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

Daniel Godoy
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Introduction

If you are training a **binary classifier**, chances are you are using **binary cross-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 Data Science Retreat. 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***.

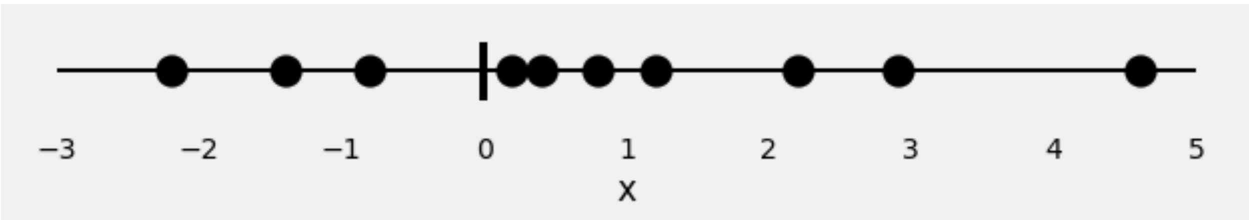


Figure 0: the feature

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

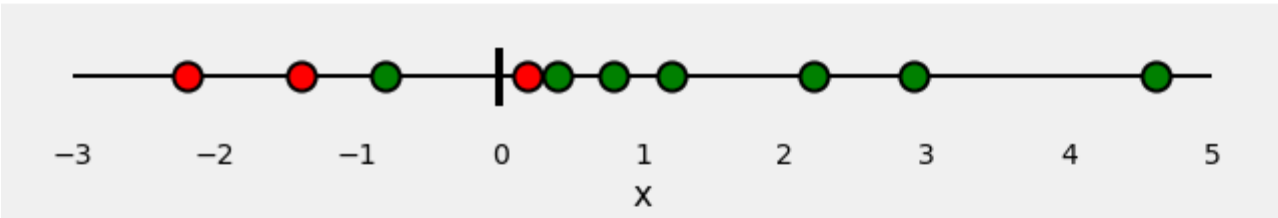


Figure 1: the data

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.

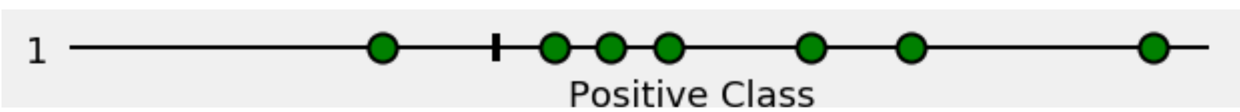
Reading this formula, it tells you that, for each **green** point (*y=1*), it adds *log(p(y))* to the loss, that is, the **log probability of it being green**. Conversely, it adds *log(1-p(y))*, that is, the **log probability of it being red**, for each **red** point (*y=0*). Not necessarily difficult, 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:



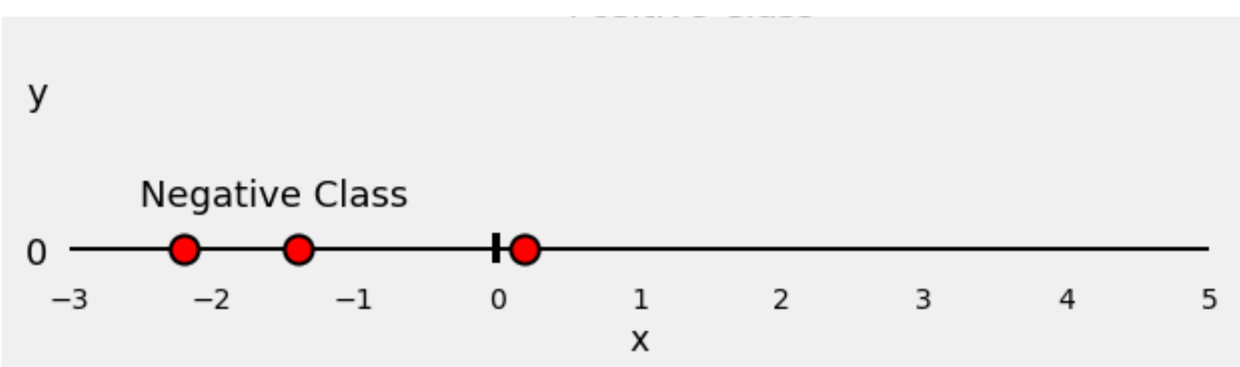


Figure 2: splitting the data!

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:

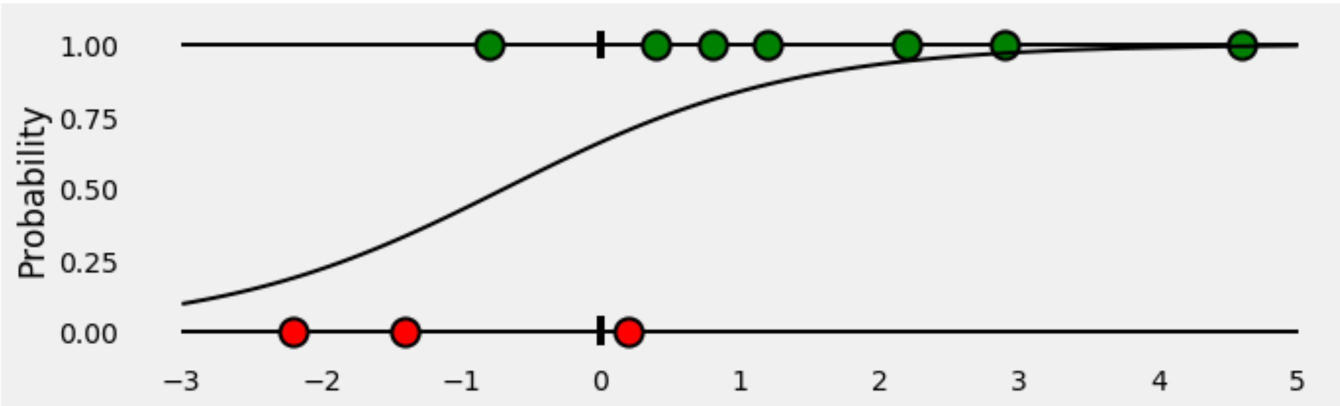


Figure 3: fitting a Logistic Regression

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.

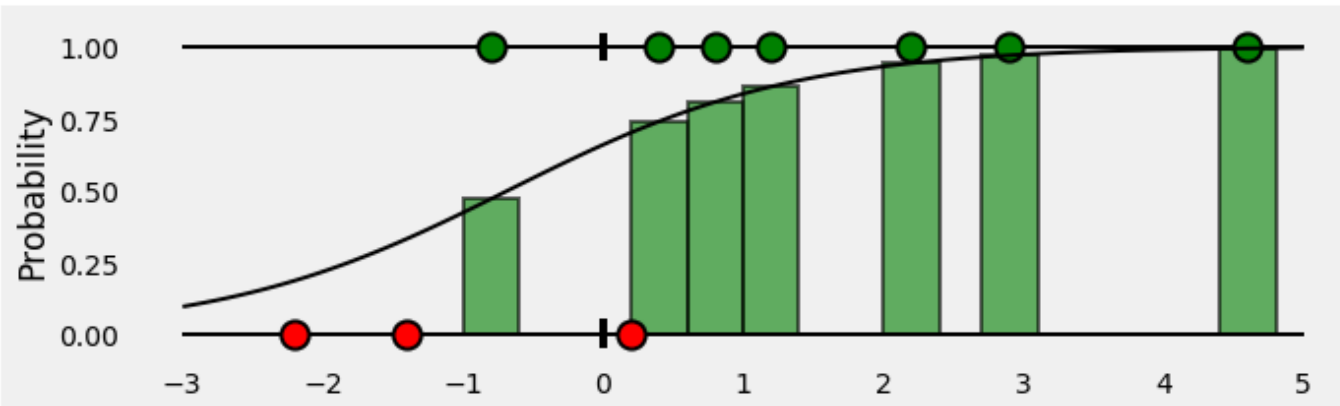


Figure 4: probabilities of classifying points in the POSITIVE class correctly

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 :-)

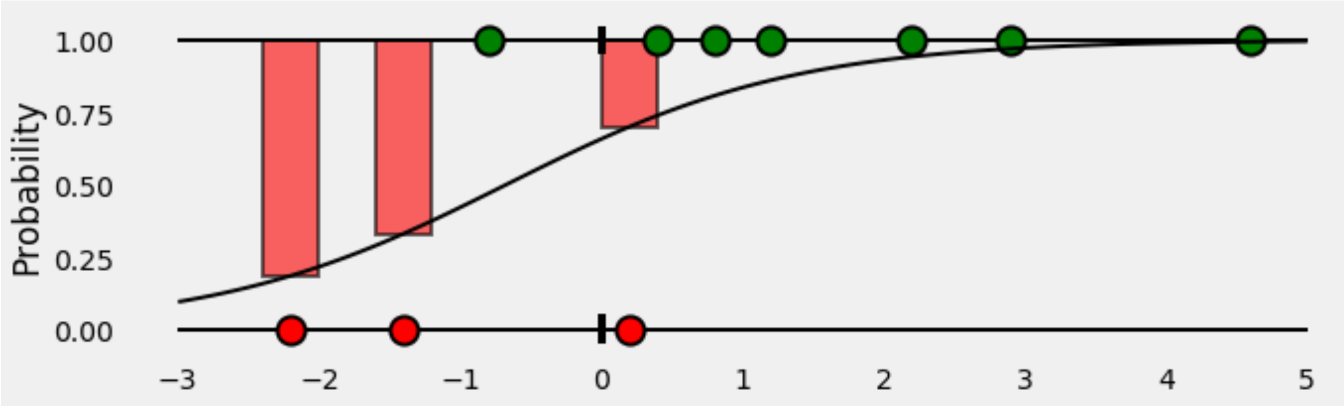


Figure 5: probabilities of classifying points in the NEGATIVE class correctly

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

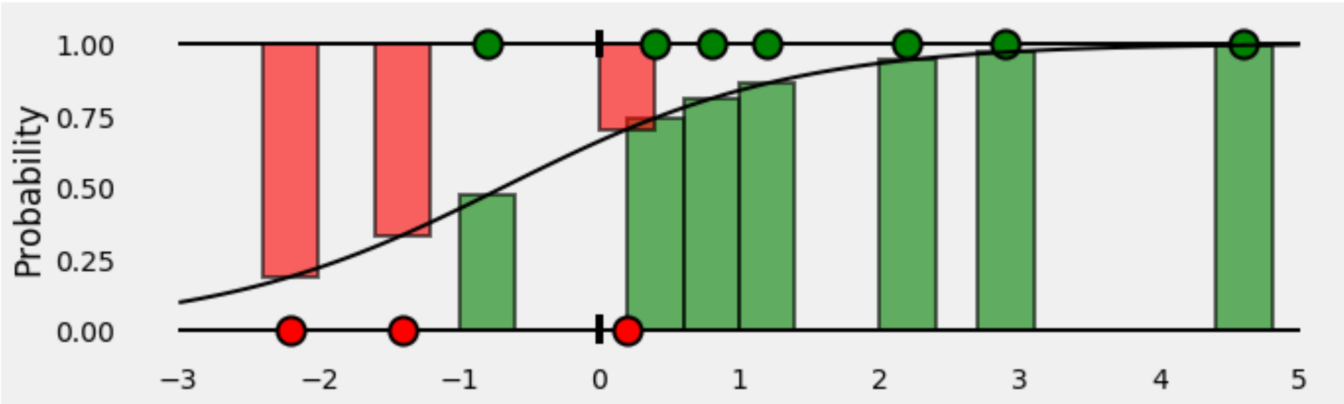
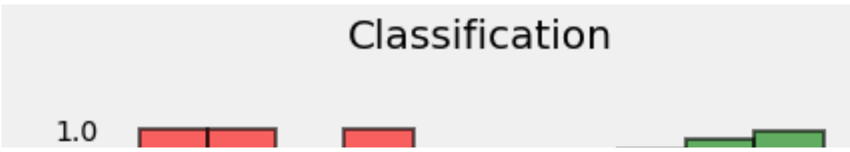


Figure 6: all probabilities put together!

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:



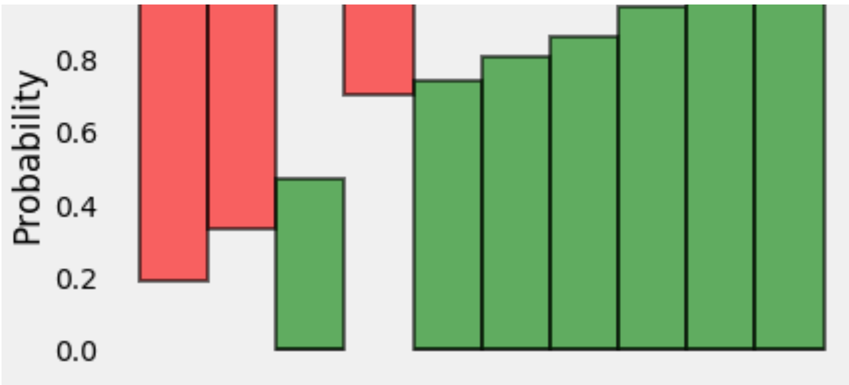


Figure 7: probabilities of all points

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

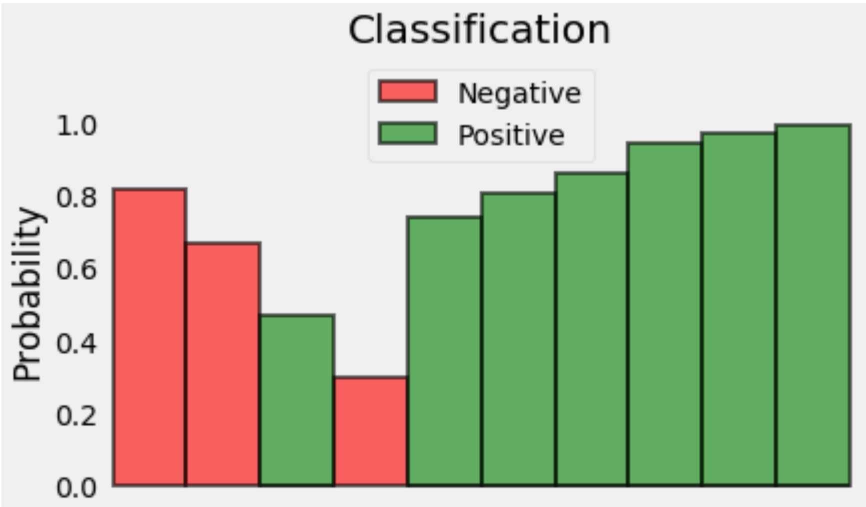


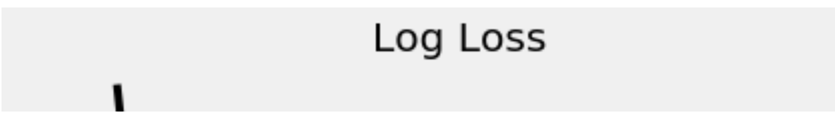
Figure 8: probabilities of all points — much better :-)

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**:



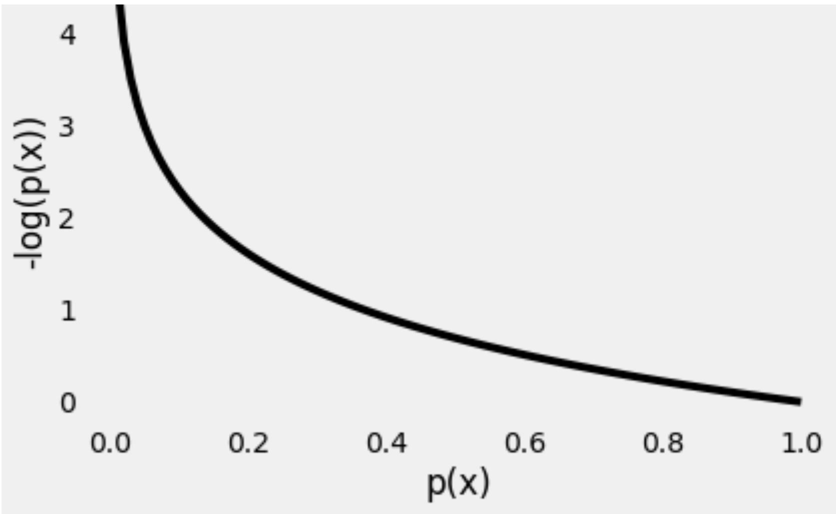


Figure 9: Log Loss for different probabilities

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**.

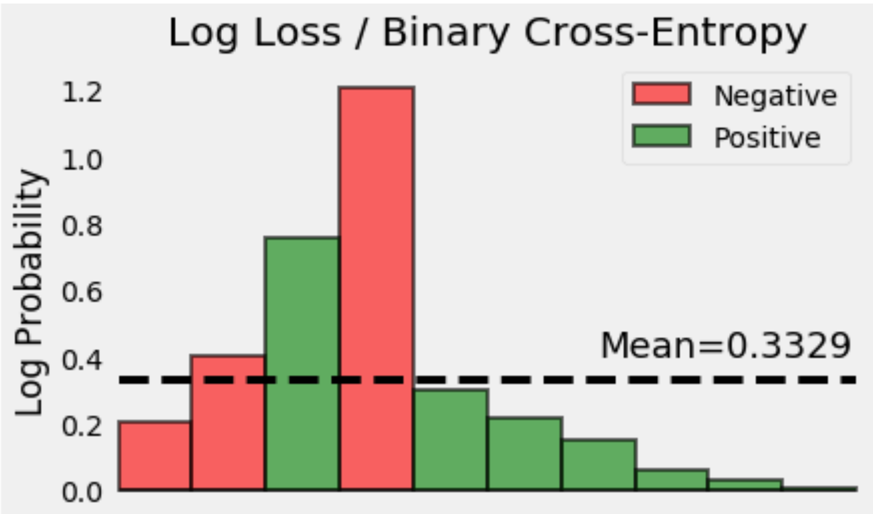


Figure 10: finally, the loss!

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 :-)

```
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import log_loss
import numpy as np
```

```python

x = np.array([-2.2, -1.4, -.8, .2, .4, .8, 1.2, 2.2, 2.9, 4.6])
y = np.array([0.0, 0.0, 1.0, 0.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0])

logr = LogisticRegression(solver='lbfgs')
logr.fit(x.reshape(-1, 1), y)

y_pred = logr.predict_proba(x.reshape(-1, 1))[:, 1].ravel()
loss = log_loss(y, y_pred)

print('x = {}'.format(x))
print('y = {}'.format(y))
print('p(y) = {}'.format(np.round(y_pred, 2)))
print('Log Loss / Cross Entropy = {:.4f}'.format(loss))
```


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 post** 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:

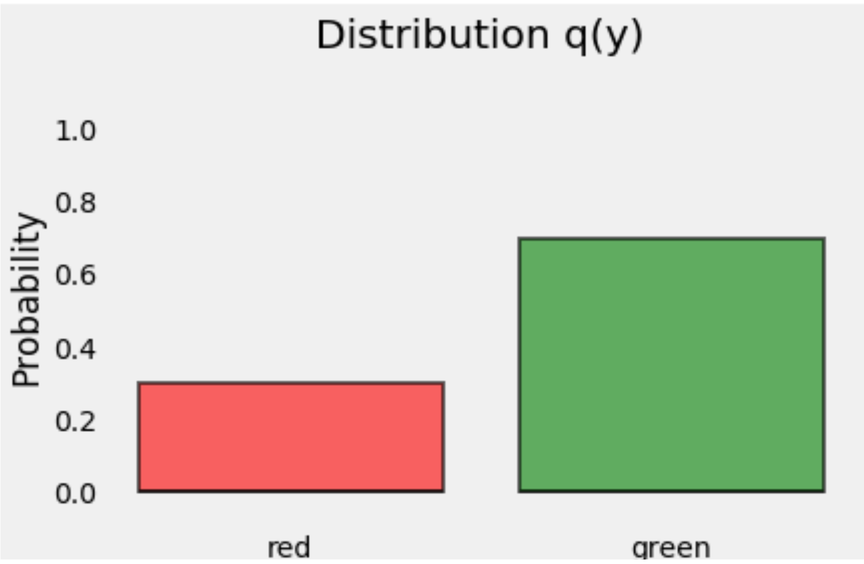


Figure 11: q(y), the distribution of our points

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***):

$$H(q) = log(2)$$

Entropy for a half-half distribution

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.

$$H_p(q) - H(q) >= 0$$

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:

$$\begin{aligned} y_i &= 1 \Rightarrow log(p(y_i)) \\ y_i &= 0 \Rightarrow log(1 - p(y_i)) \end{aligned}$$

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** :-)