

CS 466/566

Introduction to Deep Learning

Lecture 8 – Back Propagation

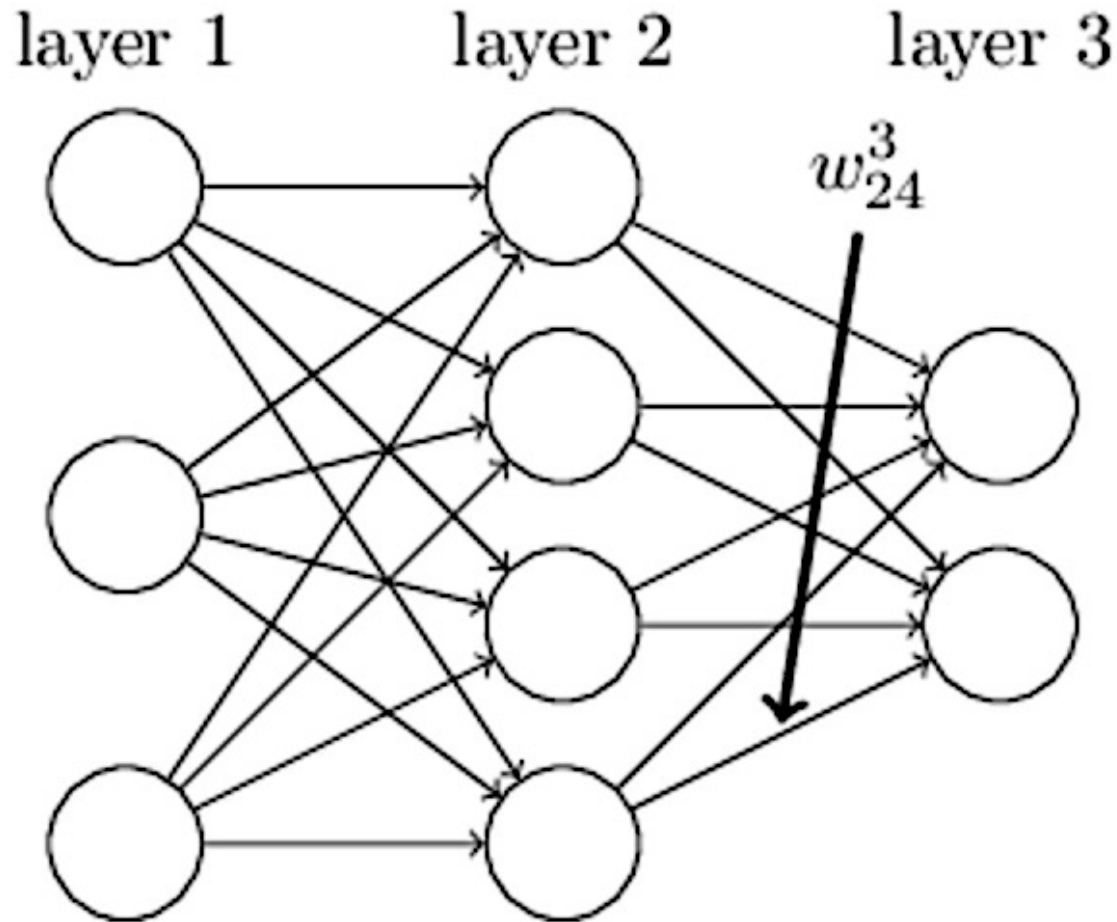
Neural Network Notation

- For each neuron j , its output a_j is defined as

$$a_j = \sigma(z_j) = \sigma\left(\sum_{k=1}^n w_{jk} a_k\right)$$

- where
 - z_j is the input to a neuron: weighted sum of outputs of previous neurons
 - a_j is the activated value of z_j .
 - n is the number of input units to the neuron.
 - w_{ij} denotes the weight between neuron i and neuron j .

Neural Network Notation



$\left\{ \begin{array}{l} w_{jk}^l \text{ is the weight from the } k^{th} \text{ neuron} \\ \text{in the } (l-1)^{th} \text{ layer to the } j^{th} \text{ neuron} \\ \text{in the } l^{th} \text{ layer} \end{array} \right.$

A naïve approach for updating weights

- Imagine that back-propagation hasn't been derived yet.
- You want to use gradient descent for learning.
- You need a way of computing the gradient of the cost function.
- You think back to your knowledge of calculus, and decide to see if you can use the chain rule to compute the gradient.
- But after playing around a bit, the algebra looks complicated, and you get discouraged.
- You decide to regard the cost as a function of the weights $C = C(w)$ alone.

A naïve approach for updating weights

- An obvious way of doing that is to use the numerical approximation of the derivative at a specific weight.

$$\frac{\partial C}{\partial w_j} \approx \frac{C(w + \epsilon e_j) - C(w)}{\epsilon}$$

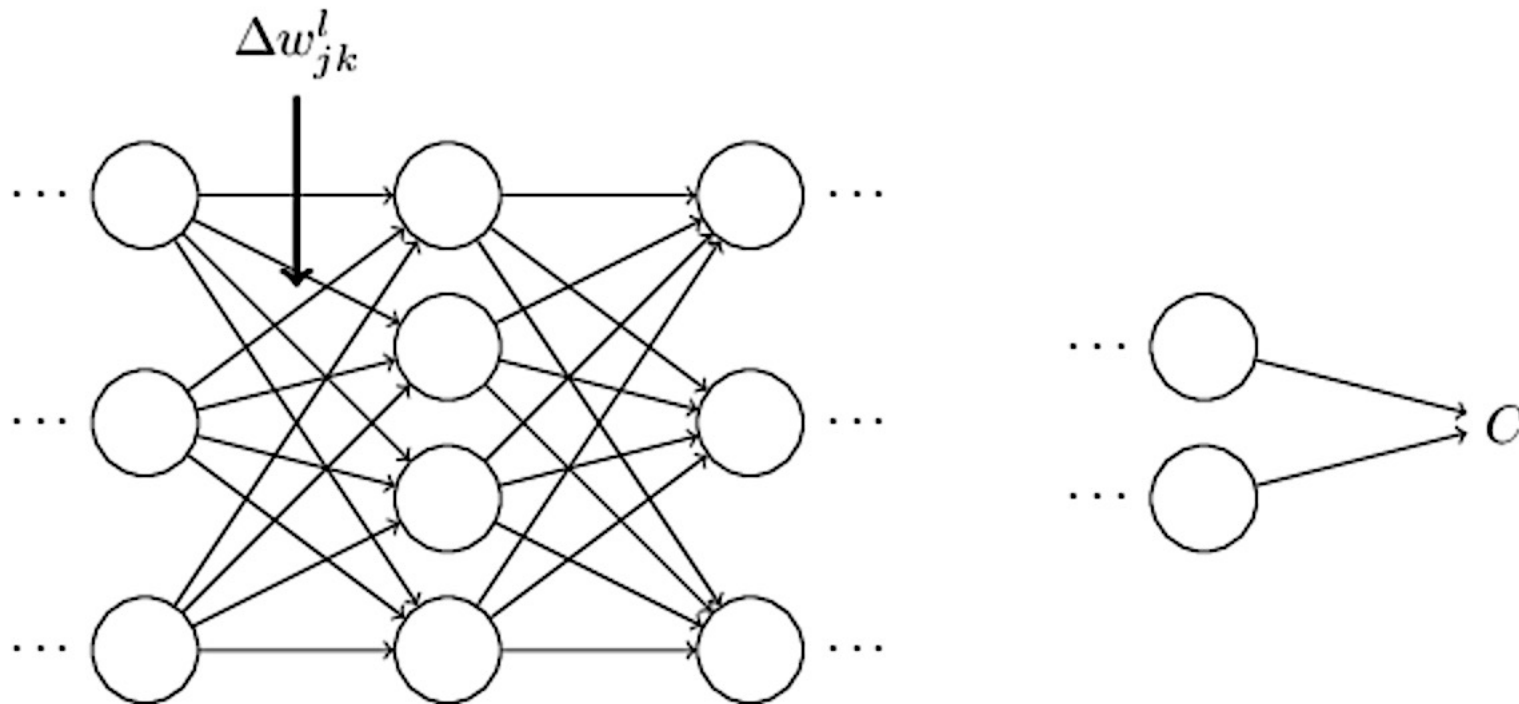
- where $\epsilon > 0$ is a small positive number, and e_j is the unit vector in the j^{th} direction.
- This approach looks very promising.
- It's simple conceptually, and extremely easy to implement, using just a few lines of code.
- Certainly, it looks much more promising than the idea of using the chain rule to compute the gradient!

A naïve approach for updating weights

- Unfortunately, while this approach appears promising, when you implement the code it turns out to be extremely slow.
- To understand why, imagine we have a **million weights** in our network.
- Then for each distinct weight w_j we need to compute $C(w + \epsilon e_j)$ in order to compute its partial effect on ultimate cost.
- That means that to compute the gradient we need to compute the cost function a million different times, requiring **a million forward passes** through the network (**per training example**)!
- We need a more efficient strategy.

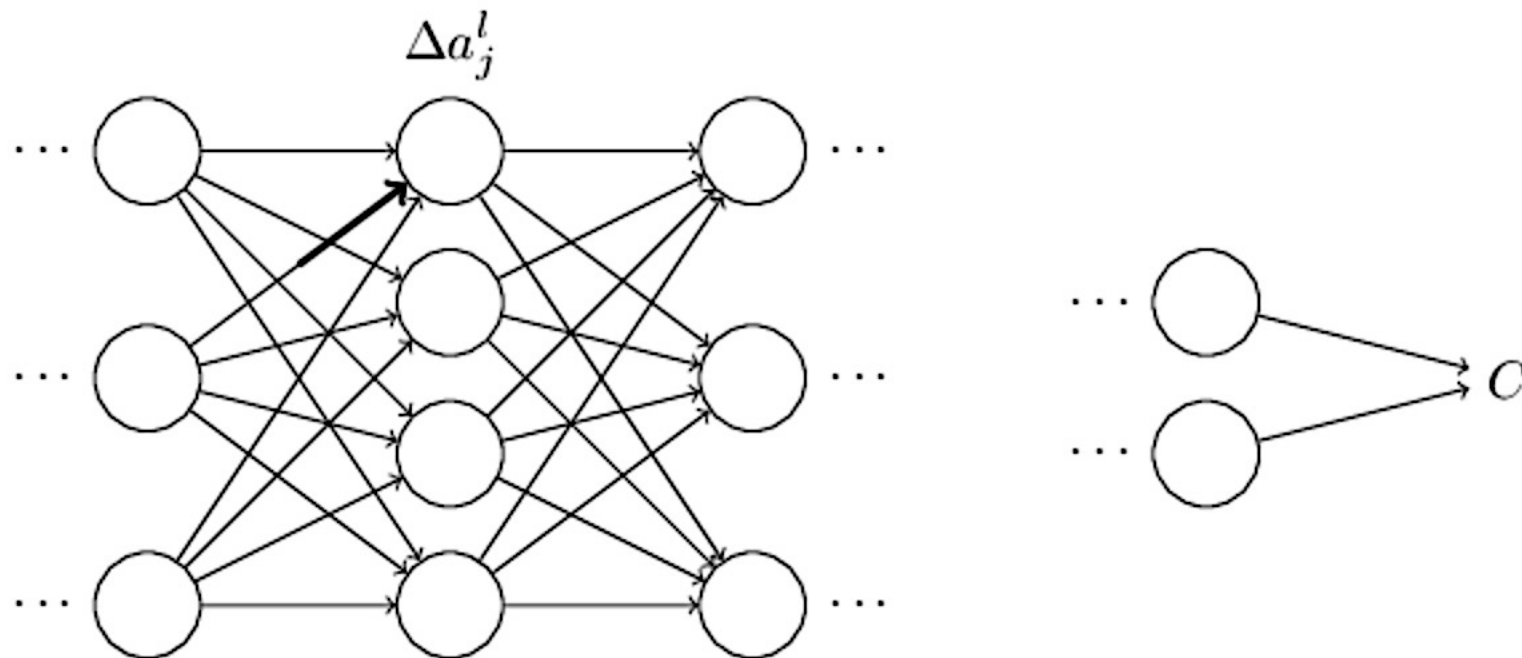
Intuition before derivation of back propagation

- To improve our intuition about what the algorithm is doing, let's imagine that we've made a small change to some weight in the network:



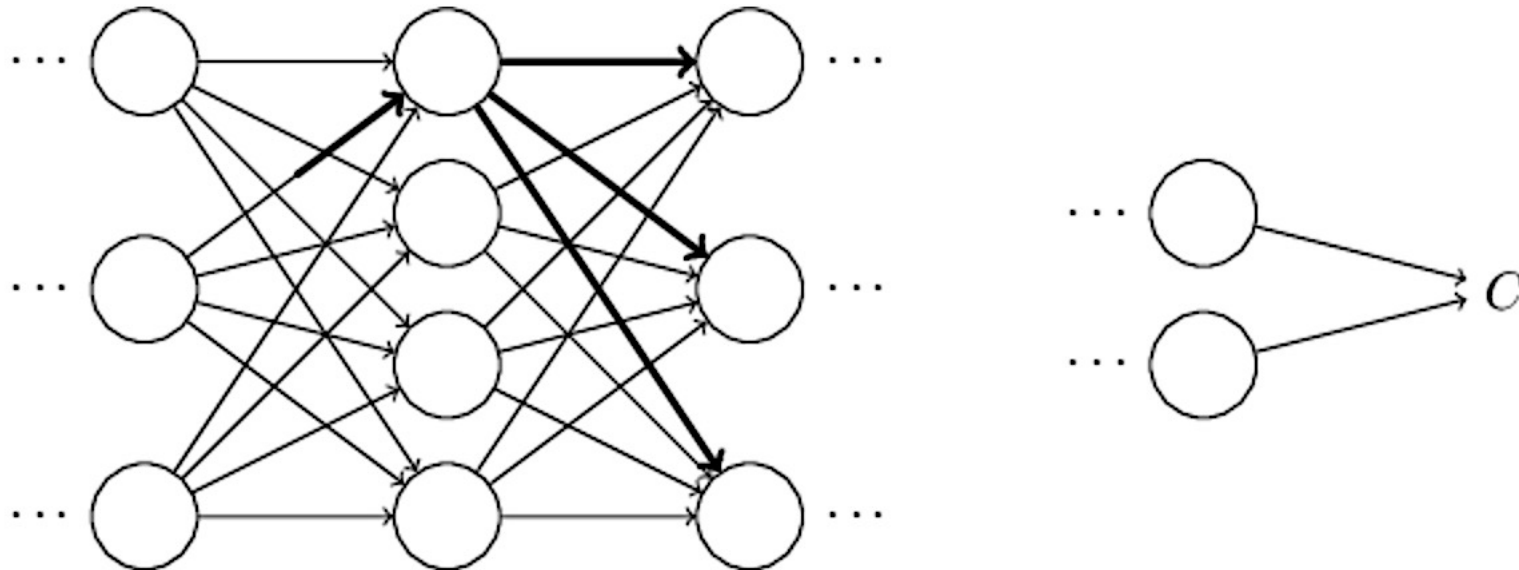
Intuition before derivation of back propagation

- That change in weight will cause a change in the output activation from the corresponding neuron:



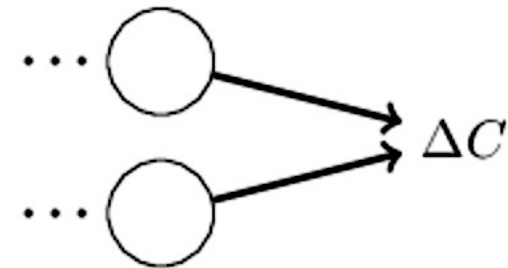
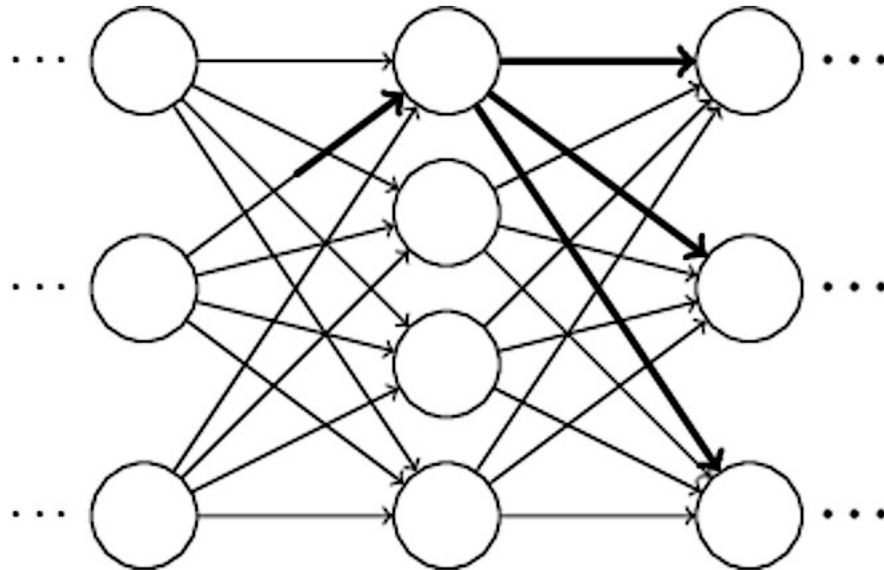
Intuition before derivation of back propagation

- That, in turn, will cause a change in *all* the activations in the next layer:



Intuition before derivation of back propagation

- Those changes will in turn cause changes in the next layer, and then the next, and so on all the way through to causing a change in the final layer, and then in the cost function:



Intuition before derivation of back propagation

- The change ΔC in the cost is related to the change in the weight by the equation:

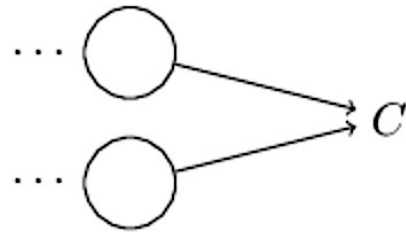
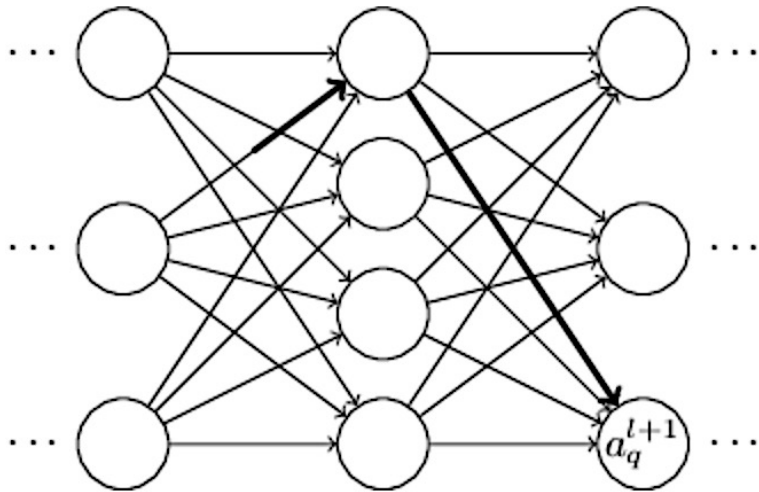
$$\Delta C \approx \frac{\partial C}{\partial w_{jk}^l} \Delta w_{jk}^l$$

- Let's try to carry this out. The change in w causes a small change in the activation of the j^{th} neuron in the l^{th} layer. This change is given by:

$$\Delta a_j^l \approx \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l$$

Intuition before derivation of back propagation

- The change in activation will cause changes in **all** the activations in the next layer, i.e., the $(l+1)^{th}$ layer.
- We'll concentrate on the way **just a single one of those activations** is affected



$$\Delta a_j^l \approx \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l$$

- in fact,
it'll cause a change
like this:

$$\Delta a_q^{l+1} \approx \frac{\partial a_q^{l+1}}{\partial a_j^l} \Delta a_j^l$$

Intuition before derivation of back propagation

- We have:

$$\boxed{\Delta a_j^l} \approx \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l$$

$$\Delta a_q^{l+1} \approx \frac{\partial a_q^{l+1}}{\partial a_j^l} \boxed{\Delta a_j^l}$$

- Substituting

$$\Delta a_q^{l+1} \approx \frac{\partial a_q^{l+1}}{\partial a_j^l} \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l$$

Intuition before derivation of back propagation

- This change will, in turn, cause changes in the activations in the next layer.
- In fact, we can imagine a path all the way through the network from ***our initial weight*** to ***C***, with each change in activation causing a change in the next activation, and, finally, a change in the **cost** at the output.
- If the path goes through some activations then the resulting expression can be:

$$\Delta C \approx \frac{\partial C}{\partial a_m^L} \frac{\partial a_m^L}{\partial a_n^{L-1}} \frac{\partial a_n^{L-1}}{\partial a_p^{L-2}} \cdots \frac{\partial a_q^{l+1}}{\partial a_j^l} \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l$$

- This represents the change in **C** due to changes in the activations along this particular path through the network.

Intuition before derivation of back propagation

- Of course, there's many paths by which a change in **our weight** can propagate to affect the cost, and **we've been considering just a single path**.
- To compute the total change in C it is plausible that we should sum over all the possible paths between the weight and the final cost, i.e.,

$$\Delta C \approx \sum_{mnp\dots q} \frac{\partial C}{\partial a_m^L} \frac{\partial a_m^L}{\partial a_n^{L-1}} \frac{\partial a_n^{L-1}}{\partial a_p^{L-2}} \cdots \frac{\partial a_q^{l+1}}{\partial a_j^l} \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l$$

- where we've summed over all possible choices for the intermediate neurons along the path. But remember how we started all this:

$$\Delta C \approx \frac{\partial C}{\partial w_{jk}^l} \Delta w_{jk}^l$$

Intuition before derivation of back propagation

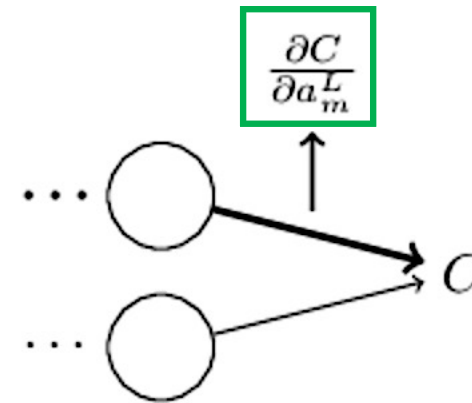
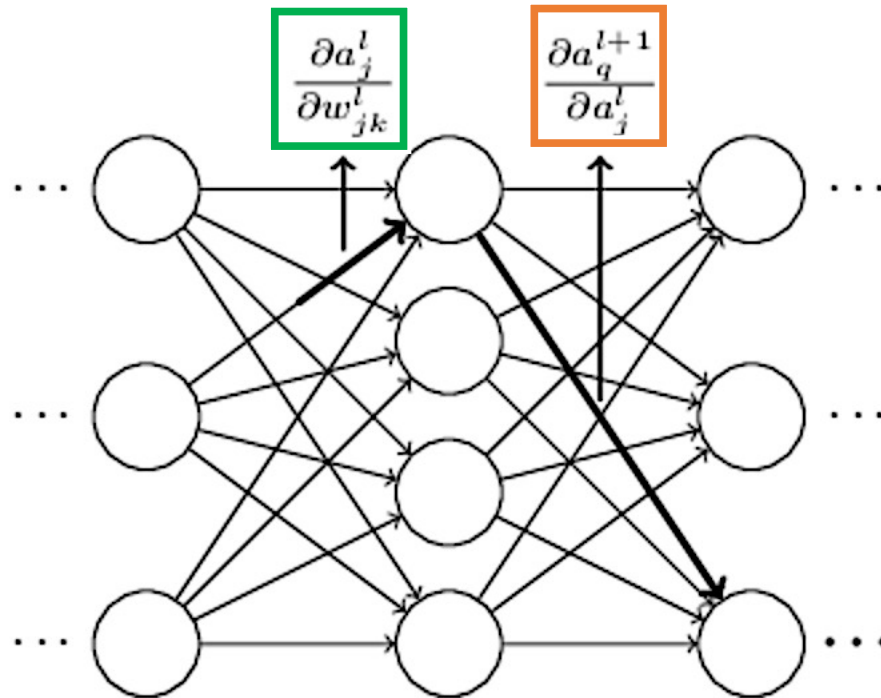
- At last, we have:

$$\frac{\partial C}{\partial w_{jk}^l} = \sum_{mnp\dots q} \boxed{\frac{\partial C}{\partial a_m^L}} \boxed{\frac{\partial a_m^L}{\partial a_n^{L-1}}} \boxed{\frac{\partial a_n^{L-1}}{\partial a_p^{L-2}}} \cdots \boxed{\frac{\partial a_q^{l+1}}{\partial a_j^l}} \boxed{\frac{\partial a_j^l}{\partial w_{jk}^l}}$$

- This looks complicated! However, it has a nice intuitive interpretation.
- We're computing the rate of change of C with respect to **a weight** in the network.
- What the equation tells us is that *every edge between two neurons in the network is associated with a rate factor which is just the partial derivative of one neuron's activation with respect to the other neuron's activation.*

Intuition before derivation of back propagation

$$\frac{\partial C}{\partial w_{jk}^l} = \sum_{mnp\dots q} \boxed{\frac{\partial C}{\partial a_m^L}} \boxed{\frac{\partial a_m^L}{\partial a_n^{L-1}}} \boxed{\frac{\partial a_n^{L-1}}{\partial a_p^{L-2}}} \cdots \boxed{\frac{\partial a_q^{l+1}}{\partial a_j^l}} \boxed{\frac{\partial a_j^l}{\partial w_{jk}^l}}$$



Back propagation

Now that we have an intuition about the effect of changing a single weight in our network,

Let's start the real derivation;
starting from the output layer,
going towards the input layer

Back propagation: Cost function assumptions

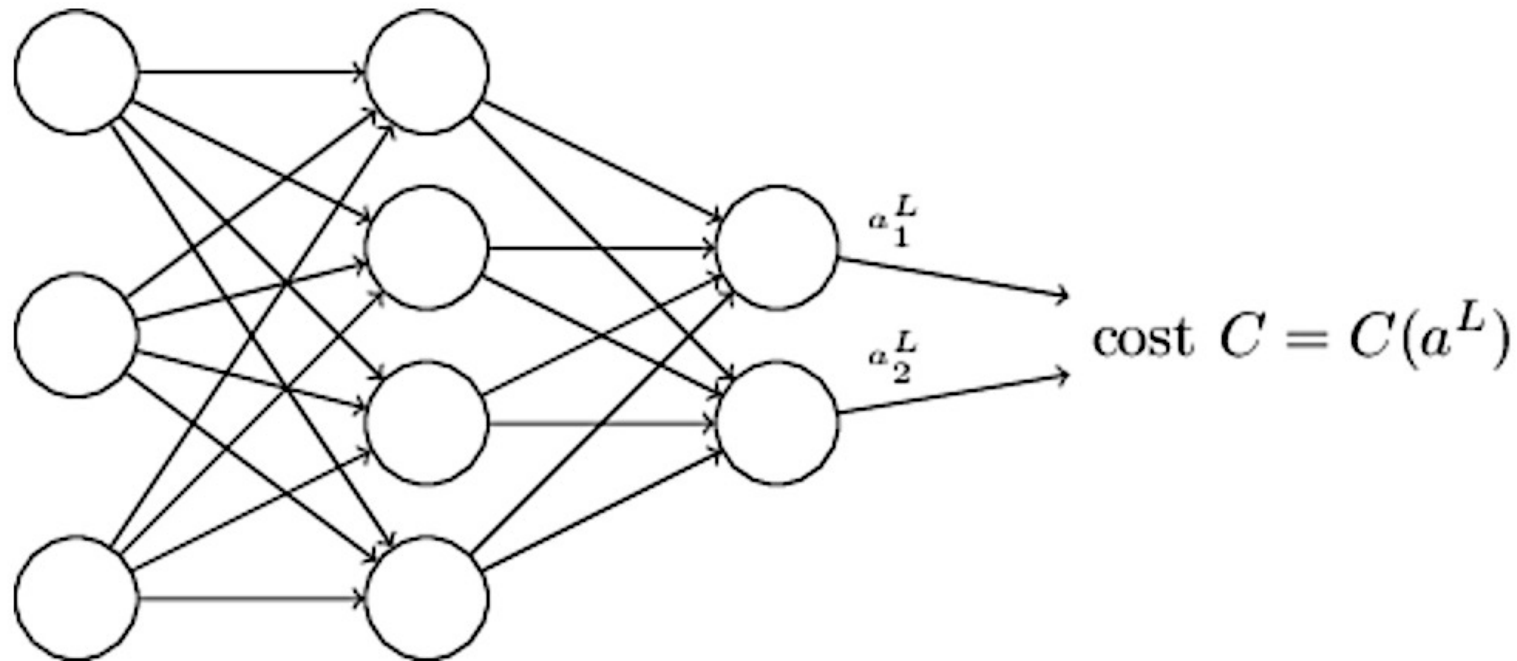
First Assumption

- Cost must be written as an average over cost functions for individual training examples.
- The reason for this assumption is that the backpropagation algorithm calculates the gradient of the error function for a single training example, which needs to be generalized to the overall error function.
- In practice, training examples are placed in batches, and the error is averaged at the end of the batch, which is then used to update the weights.

Back propagation: Cost function assumptions

Second Assumption

- Cost must be written as a function of the outputs from the neural network.



Back propagation: Idea

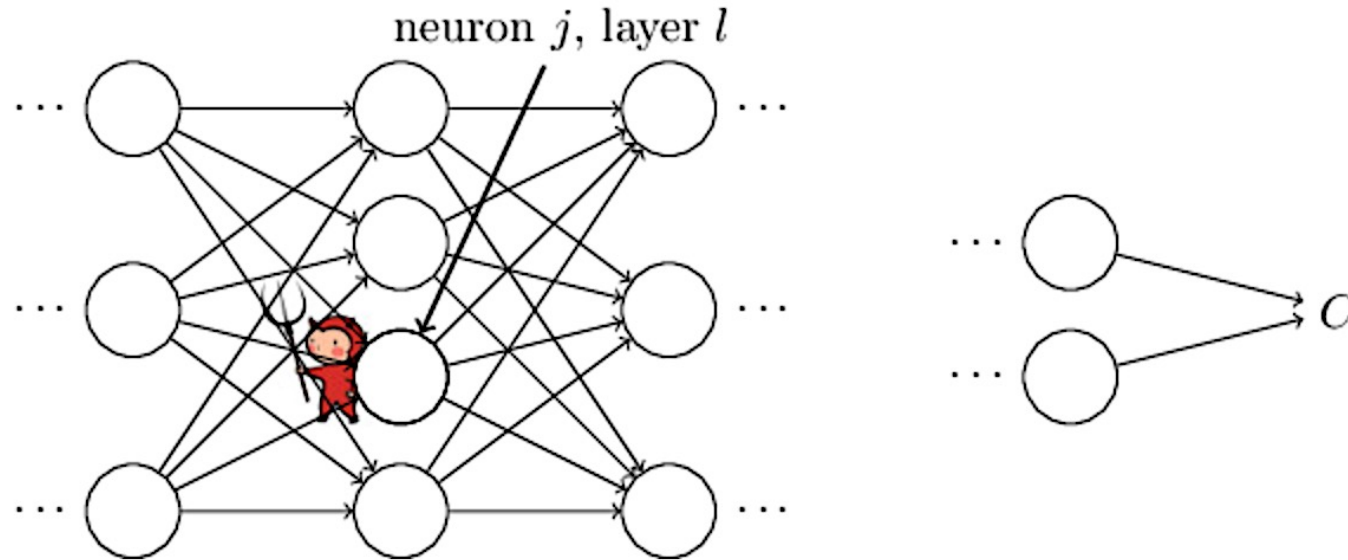
- Backpropagation is about calculating how changing the weights and biases in a network changes the cost function, *effectively*.
- Ultimately, this will mean computing the partial derivatives.
- But to compute those, we first introduce an intermediate quantity which we call the *local error* in the j^{th} neuron in the l^{th} layer.

$$\delta_j^{(l)} = \frac{\partial C}{\partial z_j^{(l)}}$$

- Backpropagation will give us a procedure to compute the error and then will relate it to the ultimate cost function.

Back propagation: Idea

- To understand how the *local error* is defined, imagine there is a **demon** in our neural network:



$$\delta_j^{(l)} = \frac{\partial C}{\partial z_j^{(l)}}$$

$$\sigma(z_j^l + \Delta z_j^l)$$

$$\frac{\partial C}{\partial z_j^{(l)}} \Delta z_j^l$$

- The **demon** sits at the j^{th} neuron in layer l . As the input to the neuron comes in, the demon messes with the neuron's operation. It adds a little change to the neuron's weighted input z_j .
- This change propagates through later layers in the network, finally causing the overall cost to change by an amount.

Back propagation: Regression with squared cost

- Since backpropagation uses the gradient descent method, one needs to calculate the derivative of the squared cost function with respect to the weights of the network.
- Assuming one output neuron, the squared cost function is:

$$C = \frac{1}{2}(t - y)^2$$

- where
 - C is the squared cost,
 - t is the target output for a training sample
 - y is the actual output of the output neuron.

Back propagation

- The activation function σ is in general non-linear and differentiable. A commonly used activation function is the logistic function:

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

- which has a nice derivative of:

$$\frac{d\sigma}{dz} = \sigma(z)(1 - \sigma(z))$$

Recall: Derivative of division

$$\frac{\partial \frac{g(x)}{h(x)}}{\partial x} = \frac{\partial g(x)}{\partial x} \frac{1}{h(x)} - \frac{g(x)}{h(x)^2} \frac{\partial h(x)}{\partial x}$$

Back propagation

- Finding the derivative of the cost:
 - Calculating the partial derivative of the cost with respect to a weight w_{ij} is done using the chain rule twice:

$$\frac{\partial C}{\partial w_{ij}} = \boxed{\frac{\partial C}{\partial a_i}} \frac{\partial a_i}{\partial z_i} \frac{\partial z_i}{\partial w_{ij}}$$

- a_i can be either at the **output layer**, or in **an arbitrary inner layer** of the network.

Back propagation

$$\frac{\partial C}{\partial w_{ij}} = \frac{\partial C}{\partial a_i} \frac{\partial a_i}{\partial z_i} \boxed{\frac{\partial z_i}{\partial w_{ij}}}$$

- In the last factor of the right-hand side of the above, only one term depends on w_{ij} , so that

$$\boxed{\frac{\partial z_i}{\partial w_{ij}}} = \frac{\partial}{\partial w_{ij}} \left(\sum_{k=1}^n w_{ik} a_k \right) = \boxed{a_j}$$

Back propagation

$$\frac{\partial C}{\partial w_{ij}} = \frac{\partial C}{\partial a_i} \frac{\partial a_i}{\partial z_i} \frac{\partial z_i}{\partial w_{ij}}$$

- If the neuron is in the **first layer** after the input layer, a_i is just x_i .
- The derivative of the output of neuron j (a_i) with respect to its input (z_i) is simply the partial derivative of the activation function (assuming here that the logistic function is used):

$$\frac{\partial a_i}{\partial z_i} = \frac{\partial}{\partial z_i} \sigma(z_i) = \sigma(z_i)(1 - \sigma(z_i))$$

- This is the reason why backpropagation requires the activation function to be differentiable.

Back propagation

$$\frac{\partial C}{\partial w_{ij}} = \boxed{\frac{\partial C}{\partial a_i}} \frac{\partial a_i}{\partial z_i} \frac{\partial z_i}{\partial w_{ij}}$$

- The first factor is straightforward to evaluate if the neuron is in the output layer, because then $a_i = y$ and

$$\boxed{\frac{\partial C}{\partial a_i}} = \frac{\partial C}{\partial y} = \frac{\partial}{\partial y} \frac{1}{2} (t - y)^2 = y - t = \boxed{a_i - t}$$

- However, if i is in an arbitrary inner layer of the network, it is less obvious.

Back propagation

$$\frac{\partial C}{\partial w_{ij}} = \boxed{\frac{\partial C}{\partial a_i}} \frac{\partial a_i}{\partial z_i} \frac{\partial z_i}{\partial w_{ij}}$$

- Considering C as a function of the inputs of all neurons $L=u, v, \dots, w$ receiving input from neuron i ,

$$\boxed{\frac{\partial C(a_i)}{\partial a_i}} = \frac{\partial C(z_u, z_v, \dots, z_w)}{\partial a_i}$$

- and taking the **total derivative** with respect to a_i , a recursive expression for the derivative is obtained:

$$\boxed{\frac{\partial C}{\partial a_i}} = \sum_{l \in L} \left(\frac{\partial C}{\partial z_l} \frac{\partial z_l}{\partial a_i} \right) = \boxed{\sum_{l \in L} \left(\frac{\partial C}{\partial a_l} \frac{\partial a_l}{\partial z_l} w_{li} \right)}$$

- Therefore, the derivative with respect to a_i can be calculated if all the derivatives with respect to the outputs a_l of the next layer are known.

Back propagation

$$\frac{\partial C}{\partial w_{ij}} = \frac{\partial C}{\partial a_i} \frac{\partial a_i}{\partial z_i} \frac{\partial z_i}{\partial w_{ij}}$$

- Putting it all together from previous slides:

$$\frac{\partial C}{\partial w_{ij}} = \delta_i a_j$$

- where

$$\delta_i = \frac{\partial C}{\partial a_i} \frac{\partial a_i}{\partial z_i} = \begin{cases} (a_i - t_i) a_i (1 - a_i) & \text{if } i \text{ is an output neuron} \\ (\sum_{l \in L} \delta_l w_{li}) a_i (1 - a_i) & \text{if } i \text{ is an inner neuron} \end{cases}$$

Back propagation: Final

$$\frac{\partial C}{\partial w_{ij}} = \delta_i a_j$$

$$\delta_i = \frac{\partial C}{\partial a_i} \frac{\partial a_i}{\partial z_i} = \begin{cases} (a_i - t_i) a_i (1 - a_i) & \text{if } i \text{ is an output neuron} \\ (\sum_{l \in L} \delta_l w_{li}) a_i (1 - a_i) & \text{if } i \text{ is an inner neuron} \end{cases}$$

- To update the weight w_{ij} using gradient descent, one must choose a learning rate, α .
- The change in weight, which is added to the old weight, is equal to the product of the learning rate and the gradient, multiplied by -1 :

$$\Delta w_{ij} = -\alpha \frac{\partial C}{\partial w_{ij}} = \begin{cases} -\alpha a_j (a_i - t_i) a_i (1 - a_i) & \text{if } i \text{ is an output neuron} \\ -\alpha a_j (\sum_{l \in L} \delta_l w_{li}) a_i (1 - a_i) & \text{if } i \text{ is an inner neuron} \end{cases}$$