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Simeon Kostadinov Follow
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Understanding Backpropagation Algorithm

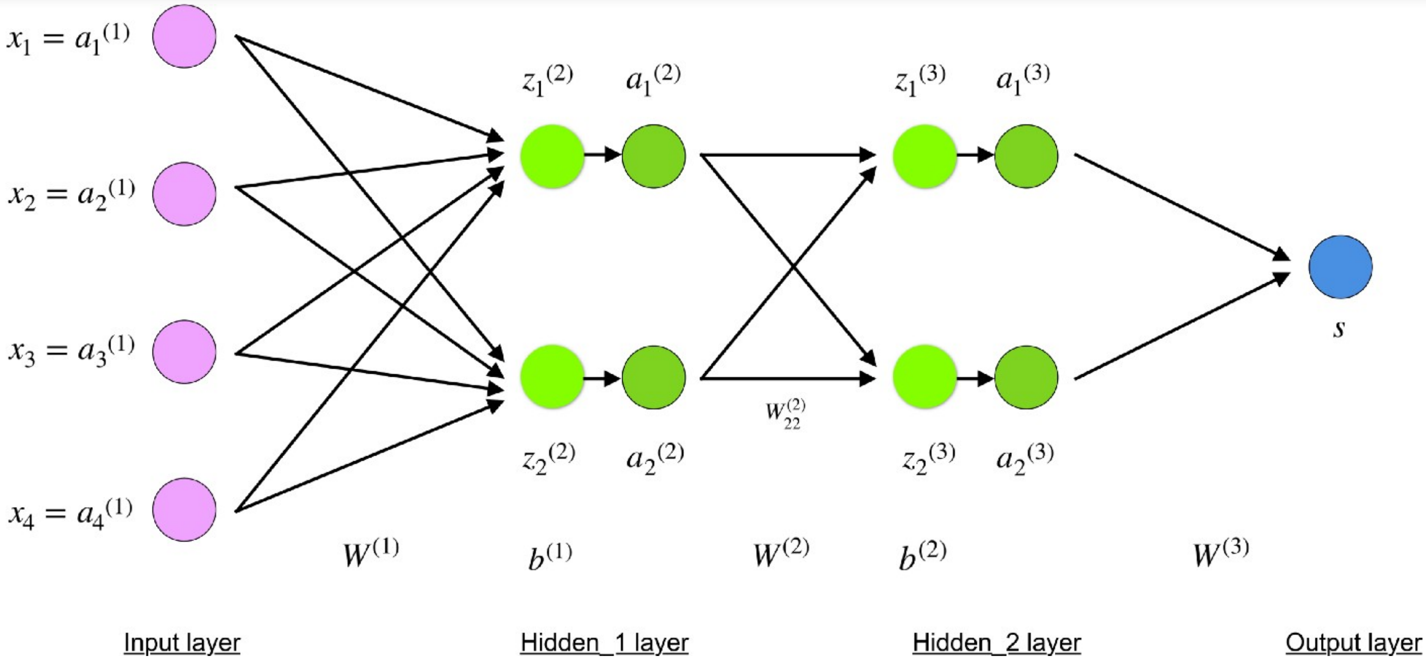
Learn the nuts and bolts of a neural network's most important ingredient

"A man is running on a highway" — photo by Andrea Leopardi on Unsplash

Backpropagation algorithm is probably the most fundamental building block in a neural network. It was first introduced in 1960s and almost 30 years later (1989) popularized by Rumelhart, Hinton and Williams in a paper called *"Learning representations by back-propagating errors"*.

The algorithm is used to effectively train a neural network through a method called chain rule. In simple terms, after each forward pass through a network, backpropagation performs a backward pass while adjusting the model's parameters (weights and biases).

In this article, I would like to go over the mathematical process of training and optimizing a simple 4-layer neural network. *I believe this would help the reader understand how backpropagation works as well as realize its importance.*



Simple 4-layer neural network illustration

Input layer

The neurons, colored in **purple**, represent the input data. These can be as simple as scalars or more complex like vectors or multidimensional matrices.

$$x_i = a_i^{(1)}, i \in 1,2,3,4$$

Equation for input x_i

The first set of activations (a) are equal to the input values. *NB: "activation" is the neuron's value after applying an activation function. See below.*

Hidden layers

The final values at the hidden neurons, colored in **green**, are computed using z^l — weighted inputs in layer l, and a^l— activations in layer l. For layer 2 and 3 the equations are:

- $l = 2$

$$z^{(2)} = W^{(1)}x + b^{(1)}$$

$$a^{(2)} = f(z^{(2)})$$

Equations for z² and a²

- $l = 3$

$$z^{(3)} = W^{(2)}a^{(2)} + b^{(2)}$$

$$a^{(3)} = f(z^{(3)})$$

Activations a^2 and a^3 are computed using an activation function *f*. Typically, this **function *f* is non-linear** (e.g. sigmoid, ReLU, tanh) and allows the network to learn complex patterns in data. We won't go over the details of how activation functions work, but, if interested, I strongly recommend reading this great article.

Looking carefully, you can see that all of x, z^2, a^2, z^3, a^3, W^1, W^2, b^1 and b^2 are missing their subscripts presented in the 4-layer network illustration above. **The reason is that we have combined all parameter values in matrices, grouped by layers.** This is the standard way of working with neural networks and one should be comfortable with the calculations. However, I will go over the equations to clear out any confusion.

Let's pick layer 2 and its parameters as an example. The same operations can be applied to any layer in the network.

- W^1 is a weight matrix of shape *(n, m)* where *n* is the number of output neurons (neurons in the next layer) and *m* is the number of input neurons (neurons in the previous layer). For us, $n = 2$ and $m = 4$.

$$W^{(1)} = \begin{bmatrix} W_{11}^{(1)} & W_{12}^{(1)} & W_{13}^{(1)} & W_{14}^{(1)} \\ W_{21}^{(1)} & W_{22}^{(1)} & W_{23}^{(1)} & W_{24}^{(1)} \end{bmatrix}$$

Equation for W¹

NB: The first number in any weight's subscript matches the index of the neuron in the next layer (in our case this is the *Hidden_2 layer*) **and the second number matches the index of the neuron in previous layer** (in our case this is the *Input layer*).

- x is the input vector of shape *(m, 1)* where *m* is the number of input neurons. For us, $m = 4$.

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

Equation for x

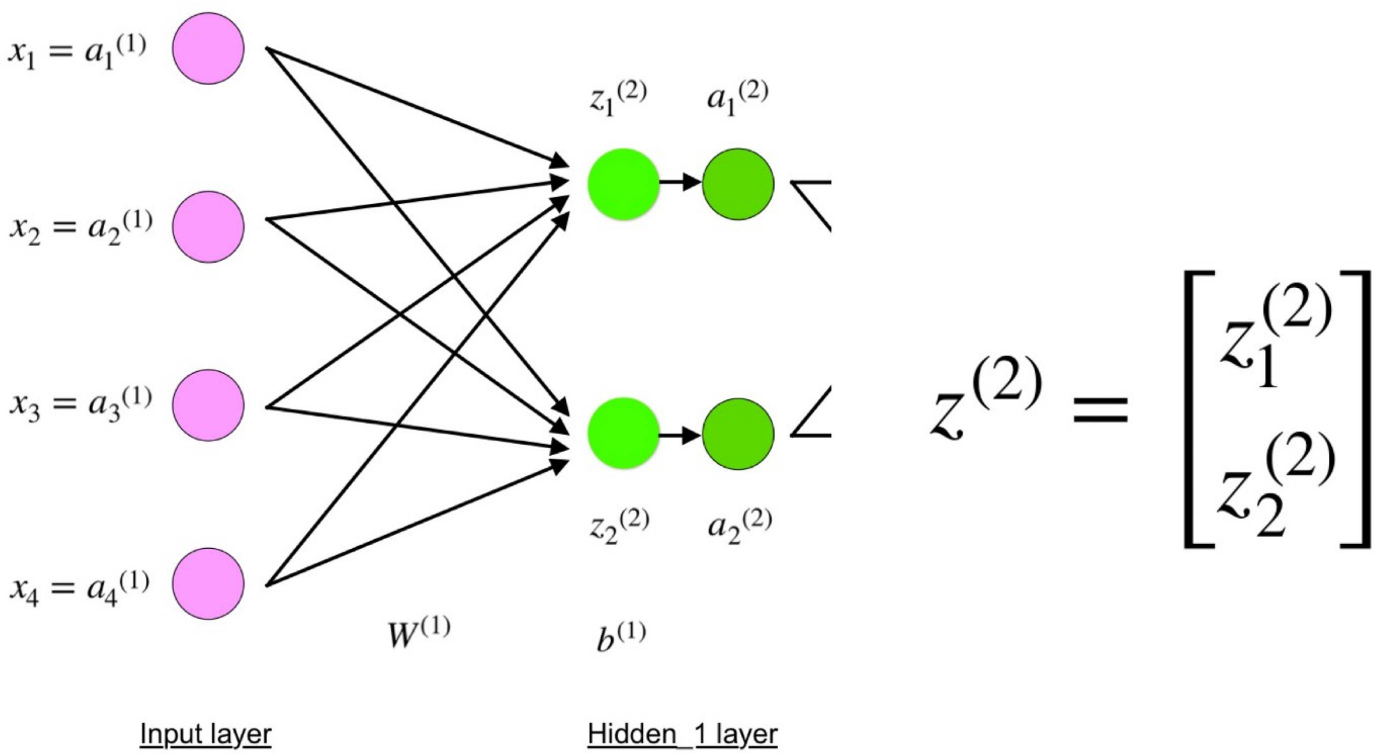
- b^1 is a bias vector of shape *(n , 1)* where *n* is the number of neurons in the current layer. For us, $n = 2$.

$$b^{(1)} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \end{bmatrix}$$

Equation for b¹

Following the equation for z^2, we can use the above definitions of W^1, x and b^1 to derive "*Equation for z^2*":

$$z^{(2)} = \begin{bmatrix} W_{11}^{(1)}x_1 + W_{12}^{(1)}x_2 + W_{13}^{(1)}x_3 + W_{14}^{(1)}x_4 \\ W_{21}^{(1)}x_1 + W_{22}^{(1)}x_2 + W_{23}^{(1)}x_3 + W_{24}^{(1)}x_4 \end{bmatrix} + \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \end{bmatrix}$$



Input and Hidden_1 layers

You will see that z^2 can be expressed using $(z_1)^2$ and $(z_2)^2$ where $(z_1)^2$ and $(z_2)^2$ are the sums of the multiplication between every input x_i with the corresponding weight $(W_{ij})^1$.

This leads to the same "*Equation for* z^2" and proofs that the matrix representations for z^2, a^2, z^3 and a^3 are correct.

Output layer

The final part of a neural network is the output layer which produces the predicated value. In our simple example, it is presented as a single neuron, colored in **blue** and evaluated as follows:

$$s = W^{(3)} a^{(3)}$$

Equation for output s

Again, we are using the matrix representation to simplify the equation. One can use the above techniques to understand the underlying logic. **Please leave any comments below if you find yourself lost in the equations — I would love to help!**

Forward propagation and evaluation

The equations above form network's forward propagation. Here is a short overview:

$$z^{(2)} = W^{(1)}x + b^{(1)} \quad \text{neuron value at } Hidden_1 \text{ layer}$$

$$a^{(2)} = f(z^{(2)}) \quad \text{activation value at } Hidden_1 \text{ layer}$$

$$z^{(3)} = W^{(2)}a^{(2)} + b^{(2)} \quad \text{neuron value at } Hidden_2 \text{ layer}$$

$$a^{(3)} = f(z^{(3)}) \quad \text{activation value at } Hidden_2 \text{ layer}$$

$$s = W^{(3)}a^{(3)} \quad \text{Output layer}$$

Overview of forward propagation equations colored by layer

The final step in a forward pass is to evaluate the **predicted output** ***s*** against an **expected output** ***y***.

The output *y* is part of the training dataset *(x, y)* where *x* is the input (as we saw in the previous section).

Evaluation between *s* and *y* happens through a **cost function**. This can be as simple as MSE (mean squared error) or more complex like cross-entropy.

We name this cost function *C* and denote it as follows:

$$C = cost(s, y)$$

Equation for cost function C

were *cost* can be equal to MSE, cross-entropy or any other cost function.

Based on *C*'s value, the model "knows" how much to adjust its parameters in order to get closer to the expected output *y*. This happens using the backpropagation algorithm.

Backpropagation and computing gradients

According to the paper from 1989, backpropagation:

> *repeatedly adjusts the weights of the connections in the network so as to minimize a measure of the difference between the actual output vector of the net and the desired output vector.*

and

> *the ability to create useful new features distinguishes back-propagation from earlier, simpler methods…*

In other words, **backpropagation aims to minimize the cost function by adjusting network's weights and biases.** The level of adjustment is determined by the gradients of the cost function with respect to those parameters.

One question may arise — **why computing gradients?**

- *Gradient of a function C(x_1, x_2, …, x_m) in point x is a vector of the partial derivatives of C in x.*

$$\frac{\partial C}{\partial x} = [\frac{\partial C}{\partial x_1}, \frac{\partial C}{\partial x_2}, \ldots, \frac{\partial C}{\partial x_m}]$$

Equation for derivative of C in x

- *The derivative of a function C measures the sensitivity to change of the function value (output value) with respect to a change in its argument x (input value). In other words, the derivative tells us the direction C is going.*
- *The gradient shows how much the parameter x needs to change (in positive or negative direction) to minimize C.*

Compute those gradients happens using a technique called chain rule.

For a single weight *(w_jk)^l,* the gradient is:

$$\frac{\partial C}{\partial w^l_{jk}} = \frac{\partial C}{\partial z^l_j}\frac{\partial z^l_j}{\partial w^l_{jk}} \qquad chain\ rule$$

$$z^l_j = \sum_{k=1}^{m} w^l_{jk} a^{l-1}_k + b^l_j \qquad by\ definition$$

$$m \ - \ number\ of\ neurons\ in\ l-1\ layer$$

$$\frac{\partial z^l_j}{\partial w^l_{jk}} = a^{l-1}_k \qquad by\ differentiation\ (calculating\ derivative)$$

$$\frac{\partial C}{\partial w^l_{jk}} = \frac{\partial C}{\partial z^l_j} a^{l-1}_k \qquad final\ value$$

Equations for derivative of C in a single weight (w_jk)^l

Similar set of equations can be applied to *(b_j)^l*:

$$\partial b_j^l \qquad \partial z_j^l \, \partial b_j^l$$

$$\frac{\partial z_j^l}{\partial b_j^l} = 1 \qquad by\ differentiation\ (calculating\ derivative)$$

$$\frac{\partial C}{\partial b_j^l} = \frac{\partial C}{\partial z_j^l} 1 \qquad final\ value$$

Equations for derivative of C in a single bias (b_j)^l

The common part in both equations is often called *"local gradient"* and is expressed as follows:

$$\delta_j^l = \frac{\partial C}{\partial z_j^l} \qquad local\ gradient$$

Equation for local gradient

The *"local gradient"* can easily be determined using the chain rule. I won't go over the process now but if you have any questions, please comment below.

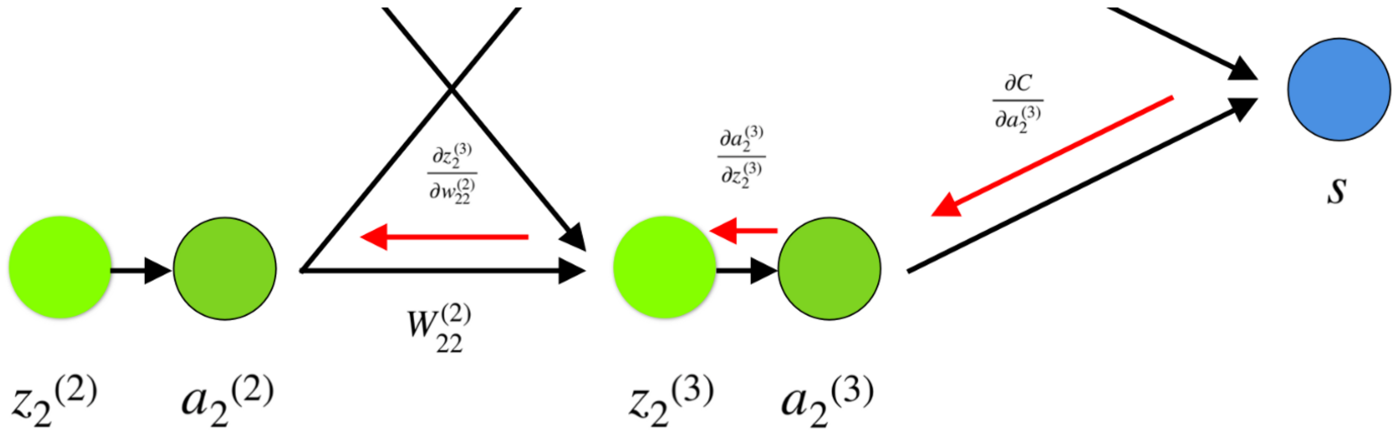
The gradients allow us to optimize the model's parameters:

$$\begin{aligned} & while\ (termination\ condition\ not\ met) \\ & \qquad w := w - \epsilon \frac{\partial C}{\partial w} \\ & \qquad b := b - \epsilon \frac{\partial C}{\partial b} \\ & end \end{aligned}$$

Algorithm for optimizing weights and biases (also called "Gradient descent")

- Initial values of w and b are randomly chosen.
- Epsilon (e) is the learning rate. It determines the gradient's influence.
- w and b are matrix representations of the weights and biases. Derivative of C in w or b can be calculated using partial derivatives of C in the individual weights or biases.
- Termination condition is met once the cost function is minimized.

Let's zoom in on the bottom part of the above neural network:



Visual representation of backpropagation in a neural network

Weight *(w_22)²* connects *(a_2)²* and *(z_2)²*, so computing the gradient requires applying the chain rule through *(z_2)³* and *(a_2)³*:

$$\frac{\partial C}{\partial w_{22}^{(2)}} = \frac{\partial C}{\partial z_2^{(3)}} \cdot \frac{\partial z_2^{(3)}}{\partial w_{22}^{(2)}} = \frac{\partial C}{\partial a_2^{(3)}} \cdot \frac{\partial a_2^{(3)}}{\partial z_2^{(3)}} \cdot a_2^{(2)} = \frac{\partial C}{\partial a_2^{(3)}} \cdot f'(z_2^{(3)}) \cdot a_2^{(2)}$$

Equation for derivative of C in (w_22)²

Calculating the final value of derivative of *C* in *(a_2)³* requires knowledge of the function *C*. Since *C* is dependent on *(a_2)³*, calculating the derivative should be fairly straightforward.

I hope this example manages to throw some light on the mathematics behind computing gradients. To further enhance your skills, I strongly recommend watching Stanford's NLP series where Richard Socher gives 4 great explanations of backpropagation.

Final remarks

In this article, I went through a detailed explanation of how backpropagation works under the hood using mathematical techniques like computing gradients, chain rule etc. *Knowing the nuts and bolts of this algorithm will fortify your neural networks knowledge and make you feel comfortable to take on more complex models. Enjoy your deep learning journey!*

Thank you for the reading. Hope you enjoyed the article 🤩 and I wish you a great day!