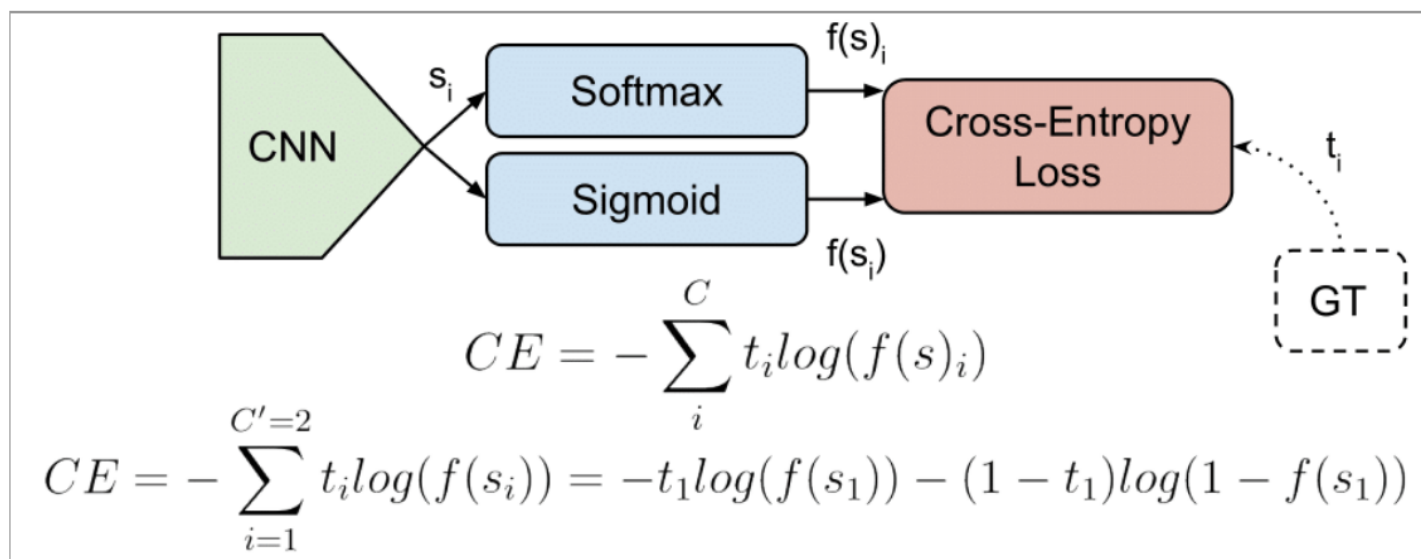




Understanding Categorical Cross-Entropy Loss, Binary Cross-Entropy Loss, Softmax Loss, Logistic Loss, Focal Loss and all those confusing names

May 23, 2018

People like to use cool names which are often confusing. When I started playing with CNN beyond single label classification, I got confused with the different names and formulations people write in their papers, and even with the loss layer names of the deep learning frameworks such as Caffe, Pytorch or TensorFlow. In this post I group up the different names and variations people use for **Cross-Entropy Loss**. I explain their main points, use cases and the implementations in different deep learning frameworks.



First, let's introduce some concepts:

Tasks

Multi-Class Classification







One-of-many classification. Each sample can belong to ONE of C classes. The CNN will have C output neurons that can be gathered in a vector s (Scores). The target (ground truth) vector t will be a one-hot vector with a positive class and $C - 1$ negative classes.

This task is treated as a single classification problem of samples in one of C classes.

Multi-Label Classification

Each sample can belong to more than one class. The CNN will have as well C output neurons. The target vector t can have more than a positive class, so it will be a vector of 0s and 1s with C dimensionality.

This task is treated as C different binary ($C' = 2, t' = 0$ or $t' = 1$) and independent classification problems, where each output neuron decides if a sample belongs to a class or not.

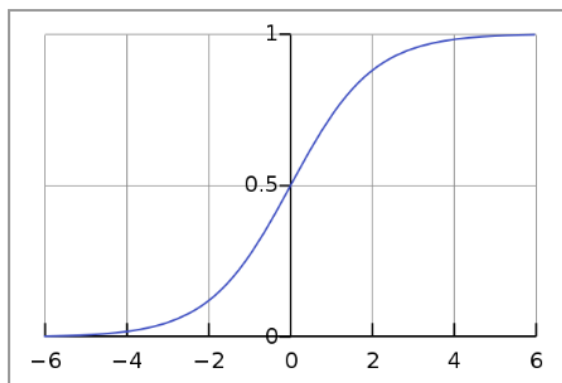
| Multi-Class | | Multi-Label | |
|-------------|--|---|--|
| $C = 3$ | <p>Samples</p> <div></div> <p>Labels (t)</p> <div>$[0\ 0\ 1]$$[1\ 0\ 0]$$[0\ 1\ 0]$</div> | <p>Samples</p> <div></div> <p>Labels (t)</p> <div>$[1\ 0\ 1]$$[0\ 1\ 0]$$[1\ 1\ 1]$</div> | |

Output Activation Functions

These functions are transformations we apply to vectors coming out from CNNs (s) before the loss computation.

Sigmoid

It squashes a vector in the range (0, 1). It is applied independently to each element of s s_i . It's also called **logistic function**.



$$f(s_i) = \frac{1}{1 + e^{s_i}}$$

Softmax

Softmax it's a function, not a loss. It squashes a vector in the range (0, 1) and all the resulting elements add up to 1. It is applied to the output scores s . As elements represent a class, they can be interpreted as class probabilities.

The Softmax function cannot be applied independently to each s_i , since it depends on all elements of s . For a given class s_i , the Softmax function can be computed as:

$$f(s)_i = \frac{e^{s_i}}{\sum_j^C e^{s_j}}$$

Where s_j are the scores inferred by the net for each class in C . Note that the Softmax activations for a class s_i depends on all the scores in s .

An extense comparison of this two functions can be found [here](#)

Activation functions are used to transform vectors before computing the loss in the training phase. In testing, when the loss is no longer applied, activation functions are also used to get the CNN outputs.

Losses

Cross-Entropy loss

The **Cross-Entropy Loss** is actually the only loss we are discussing here. The other losses names written in the title are other names or variations of it. The CE Loss is defined as:

$$CE = - \sum_i^C t_i \log(s_i)$$

Where t_i and s_i are the groundtruth and the CNN score for each class i in C . As **usually an activation function (Sigmoid / Softmax) is applied to the scores before the CE Loss computation**, we write $f(s_i)$ to

refer to the activations.

In a **binary classification problem**, where $C' = 2$, the Cross Entropy Loss can be defined also as [\[discussion\]](#):

$$CE = - \sum_{i=1}^{C'=2} t_i \log(s_i) = -t_1 \log(s_1) - (1 - t_1) \log(1 - s_1)$$

Where it's assumed that there are two classes: C_1 and C_2 . t_1 $[0,1]$ and s_1 are the groundtruth and the score for C_1 , and $t_2 = 1 - t_1$ and $s_2 = 1 - s_1$ are the groundtruth and the score for C_2 . That is the case when we split a Multi-Label classification problem in C' binary classification problems. See next Binary Cross-Entropy Loss section for more details.

Logistic Loss and **Multinomial Logistic Loss** are other names for **Cross-Entropy loss**. [\[Discussion\]](#)

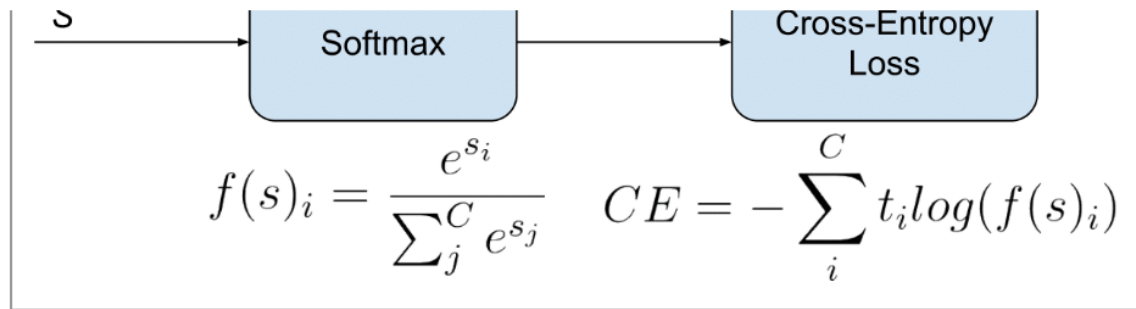
The layers of Caffe, Pytorch and Tensorflow than use a Cross-Entropy loss without an embedded activation function are:

- Caffe: [Multinomial Logistic Loss Layer](#). Is limited to multi-class classification (does not support multiple labels).
- Pytorch: [BCELoss](#). Is limited to binary classification (between two classes).
- TensorFlow: [log_loss](#).

Categorical Cross-Entropy loss

Also called **Softmax Loss**. It is a **Softmax activation** plus a **Cross-Entropy loss**. If we use this loss, we will train a CNN to output a probability over the C classes for each image. It is used for multi-class classification.





In the specific (and usual) case of Multi-Class classification the labels are one-hot, so only the positive class C_p keeps its term in the loss. There is only one element of the Target vector t which is not zero $t_i = t_p$. So discarding the elements of the summation which are zero due to target labels, we can write:

$$CE = -\log \left(\frac{e^{s_p}}{\sum_j^C e^{s_j}} \right)$$

Where s_p is the CNN score for the positive class.

Defined the loss, now we'll have to compute its **gradient respect to the output neurons** of the CNN in order to backpropagate it through the net and optimize the defined loss function tuning the net parameters. So we need to compute the gradient of CE Loss respect each CNN class score in s . The loss terms coming from the negative classes are zero. However, the loss gradient respect those negative classes is not cancelled, since the Softmax of the positive class also depends on the negative classes scores.

The gradient expression will be the same for all C except for the ground truth class C_p , because the score of C_p (s_p) is in the nominator.

After some calculus, the derivative respect to the positive class is:

$$\frac{\partial}{\partial s_p} \left(-\log \left(\frac{e^{s_p}}{\sum_j^C e^{s_j}} \right) \right) = \left(\frac{e^{s_p}}{\sum_j^C e^{s_j}} - 1 \right)$$

And the derivative respect to the other (negative) classes is:

$$\frac{\partial}{\partial s_n} \left(-\log \left(\frac{e^{s_p}}{\sum_j^C e^{s_j}} \right) \right) = \left(\frac{e^{s_n}}{\sum_j^C e^{s_j}} \right)$$

Where s_n is the score of any negative class in C different from C_p .

- Caffe: [SoftmaxWithLoss Layer](#). Is limited to multi-class classification.
- Pytorch: [CrossEntropyLoss](#). Is limited to multi-class classification.
- TensorFlow: [softmax_cross_entropy](#). Is limited to multi-class classification.

*In [this Facebook work](#) they claim that, despite being counter-intuitive, **Categorical Cross-Entropy loss**, or **Softmax loss** worked better than **Binary Cross-Entropy loss** in their multi-label classification problem.*

→ **Skip this part if you are not interested in Facebook or me using Softmax Loss for multi-label classification, which is not standard.**

When Softmax loss is used in a multi-label scenario, the gradients get a bit more complex, since the loss contains an element for each positive class. Consider M are the positive classes of a sample. The CE Loss with Softmax activations would be:

$$CE = \frac{1}{M} \sum_p^M -\log \left(\frac{e^{s_p}}{\sum_j^C e^{s_j}} \right)$$

Where each s_p in M is the CNN score for each positive class. As in Facebook paper, I introduce a scaling factor $1/M$ to make the loss invariant to the number of positive classes, which may be different per sample.

The gradient has different expressions for positive and negative classes. For positive classes:

$$\frac{\partial}{\partial s_{pi}} \left(\frac{1}{M} \sum_p^M -\log \left(\frac{e^{s_p}}{\sum_j^C e^{s_j}} \right) \right) = \frac{1}{M} \left(\left(\frac{e^{s_{pi}}}{\sum_j^C e^{s_j}} - 1 \right) + (M-1) \frac{e^{s_{pi}}}{\sum_j^C e^{s_j}} \right)$$

Where s_{pi} is the score of any positive class.

For negative classes:

$$\frac{\partial}{\partial s_n} \left(\frac{1}{M} \sum_p^M -\log \left(\frac{e^{s_p}}{\sum_j^C e^{s_j}} \right) \right) = \frac{e^{s_n}}{\sum_j^C e^{s_j}}$$

This expressions are easily inferable from the single-label gradient expressions.

As Caffe Softmax with Loss layer nor Multinomial Logistic Loss Layer accept multi-label targets, I implemented my own PyCaffe Softmax loss layer, following the specifications of the Facebook paper. Caffe python layers let's us easily customize the operations done in the forward and backward passes of the layer:

Forward pass: Loss computation

```
def forward(self, bottom, top):
    labels = bottom[1].data
    scores = bottom[0].data
    # Normalizing to avoid instability
    scores -= np.max(scores, axis=1, keepdims=True)
    # Compute Softmax activations
    exp_scores = np.exp(scores)
    probs = exp_scores / np.sum(exp_scores, axis=1, keepdims=True)
```



```

logprobs = np.zeros([bottom[0].num,1])
# Compute cross-entropy Loss
for r in range(bottom[0].num): # For each element in the batch
    scale_factor = 1 / float(np.count_nonzero(labels[r, :]))
    for c in range(len(labels[r,:])): # For each class
        if labels[r,c] != 0: # Positive classes
            logprobs[r] += -np.log(probs[r,c]) * labels[r,c] * scale_factor # We sum the loss

data_loss = np.sum(logprobs) / bottom[0].num

self.diff[...] = probs # Store softmax activations
top[0].data[...] = data_loss # Store Loss

```

We first compute Softmax activations for each class and store them in *probs*. Then we compute the loss for each image in the batch considering there might be more than one positive label. We use an *scale_factor* (M) and we also multiply losses by the labels, which can be binary or real numbers, so they can be used for instance to introduce class balancing. The batch loss will be the mean loss of the elements in the batch. We then save the *data_loss* to display it and the *probs* to use them in the backward pass.

Backward pass: Gradients computation

```

def backward(self, top, propagate_down, bottom):
    delta = self.diff # If the class label is 0, the gradient is equal to probs
    labels = bottom[1].data
    for r in range(bottom[0].num): # For each element in the batch
        scale_factor = 1 / float(np.count_nonzero(labels[r, :]))
        for c in range(len(labels[r,:])): # For each class
            if labels[r, c] != 0: # If positive class
                delta[r, c] = scale_factor * (delta[r, c] - 1) + (1 - scale_factor) * delta[r, c]

```

```
bottom[0].diff[...] = delta / bottom[0].num
```

In the backward pass we need to compute the gradients of each element of the batch respect to each one of the classes scores s . As the gradient for all the classes C except positive classes M is equal to $probs$, we assign $probs$ values to $delta$. For the positive classes in M we subtract 1 to the corresponding $probs$ value and use $scale_factor$ to match the gradient expression. We compute the mean gradients of all the batch to run the backpropagation.

The Caffe Python layer of this Softmax loss supporting a multi-label setup with real numbers labels is available [here](#)

Binary Cross-Entropy Loss

Also called **Sigmoid Cross-Entropy loss**. It is a **Sigmoid activation** plus a **Cross-Entropy loss**. Unlike **Softmax loss** it is independent for each vector component (class), meaning that the loss computed for every vector component is not affected by other component values. That's why it is used for **multi-label classification**, where the insight of an element belonging to a certain class should not influence the decision for another class. It's called **Binary Cross-Entropy Loss** because it sets up a binary classification problem between $C' = 2$ classes for every class in C , as explained above. So when using this Loss, the formulation of **Cross Entropy Loss** for binary problems is often used:

$$CE = - \sum_{i=1}^{C'=2} t_i \log(f(s_i)) = -t_1 \log(f(s_1)) - (1 - t_1) \log(1 - f(s_1))$$



LOSS

$$f(s_i) = \frac{1}{1 + e^{s_i}} \quad CE = -t_1 \log(f(s_1)) - (1 - t_1) \log(1 - f(s_1))$$

This would be the pipeline for each one of the C classes. We set C independent binary classification problems ($C' = 2$). Then we sum up the loss over the different binary problems. s_1 and t_1 are the score and the groundtruth label for the class C_1 , which is also the class C_i in C . $s_2 = 1 - s_1$ and $t_2 = 1 - t_1$ are the score and the groundtruth label of the class C_2 , which is not a “class” in our original problem with C classes, but a class we create to set up the binary problem with $C_1 = C_i$. We can understand it as a background class.

The loss can be expressed as:

$$CE = \begin{cases} -\log(f(s_1)) & \text{if } t_1 = 1 \\ -\log(1 - f(s_1)) & \text{if } t_1 = 0 \end{cases}$$

Where $t_1 = 1$ means that the class $C_1 = C_i$ is positive for this sample.

In this case, the activation function does not depend in scores of other classes in C more than $C_1 = C_i$. So the gradient respect to the each score s_i in s will only depend on the loss given by its binary problem.

The gradient respect to the score $s_i = s_1$ can be written as:

$$\frac{\partial}{\partial s_i} (CE(f(s_i))) = t_1(f(s_1) - 1) + (1 - t_1)f(s_1)$$

Where $f()$ is the **sigmoid** function. It can also be written as:

$$\frac{\partial}{\partial s_i} (CE(f(s_i))) = \begin{cases} f(s_i) - 1 & \text{if } t_i = 1 \\ f(s_i) & \text{if } t_i = 0 \end{cases}$$

Refer [here](#) for a detailed loss derivation.

- Caffe: [Sigmoid Cross-Entropy Loss Layer](#)
- Pytorch: [BCEWithLogitsLoss](#)
- TensorFlow: [sigmoid_cross_entropy](#).

Focal Loss

Focal Loss was introduced by Lin et al., from Facebook, in [this paper](#). They claim to improve one-stage object detectors using **Focal Loss** to train a detector they name RetinaNet. **Focal loss** is a **Cross-Entropy Loss** that weighs the contribution of each sample to the loss based in the classification error. The idea is that, if a sample is already classified correctly by the CNN, its contribution to the loss decreases. With this strategy, they claim to solve the problem of class imbalance by making the loss implicitly focus in those problematic classes. Moreover, they also weight the contribution of each class to the lose in a more explicit class balancing. They use Sigmoid activations, so **Focal loss** could also be considered a **Binary Cross-Entropy Loss**. We define it for each binary problem as:

$$FL = - \sum_{i=1}^{C=2} (1 - s_i)^{\gamma} t_i \log(s_i)$$

Where $(1 - s_i)^{\gamma}$, with the focusing parameter $\gamma \geq 0$, is a modulating factor to reduce the influence of correctly classified samples in the loss. With $\gamma = 0$, **Focal Loss** is equivalent to **Binary Cross Entropy Loss**.

The loss can be also defined as :

$$FL = \begin{cases} -(1 - s_1)^\gamma \log(s_1) & \text{if } t_1 = 1 \\ -(1 - (1 - s_1))^\gamma \log(1 - s_1) & \text{if } t_1 = 0 \end{cases}$$

Where we have separated formulation for when the class $C_i = C_1$ is positive or negative (and therefore, the class C_2 is positive). As before, we have $s_2 = 1 - s_1$ and $t_2 = 1 - t_1$.

The gradient gets a bit more complex due to the inclusion of the modulating factor $(1 - s_i)^\gamma$ in the loss formulation, but it can be deduced using the **Binary Cross-Entropy** gradient expression.

In case C_i is positive ($t_i = 1$), the gradient expression is:

$$\frac{\partial}{\partial s_i} (FL(f(s_i))) = (1 - f(s_i))^\gamma (\gamma f(s_i) \log(f(s_i)) + f(s_i) - 1) \quad \text{if } t_1 = 1$$

Where $f()$ is the **sigmoid** function. To get the gradient expression for a negative C_i ($t_i = 0$), we just need to replace $f(s_i)$ with $(1 - f(s_i))$ in the expression above.

*Notice that, if the modulating factor $\gamma = 0$, the loss is equivalent to the **CE Loss**, and we end up with the same gradient expression.*

I implemented **Focal Loss** in a PyCaffe layer:

Forward pass: Loss computation

```
def forward(self, bottom, top):
    labels = bottom[1].data
    scores = bottom[0].data
    scores = 1 / (1 + np.exp(-scores)) # Compute sigmoid activations
```

```

logprobs = np.zeros([bottom[0].num, 1])

# Compute cross-entropy Loss
for r in range(bottom[0].num): # For each element in the batch
    for c in range(len(labels[r, :])):
        # For each class we compute the binary cross-entropy Loss
        # We sum the loss per class for each element of the batch
        if labels[r, c] == 0: # Loss form for negative classes
            logprobs[r] += self.class_balances[str(c+1)] * -np.log(1-scores[r, c]) * scores[r, c]
        else: # Loss form for positive classes
            logprobs[r] += self.class_balances[str(c+1)] * -np.log(scores[r, c]) * (1 - scores[r, c])
        # The class balancing factor can be included in Labels by using scaled real values

data_loss = np.sum(logprobs) / bottom[0].num
top[0].data[...] = data_loss

```

Where $\text{logprobs}[r]$ stores, per each element of the batch, the sum of the binary cross entropy per each class. The *focusing_parameter* is γ , which by default is 2 and should be defined as a layer parameter in the net prototxt. The *class_balances* can be used to introduce different loss contributions per class, as they do in the Facebook paper.

Backward pass: Gradients computation

```

def backward(self, top, propagate_down, bottom):
    delta = np.zeros_like(bottom[0].data, dtype=np.float32)
    labels = bottom[1].data
    scores = bottom[0].data
    # Compute sigmoid activations

```



```

scores = 1 / (1 + np.exp(-scores))

for r in range(bottom[0].num): # For each element in the batch
    for c in range(len(labels[r, :])): # For each class
        p = scores[r, c]
        if labels[r, c] == 0:
            delta[r, c] = self.class_balances[str(c+1)] * -(p ** self.focusing_parameter) *
        else: # If the class label != 0
            delta[r, c] = self.class_balances[str(c+1)] * (((1 - p) ** self.focusing_parameter) *
            self.focusing_parameter * p * np.log(
                p) + p - 1)) # Gradient for classes with positive labels

bottom[0].diff[...] = delta / bottom[0].num

```

The Focal Loss Caffe python layer is available [here](#).