Big Data and AI Strategies

Neural Network Explained, Part V: Backpropagation

In the previous note, we discussed the importance of data pre-processing and suggested a few common practices. So far, we have largely covered what is known as the 'forward propagation' process. That is, the computation goes from left to right: the neural net accepts the inputs and transforms them as per the activation functions to produce outputs. In reality, we can observe the outputs but do not know the parameters of the activation functions. Therefore our goal is to figure out the best-fitting parameter values using the observed outputs. This process is known as training the neural net, and a particular method has become very prevalent. It is known as **backpropagation** and is the topic of this note.

In order to train the neural net, we first need to identify an objective, also known as a loss function. A plausible choice would be to minimize the squared difference between the neural net outputs and the observed values, similar to an ordinary least squares (OLS) regression. However, unlike for OLS, where the parameters can be solved analytically, for neural nets we generally have to resort to numerical solutions. The numerical procedure of choice is gradient descent.

Gradient Descent

Given some initial guess of the parameters, we want to move the values in the direction that causes the loss function to decrease most rapidly. It turns out that the direction of the steepest descent is the negative gradient of the loss function. Since the gradient only describes the condition locally, it needs to be re-evaluated once we move away from the initial guess. How far to move before re-evaluation is known as the **learning rate**. To summarize, we compute the gradient of the loss function at some initial parameter values, then move the parameter values in the negative gradient direction for a small distance. The procedure is repeated until the value of objective function no longer decreases (convergence).

Stochastic gradient descent (SGD): The loss function is complex and there is no guarantee the gradient descent will reach the global minimum. It is not uncommon for the algorithm to get stuck in some local minima. When faced with such problems, stochastic optimization is often preferred to deterministic methods. In other words, we artificially inject randomness into the process. The idea is to perturb a candidate solution and see if it remains robust. By doing so we may stand a better chance of getting out of the local minima and reach the global minimum. SGD, specifically, introduces randomness by performing iterations on different random subsets of the data. Since not all observations are included in an iteration, another term, **epoch**, is used to denote the number of times all observations have been utilized at least once.

Choice of learning rate: A learning rate that is either too big or too small is both at risk of causing non-convergence. Theoretically, there exists an optimal learning rate for every iteration. However, finding the optimal learning rate is a computationally expensive operation itself. Therefore, in practice the learning rate is determined somewhat heuristically, and remains an area of active research. Common algorithms determine the learning rate adaptively, i.e., decrease the value as the number of iteration increases.

Gradient descent forms the basis of backpropagation, but it is not the only way to train a neural network. There are methods that promise faster convergence, but require computing the much more expensive second derivatives, and then there are those that promise more robust convergence, but take too much time. In this author’s view, gradient descent has attained such popularity because it strikes a balance between computational cost and convergence speed. Additionally, the relatively straightforward computation also means it is friendly to parallel processing and can be sped up significantly with the help of GPUs.

Vanishing Gradient

Gradient descent is not without its issues, with vanishing gradient being a major one. To illustrate, assuming we have a simple network with two hidden layers, and each has a sigmoid activation functions. To find the gradient of the loss function with respect to a parameter, β_1, we arrive at the bottom equation below, by chain rule. Note the overall gradient is a product of the two sigmoid gradients, among other terms.

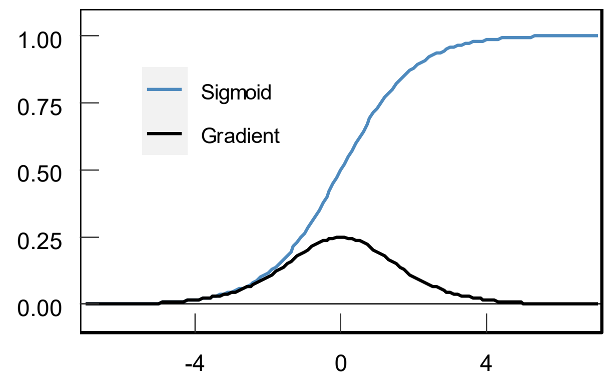
$$L = \sum (y - \hat{y})^2$$

$$\hat{y} = \beta_y \sigma_2\left(\beta_2 \sigma_1(\beta_1 x)\right)$$

$$\frac{\partial L}{\partial \beta_1} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma_2} \cdot \frac{\partial \sigma_2}{\partial \sigma_1} \cdot \frac{\partial \sigma_1}{\partial \beta_1}$$

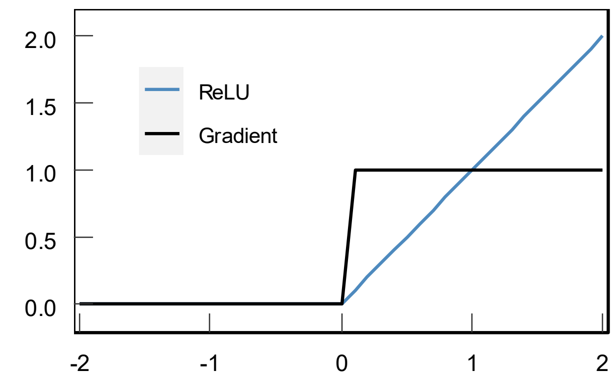
As shown in Figure 1, the gradient values of the sigmoid function are small, because sigmoid is a relatively slow-changing function. Since the gradient is always less than 1, the product of the two gradients will be shrunk further toward 0. As one can imagine, if a network has many layers, the end product of many sigmoid gradients multiplied together may end up being very close to 0, regardless of the inputs. This is not helpful for what we are trying to do.

Figure 1: Sigmoid and its gradient



Source: J.P. Morgan

Figure 2: ReLU and its gradient



Source: J.P. Morgan

There are a couple of common ways to remedy the issue. A simple way is to use a different activation function. For instance, the ReLU function has a gradient of exactly 1 for x > 0 (Figure 2). Alternatively, architectures such as Recurrent Neural Network are designed specifically to counter the vanishing gradient problem. Readers can refer to our earlier notes on network architectures for more details.

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