$.

- 1 The model inputs a sample x_i
- 2 And outputs a prediction h_i which should be close to y_i

To Train a Model means minimizing a loss function



Goals

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The goals of this lecture are:

- 1 To demonstrate the grounds of loss functions in AI
- 2 To generalize the loss functions intuition



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Section 2. Recap



Probability Mass Distribution

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A **probability mass distribution** is a function $p(x_i)$ that satisfies the following two properties:

1 Non-Negativity: The probability mass function is non-negative for all possible values of x_i :

$$p(x_i) \ge 0$$
 for all x_i .

Normalization: The sum of the probabilities over all possible values of x is equal to one:

$$\sum_{i} p(x_{i}) = 1.$$



Product Rule for the joint probability

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The **product rule** (or chain rule) for the joint probability of N variables x_1, x_2, \ldots, x_N is given by:

$$p(x_1, x_2, \ldots, x_N) = p(x_1) \cdot p(x_2 \mid x_1) \cdot p(x_3 \mid x_1, x_2) \ldots p(x_N \mid x_1, x_2, \ldots, x_{N-1}).$$

If the variables $x_1, x_2, ..., x_N$ are <u>independent and identically distributed</u> (i.i.d.), the joint probability takes the form:

$$p(x_1,x_2,\ldots,x_N)=p(x_1)\cdot p(x_2)\cdot p(x_3)\ldots p(x_N).$$



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Section 3. Loss Functions



Binary Cross-Entropy (BCE) Loss Intuition

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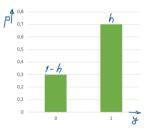


Figure: The Bernoulli distribution Bishop and Nasrabadi (2006); Prince (2023).

Derivation of BCE Loss from MLE

For a pair (x_i, y_i) , the Bernoulli distribution takes the form:

$$p(y_i \mid h_i) = h_i^{y_i} (1 - h_i)^{1 - y_i}.$$

This represents the probability of observing y_i given the predicted probability h_i .

For a dataset of N i.i.d. pairs, the joint probability is:

$$P(y_1, y_2, \dots, y_N \mid h_1, h_2, \dots, h_N) = \prod_{i=1}^N h_i^{y_i} (1 - h_i)^{1 - y_i} \to \max.$$

Then we take the negative logarithm of the joint probability:

$$-\log P = -\sum_{i=1}^N \left[y_i \log h_i + (1-y_i) \log (1-h_i)\right] o \min.$$





Binary Cross-Entropy (BCE) Loss Intuition

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Figure: The BCE loss values intuition concerning the predictions and labels Prince (2023); Goodfellow et al. (2016).

Derivation of BCE Loss from MLE

The Binary Cross-Entropy (BCE) loss can be derived from Maximum Likelihood Estimation (MLE) for binary classification problems. Given a set of predictions \hat{y}_i and true labels y_i , the BCE loss is defined as:

$$\mathcal{L}_{BCE} = -\frac{1}{N} \sum_{i=1}^{N} \left[y_i \log h_i + (1 - y_i) \log(1 - h_i) \right],$$

where:

- N is the number of samples,
- $y_i \in \{0,1\}$ is the true label,
- $h_i \in (0,1)$ is the predicted probability.



An Uncertainty Aware Binary Cross-Entropy (UBCE) Loss Intuition

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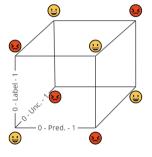


Figure: The UBCE loss values intuition concerning the predictions, the labels, and the uncertainties .

Derivation of BCE Loss from MLE

The Binary Cross-Entropy (BCE) loss can be derived from Maximum Likelihood Estimation (MLE) for binary classification problems. Given a set of predictions \hat{y}_i and true labels y_i , the BCE loss is defined as:

$$\mathcal{L}_{\mathsf{UBCE}} = -?$$

where:

- N is the number of samples.
- $y_i \in \{0,1\}$ is the true label,
- $h_i \in (0,1)$ is the predicted probability,
- $u_i \in (0,1)$ is the uncertainty of the prediction.



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Recipe for constructing loss functions by Prince (2023)

- Choose a suitable probability distribution defined over the domain of the predictions
- 2 Set the machine learning model to predict
- 3 To train the model, find the model parameters that minimize the negative log-likelihood loss function over the training dataset pairs
- 4 to perform inference for a new test sample, return either the full distribution or the value where this distribution is maximized.



Bibliography

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