I, Deep Learning

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## Feedforward Neural Networks in Depth, Part 1: Forward and Backward Propagations Dec 10, 2021

This post is the first of a three-part series in which we set out to derive the mathematics behind feedforward neural networks. They have an input and an output layer with at least one hidden layer in between,

- fully-connected layers, which means that each node in one layer connects to every node in the
- following layer, and • ways to introduce nonlinearity by means of activation functions.
- We start with forward propagation, which involves computing predictions and the associated cost of

these predictions. Forward Propagation

Settling on what notations to use is tricky since we only have so many letters in the Roman alphabet. As

## you browse the Internet, you will likely find derivations that have used different notations than the ones we are about to introduce. However, and fortunately, there is no right or wrong here; it is just a matter of

taste. In particular, the notations used in this series take inspiration from Andrew Ng's Standard notations for Deep Learning. If you make a comparison, you will find that we only change a couple of the details. Now, whatever we come up with, we have to support multiple layers, several nodes in each layer,

 various types of cost functions, and mini-batches of training examples.

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As a result, our definition of a node ends up introducing a fairly large number of notations:

various activation functions,

 $z_{j,i}^{[l]} = \sum_k w_{j,k}^{[l]} a_{k,i}^{[l-1]} + b_j^{[l]},$  $a_{j,i}^{[l]} = g_j^{[l]}(z_{1,i}^{[l]}, \dots, z_{j,i}^{[l]}, \dots, z_{n^{[l]},i}^{[l]}).$ 

more sense once we have explained the notations, which we shall do next: **Entity Description** 

Does the node definition look intimidating to you at first glance? Do not worry. Hopefully, it will make

**Description** The current layer 
$$l=1,\ldots,L$$
 , where  $L$  is the number of layers that have weights and biases. We use  $l=0$  and  $l=L$  to denote the input and output layers.

 $n^{[l]}$ The number of nodes in the current layer.  $n^{[l-1]}$ The number of nodes in the previous layer.

The jth node of the current layer,  $j=1,\ldots,n^{[l]}$ .

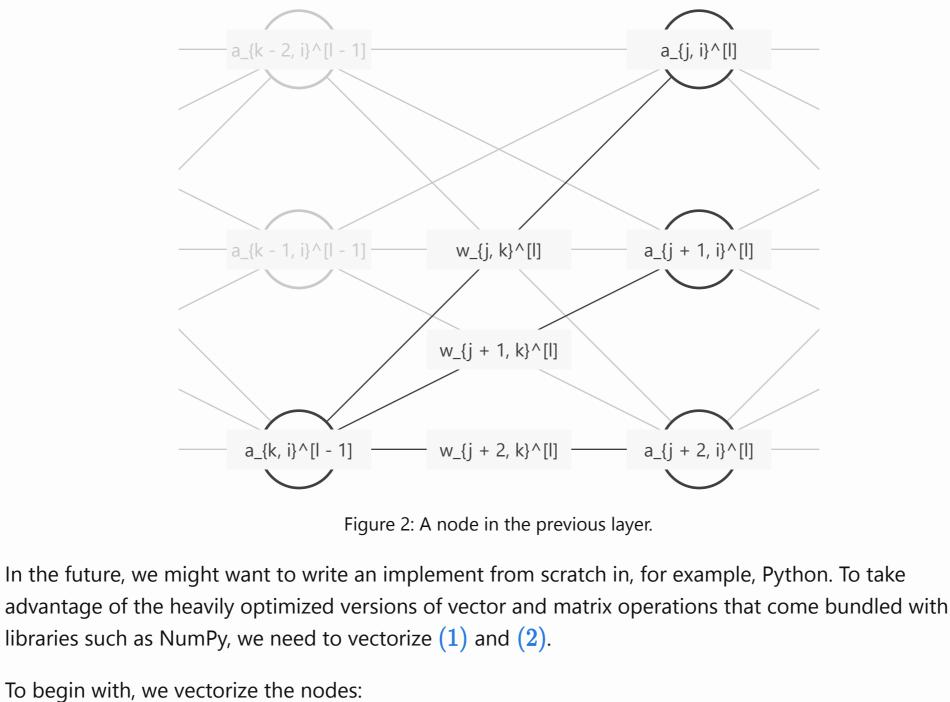
The kth node of the previous layer,  $k=1,\ldots,n^{[l-1]}$ .  ${m k}$  $\boldsymbol{i}$ The current training example  $i=1,\ldots,m$ , where m is the number of training examples.  $z_{j,i}^{[l]}$ A weighted sum of the activations of the previous layer, shifted by a bias.  $w_{j,k}^{\left[l
ight]}$ A weight that scales the kth activation of the previous layer.  $b_j^{[l]}$ A bias in the current layer.  $a_{j,i}^{\left[l
ight]}$ An activation in the current layer.  $a_{k,i}^{\left[l-1\right]}$ An activation in the previous layer.  $g_j^{[l]}$ An activation function  $g_j^{[l]} \colon \mathbb{R}^{n^{[l]}} o \mathbb{R}$  used in the current layer. To put it concisely, a node in the current layer depends on every node in the previous layer, and the following visualization can help us see that more clearly: a\_{j, i}^[l]  $a_{k - 2, i}^{l - 1}$  $w_{j, k - 2}^{l}$  $w_{j, k - 1}^{l}$  $W_{j, k}^{[j]}$ a\_{k - 1, i}^[l - 1]  $a_{j} + 1, i^{[l]}$ 

a\_{k, i}^[l - 1]  $a_{j} + 2, i^{[j]}$ 

Figure 1: A node in the current layer.

Moreover, a node in the previous layer affects every node in the current layer, and with a change in

highlighting, we will also be able to see that more clearly:



 $egin{bmatrix} z_{1,i}^{[l]} \ dots \ z_{1,i}^{[l]} \ dots \ z_{j,i}^{[l]} \ dots \ z_{n^{[l]},i}^{[l]} \ \end{bmatrix} = egin{bmatrix} w_{1,1}^{[l]} & \cdots & w_{1,k}^{[l]} & \cdots & w_{1,n^{[l-1]}}^{[l]} \ dots \ z_{n^{[l]},i}^{[l-1]} \ dots \ z_{n^{[l]},i}^{[l]} \ \end{bmatrix} & egin{bmatrix} a_{1,i}^{[l-1]} \ dots \ a_{1,i}^{[l-1]} \ dots \ a_{1,i}^{[l-1]} \ dots \ a_{1,i}^{[l-1]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l-1]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ dots \ a_{1,i}^{[l]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ \ a_{1,i}^{[l]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ \ a_{1,i}^{[l]} \ \ a_{1,i}^{[l]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ \ a_{1,i}^{[l]} \ \ a_{1,i}^{[l]} \ \ a_{1,i}^{[l]} \ \end{matrix} + egin{bmatrix} b_{1}^{[l]} \ \ a_{1,i}^{[l]} \ \ a_{1,$ 

 $egin{bmatrix} a_{1,i}^{[l]} & egin{bmatrix} g_1^{[l]}(z_{1,i}^{[l]},\ldots,z_{j,i}^{[l]},\ldots,z_{n^{[l]},i}^{[l]}) \ & dots \ a_{j,i}^{[l]} & egin{bmatrix} g_j^{[l]}(z_{1,i}^{[l]},\ldots,z_{j,i}^{[l]},\ldots,z_{n^{[l]},i}^{[l]}) \ & dots \ g_{n^{[l]},i}^{[l]}(z_{1,i}^{[l]},\ldots,z_{j,i}^{[l]},\ldots,z_{n^{[l]},i}^{[l]}) \end{bmatrix}, \ & dots \$ 

 $\mathbf{z}_{:,i}^{[l]} = \mathbf{W}^{[l]} \mathbf{a}_{:,i}^{[l-1]} + \mathbf{b}^{[l]},$ 

where  $\mathbf{z}_{:,i}^{[l]} \in \mathbb{R}^{n^{[l]}}$ ,  $\mathbf{W}^{[l]} \in \mathbb{R}^{n^{[l]} \times n^{[l-1]}}$ ,  $\mathbf{b}^{[l]} \in \mathbb{R}^{n^{[l]}}$ ,  $\mathbf{a}_{:,i}^{[l]} \in \mathbb{R}^{n^{[l]}}$ ,  $\mathbf{a}_{:,i}^{[l-1]} \in \mathbb{R}^{n^{[l-1]}}$ , and lastly,  $\mathbf{g}^{[l]} \colon \mathbb{R}^{n^{[l]}} \to \mathbb{R}^{n^{[l]}}$ 

 $\mathbf{a}^{[l]}_{\cdot,i} = \mathbf{g}^{[l]}(\mathbf{z}^{[l]}_{\cdot,i}),$ 

. We have used a colon to clarify that  $\mathbf{z}_{:,i}^{[l]}$  is the ith column of  $\mathbf{Z}^{[l]}$ , and so on.

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which we can write as

Next, we vectorize the training examples: 
$$\begin{aligned} \mathbf{Z}^{[l]} &= \begin{bmatrix} \mathbf{z}_{:,1}^{[l]} & \dots & \mathbf{z}_{:,i}^{[l]} & \dots & \mathbf{z}_{:,m}^{[l]} \end{bmatrix} \\ &= \mathbf{W}^{[l]} \begin{bmatrix} \mathbf{a}_{:,1}^{[l-1]} & \dots & \mathbf{a}_{:,i}^{[l-1]} & \dots & \mathbf{a}_{:,m}^{[l-1]} \end{bmatrix} + \begin{bmatrix} \mathbf{b}^{[l]} & \dots & \mathbf{b}^{[l]} & \dots & \mathbf{b}^{[l]} \end{bmatrix} \\ &= \mathbf{W}^{[l]} \mathbf{A}^{[l-1]} + \mathbf{broadcast}(\mathbf{b}^{[l]}), \\ \mathbf{A}^{[l]} &= \begin{bmatrix} \mathbf{a}_{:,1}^{[l]} & \dots & \mathbf{a}_{:,i}^{[l]} & \dots & \mathbf{a}_{:,m}^{[l]} \end{bmatrix}, \end{aligned}$$
 where 
$$\begin{aligned} \mathbf{Z}^{[l]} &\in \mathbb{R}^{n^{[l]} \times m}, & \mathbf{A}^{[l]} &\in \mathbb{R}^{n^{[l]} \times m}, & \text{and } \mathbf{A}^{[l-1]} &\in \mathbb{R}^{n^{[l-1]} \times m}. & \text{In addition, have a look at the NumPy documentation if you want to read a well-written explanation of broadcasting.} \end{aligned}$$
 We would also like to establish two additional notations:

 $\mathbf{A}^{[0]}=\mathbf{X},$ 

 $\mathbf{A}^{[L]} = \mathbf{\hat{Y}},$ 

 $J=f(\mathbf{\hat{Y}},\mathbf{Y})=f(\mathbf{A}^{[L]},\mathbf{Y}),$ 

where  $\mathbf{X} \in \mathbb{R}^{n^{[0]} \times m}$  denotes the inputs and  $\mathbf{\hat{Y}} \in \mathbb{R}^{n^{[L]} \times m}$  denotes the predictions/outputs.

where  $\mathbf{Y} \in \mathbb{R}^{n^{[L]} \times m}$  denotes the targets and  $f \colon \mathbb{R}^{2n^{[L]}} \to \mathbb{R}$  can be tailored to our needs.

Finally, we are ready to define the cost function:

apply the chain rule to the following example:

Now, let us concentrate on the task at hand:

Vectorization results in

We are done with forward propagation! Next up: backward propagation, also known as backpropagation, which involves computing the gradient of the cost function with respect to the weights and biases. **Backward Propagation** 

We will make heavy use of the chain rule in this section, and to understand better how it works, we first

 $u_i = g_i(x_1, \ldots, x_i, \ldots, x_n),$ 

 $y_k = f_k(u_1, \ldots, u_i, \ldots, u_m).$ 

 $rac{\partial y_k}{\partial x_i} = \sum_i rac{\partial y_k}{\partial u_i} rac{\partial u_i}{\partial x_i}.$ 

 $rac{\partial J}{\partial w_{j,k}^{[l]}} = \sum_i rac{\partial J}{\partial z_{j,i}^{[l]}} rac{\partial z_{j,i}^{[l]}}{\partial w_{j,k}^{[l]}} = \sum_i rac{\partial J}{\partial z_{j,i}^{[l]}} a_{k,i}^{[l-1]},$ 

 $-\sum_{i}rac{\overline{\partial z_{j,i}^{[l]}}}{\partial z_{j,i}^{[l]}}rac{\overline{\partial b_{j}^{[l]}}}{\overline{\partial b_{j}^{[l]}}}-\sum_{i}rac{\overline{\partial z_{j,i}^{[l]}}}{\overline{\partial z_{j,i}^{[l]}}}$ 

 $\frac{\partial J}{\partial z} = \sum_{i} \frac{\partial J}{\partial z_{j,i}^{[l]}} = \sum_{i} \frac{\partial J}{\partial z_{j,i}^{[l]}}$ 

Note that  $x_j$  may affect  $u_1,\ldots,u_i,\ldots,u_m$ , and  $y_k$  may depend on  $u_1,\ldots,u_i,\ldots,u_m$ ; thus,

Great! If we ever get stuck trying to compute or understand some partial derivative, we can always go back to (10), (11), and (12). Hopefully, these equations will provide the clues necessary to move forward. However, be extra careful not to confuse the notation used for the chain rule example with the

notation we use elsewhere in this series. The overlap is unintentional.

 $\partial J$  $\partial J$  $\partial J$  $\partial J$  $\overline{\partial w_{n^{[l]},k}^{[l]}}$ 

 $\partial z_{1,m}^{[l]}$ 

 $\partial J$ 

 $\partial z_{1,i}^{[l]}$ 

 $\partial J$ 

 $\partial J$ 

(15)

(16)

(17)

(18)

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(21)

(22)

 $\partial J$ 

 $\partial J$ 

 $egin{bmatrix} rac{\partial J}{\partial a_{1,1}^{[l-1]}} & \cdots & rac{\partial J}{\partial a_{1,i}^{[l-1]}} & \cdots & rac{\partial J}{\partial a_{1,m}^{[l-1]}} \ dots & dots & dots & dots & dots \ rac{\partial J}{\partial a_{k,1}^{[l-1]}} & \cdots & rac{\partial J}{\partial a_{k,m}^{[l-1]}} & \cdots & rac{\partial J}{\partial a_{k,m}^{[l-1]}} \ \end{pmatrix}$  $\partial J$ 

On purpose, we have omitted the details of  $g_j^{[l]}(z_{1,i}^{[l]},\ldots,z_{j,i}^{[l]},\ldots,z_{n^{[l]},i}^{[l]})$ ; consequently, we cannot derive

Furthermore, according to (17), we see that  $\partial J/\partial z_{j,i}^{[l]}$  also depends on  $\partial J/\partial a_{j,i}^{[l]}$ . Now, it might come as

 $rac{\partial J}{\partial a_{k,i}^{[l-1]}} = \sum_{j} rac{\partial J}{\partial z_{j,i}^{[l]}} rac{\partial z_{j,i}^{[l]}}{\partial a_{k,i}^{[l-1]}} = \sum_{j} rac{\partial J}{\partial z_{j,i}^{[l]}} w_{j,k}^{[l]}.$ 

a surprise, but  $\partial J/\partial a^{[l]}_{j,i}$  has already been computed when we reach the lth layer during backward

propagation. How did that happen, you may ask. The answer is that every layer paves the way for the

an analytic expression for  $\partial a_{j,i}^{[l]}/\partial z_{j,i'}^{[l]}$  which we depend on in (17). However, since the second post of

this series will be dedicated to activation functions, we will instead derive  $\partial a_{j,i}^{[l]}/\partial z_{j,i}^{[l]}$  there.

previous layer by also computing  $\partial J/\partial a_{k,i}^{[l-1]}$  , which we shall do now:

where  $\partial J/\partial \mathbf{A}^{[l]} \in \mathbb{R}^{n^{[l]} \times m}$ .

As usual, our next step is vectorization:

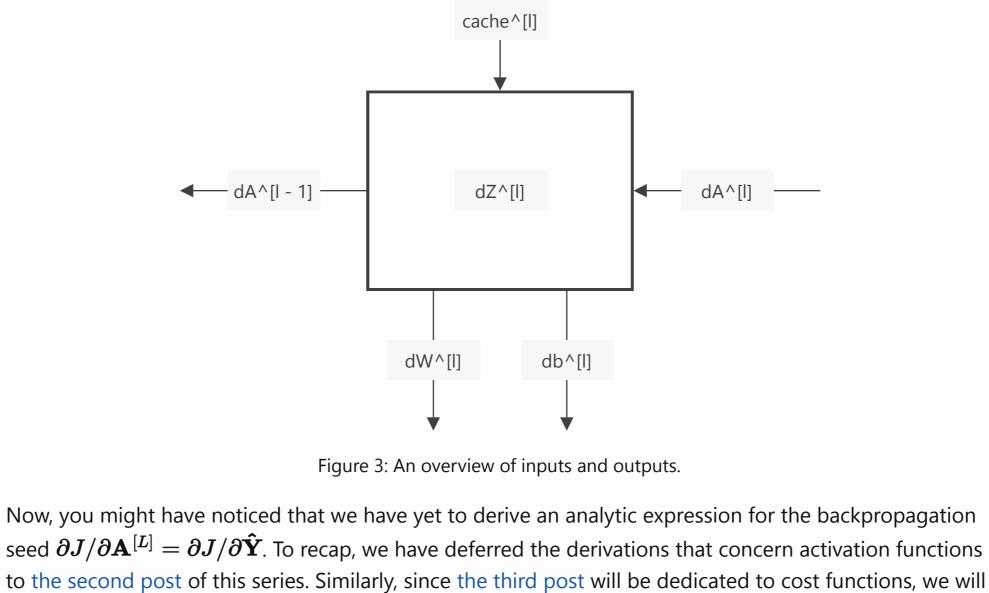
which we can write as

Summary

where  $\partial J/\partial \mathbf{A}^{[l-1]} \in \mathbb{R}^{n^{[l-1]} \times m}$ . Forward propagation is seeded with  $\mathbf{A}^{[0]} = \mathbf{X}$  and evaluates a set of recurrence relations to compute the predictions  $\mathbf{A}^{[L]} = \mathbf{\hat{Y}}$ . We also compute the cost  $J = f(\mathbf{\hat{Y}}, \mathbf{Y}) = f(\mathbf{A}^{[L]}, \mathbf{Y})$ . Backward propagation, on the other hand, is seeded with  $\partial J/\partial {\bf A}^{[L]}=\partial J/\partial {\bf \hat{Y}}$  and evaluates a different set of recurrence relations to compute  $\partial J/\partial \mathbf{W}^{[l]}$  and  $\partial J/\partial \mathbf{b}^{[l]}$ . If not stopped prematurely, it eventually computes  $\partial J/\partial {\bf A}^{[0]}=\partial J/\partial {\bf X}$ , a partial derivative we usually ignore. Moreover, let us visualize the inputs we use and the outputs we produce during the forward and backward propagations:

W^[l]

b^[l]



Yet another blog about deep learning.

instead address the derivation of the backpropagation seed there.

Last but not least: congratulations! You have made it to the end (of the first post).

**in** jonaslalin