NEURAL NETWORKS AND DEEP LEARNING CST 395 CS 5TH SEMESTER HONORS COURSE- Dr Binu V P, 9847390760

CS 5th Semester Honors course for the Computer Science at KTU- Dr Binu V P

Differentiation of the Sigmoid activation and cross-entropy loss function

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A step-by-step differentiation of the Sigmoid activation and cross-entropy loss function is discussed here.
The understanding of derivatives of these two functions is essential in the area of machine learning when performing back-propagation during model training.

Derivative of Sigmoid Function

Sigmoid/ Logistic function is defined as:
$g(x) = \frac{1}{1+e^{-x}} \in (0, 1)$

For any value of x, the Sigmoid function $g(x)$ falls in the range $(0, 1)$. As the value of x decreases, g(x) approaches 0, whereas as x grows bigger, $g(x)$tends to 1. Examples,

$g(-5.5) = 0.0040$
$g(6.5) = 0.9984$
$g(0.4) = 0.5986$

$$\frac{dg}{dx} = \frac{d}{dx}\left(\frac{1}{1+e^{-x}}\right) = \frac{vu^{'} - uv^{'}}{v^2}$$
$$= \frac{(0)(1-e^{-x}) - 1(-e^{-x})}{(1-e^{-x})^2}$$
$$= \frac{e^{-x}}{(1-e^{-x})^2}$$

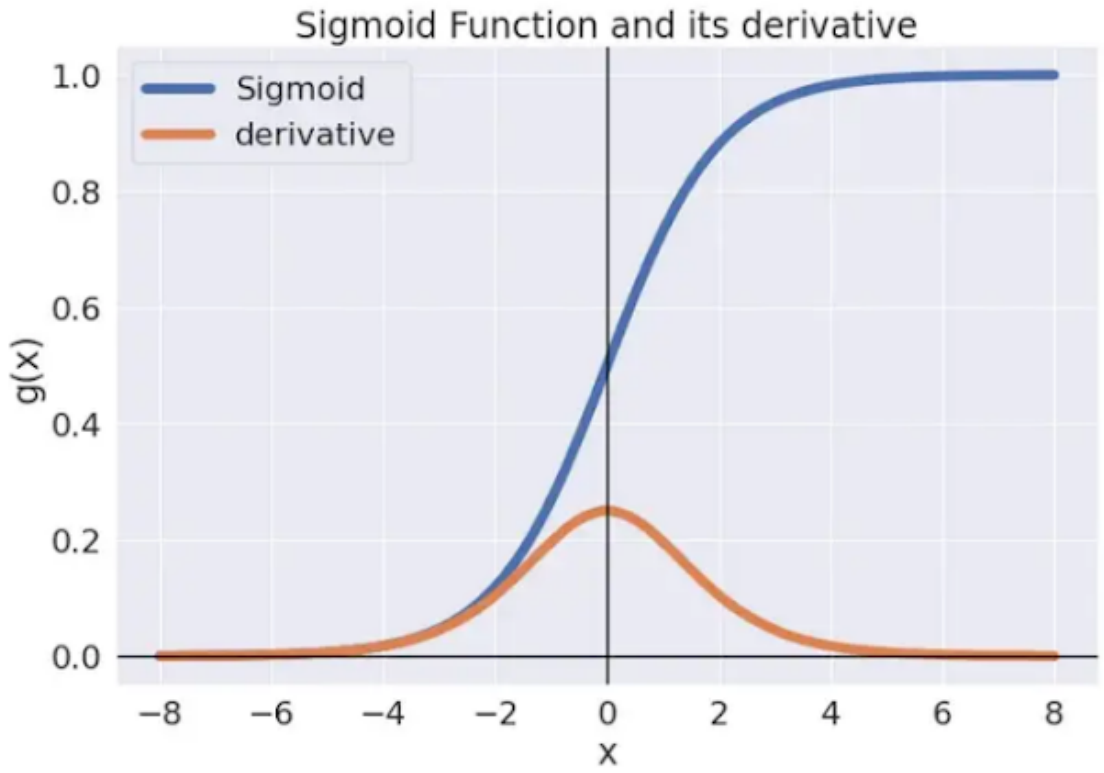
It is noted that we can further simplify the derivative and write in term of g(x)

$$\frac{dg}{dx} = \frac{d}{dx}\left(\frac{1}{1+e^{-x}}\right) = \frac{e^{-x}}{(1+e^{-x})^2}$$
$$= \frac{1}{1+e^{-x}} \cdot \frac{e^{-x}}{1+e^{-x}}$$
$$= \frac{1}{1+e^{-x}} \cdot \frac{1+e^{-x}-1}{1+e^{-x}}$$
$$= \frac{1}{1+e^{-x}} \cdot \frac{\cancel{1+e^{-x}}}{\cancel{1+e^{-x}}} - \frac{1}{1+e^{-x}}$$
$$= \frac{1}{1+e^{-x}} \cdot 1 - \frac{1}{1+e^{-x}}$$
$$\therefore \frac{dg}{dx} = g(x)(1-g(x))$$

Why do we use this version of the derivative?

In the forward propagation step, you compute the sigmoid function $(g(x))$ and have its value handy. While computing the derivative in the backpropagation step, all you have to do is plug in the value of $g(x)$ in the formula derived above.

Here is the plot of sigmoid function and its derivative



Derivative of Cross-Entropy Function

Cross-Entropy loss function is a very important cost function used for classification problems.The concept of cross-entropy traces back into the field of Information Theory where Claude Shannon introduced the concept of entropy in 1948. Before diving into Cross-Entropy cost function, let us introduce entropy .

Entropy

Entropy of a random variable X is the level of uncertainty inherent in the variables possible outcome.

For $p(x)$ — probability distribution and a random variable X, entropy is defined as follows

$$H(X) = \begin{cases} -\int_x p(x) \log p(x), & \text{if } X \text{ is continous} \\ -\sum_x p(x) \log p(x), & \text{if } X \text{ is discrete} \end{cases}$$

Cross-Entropy Loss Function is also called **logarithmic loss, log loss** or **logistic loss.**

Each predicted class probability is compared to the actual class desired output 0 or 1 and a score/loss is calculated that penalizes the probability based on how far it is from the actual expected value. The penalty is logarithmic in nature yielding a large score for large differences close to 1 and small score for small differences tending to 0.

Cross-entropy loss is used when adjusting model weights during training. The aim is to minimize the loss, i.e, the smaller the loss the better the model. A perfect model has a cross-entropy loss of 0.

Cross-entropy is defined as

$E_g = -\sum_{i=1}^{n} t_i ln(p_i)$
where t_i is the truth value and p_i is the probability of the i^{th} class.

For classification with two classes, we have binary cross-entropy loss which is defined as follows

$$E_b = -[t_n ln(\bar{y}) + (1-t) ln(1-\hat{y})]$$

The truth label, t, on the binary loss is a known value, whereas $\hat{y}$ is a variable. This means that the function will be differentiated with respect to $\hat{y}$ and treat t as a constant. Let's go ahead and work on the derivative now.

$$\begin{aligned}\frac{\partial}{\partial \hat{y}}(t \ln \hat{y}) &= t\frac{\partial}{\partial \hat{y}}(\ln \hat{y}) + \ln(\hat{y})\frac{\partial}{\partial \hat{y}}(t) \\ &= \frac{t}{\hat{y}} + \ln \hat{y}(0) \\ &= \frac{t}{\hat{y}}\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial \hat{y}}((1-t)\ln(1-\hat{y})) &= (1-t)\frac{\partial}{\partial \hat{y}}(\ln(1-\hat{y})) + \ln((1-\hat{y}))\frac{\partial}{\partial \hat{y}}(1-t) \\ &= -\frac{1-t}{1-\hat{y}} + \ln(1-\hat{y})(0) \\ &= -\frac{1-t}{1-\hat{y}}\end{aligned}$$

And therefore, the derivative of the binary cross-entropy loss function becomes

$$\therefore \frac{\partial E_b}{\partial \hat{y}} = -\left(\frac{t}{\hat{y}} - \frac{1-t}{1-\hat{y}}\right)$$
$$= \left(\frac{t}{\hat{y}} + \frac{1-t}{1-\hat{y}}\right)$$

Partial Derivative of cost function for linear regression

First, here are the elements in the hypothesis:

- x is an mxn matrix containing one row for each training record and one column for each feature
- θ is a 1xn matrix containing the weights for the hypothesis
- y is an mx1 matrix containing the response values

So n represents the number of features in the training set and m represents the number of rows in the training set.

The hypothesis is:

$$h_\theta = \theta^T x$$

This is the cost function in its simplest form (the superscript i's refer to a particular feature):

$$J(\theta) = \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

This simply gives the total of the squared errors. To get the mean of the squared errors:

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

We can also multiply this by $\frac{1}{2}$ for a purely arbitrary reason, to make the derivative easier to calculate, as we'll see below. Note that this is *not* now the mean of the squared errors, but rather one-half of the mean, but this is not important, because we will only be comparing various calculations of one-half the mean against each other.

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

Now we can take the partial derivative for any one feature in x.

$$\frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 = ?$$

First, the $\frac{1}{2m}$ is outside of the $\sum$, so it acts as a constant that will not change. So we need to take the partial derivative of everything inside the $\sum$. We have a quantity that is squared, so the first step is to apply the chain rule, which effectively means:

$$\frac{\partial}{\partial_{\text{stuff}}} (\text{stuff})^2 = 2(\text{stuff}) \times \frac{\partial}{\partial_{\text{stuff}}} \text{stuff}$$

So:

$$\frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 = \frac{1}{2m} \sum_{i=1}^{m} 2(h_\theta(x^{(i)}) - y^{(i)}) \times \frac{\partial}{\partial \theta_j} h_\theta(x^{(i)})$$

We know from above that the function h_θ is:

$$h_\theta = \theta^T x$$

So:

$$\frac{\partial}{\partial \theta_j} h_\theta = \frac{\partial}{\partial \theta_j} \theta_j^T x_j$$

Here, x_j is a constant, and the derivative of θ_j with respect to θ_j is 1, so we are left with:

$$\frac{\partial}{\partial \theta_j} h_\theta = x_j$$

Plug this back into the above equation and we have:

$$\frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 = \frac{1}{2m} \sum_{i=1}^{m} 2(h_\theta(x^{(i)}) - y^{(i)}) \cdot x_j^{(i)}$$

As the final step, the 2 in the denominator outside of the $\sum$ and the 2 inside the $\sum$ cancel each other out, leaving:

$$\frac{\partial}{\partial \theta_j} = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_j^{(i)}$$

Partial Derivative of Cost Function for Logistic Regression

Cost function

The cost function for logistic regression is:

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} y^{(i)} \log(h_\theta(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$$

Minimized cost function

This is what we know . to be the partial derivative of the cost function. Can we find it?

$$\frac{\partial}{\partial \theta_j} = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

Hypothesis (sigmoid) function

$$h_\theta(x^{(i)}) = \frac{1}{1 + e^{-\theta^T x}}$$

Rules for logarithmic expressions

$$\log\left(\frac{x}{y}\right) = \log(x) - \log(y)$$

$$\log(e^a) = a$$

Finding the partial derivatives for each j in θ

1. Simplify the cost function

$$J(\theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\left(y^{(i)}(\log h_\theta(x^{(i)})) + (1-y^{(i)})\log(1-h_\theta(x^{(i)}))\right)\right]$$

Replace $h_\theta(x^{(i)})$ with sigmoid

$$= -\frac{1}{m}\left[\sum_{i=1}^{m}\left(y^{(i)}\log(\frac{1}{1+e^{-\theta^T x^{(i)}}}) + (1-y^{(i)})\log(1-\frac{1}{1+e^{-\theta^T x^{(i)}}})\right)\right]$$

Convert right term to single rational expression

$$= -\frac{1}{m}\left[\sum_{i=1}^{m}\left(y^{(i)}\log(\frac{1}{1+e^{-\theta^T x^{(i)}}}) + (1-y^{(i)})\log(\frac{e^{-\theta^T x^{(i)}}}{1+e^{-\theta^T x^{(i)}}})\right)\right]$$

Apply $\log(\frac{a}{b}) = \log(a) - \log(b)$ on left term

$$= -\frac{1}{m}\left[\sum_{i=1}^{m}\left(y^{(i)}(\log(1) - \log(1+e^{-\theta^T x^{(i)}})) + (1-y^{(i)})\log(\frac{e^{-\theta^T x^{(i)}}}{1+e^{-\theta^T x^{(i)}}})\right)\right]$$

$$= -\frac{1}{m}\left[\sum_{i=1}^{m}\left(-y^{(i)}\log(1+e^{-\theta^T x^{(i)}}) + (1-y^{(i)})\log(\frac{e^{-\theta^T x^{(i)}}}{1+e^{-\theta^T x^{(i)}}})\right)\right]$$

Apply $\log(\frac{a}{b}) = \log(a) - \log(b)$ to right term

$$= -\frac{1}{m}\left[\sum_{i=1}^{m}\left(-y^{(i)}\log(1+e^{-\theta^T x^{(i)}}) + (1-y^{(i)})\log(e^{-\theta^T x^{(i)}}) - (1-y^{(i)})(\log(1+e^{-\theta^T x^{(i)}}))\right)\right]$$

Apply $\log(e^a) = a$ to right term

$$= -\frac{1}{m}\left[\sum_{i=1}^{m}\left(-y^{(i)}\log(1+e^{-\theta^T x^{(i)}}) + (1-y^{(i)})(-\theta^T x^{(i)}) - (1-y^{(i)})(\log(1+e^{-\theta^T x^{(i)}}))\right)\right]$$

Move minus sign inside $\sum$

$$= \frac{1}{m}\left[\sum_{i=1}^{m}\left(y^{(i)}\log(1+e^{-\theta^T x^{(i)}}) + (1-y^{(i)})(\theta^T x^{(i)}) + (1-y^{(i)})(\log(1+e^{-\theta^T x^{(i)}}))\right)\right]$$

Combine first and third terms

$$= \frac{1}{m}\left[\sum_{i=1}^{m}\left(\log(1+e^{-\theta^T x^{(i)}}) + (1-y^{(i)})(\theta^T x^{(i)})\right)\right]$$

2. Take the partial derivative

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m}\left[\sum_{i=1}^{m}\left(\frac{e^{-\theta^T x^{(i)}}(-x_j^{(i)})}{1+e^{-\theta^T x^{(i)}}} + (1-y^{(i)})x_j^{(i)}\right)\right]$$

Now factor out $x^{(i)}{}_j$

$$= \frac{1}{m}\left[\sum_{i=1}^{m}\left(\frac{-e^{-\theta^T x^{(i)}}}{1+e^{-\theta^T x^{(i)}}} + 1 - y^{(i)}\right)x_j^{(i)}\right]$$

Combine first two terms

$$= \frac{1}{m}\left[\sum_{i=1}^{m}\left(\frac{1}{1+e^{-\theta^T x^{(i)}}} - y^{(i)}\right)x_j^{(i)}\right]$$

Substitute $h_\theta(x^{(i)})$ for sigmoid function

$$= \frac{1}{m}\left[\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)x_j^{(i)}\right]$$

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