1 Introduction

In my GitHub project general purpose network I tried to figure out, how to apply backpropagation to a network of previously unspecified size. I wanted someone to be able to create a network with a size of his choosing, without the backpropagation algorithm I implemented being broken (unlike my previous project).

Most of the resources about backpropagation I found extremely confusing and the few that were helpful, like this amazing blogpost, derived the gradients per hand for every single weights, not something that I would like to do for large networks.

So I decided to try and figure out an algorithm that works for a network of any size without it having to be specified before and doesn't calculate the gradient for every single weights one after another. This is basically my attempt at explaining backpropagation, with an example, in a more understandable way than most resources I found.

I should note that while I am pretty sure that the algorithm I came up with works, and that I found that it is done pretty much the same way in this book, I don't know about the differences to more advanced projects than my simple exercise project. If you find any error or have some helpful/interesting resource to share, feel free to contact me/create an issue on GitHub.

I will not include biases in this example (or not yet), but once you understood this article, or rather the principle I'm trying to explain, including biases into the backpropagation is very simple.

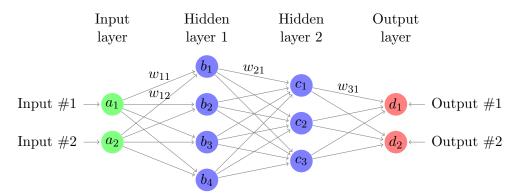
2 Requirements

To understand what I'm doing in this article, you need to know what the partial derivative is and how to derive it (unless you want to take my word for it).

Also some knowledge about matrix-vector multiplication or a cheatsheet would be helpful. The german wikipedia page has some great images displaying how different multiplications between matrices and vectors work. The network used in this example is the same as for the other documents in

this project and can also be found here (with slight notational differences), but for the sake of completeness, I added it in section 3.

3 The network



The notation of the network should mostly be self explanatory. Each layer is denoted by a letter, starting with "a" at the input layer and then going upwards until "d" for the output layer.

The neurons in each layer are labeled by the letter of its layer and a number as its index, starting with 1 at the top of the layer and counting upwards, so a_1 would be the first neuron in layer a.

A weight is denoted by the letter w and indexed by a letter and a number. The letter is layer the weight leads to and the number the weights position in the layer. For example w_{a1} is the first weight in the first layer, connecting a_1 and b_1 . Weight w_{a2} would be the weight connecting a_2 and b_1 , w_{a3} the neurons a_1 and a_2 and so on.

4 Forward propagation

Before starting with the backpropagation part, let's look at how we forward propagate inputs to get our corresponding output. Here I will establish the terminology needed when explaining backpropagation and it will help to understand the process of getting the gradient.

We have two inputs a_1 and a_2 , lets say we use two binary inputs

$$a_1 = 1, a_2 = 0,$$

that we could use when learning a logic gate.

As weights we will use:

$$W_{b} = \begin{bmatrix} w_{b1} & w_{b2} \\ w_{b3} & w_{b4} \\ w_{b5} & w_{b6} \\ w_{b7} & w_{b8} \end{bmatrix} = \begin{bmatrix} 0.1 & 0.2 \\ 0.3 & 0.4 \\ 0.5 & 0.6 \\ 0.7 & 0.8 \end{bmatrix}$$

$$W_{c} = \begin{bmatrix} w_{c1} & w_{c2} & w_{c3} & w_{c4} \\ w_{c5} & w_{c6} & w_{c7} & w_{c8} \\ w_{c9} & w_{c10} & w_{c11} & w_{c12} \end{bmatrix} = \begin{bmatrix} 0.25 & 0.30 & 0.35 & 0.40 \\ 0.45 & 0.50 & 0.55 & 0.60 \\ 0.65 & 0.70 & 0.75 & 0.80 \end{bmatrix}$$

$$W_{d} = \begin{bmatrix} w_{d1} & w_{d2} & w_{d3} \\ w_{d4} & w_{d5} & w_{d6} \end{bmatrix} = \begin{bmatrix} 0.3 & 0.4 & 0.5 \\ 0.6 & 0.7 & 0.8 \end{bmatrix}$$

Since the net value (before applying an activation function like sigmoid) of a neuron is the sum of all its weights multiplied with its corresponding inputs (e.g. the net value of the neuron b_1 $net_{b_1} = w_{b_1} * a_1 + w_{b_2} * a_2$, we can use matrix multiplication to calculate all net values for a layer in a single step. When using matrix multiplication to calculate all net inputs for layer b it looks like this

$$net_b = W_b * a = \begin{bmatrix} 0.1 & 0.2 \\ 0.3 & 0.4 \\ 0.5 & 0.6 \\ 0.7 & 0.8 \end{bmatrix} * \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0.1 * 1 + 0.2 * 0 \\ 0.3 * 1 + 0.4 * 0 \\ 0.5 * 1 + 0.6 * 0 \\ 0.7 * 1 + 0.8 * 0 \end{bmatrix} = \begin{bmatrix} 0.1 \\ 0.3 \\ 0.5 \\ 0.7 \end{bmatrix}$$

Next we want the output out_b of layer b, so we have to apply our activation function, in this case the sigmoid function, to every single element in the vector net_b .

Just as a reminder, the sigmoid function is $sig(x) = \frac{1}{1+e^{-x}}$, so if you are following this example you are probably going to need a calculation from here on out.

Applying the sigmoid function we get

$$out_b = sig(net_b) = sig(\begin{bmatrix} 0.1\\0.3\\0.5\\0.7 \end{bmatrix}) = \begin{bmatrix} 0.5250\\0.5744\\0.6225\\0.6682 \end{bmatrix}$$

I rounded the results to 4 decimals and will continue the calculations with the rounded values. This goes for both this current calculation, as well as the rest of the article. If we continue propagating these results forward until the output layer we get

$$net_c = W_c * out_b = \begin{bmatrix} 0.25 & 0.30 & 0.35 & 0.40 \\ 0.45 & 0.50 & 0.55 & 0.60 \\ 0.65 & 0.70 & 0.75 & 0.80 \end{bmatrix} * \begin{bmatrix} 0.5250 \\ 0.5744 \\ 0.6225 \\ 0.6682 \end{bmatrix} = \begin{bmatrix} 0.7887 \\ 1.2667 \\ 1.7448 \end{bmatrix}$$

$$out_c = sig(net_c) = sig(\begin{bmatrix} 0.7887 \\ 1.2667 \\ 1.7448 \end{bmatrix}) = \begin{bmatrix} 0.6876 \\ 0.7802 \\ 0.8513 \end{bmatrix}$$

$$net_d = W_d * out_c = \begin{bmatrix} 0.3 & 0.4 & 0.5 \\ 0.6 & 0.7 & 0.8 \end{bmatrix} * \begin{bmatrix} 0.6876 \\ 0.7802 \\ 0.8513 \end{bmatrix} = \begin{bmatrix} 0.9441 \\ 1.6397 \end{bmatrix}$$

$$out_d = sig(net_d) = sig(\begin{bmatrix} 0.9441 \\ 1.6397 \end{bmatrix}) = \begin{bmatrix} 0.7199 \\ 0.8375 \end{bmatrix}$$

Now that we reached the output of layer d we also have the output of our network. Our first output neuron d_1 has the value 0.7199 and our second one d_2 the value 0.8375.

These two values are our networks guess for what the output should be when the input values we chose earlier are plugged in. With that we are basically done with the forward propagation part, since no matter the weights, the process will remain the same. Before moving on to the backpropagation part though, I would like to mention something noteworthy, that will be helpful for understanding backpropagation.

When forward propagating, we started with our inputs and in the end got our outputs. The way we calculated them is by multiplying matrices, applying an activation function, then again multiplying matrices and so on. Basically the entire forward propagation process is nothing but the chaining of functions, the matrix multiplication being one and the activation function being another. Every intermediate result, e.g. net_b is immediately passed on to the next function until we get the output.

This is noteworthy, because later we will need to derive this gigantic chain of functions, so we can train our network. For this, as you might have guessed, the chain rule is perfect.

5 Backpropagation

5.1 The error

Before we can start with the backpropagation itself, we need something we can actually propagate back. Since we want to train the network, we need to know how wrong our guesses were for those inputs and then use the gradient (derivative) to move into the right direction, so it improves.

For this we will use an error function, the squared error

$$E_{total} = \sum_{i=1}^{\infty} \frac{1}{2} (target - out)^2 \tag{1}$$

In this equation we subtract the actual value we got from the target value we wanted. I multiplied by 1/2 here so it cancels out with the square when deriving the function later on.

The total error E_{total} is the sum of all those errors calculated for every single output neuron. For different inputs we could get a totally different output and so our error could be totally different as well.

If we wanted only the error for d_1 (for the inputs we chose earlier) it would be

$$E_{d_1} = \sum \frac{1}{2} (target_{d_1} - out_{d_1})$$

From here on out it will be hard to continue without a target output for out network, so let's say it takes the two inputs a_1 and a_2 and its job is to reverse, or rather switch them. This would mean our inputs and corresponding outputs are.

a_1	a_2		out_{d_1}	out_{d_2}
1	1	=	1	1
1	0	=	0	1
0	1	=	1	0
0	0	=	0	0

Our goal is to make the network learn, which simply means we want its guesses to be as close to the correct output as possible. But you could also put it in other word, we want our error to be as low as possible. Since we have a function 1 that calculates the error, our goal will be to find the minimal possible value for the function.

For this we will use gradient descent (I will not go into detail here, so if you need a refreshed, feel free to look it up) and for that we will calculate the first derivative of the error function. The only value in the function that we can really influence is the output, therefore we will take the partial derivative with respect to it.

$$\frac{\partial E_{total}}{\partial out} = \frac{1}{2} * 2 * (target - out) * (-1) = (out - target)$$
 (2)

Now that we have both our error function and its derivative and, in theory, can minimize the error. But right now we only derived with respect to the output, so how do we tell the network how it can get closer to that output? For that let's look at what our network consists of.

We have our inputs and our weights, as well as an activation function. Changing the inputs would make no sense, after all we want to come closer to our target values for exactly those inputs.

Similar for the activation function, while we can choose between several functions and could even choose different ones for different layers, they are fixed once chosen and we can't change them.

So all that is left to change are out weights, which makes sense, since those are the only values that are indepentent for each layer and since they do the actual work in our network.

In other words, the variables we want to derive the error with respect to are the weights. This means we have to derive the error with respect to every single weight to get its gradient and then adjust the network accordingly. Let's derive for a weight in the last layer, for example w_{d1} . We then, without yet plugging in values or variables, get

$$\frac{\partial E_{total}}{\partial w_{d1}} = \frac{\partial E_{total}}{\partial out_{d_1}} \frac{\partial out_{d_1}}{\partial net_{d_1}} \frac{\partial net_{d_1}}{\partial w_{d1}}$$
(3)

If this step isn't clear think about what I wrote at the end of section 4. The entire network is nothing but a chaining of functions and when deriving the error with respect to w_{d1} , we therefore apply the chain rule. When looking at it from the right (the weight first) we have all weights of the neuron multiplied, equaling the net value of d_1 . This net value is chained with the activation function, equaling the out value of d_1 . This again is chained, this time with the error function.

As we are deriving with respect to w_{d1} , every connection that does not contain this weight will result in 0 when derived, that is why in 3, only

 out_{d_1} and net_{d_1} are relevant. Every other connection doesn't contain w_{d_1} and will therefore drop out anyway.

Now let's plug in our formulas. We then get

$$\frac{\partial E_{total}}{\partial w_{d1}} = (out_{d_1} - target_{d_1}) * (out_{d_1} * (1 - out_{d_1})) * out_{c_1}$$

If you are wondering where the second parameter comes from, this is the derivative of the sigmoid function, our activation function.

The sigmoid function is $sig(x) = \frac{1}{1+e^{-x}}$ and it's derivative is sig'(x) = sig(x) * (1 - sig(x)). The value we plug into sig(x) as x is (for this neuron) net_{d_1} . But since $sig(net_{d_1}) = out_{d_1}$, we can just write out_{d_1} instead.

This process is similar for all output neurons, for example

$$\frac{\partial E_{total}}{\partial w_{d4}} = \frac{\partial E_{total}}{\partial out_{d_2}} \frac{\partial out_{d_2}}{\partial net_{d_2}} \frac{\partial net_{d_2}}{\partial w_{d4}}$$

and with the values plugged in

$$\frac{\partial E_{total}}{\partial w_{d1}} = (out_{d_2} - target_{d_2}) * (out_{d_2} * (1 - out_{d_2})) * out_{c_1}$$

For the first layer (or the last, depending on the point of view) this process is relatively easy, most terms just drop out. If you go to the next layer it already gets harder, as more neurons are being influenced by the chosen weight. Continuing this by hand is tedious, but for a few layers with only a few neurons still possible without too much effort. Most networks are far more complex though and would need an overwhelming amount of work to be derived by hand. And even more important, the network would be fixed to it's current size, for every different combination of layers and neurons you would have to do the entire process again.

We would like a more generic solution, one that we can apply no matter the size of the network, just like the simply matrix multiplication when propagating forward.

In other words, we need to find some pattern that we can use and put into a formula.

5.2 Finding a pattern for backpropagation