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Backpropagation Algorithm

Course Notes

365√DataScience

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Abstract

In order to get a truly deep understanding of deep neural networks, one must look at the mathematics of it. The backpropagation algorithm trains a neural network through a method called chain rule. As it is at the core of the optimization process, we wanted to introduce you to it. This is definitely not a necessary part of the course, as in TensorFlow, sk-learn, or any other machine learning package (as opposed to simply NumPy), will have backpropagation methods incorporated.

Keywords: backpropagation algorithm, chain rule, TensorFlow, deep learning , deep neural networks

1. The Specific Net and Notation We Will Examine

Here's our simple network:

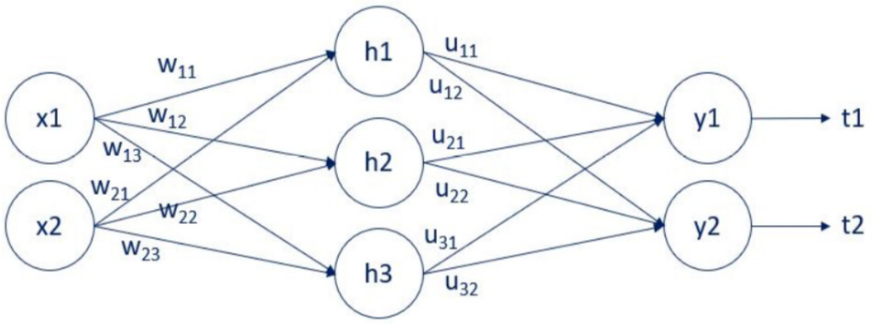

Figure 1: Backpropagation

We have two inputs: x_1 and x_2. There is a single hidden layer with 3 units (nodes): h_1, h_2, and h_3. Finally, there are two outputs: y_1 and y_2. The arrows that connect them are the weights. There are two weights matrices: $\boldsymbol{w}$, and $\boldsymbol{u}$. The w weights connect the input layer and the hidden layer. The $\boldsymbol{u}$ weights connect the hidden layer and the output layer. We have employed the letters $\boldsymbol{w}$, and $\boldsymbol{u}$, so it is easier to follow the computation to follow.
You can also see that we compare the outputs y_1 and y_2 with the targets t_1 and t_2.

There is one last letter we need to introduce before we can get to the compu- tations. Let a be the linear combination prior to activation. Thus, we have: $\mathbf{a^{(1)} = xw + b^{(1)}}$ and $\mathbf{a^{(2)} = hu + b^{(2)}}$.
Since we cannot exhaust all activation functions and all loss functions, we will focus on two of the most common. A **sigmoid** activation and an **L2-norm loss.**
With this new information and the new notation, the output y is equal to the ac- tivated linear combination. Therefore, for the output layer, we have $y = \sigma(a^{(2)})$, while for the hidden layer: $h = \sigma(a^{(1)})$.
We will examine backpropagation for the output layer and the hidden layer separately, as the methodologies differ

2. Useful Formulas

I would like to remind you that:

$$L = \frac{1}{2}\sum_{i}(y_i - t_i)^2$$

The sigmoid function is:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

and its derivative is:

$$\sigma'(x) = \sigma(x)\big(1 - \sigma(x)\big)$$

3. Backpropagation for the Output Layer

In order to obtain the update rule:

$$\mathbf{u} \leftarrow \mathbf{u} - \eta\nabla_{\mathbf{u}}L(\mathbf{u})$$

we must calculate

$$\nabla_{\mathbf{u}}L(\mathbf{u})$$

Let's take a single weight u_{ij}. The partial derivative of the loss w.r.t. u_{ij} equals:

$$\frac{\partial L}{\partial u_{ij}} = \frac{\partial L}{\partial y_j}\frac{\partial y_j}{\partial a_j^{(2)}}\frac{\partial a_j^{(2)}}{\partial u_{ij}}$$

where i corresponds to the previous layer (input layer for this transformation) and j corresponds to the next layer (output layer of the transformation). The partial derivatives were computed simply following the chain rule.

$$\frac{\partial L}{\partial y_j} = (y_i - t_i)$$

following the L2-norm loss derivative.

$$\frac{\partial y_j}{\partial a_j^{(2)}} = \sigma\left(a_j^{(2)}\right)\left(1 - \sigma\left(a_j^{(2)}\right)\right) = y_j\left(1 - y_j\right)$$

following the sigmoid derivative.
Finally, the third partial derivative is simply the derivative of $\mathbf{a}^{(2)} = \mathbf{hu} + \mathbf{b}^{(2)}$.
So,

$$\frac{\partial a_j^{(2)}}{\partial u_{ij}} = h_i$$

Replacing the partial derivatives in the expression above, we get:

$$\frac{\partial L}{\partial u_{ij}} = \frac{\partial L}{\partial y_j}\frac{\partial y_j}{\partial a_j^{(2)}}\frac{\partial a_j^{(2)}}{\partial u_{ij}} = \left(y_j - t_j\right)y_j\left(1 - y_j\right)h_i = \delta_j h_i$$

Therefore, the update rule for a single weight for the output layer is given by:

$$u_{ij} \leftarrow u_{ij} - \eta\delta_j h_i$$

4. Backpropagation of a Hidden Layer

Similarly to the backpropagation of the output layer, the update rule for a single weight, w_{ij} would depend on:

$$\frac{\partial L}{\partial w_{ij}} = \frac{\partial L}{\partial h_j}\frac{\partial h_j}{\partial a_j^{(1)}}\frac{\partial a_j^{(1)}}{\partial w_{ij}}$$

following the chain rule.
Taking advantage of the results we have so far for transformation using the sigmoid activation and the linear model, we get:

$$\frac{\partial h_j}{\partial a_j^{(1)}} = \sigma\left(a_j^{(1)}\right)\left(1 - \sigma\left(a_j^{(1)}\right)\right) = h_j\left(1 - h_j\right)$$

and

$$\frac{\partial a_j^{(1)}}{\partial w_{ij}} = x_i$$

The actual problem for backpropagation comes from the term $\frac{\partial L}{\partial h_j}$. That's due to the fact that there is no "hidden" target. You can follow the solution for weight w_{11} below. It is advisable to also check Figure 1, while going through the computations.

$$\frac{\partial L}{\partial h_1} = \frac{\partial L}{\partial y_1}\frac{\partial y_1}{\partial a_1^{(2)}}\frac{\partial a_1^{(2)}}{\partial h_1} + \frac{\partial L}{\partial y_2}\frac{\partial y_2}{\partial a_2^{(2)}}\frac{\partial a_1^{(2)}}{\partial h_1} =$$
$$= (y_1 - t_1)y_1(1 - y_1)u_{11} + (y_2 - t_2)y_2(1 - y_2)u_{12}$$

From here, we can calculate $\frac{\partial L}{\partial w_{11}}$, which was what we wanted. The final expression is:

$$\frac{\partial L}{\partial w_{11}} = [(y_1 - t_1)y_1(1 - y_1)u_{11} + (y_2 - t_2)y_2(1 - y_2)u_{12}]h_1(1 - h_1)x_1$$

The generalized form of this equation is:

$$\frac{\partial L}{\partial w_{ij}} = \sum_k (y_k - t_k)y_k(1 - y_k)u_{jk}\, h_j\left(1 - h_j\right)x_i$$

5. Backpropagation Generalization

Using the results for backpropagation for the output layer and the hidden layer, we can put them together in one formula, summarizing backpropagation, in the presence of L2-norm loss and sigmoid activations.

$$\frac{\partial L}{\partial w_{ij}} = \delta_j x_i$$

where for a hidden layer

$$\delta_j = \sum_k \delta_k w_{jk}\, y_j\left(1 - y_j\right)$$

Kudos to those of you who got to the end.

Thanks for reading.

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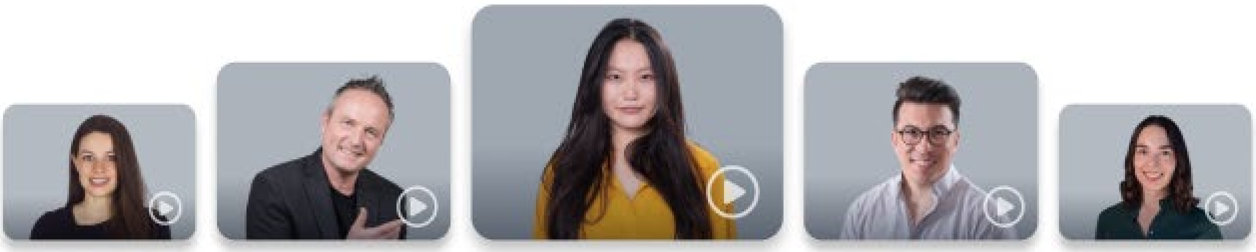

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