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Understanding binary cross-entropy / log loss: a visual explanation



Photo by G. Crescoli on Unsplash

Introduction

If you are training a **binary classifier**, chances are you are using **binary cros entropy** / **log loss** as your loss function.

Have you ever thought about **what exactly does it mean** to use this loss function? The thing is, given the ease of use of today's libraries and frameworks, it is **very easy** to **overlook the true meaning of the loss function** used.

Motivation

I was looking for a blog post that would explain the concepts behind **binary cross-entropy** / **log loss** in a **visually clear and concise manner**, so I could show it to my students at <u>Data Science Retreat</u>. Since I could not find any that would fit my purpose, I took the task of writing it myself:-)

A Simple Classification Problem

Let's start with 10 random points:

$$x = [-2.2, -1.4, -0.8, 0.2, 0.4, 0.8, 1.2, 2.2, 2.9, 4.6]$$

This is our only **feature**: *x*.

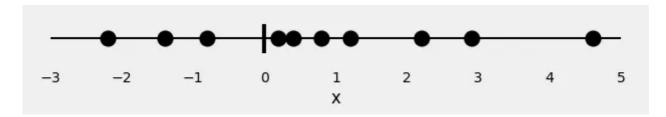


Figure 0: the feature

Now, let's assign some colors to our points: red and green. These are our labels.

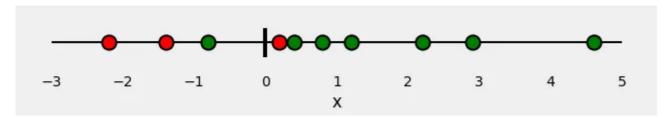


Figure 1: the data

So, our classification problem is quite straightforward: given our **feature** *x*, we need to predict its **label**: **red** or **green**.

Since this is a binary classification, we can also pose this problem as: "is the point green" or, even better, "what is the probability of the point being green"? Ideally,

green points would have a probability of 1.0 (of being green), while red points would have a probability of 0.0 (of being green).

In this setting, **green points** belong to the **positive class** (YES, they are green), while **red points** belong to the **negative class** (NO, they are not green).

If we fit a model to perform this classification, it will predict a probability of being green to each one of our points. Given what we know about the color of the points, how can we evaluate how good (or bad) are the predicted probabilities? This is the whole purpose of the loss function! It should return high values for bad predictions and low values for good predictions.

For a binary classification like our example, the typical loss function is the binary cross-entropy / log loss.

Loss Function: Binary Cross-Entropy / Log Loss

If you look this **loss function** up, this is what you'll find:

$$H_p(q) = -\frac{1}{N} \sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

Binary Cross-Entropy / Log Loss

where y is the label (1 for green points and 0 for red points) and p(y) is the predicted probability of the point being green for all N points.

Reading this formula, it tells you that, for each **green** point (y=1), it adds log(p(y)) to the loss, that is, the **log probability of it being green**. Conversely, it adds log(1-p(y)), that is, the **log probability of it being red**, for each **red** point (y=0). Not necessarily difficult, sure, but no so intuitive too...

Besides, what does **entropy** have to do with all this? Why are we taking **log of probabilities** in the first place? These are valid questions and I hope to answer them on the "*Show me the math*" section below.

But, before going into more formulas, let me show you a **visual representation** of the formula above...

Computing the Loss — the visual way

First, let's **split** the points according to their classes, **positive** or **negative**, like the figure below:

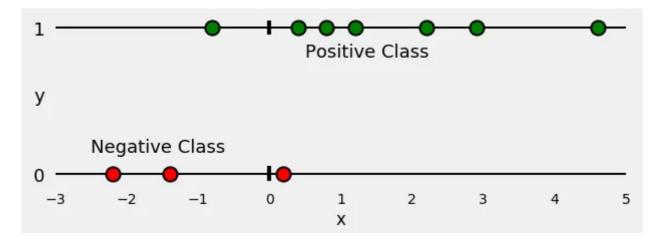


Figure 2: splitting the data!

Now, let's train a **Logistic Regression** to classify our points. The fitted regression is a *sigmoid curve* representing the **probability of a point being green for any given** x. It looks like this:

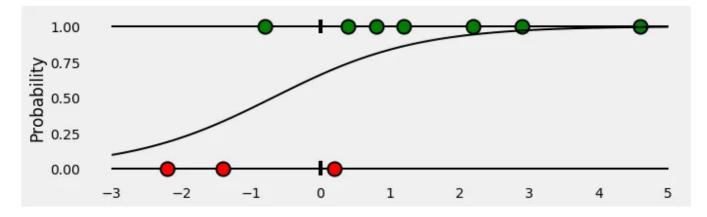


Figure 3: fitting a Logistic Regression

Then, for all points belonging to the **positive class** (**green**), what are the predicted **probabilities** given by our classifier? These are the **green bars under** the *sigmoid curve*, at the *x* coordinates corresponding to the points.

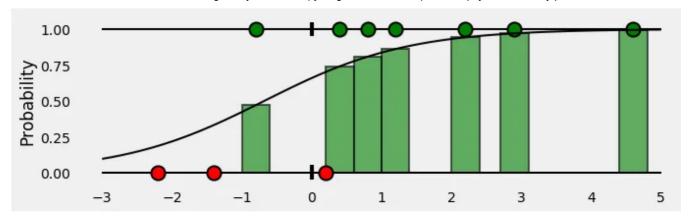


Figure 4: probabilities of classifying points in the POSITIVE class correctly

OK, so far, so good! What about the points in the **negative class**? Remember, the **green bars under** *the sigmoid curve* represent the probability of a given point being **green**. So, what is the probability of a given point being **red**? The **red bars ABOVE** *the sigmoid curve*, of course :-)

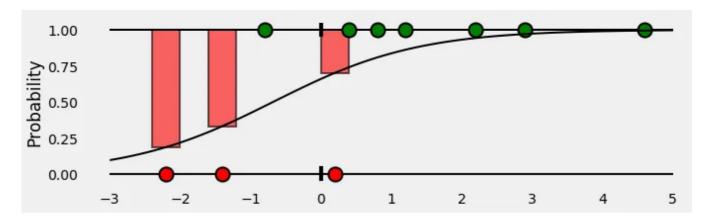


Figure 5: probabilities of classifying points in the NEGATIVE class correctly

Putting it all together, we end up with something like this:

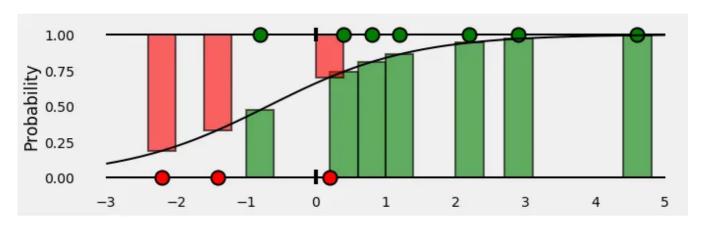


Figure 6: all probabilities put together!

The bars represent the **predicted probabilities** associated with the corresponding **true class** of each point!

OK, we have the predicted probabilities... time to **evaluate** them by computing the **binary cross-entropy** / **log loss!**

These **probabilities** are all we need, so, let's **get** rid of the *x* axis and bring the bars next to each other:

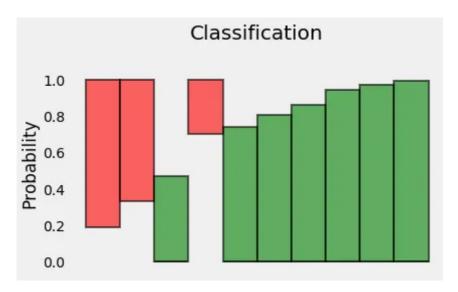


Figure 7: probabilities of all points

Well, the *hanging bars* don't make much sense anymore, so let's **reposition them**:

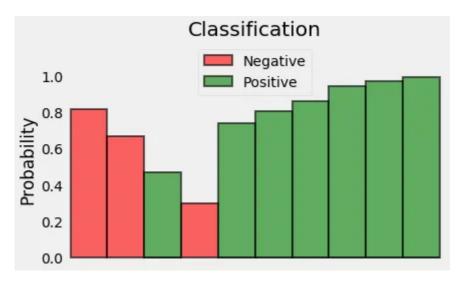


Figure 8: probabilities of all points — much better :-)

Since we're trying to compute a **loss**, we need to penalize bad predictions, right? If the **probability** associated with the **true class** is **1.0**, we need its **loss** to be **zero**. Conversely, if that **probability is low**, say, **0.01**, we need its **loss** to be **HUGE**!

It turns out, taking the (negative) log of the probability suits us well enough for this purpose (since the log of values between 0.0 and 1.0 is negative, we take the negative log to obtain a positive value for the loss).

Actually, the reason we use **log** for this comes from the definition of **cross-entropy**, please check the "Show me the math" section below for more details.

The plot below gives us a clear picture —as the **predicted probability** of the **true** class gets closer to zero, the loss increases exponentially:

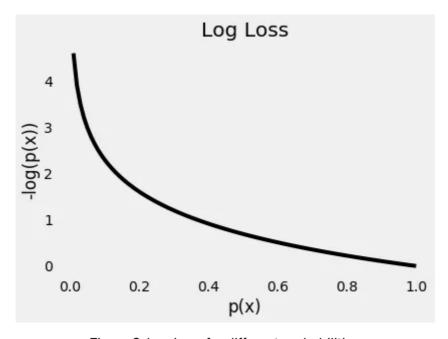
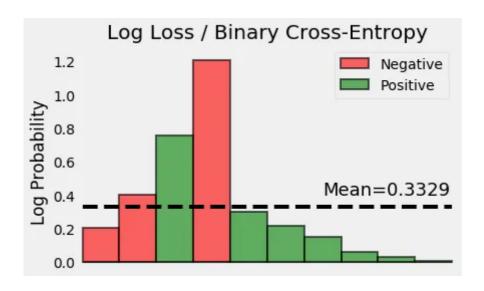


Figure 9: Log Loss for different probabilities

Fair enough! Let's take the (negative) log of the probabilities — these are the corresponding losses of each and every point.

Finally, we compute the mean of all these losses.



Voilà! We have successfully computed the binary cross-entropy / log loss of this toy example. It is 0.3329!

Show me the code

If you want to **double check the value** we found, just **run the code** below and see for yourself:-)

Show me the math (really?!)

Jokes aside, this post is **not** intended to be very mathematically inclined... but for those of you, my readers, looking to understand the role of **entropy**, **logarithms** in

all this, here we go :-)

If you want to go deeper into **information theory**, including all these concepts — entropy, cross-entropy and much, much more — check **Chris Olah's** <u>post</u> out, it is incredibly detailed!

Distribution

Let's start with the distribution of our points. Since y represents the **classes** of our points (we have 3 red points and 7 green points), this is what its distribution, let's call it q(y), looks like:

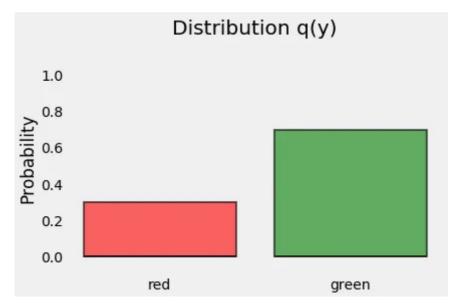


Figure 11: q(y), the distribution of our points

Entropy

Entropy is a measure of the uncertainty associated with a given distribution q(y).

What if all our points were green? What would be the uncertainty of that distribution? ZERO, right? After all, there would be no doubt about the color of a point: it is always green! So, entropy is zero!

On the other hand, what if we knew exactly **half of the points** were **green** and the **other half**, **red**? That's the **worst case** scenario, right? We would have absolutely **no edge on guessing the color** of a point: it is totally **random**! For that case, entropy is given by the formula below (*we have two classes (colors*)— *red or green* — *hence*, 2):

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For every other case in between, we can compute the entropy of a distribution, like our q(y), using the formula below, where C is the number of classes:

$$H(q) = -\sum_{c=1}^{C} q(y_c) \cdot log(q(y_c))$$

Entropy

So, if we *know* the **true distribution** of a random variable, we can compute its **entropy**. But, if that's the case, *why bother training a classifier* in the first place? After all, we **KNOW** the true distribution...

But, what if we **DON'T**? Can we try to **approximate the true distribution** with some **other distribution**, say, **p(y)**? Sure we can! :-)

Cross-Entropy

Let's assume our **points follow** this **other** distribution p(y). But we know they are **actually coming** from the **true** (unknown) distribution q(y), right?

If we compute **entropy** like this, we are actually computing the **cross-entropy** between both distributions:

$$H_p(q) = -\sum_{c=1}^{C} q(y_c) \cdot log(p(y_c))$$

Cross-Entropy

If we, somewhat miraculously, match p(y) to q(y) perfectly, the computed values for both **cross-entropy** and **entropy** will match as well.

Since this is likely never happening, **cross-entropy** will have a BIGGER value than the entropy computed on the true distribution.

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$$\bigcirc$$
 55 | $H_p(q) - H(q) >= 0$

Cross-Entropy minus Entropy

It turns out, this difference between **cross-entropy** and **entropy** has a name...

Kullback-Leibler Divergence

The Kullback-Leibler Divergence, or "KL Divergence" for short, is a measure of dissimilarity between two distributions:

$$D_{KL}(q||p) = H_p(q) - H(q) = \sum_{c=1}^{C} q(y_c) \cdot [log(q(y_c)) - log(p(y_c))]$$

KL Divergence

This means that, the **closer p**(**y**) **gets to q**(**y**), the **lower** the **divergence** and, consequently, the **cross-entropy**, will be.

So, we need to find a good p(y) to use... but, this is what our **classifier** should do, isn't it?! And indeed it does! It looks for the **best possible** p(y), which is the one that minimizes the cross-entropy.

Loss Function

During its training, the **classifier** uses each of the **N points** in its training set to compute the **cross-entropy** loss, effectively **fitting the distribution p(y)!** Since the probability of each point is 1/N, cross-entropy is given by:

$$q(y_i) = \frac{1}{N} \Rightarrow H_p(q) = -\frac{1}{N} \sum_{i=1}^{N} log(p(y_i))$$

Cross-Entropy —point by point

Remember Figures 6 to 10 above? We need to compute the **cross-entropy** on top of the *probabilities associated with the true class* of each point. It means using the **green** bars for the points in the **positive class** (y=1) and the **red** *hanging* bars for the points in the **negative class** (y=0) or, mathematically speaking:

$$y_i = 1 \Rightarrow log(p(y_i))$$

 $y_i = 0 \Rightarrow log(1 - p(y_i))$

Mathematical expression corresponding to Figure 10:-)

The final step is to compute the **average** of all points in both classes, **positive** and **negative**:

$$H_p(q) = -\frac{1}{(N_{pos} + N_{neg})} \left[\sum_{i=1}^{N_{pos}} log(p(y_i)) + \sum_{i=1}^{N_{neg}} log(1 - p(y_i)) \right]$$

Binary Cross-Entropy — computed over positive and negative classes

Finally, with a little bit of manipulation, we can take any point, **either from the positive or negative classes**, under the same formula:

$$H_p(q) = -\frac{1}{N} \sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

Binary Cross-Entropy — the usual formula

Voilà! We got back to the original formula for binary cross-entropy / log loss :-)

Final Thoughts

I truly hope this post was able **shine some new light** on a concept that is quite often taken for granted, that of **binary cross-entropy** as **loss function**. Moreover, I also hope it served to show you a little bit how **Machine Learning** and **Information Theory** are linked together.

Update July 10th, 2022: I've just published a YouTube video with an animated version of this post — check it out!

Understanding Binary Cross-Entropy / Log Loss in 5 minutes: a visual ex...



Machine Learning Classification Entropy Loss Function Towards Data Science

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