RECOD
reasoning for complex data

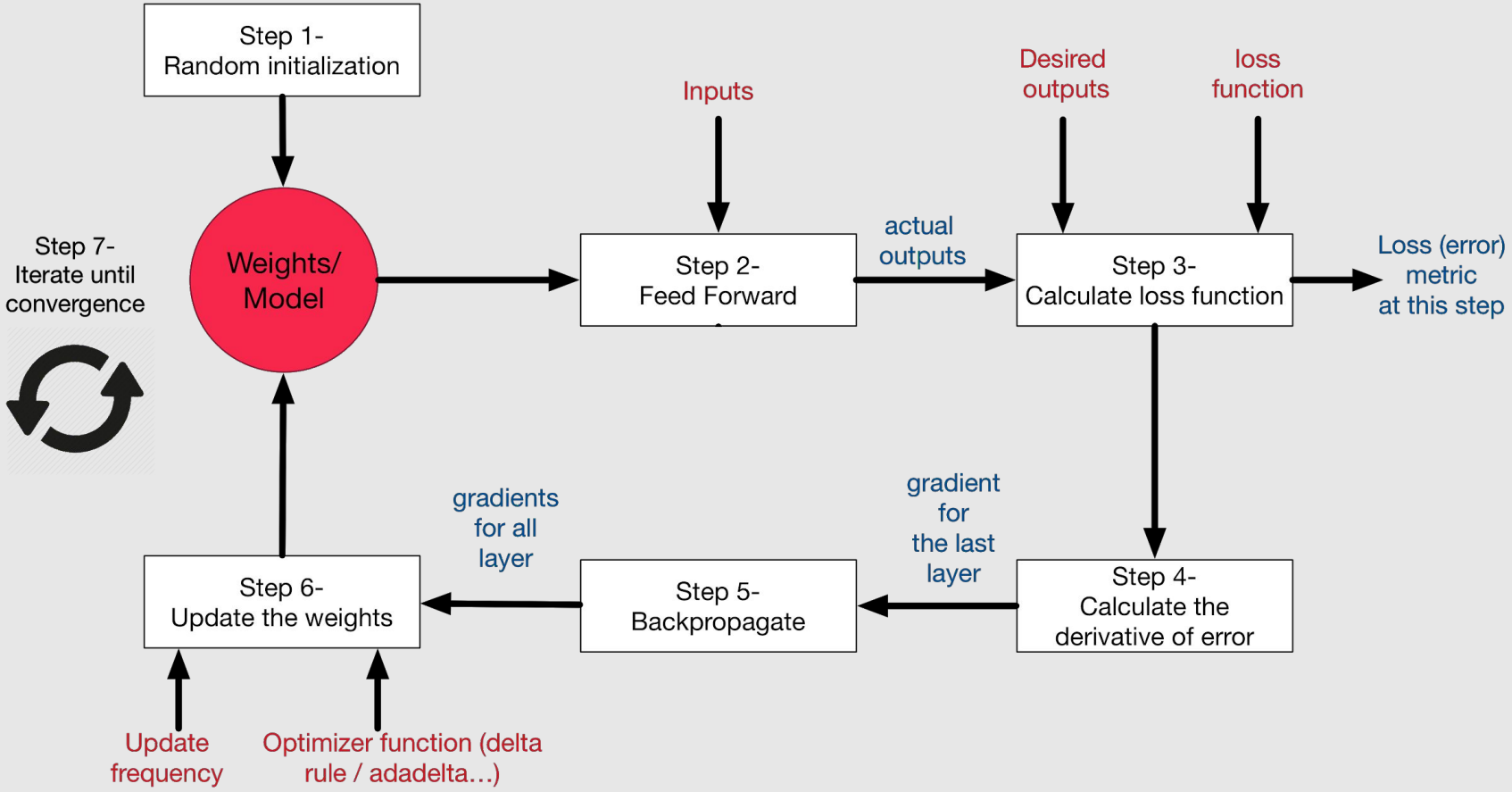
Artificial Neural Networks

Machine Learning

Prof. Sandra Avila
Institute of Computing (IC/Unicamp)

MC886, September 16, 2019

Training a Neural Network



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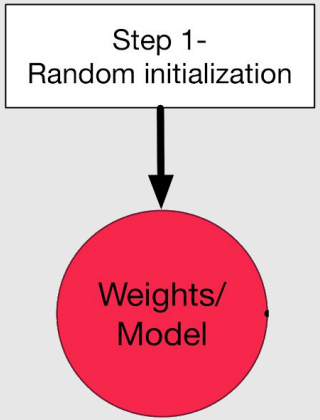
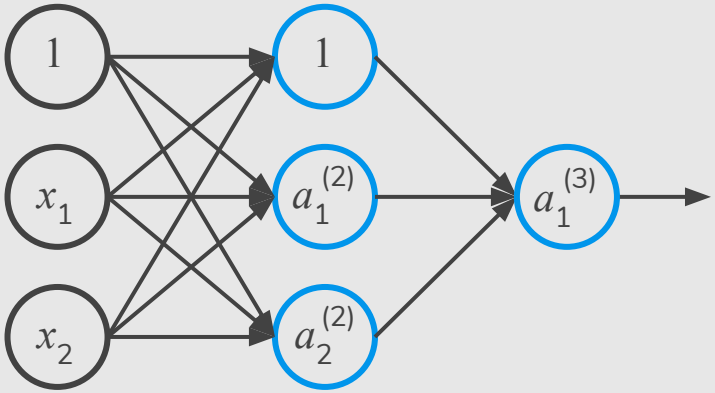


Zero Initialization

Symmetric Weights



$$a_1^{(2)} = a_2^{(2)}$$

After each update, parameters corresponding to inputs going into each of two hidden units are identical.

Symmetric Breaking

- We must initialize Θ to a **random value** in $[-\varepsilon, \varepsilon]$ (i.e. $[-\varepsilon \leq \Theta \leq \varepsilon]$)
- If the dimensions of `Theta1` is 3x4, `Theta2` is 3x4 and `Theta3` is 1x4.

```
Theta1 = random(3,4) * (2 * EPSILON) - EPSILON;
Theta2 = random(3,4) * (2 * EPSILON) - EPSILON;
Theta3 = random(1,4) * (2 * EPSILON) - EPSILON;
```

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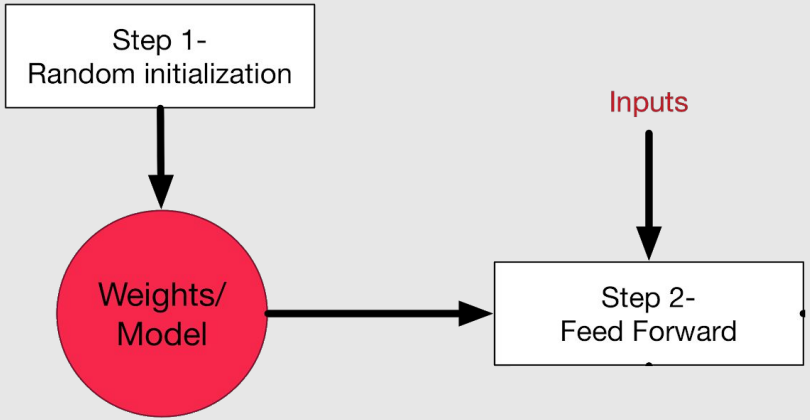


Forward Propagation

Given one training example (x, y):

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

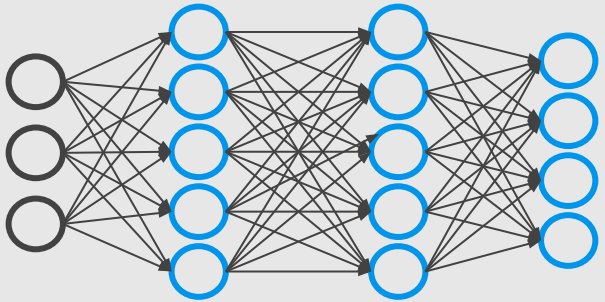
$$a^{(2)} = g(z^{(2)}) \quad (\text{add } a_0^{(2)})$$

$$z^{(3)} = \Theta^{(2)} a^{(2)}$$

$$a^{(3)} = g(z^{(3)}) \quad (\text{add } a_0^{(3)})$$

$$z^{(4)} = \Theta^{(3)} a^{(3)}$$

$$a^{(4)} = h_\Theta(x) = g(z^{(4)})$$



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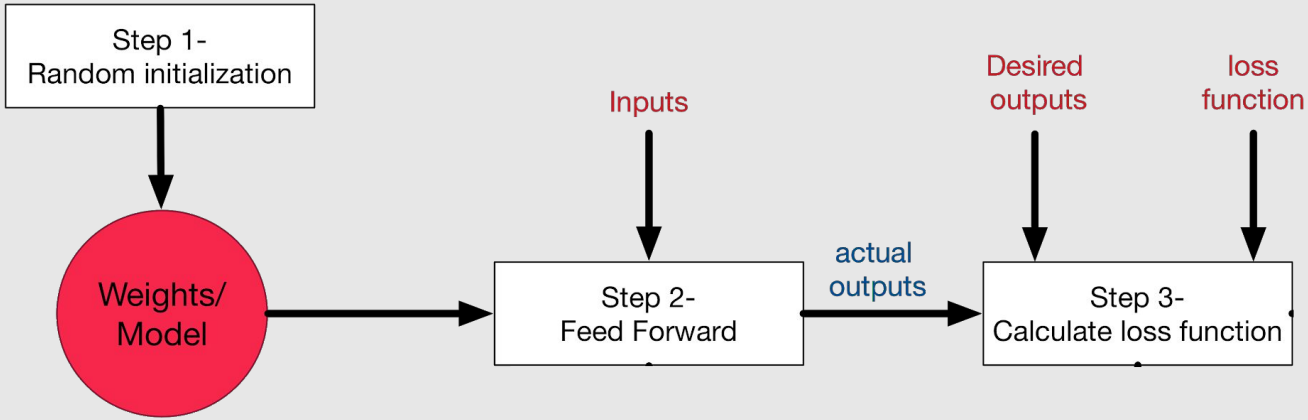

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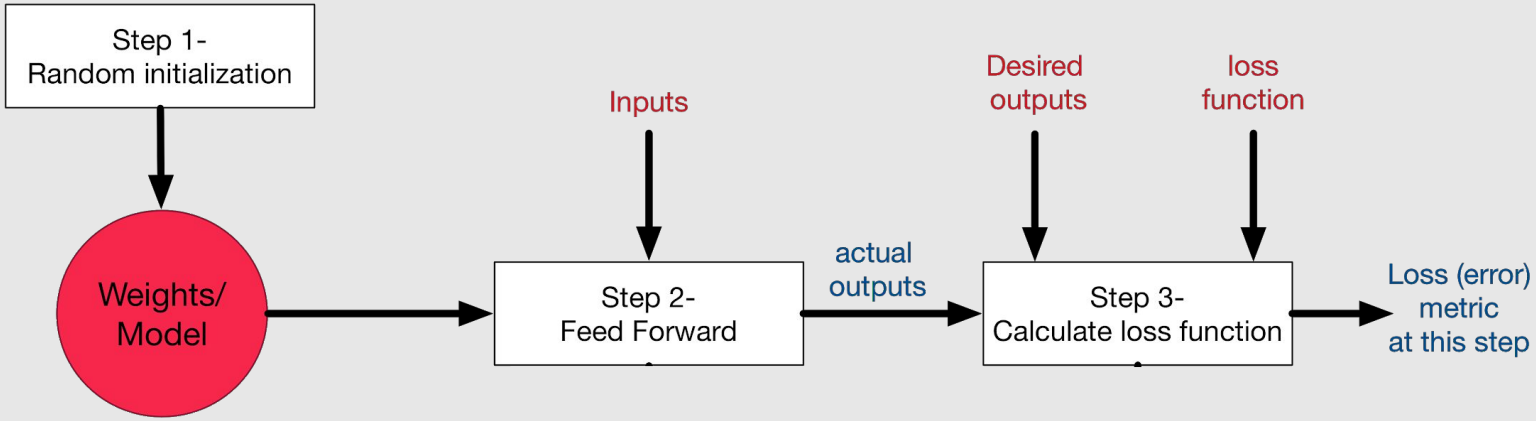

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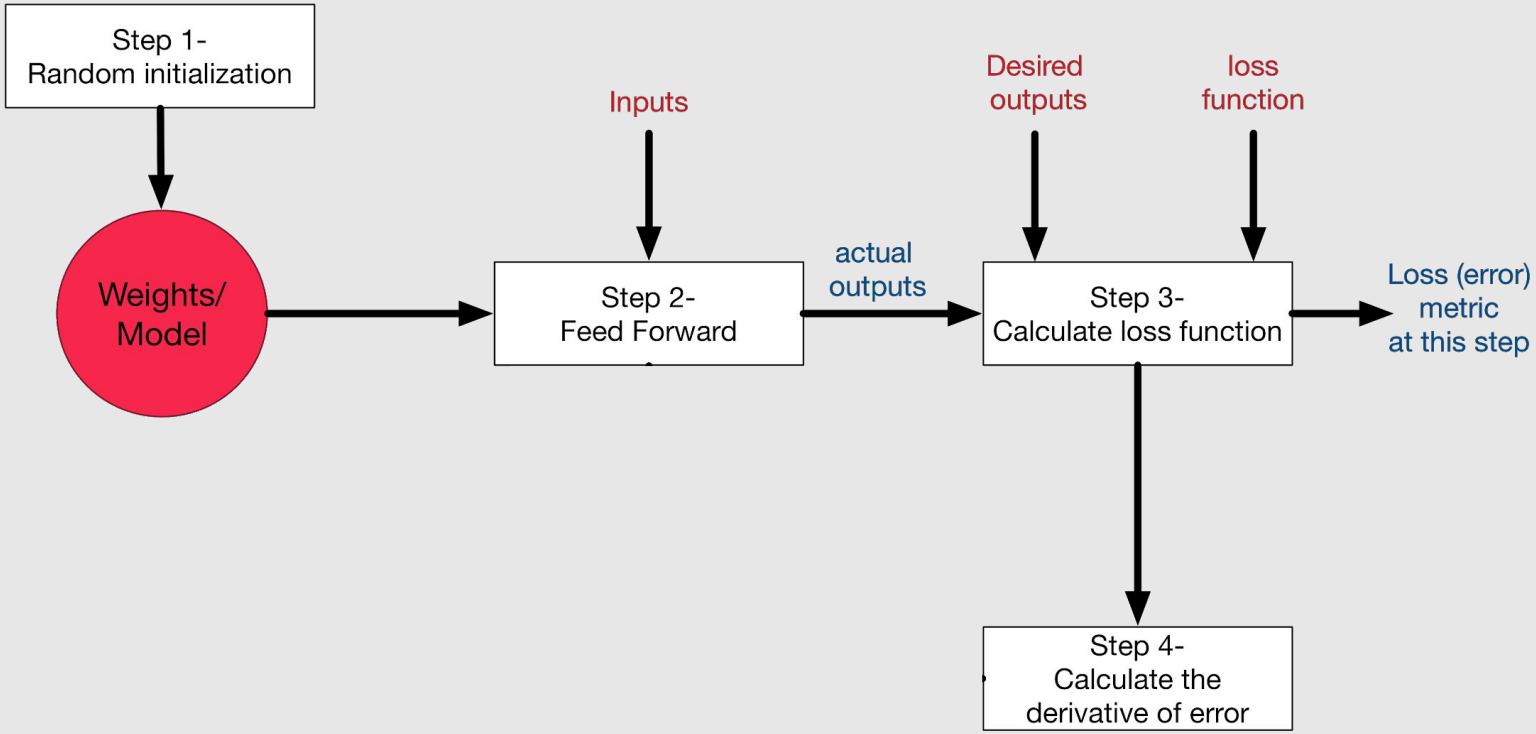
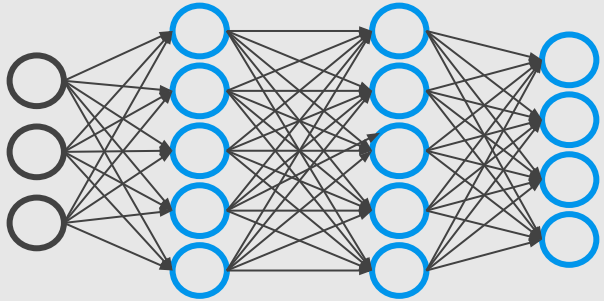


Gradient Computation: Backpropagation Algorithm

Intuition: $\delta_j^{(l)} =$ "error" of node j in layer l.



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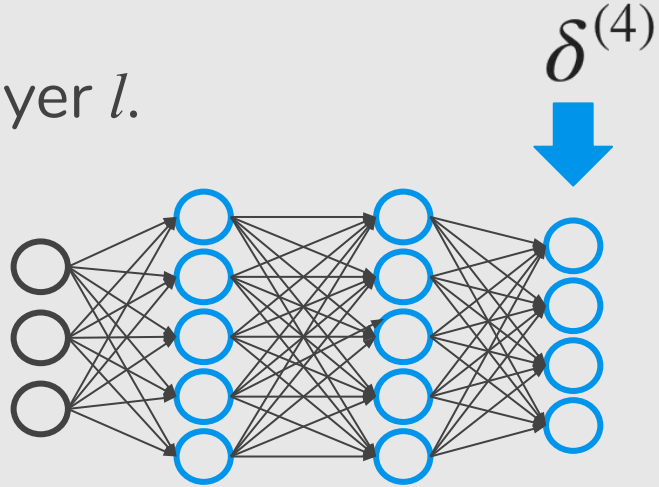
For each output unit (layer $L = 4$)

$$\delta_j^{(4)} = a_j^{(4)} - y_j$$



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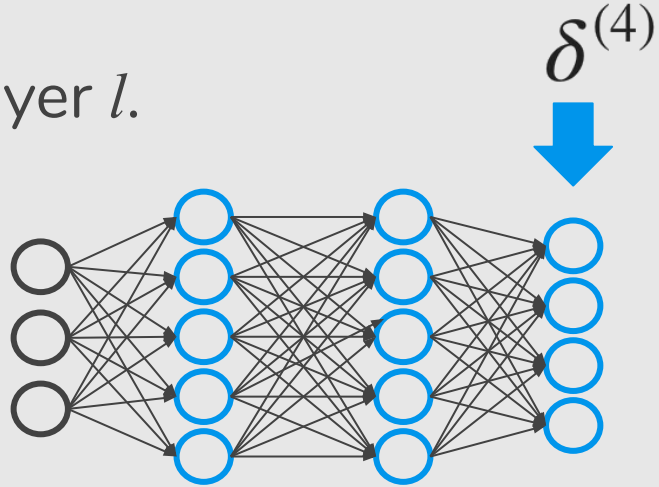
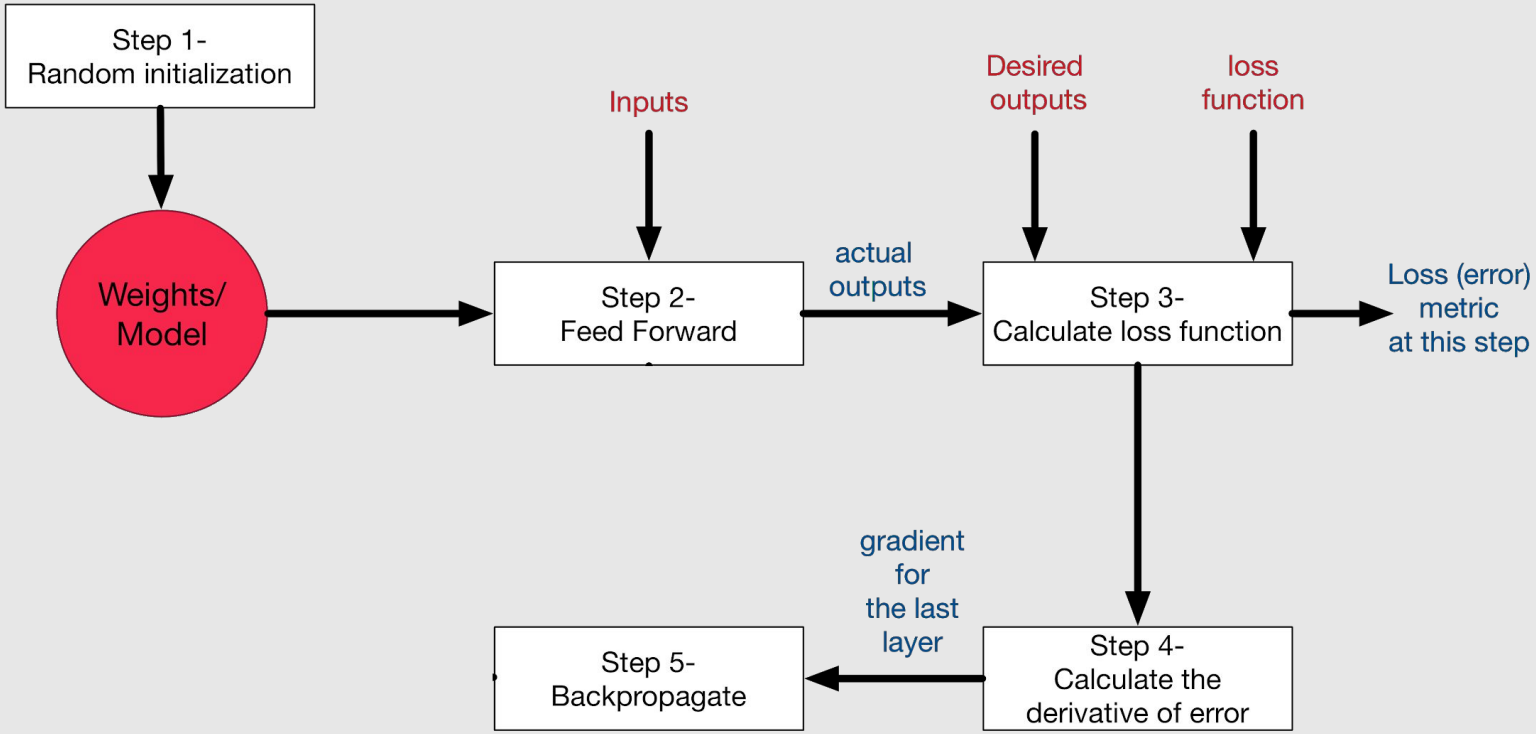


For each output unit (layer $L = 4$)

$$\delta_j^{(4)} = a_j^{(4)} - y_j$$

$$(h_\Theta(x))_j$$

Training a Neural Network



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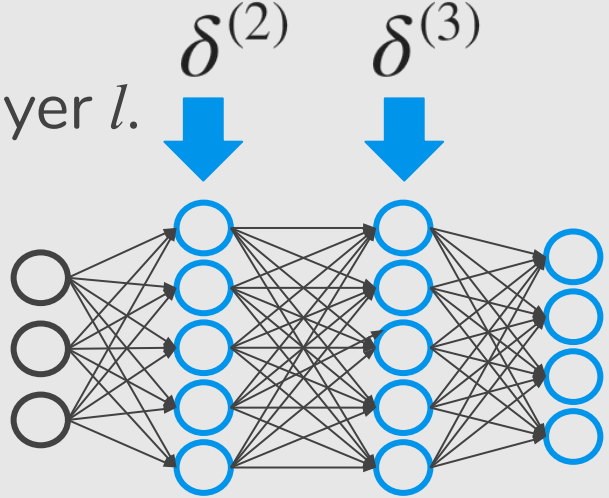

For each output unit (layer $L = 4$)

$$\delta_j^{(4)} = a_j^{(4)} - y_j$$

For each hidden unit

$$\delta^{(3)} = (\Theta^{(3)})^{\mathrm{T}} \delta^{(4)} .* g'(z^{(3)})$$

$$\delta^{(2)} = (\Theta^{(2)})^{\mathrm{T}} \delta^{(3)} .* g'(z^{(2)})$$

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = a_j^{(l)} \delta_i^{(l+1)}$$

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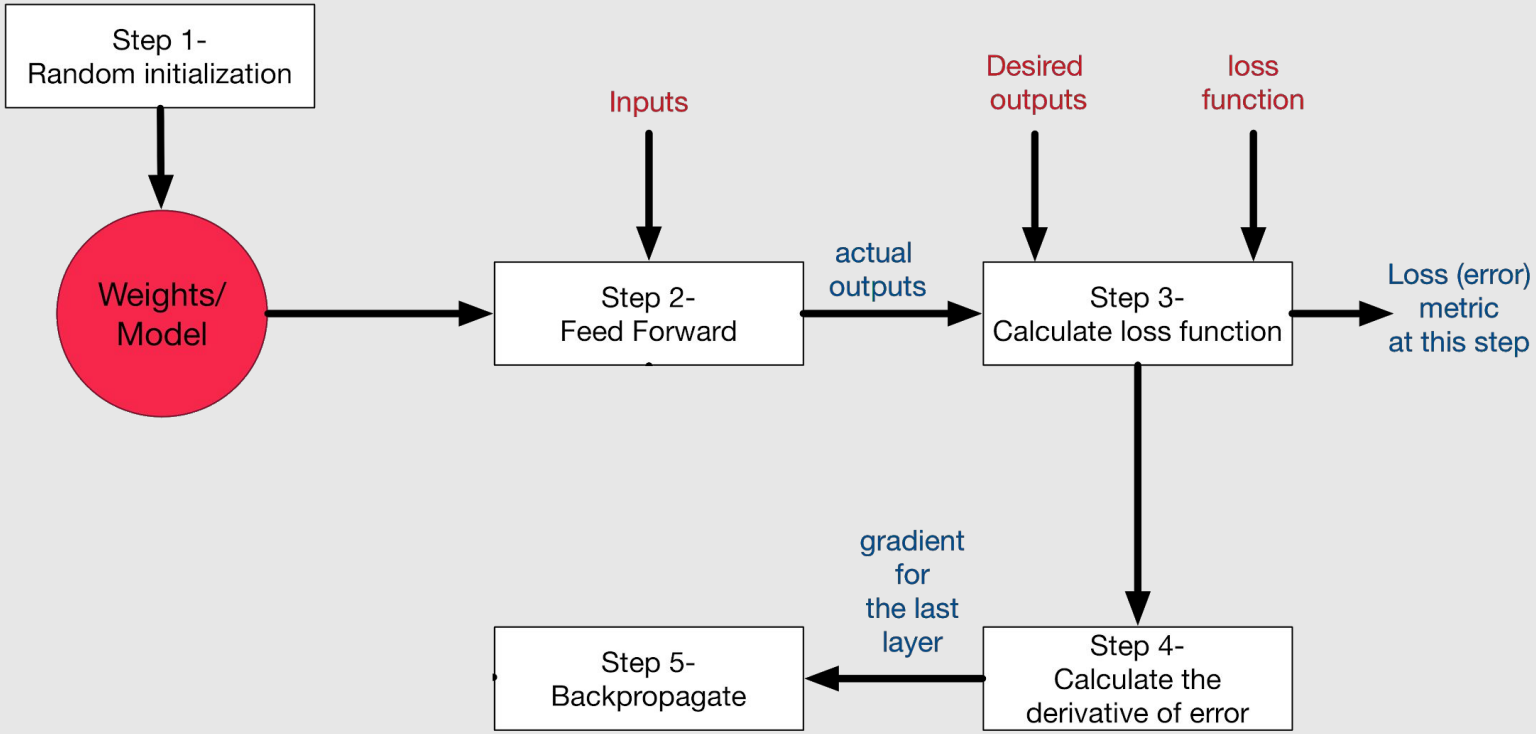

Backpropagation Algorithm

Training Set: $(x^{(1)},y^{(1)}),\ (x^{(2)},y^{(2)}),\ \ldots,\ (x^{(m)},y^{(m)})$

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Set $\Delta_{ij}^{(l)} = 0$ (for all l, i, j)

will be used as accumulators for computing $\frac{\partial}{\partial \Theta_{i,j}^{(l)}} J(\Theta)$

Backpropagation Algorithm

Training Set: $(x^{(1)},y^{(1)}),\ (x^{(2)},y^{(2)}),\ \ldots,\ (x^{(m)},y^{(m)})$

Set $\Delta_{ij}^{(l)} = 0$ (for all l, i, j)

For i = 1 to m

Set $a^{(1)} = x^{(i)}$

Performed forward propagation to compute $a^{(l)}$ for $l = 2, 3, \ldots, L$

Using $y^{(i)}$, compute $\delta^{(L)} = a^{(L)} - y^{(i)}$

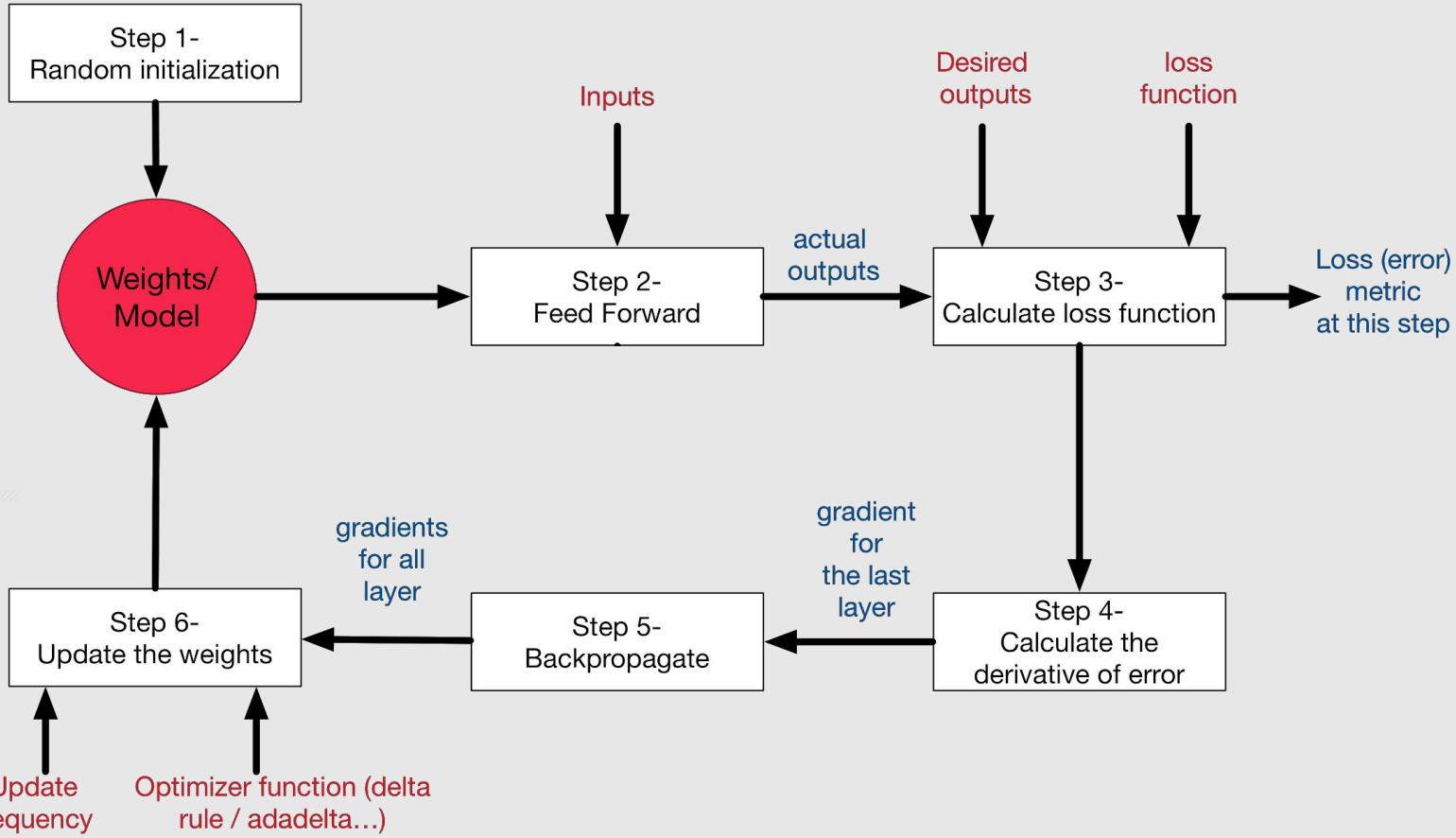
Compute $\delta^{(L-1)},\delta^{(L-2)},\ldots,\delta^{(2)}$

$$\Delta_{ij}^{(l)} := \Delta_{ij}^{(l)} + a_j^{(l)}\delta_i^{(l+1)}$$

$$D_{ij}^{(l)} := \frac{1}{m}\Delta_{ij}^{(l)}$$

$$\frac{\partial}{\partial\Theta_{i,j}^{(l)}}J(\Theta) = D_{ij}^{(l)}$$

Training a Neural Network



Gradient Descent

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log(h_\Theta(x^{(i)}))_k + (1-y_k^{(i)}) \log(1-(h_\Theta(x^{(i)}))_k)\right]$$

Want $\min_\Theta J(\Theta)$:

repeat {

$$\Theta_{ij}^{(l)} := \Theta_{ij}^{(l)} - \alpha \frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$$

}

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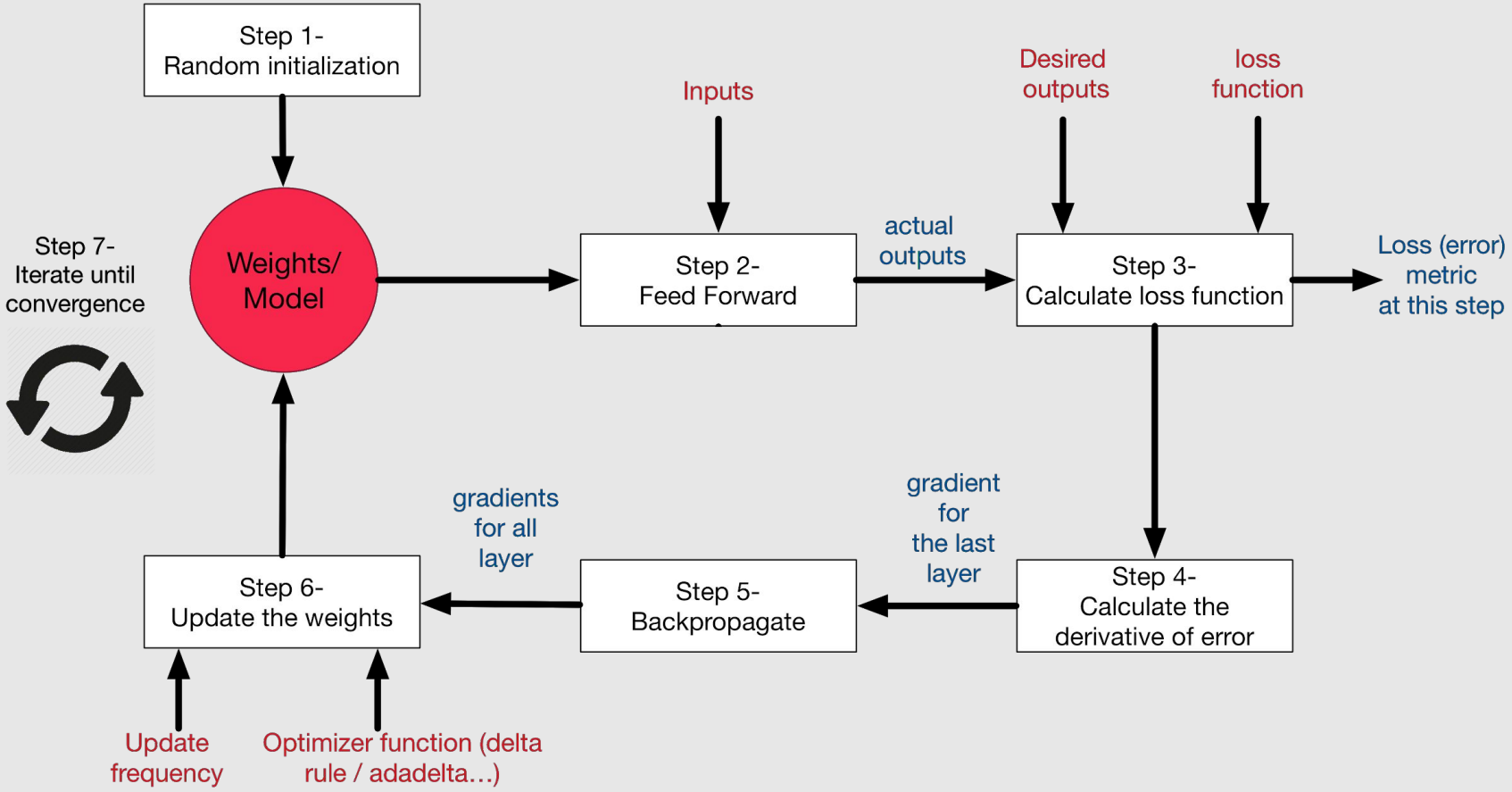

Backpropagation

A Simple Example

Backpropagation: A Simple Example

$f(x, y, z) = (x + y)z$

e.g., $x = -2$, $y = 5$, $z = -4$

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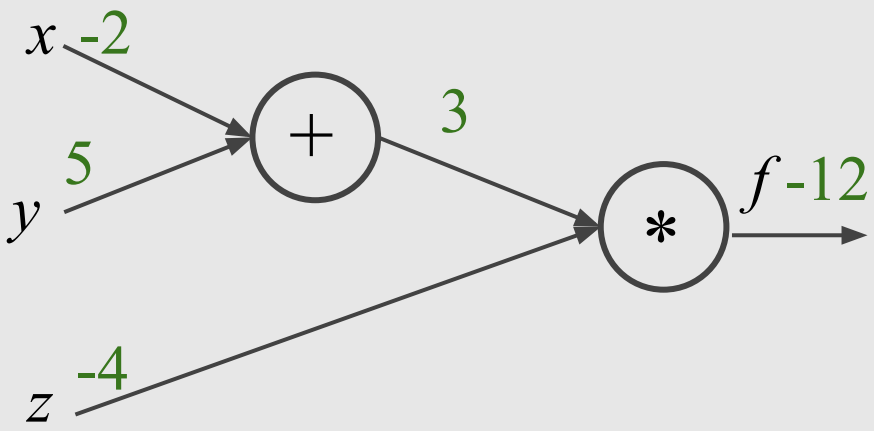

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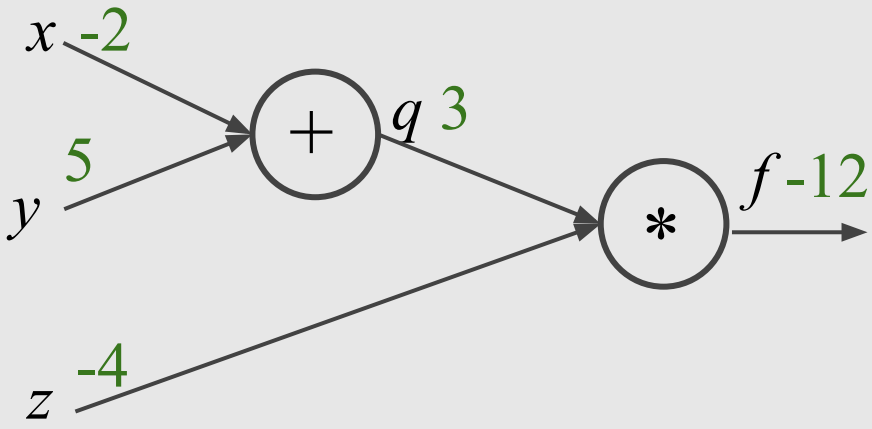

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$$f = qz \quad \frac{\partial f}{\partial q} = z \quad \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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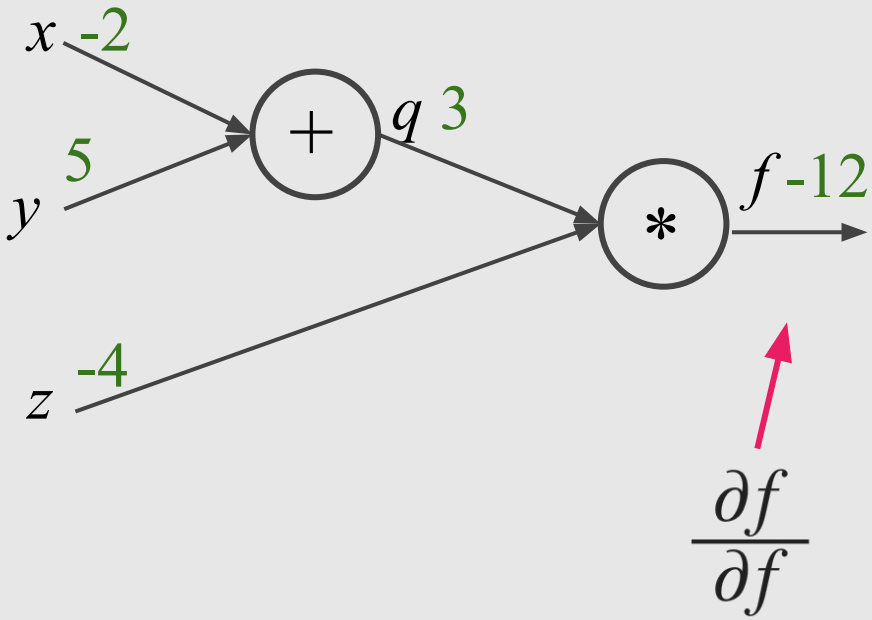

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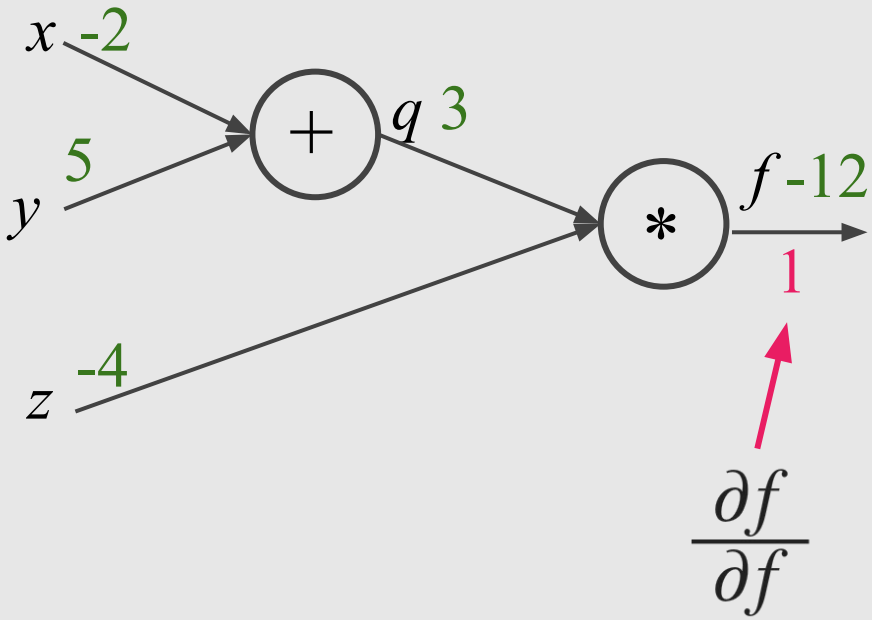

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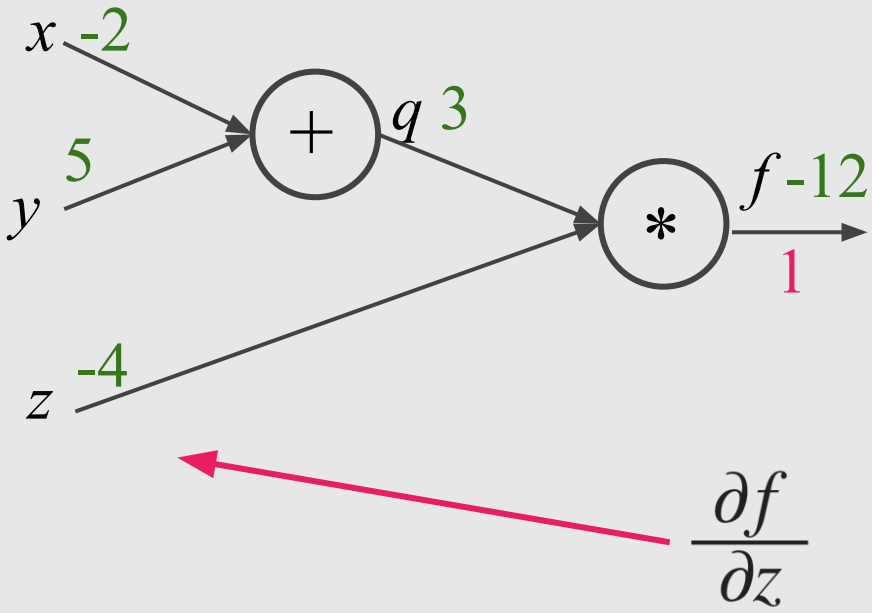

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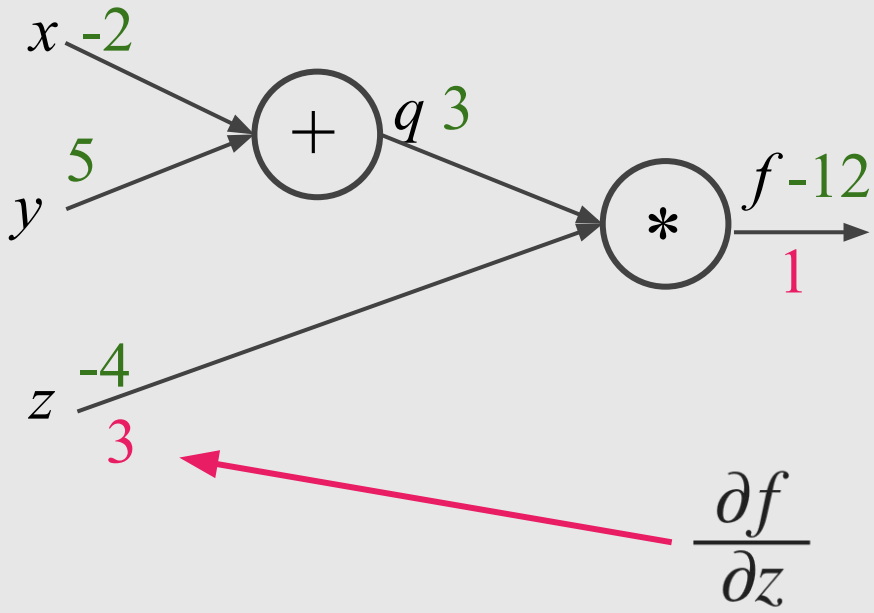

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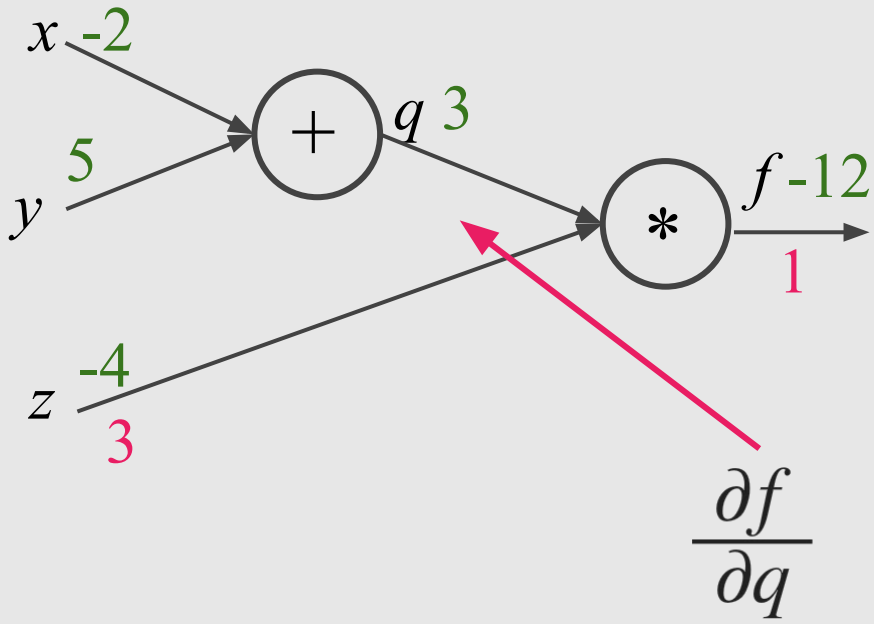

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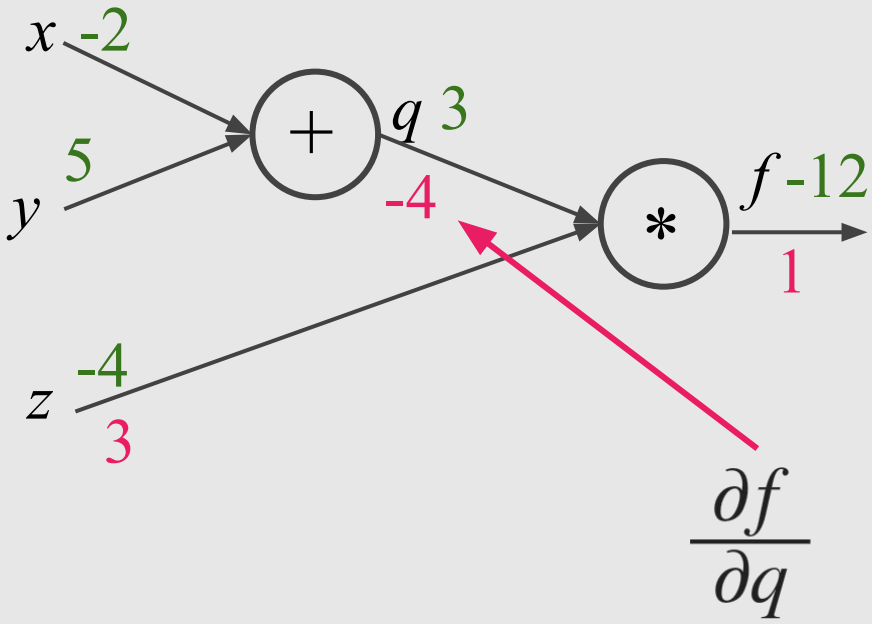

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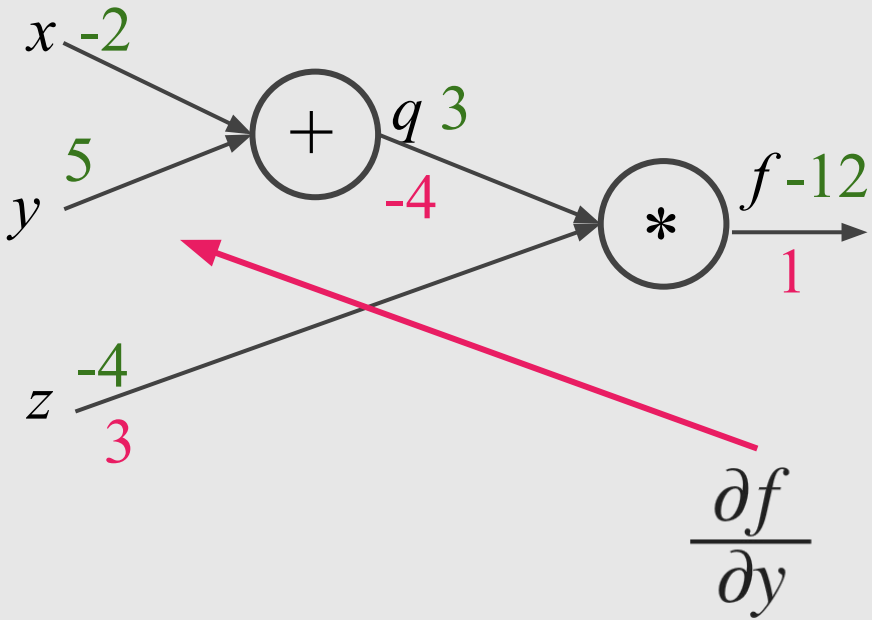

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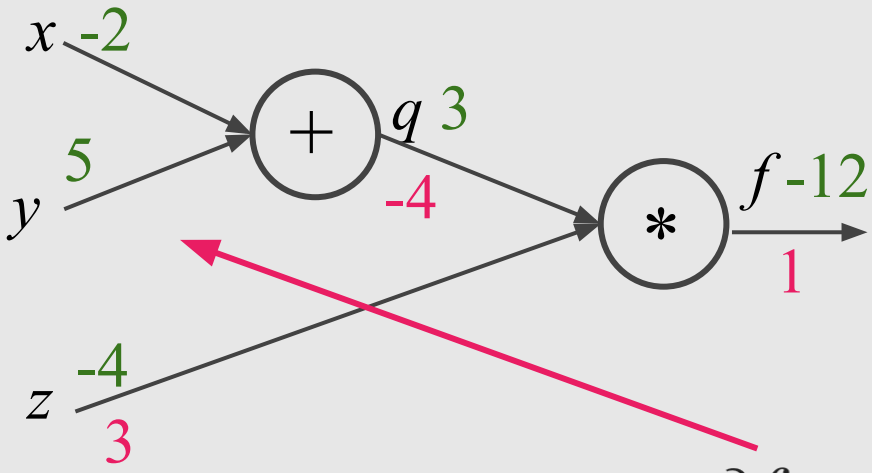

Chain rule

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial y}$$

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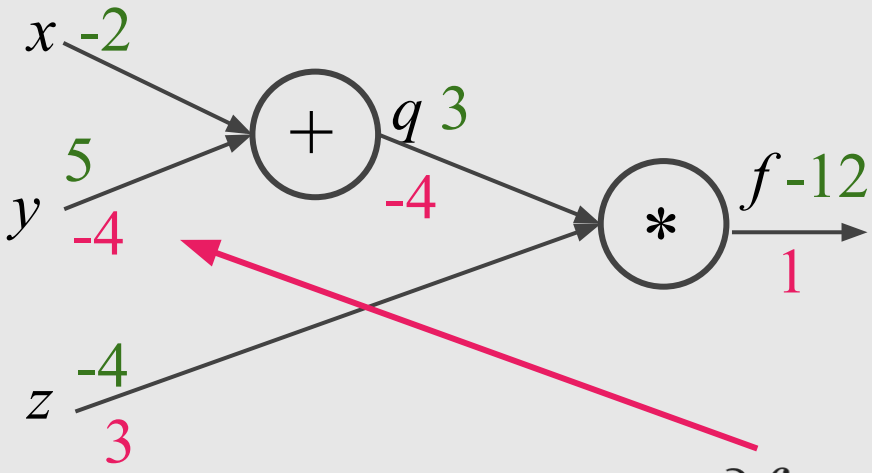

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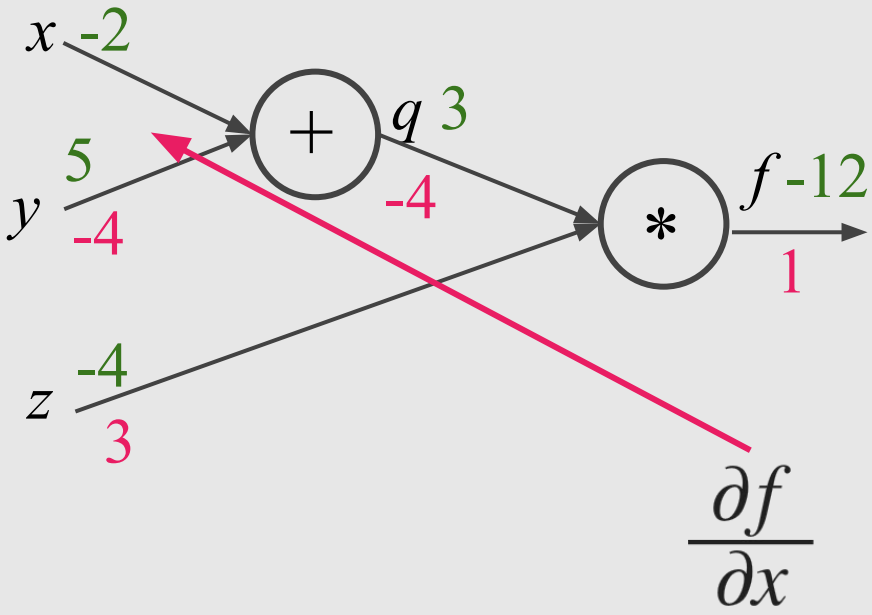

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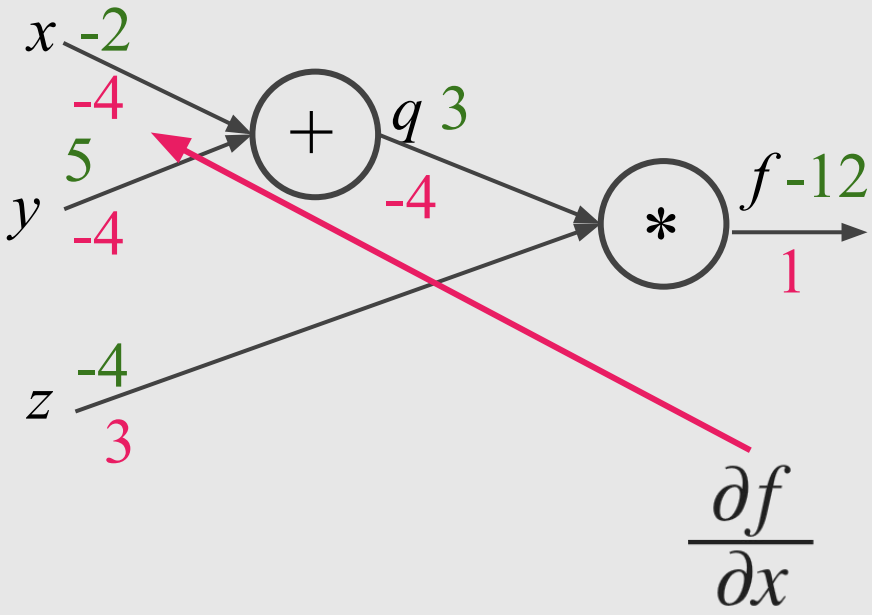
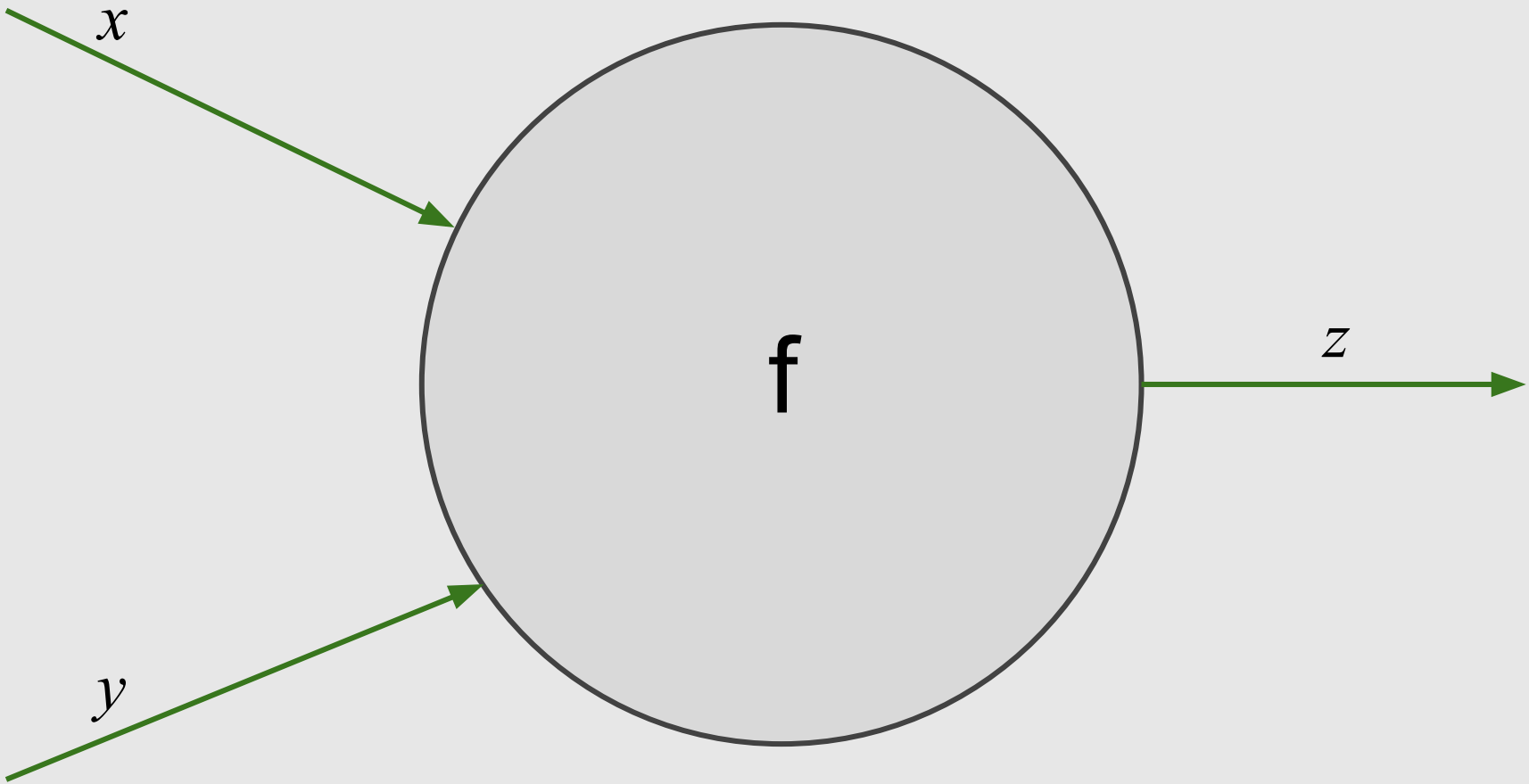
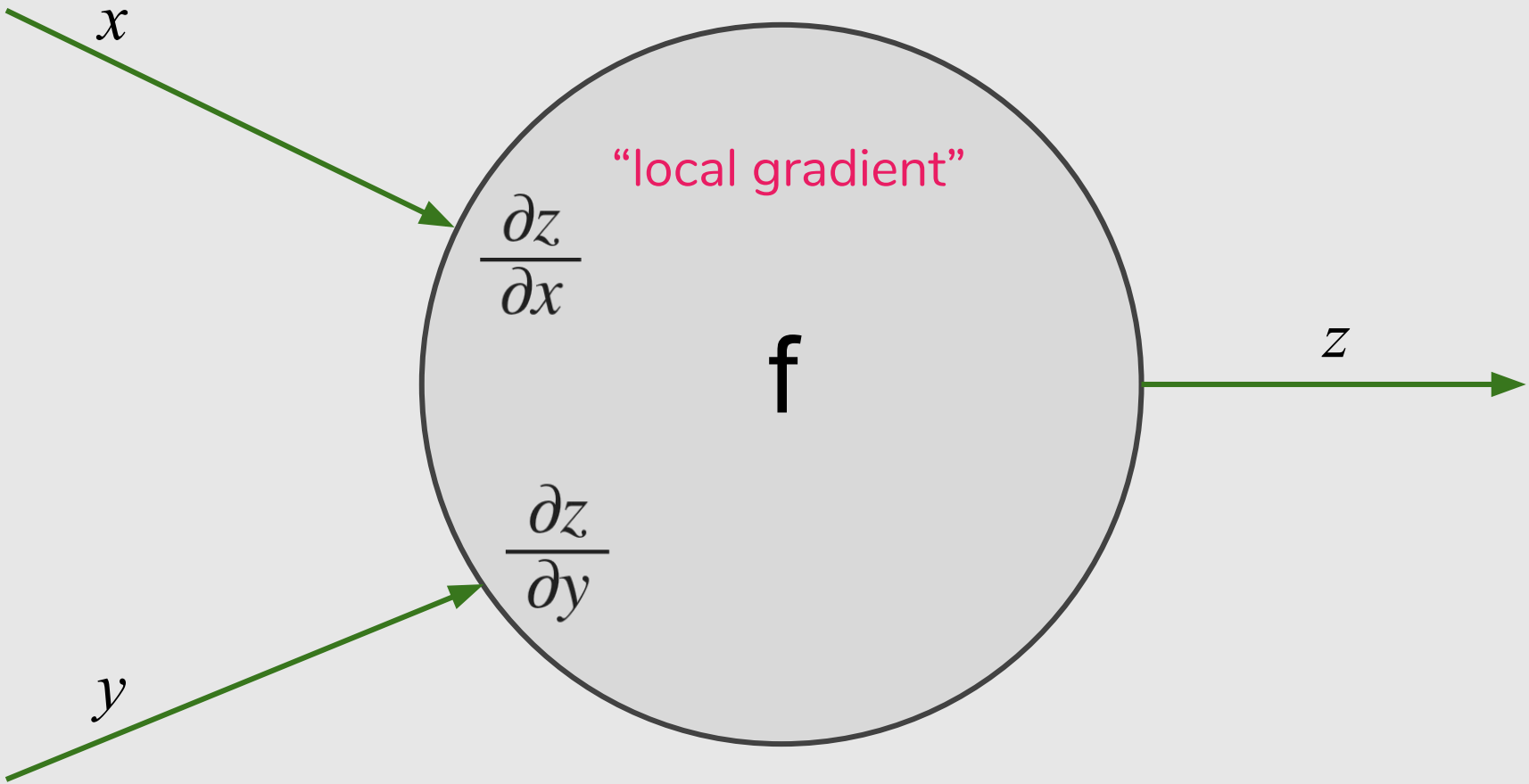
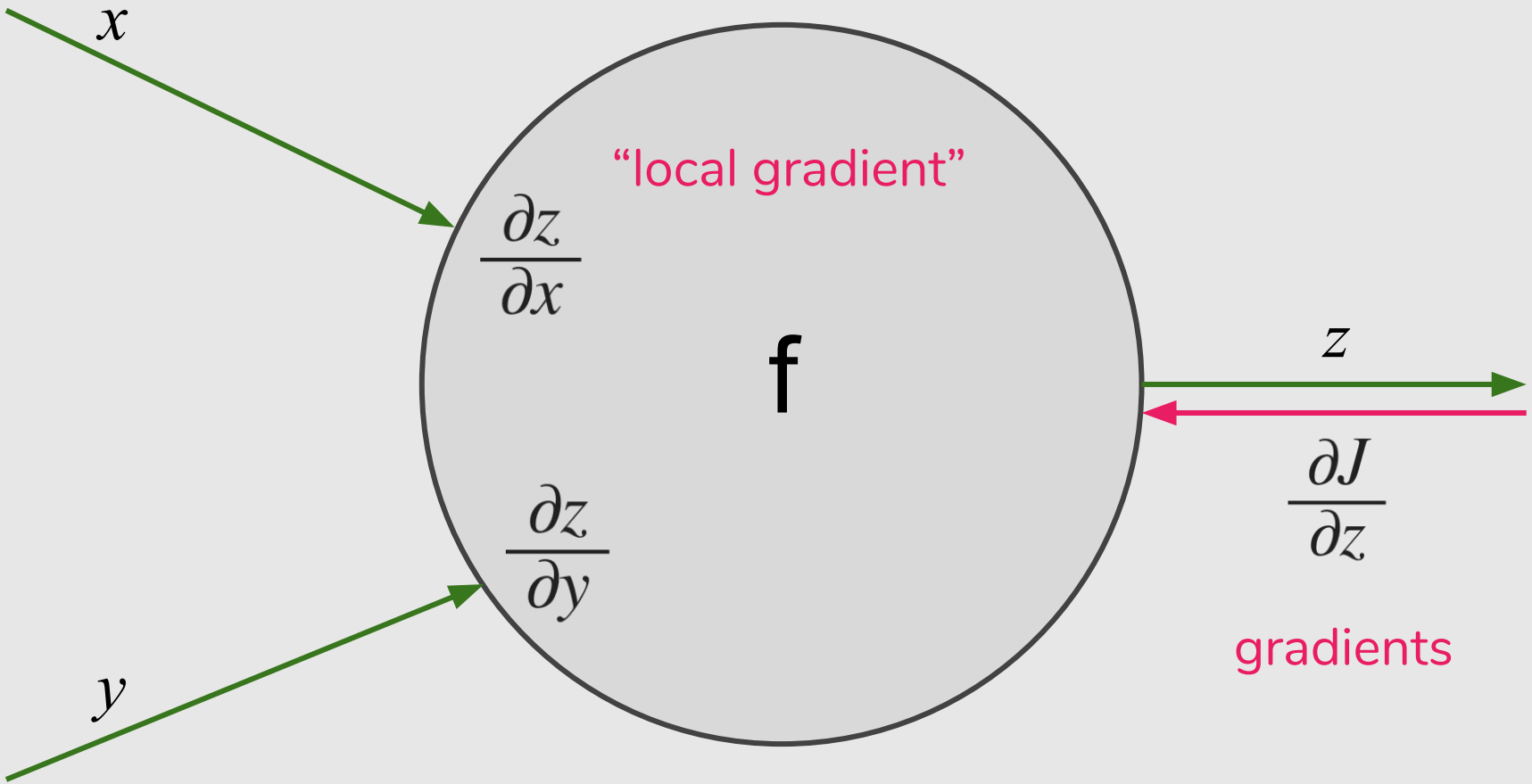



x
f
z
y


x
y
z
f
“local gradient”
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$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f
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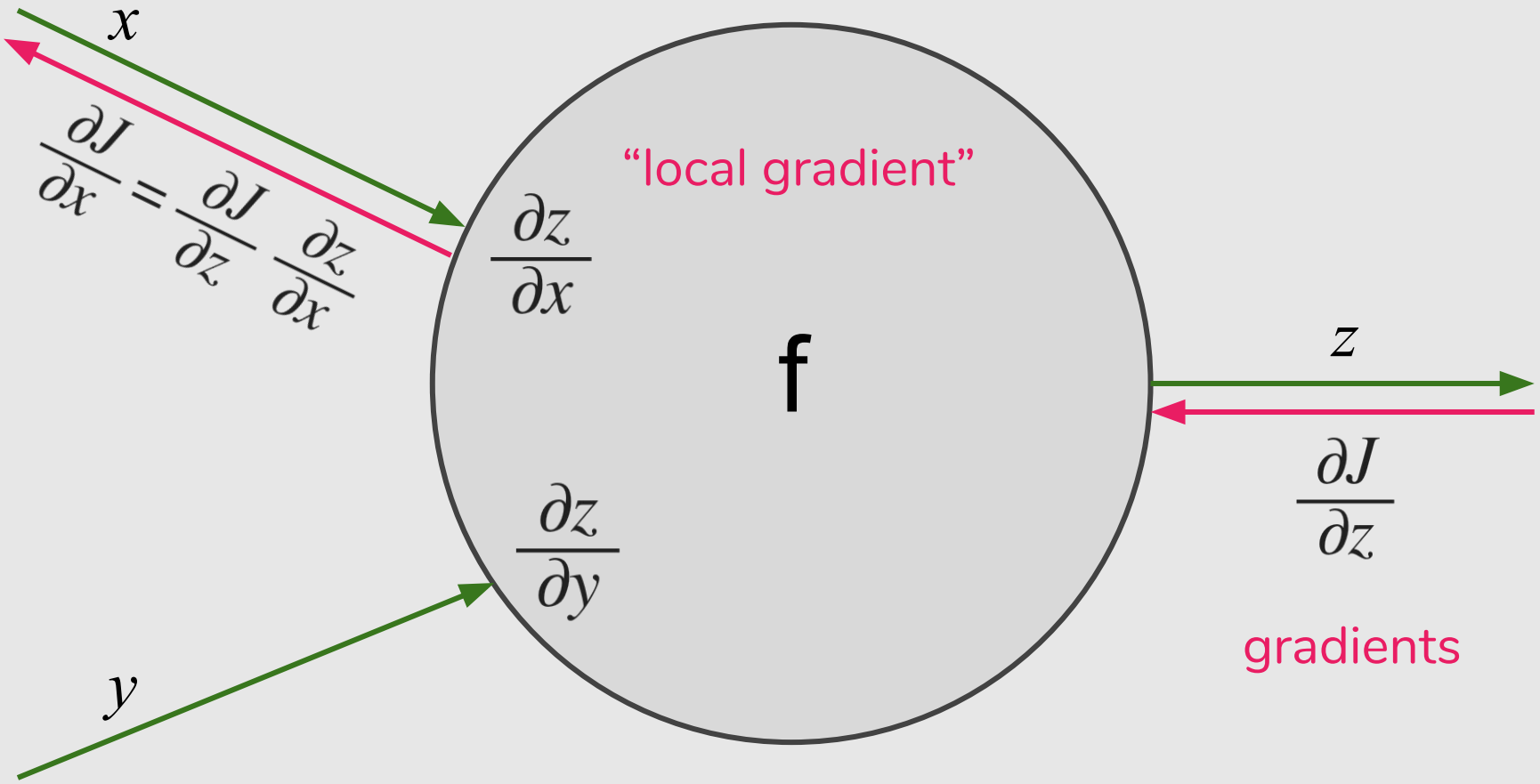
gradients


x
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"local gradient"
$\frac{\partial z}{\partial x}$
f
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y
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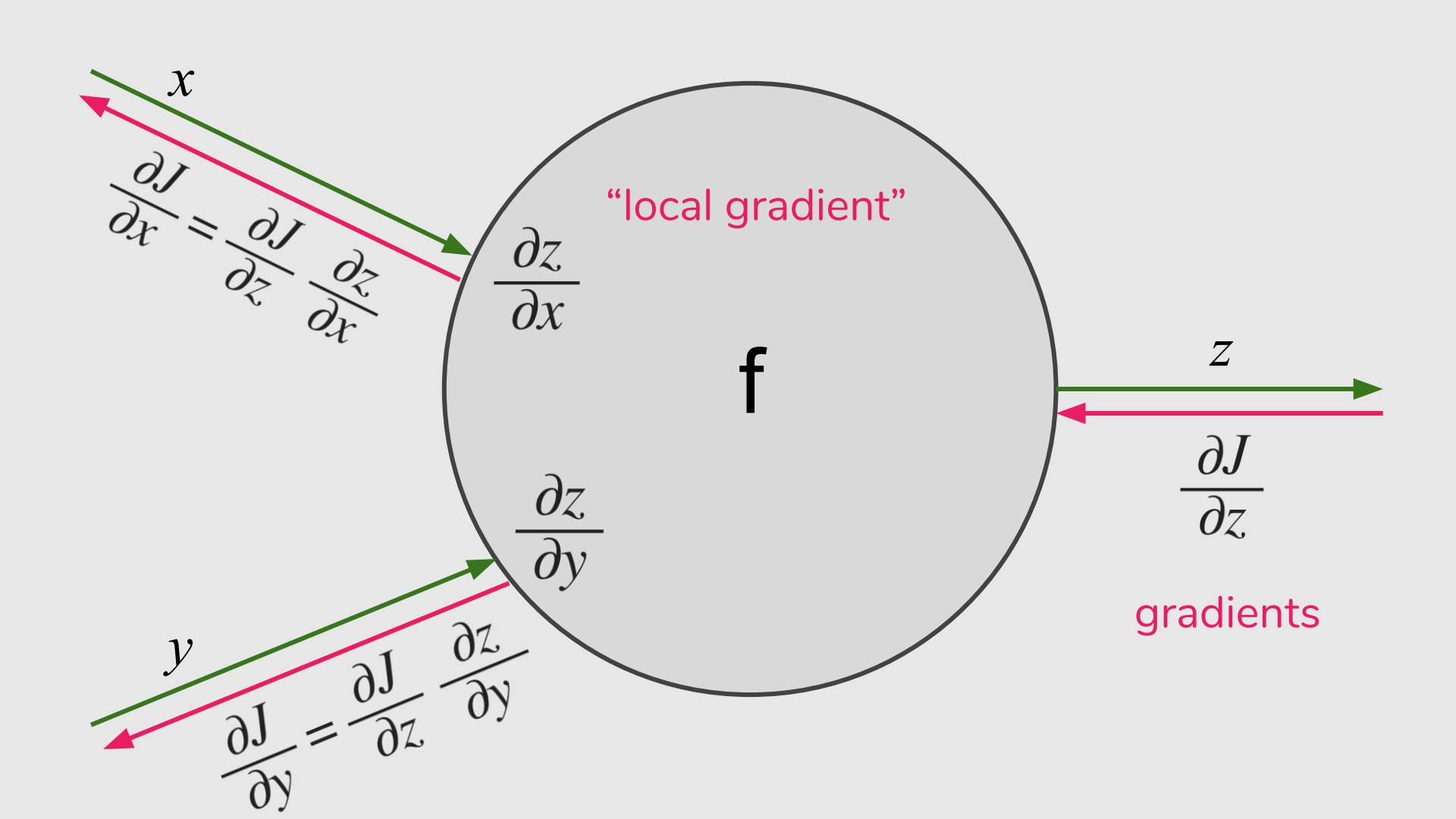
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y
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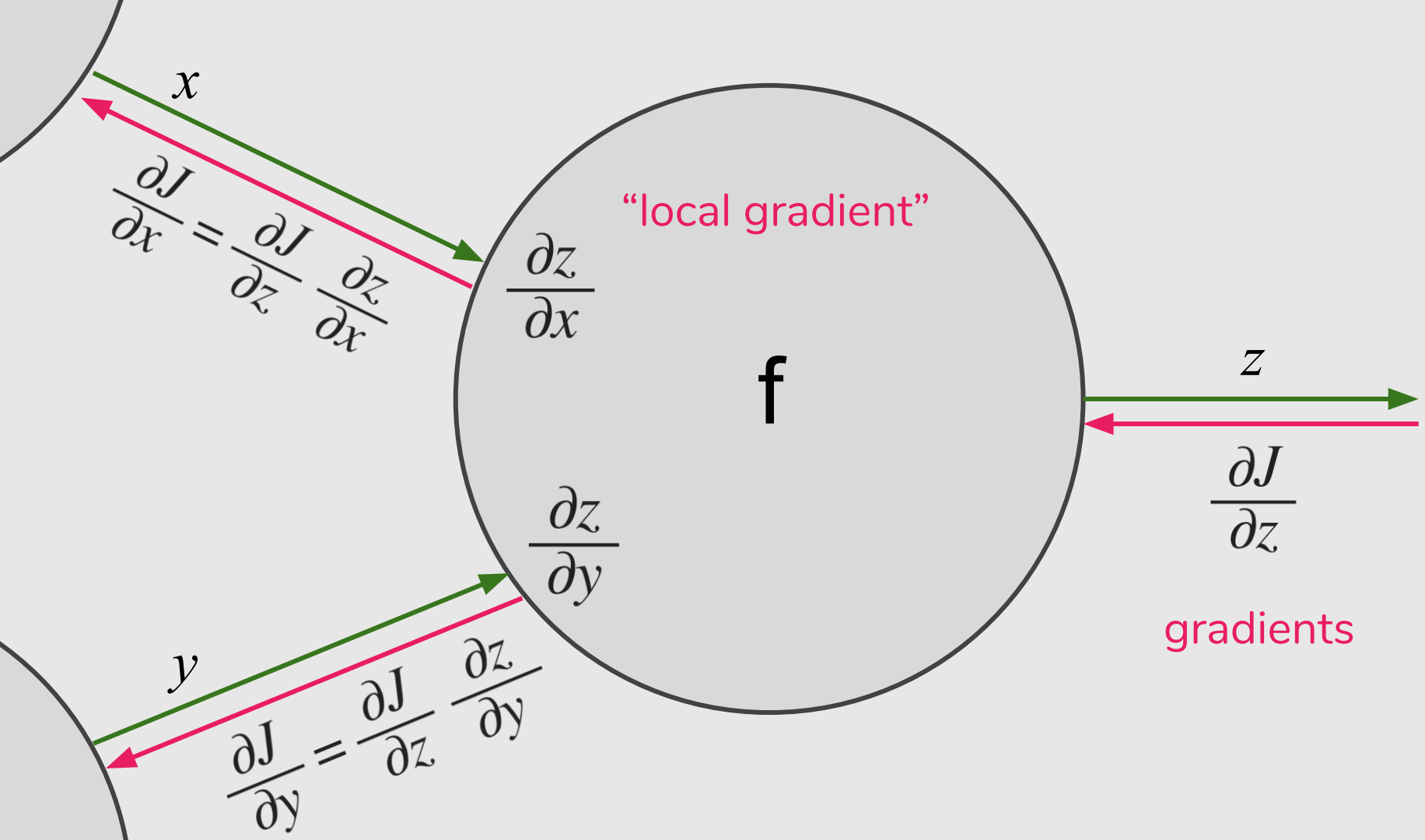
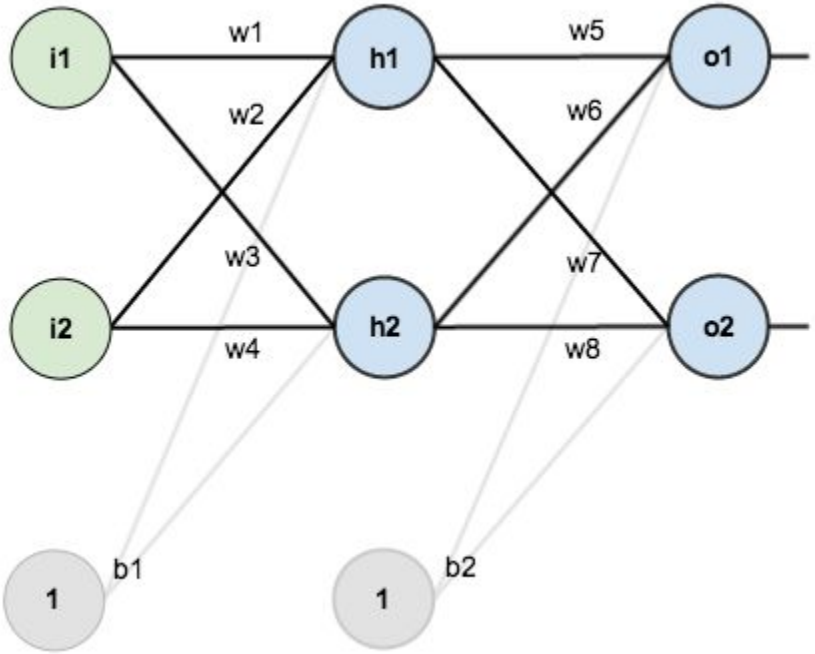
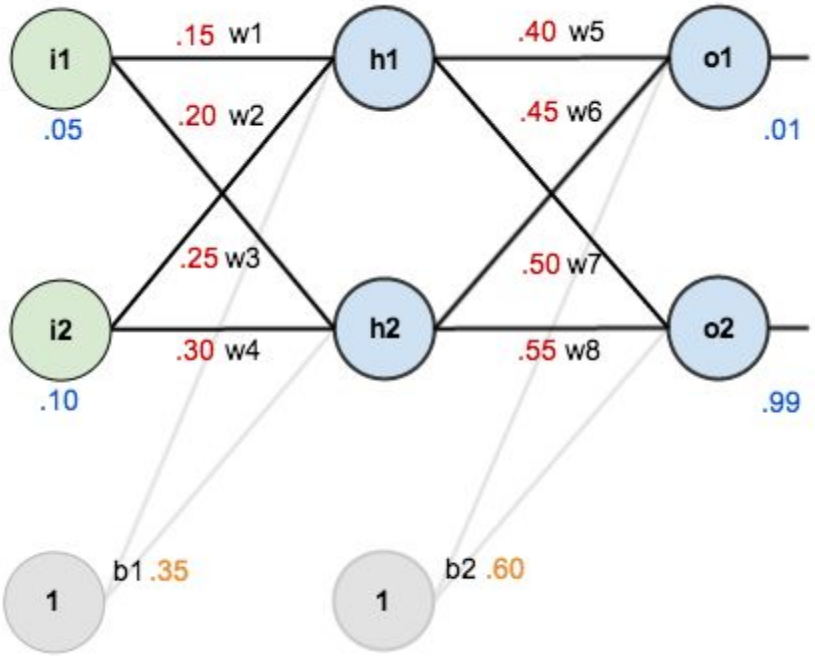

x
$\frac{\partial J}{\partial x} = \frac{\partial J}{\partial z}\frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial J}{\partial z}$
$\frac{\partial z}{\partial y}$
y
$\frac{\partial J}{\partial y} = \frac{\partial J}{\partial z}\frac{\partial z}{\partial y}$
gradients

A Step by Step Backpropagation Example



https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Given inputs 0.05 and 0.10,
we want the neural network to output 0.01 and 0.99.



Initial weights, the biases, and training inputs/outputs.

https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

The Forward Pass

Here's how we calculate the total net input for h_1:

$$net_{h1} = w_1 * i_1 + w_2 * i_2 + b_1 * 1$$

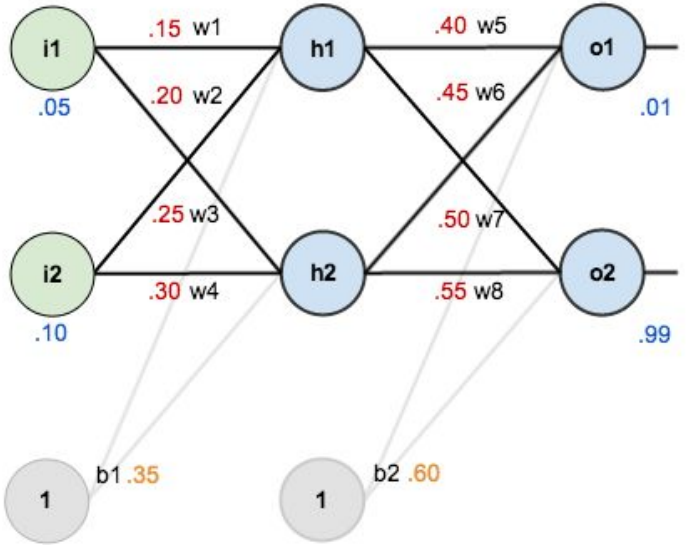
$$net_{h1} = 0.15 * 0.05 + 0.2 * 0.1 + 0.35 * 1 = 0.3775$$

We then squash it using the logistic function to get the output of h_1:

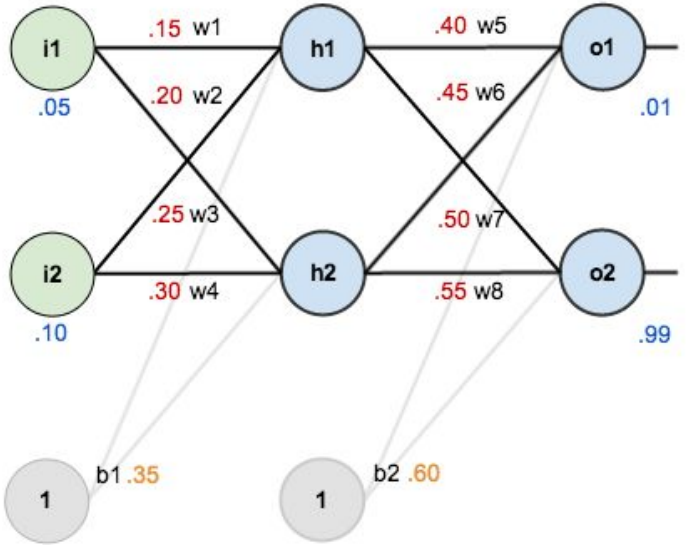
$$out_{h1} = \frac{1}{1+e^{-net_{h1}}} = \frac{1}{1+e^{-0.3775}} = 0.593269992$$

Carrying out the same process for h_2 we get:

$$out_{h2} = 0.596884378$$



The Forward Pass



We repeat this process for the output layer neurons, using the output from the hidden layer neurons as inputs.

Here's the output for o_1:

$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

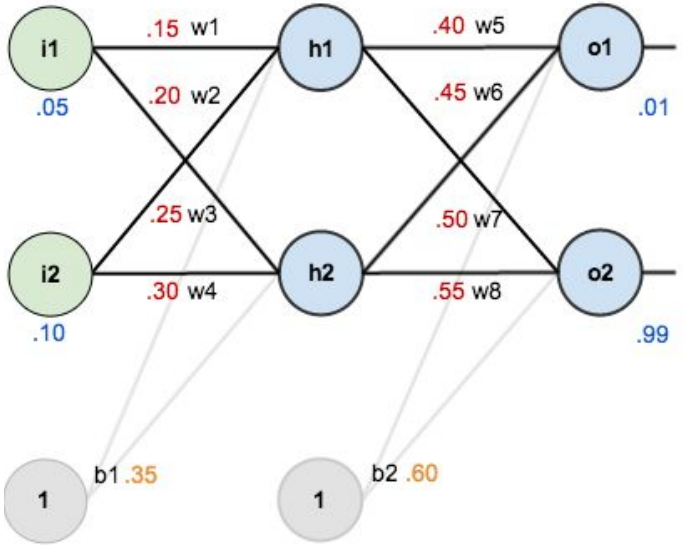
$$net_{o1} = 0.4 * 0.593269992 + 0.45 * 0.596884378 + 0.6 * 1 = 1.105905967$$

$$out_{o1} = \frac{1}{1+e^{-net_{o1}}} = \frac{1}{1+e^{-1.105905967}} = 0.75136507$$

And carrying out the same process for o_2 we get:

$$out_{o2} = 0.772928465$$

The Error



We can now calculate the error for each output neuron using the squared error function and sum them to get the total error:

$$E_{total} = \sum \frac{1}{2}(target - output)^2$$

For example, the target output for o_1 is 0.01 but the neural network output 0.75136507, therefore its error is:

$$E_{o1} = \frac{1}{2}(target_{o1} - out_{o1})^2 = \frac{1}{2}(0.01 - 0.75136507)^2 = 0.274811083$$

Repeating this process for o_2 (remembering that the target is 0.99) we get:

$$E_{o2} = 0.023560026$$

The total error for the neural network is the sum of these errors:

$$E_{total} = E_{o1} + E_{o2} = 0.274811083 + 0.023560026 = 0.298371109$$

The Backprogation Pass

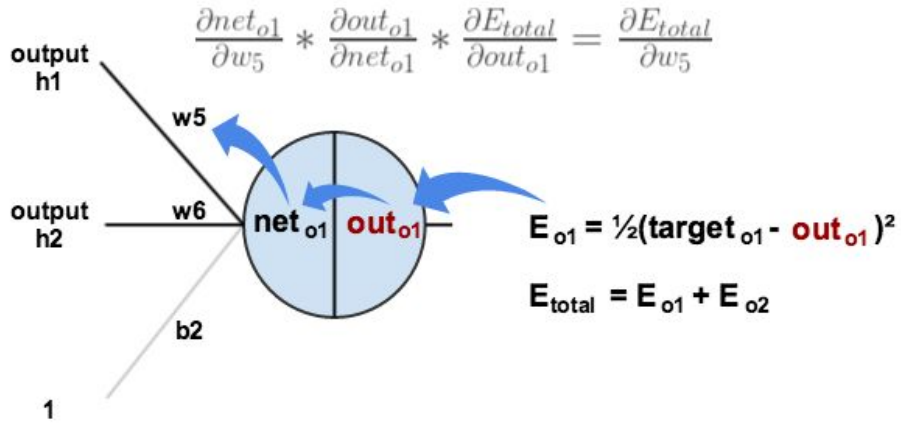
Output Layer

Consider w_5. We want to know how much a change in w_5 affects the total error, aka $\frac{\partial E_{total}}{\partial w_5}$.

> $\frac{\partial E_{total}}{\partial w_5}$ is read as "the partial derivative of E_{total} with respect to w_5". You can also say "the gradient with respect to w_5".

By applying the chain rule we know that:

$$\frac{\partial E_{total}}{\partial w_5} = \frac{\partial E_{total}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial w_5}$$



The Backprogation Pass

We need to figure out each piece in this equation.

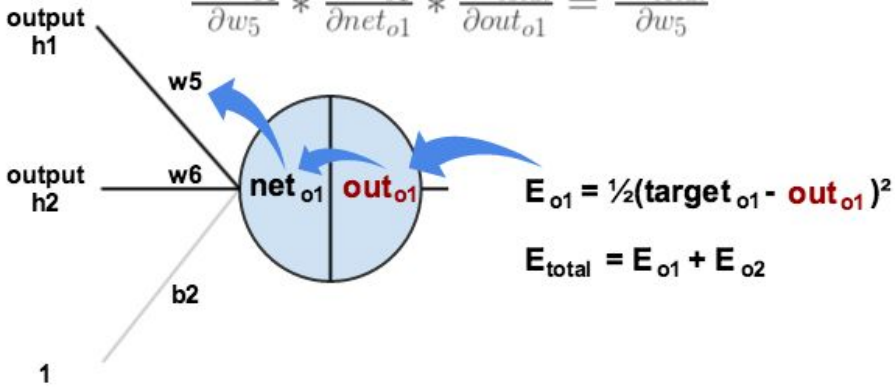
First, how much does the total error change with respect to the output?

$$E_{total} = \frac{1}{2}(target_{o1} - out_{o1})^2 + \frac{1}{2}(target_{o2} - out_{o2})^2$$

$$\frac{\partial E_{total}}{\partial out_{o1}} = 2 * \frac{1}{2}(target_{o1} - out_{o1})^{2-1} * -1 + 0$$

$$\frac{\partial E_{total}}{\partial out_{o1}} = -(target_{o1} - out_{o1}) = -(0.01 - 0.75136507) = 0.74136507$$

$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



The Backprogation Pass

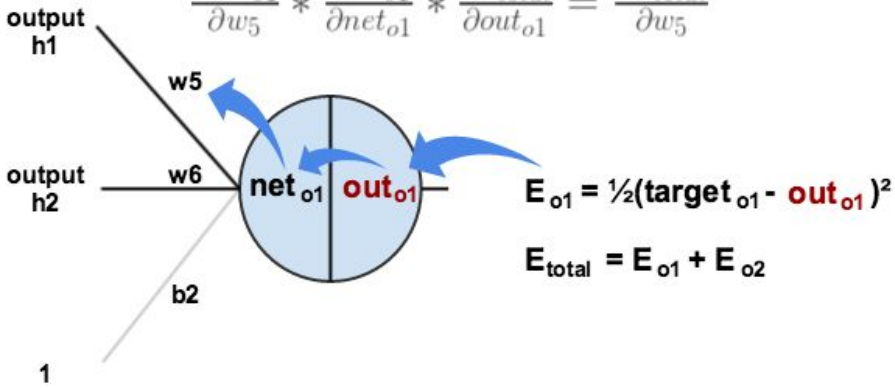
Next, how much does the output of o_1 change with respect to its total net input?

The partial derivative of the logistic function is the output multiplied by 1 minus the output:

$$out_{o1} = \frac{1}{1+e^{-net_{o1}}}$$

$$\frac{\partial out_{o1}}{\partial net_{o1}} = out_{o1}(1 - out_{o1}) = 0.75136507(1 - 0.75136507) = 0.186815602$$

$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



The Backprogation Pass

Finally, how much does the total net input of $o1$ change with respect to w_5?

$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

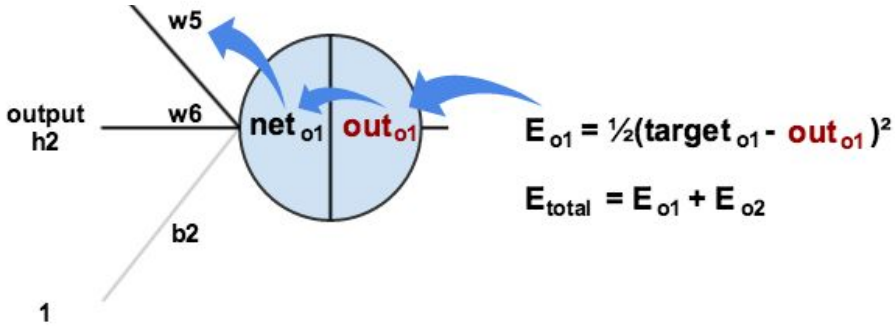
$$\frac{\partial net_{o1}}{\partial w_5} = 1 * out_{h1} * w_5^{(1-1)} + 0 + 0 = out_{h1} = 0.593269992$$

Putting it all together:

$$\frac{\partial E_{total}}{\partial w_5} = \frac{\partial E_{total}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial w_5}$$

$$\frac{\partial E_{total}}{\partial w_5} = 0.74136507 * 0.186815602 * 0.593269992 = 0.082167041$$

$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



The Backprogation Pass

You'll often see this calculation combined in the form of the delta rule:

$$\frac{\partial E_{total}}{\partial w_5} = -(target_{o1} - out_{o1}) * out_{o1}(1 - out_{o1}) * out_{h1}$$

Alternatively, we have $\frac{\partial E_{total}}{\partial out_{o1}}$ and $\frac{\partial out_{o1}}{\partial net_{o1}}$ which can be written as $\frac{\partial E_{total}}{\partial net_{o1}}$, aka δ_{o1} (the Greek letter delta) aka the *node delta*. We can use this to rewrite the calculation above:

$$\delta_{o1} = \frac{\partial E_{total}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} = \frac{\partial E_{total}}{\partial net_{o1}}$$

$$\delta_{o1} = -(target_{o1} - out_{o1}) * out_{o1}(1 - out_{o1})$$

Therefore:

$$\frac{\partial E_{total}}{\partial w_5} = \delta_{o1} out_{h1}$$

The Backprogation Pass

To decrease the error, we then subtract this value from the current weight (optionally multiplied by some learning rate, eta, which we'll set to 0.5):

$$w_5^+ = w_5 - \eta * \frac{\partial E_{total}}{\partial w_5} = 0.4 - 0.5 * 0.082167041 = 0.35891648$$

> Some sources use α (alpha) to represent the learning rate, others use η (eta), and others even use ϵ (epsilon).

We can repeat this process to get the new weights w_6, w_7, and w_8:

$$w_6^+ = 0.408666186$$

$$w_7^+ = 0.511301270$$

$$w_8^+ = 0.561370121$$

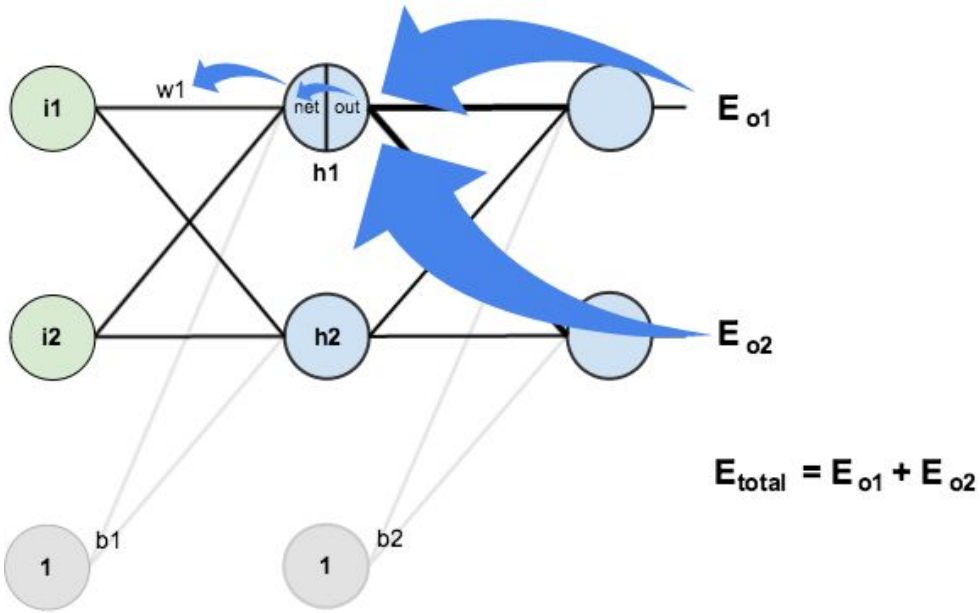
The Backprogation Pass

Hidden Layer

Next, we'll continue the backwards pass by calculating new values for w_1, w_2, w_3, and w_4.

Big picture, here's what we need to figure out:

$$\frac{\partial E_{total}}{\partial w_1} = \frac{\partial E_{total}}{\partial out_{h1}} * \frac{\partial out_{h1}}{\partial net_{h1}} * \frac{\partial net_{h1}}{\partial w_1}$$



The Backprogation Pass

We're going to use a similar process as we did for the output layer, but slightly different to account for the fact that the output of each hidden layer neuron contributes to the output (and therefore error) of multiple output neurons. We know that out_{h1} affects both out_{o1} and out_{o2} therefore the $\frac{\partial E_{total}}{\partial out_{h1}}$ needs to take into consideration its effect on the both output neurons:

$$\frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial out_{h1}} + \frac{\partial E_{o2}}{\partial out_{h1}}$$

Starting with $\frac{\partial E_{o1}}{\partial out_{h1}}$:

$$\frac{\partial E_{o1}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial out_{h1}}$$

We can calculate $\frac{\partial E_{o1}}{\partial net_{o1}}$ using values we calculated earlier:

$$\frac{\partial E_{o1}}{\partial net_{o1}} = \frac{\partial E_{o1}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} = 0.74136507 * 0.186815602 = 0.138498562$$

The Backprogation Pass

And $\frac{\partial net_{o1}}{\partial out_{h1}}$ is equal to w_5:

$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

$$\frac{\partial net_{o1}}{\partial out_{h1}} = w_5 = 0.40$$

Plugging them in:

$$\frac{\partial E_{o1}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial out_{h1}} = 0.138498562 * 0.40 = 0.055399425$$

The Backprogation Pass

Following the same process for $\frac{\partial E_{o2}}{\partial out_{h1}}$, we get:

$$\frac{\partial E_{o2}}{\partial out_{h1}} = -0.019049119$$

Therefore:

$$\frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial out_{h1}} + \frac{\partial E_{o2}}{\partial out_{h1}} = 0.055399425 + -0.019049119 = 0.036350306$$

Now that we have $\frac{\partial E_{total}}{\partial out_{h1}}$, we need to figure out $\frac{\partial out_{h1}}{\partial net_{h1}}$ and then $\frac{\partial net_{h1}}{\partial w}$ for each weight:

$$out_{h1} = \frac{1}{1+e^{-net_{h1}}}$$

$$\frac{\partial out_{h1}}{\partial net_{h1}} = out_{h1}(1 - out_{h1}) = 0.59326999(1 - 0.59326999) = 0.241300709$$

The Backprogation Pass

We calculate the partial derivative of the total net input to h_1 with respect to w_1 the same as we did for the output neuron:

$$net_{h1} = w_1 * i_1 + w_2 * i_2 + b_1 * 1$$

$$\frac{\partial net_{h1}}{\partial w_1} = i_1 = 0.05$$

Putting it all together:

$$\frac{\partial E_{total}}{\partial w_1} = \frac{\partial E_{total}}{\partial out_{h1}} * \frac{\partial out_{h1}}{\partial net_{h1}} * \frac{\partial net_{h1}}{\partial w_1}$$

$$\frac{\partial E_{total}}{\partial w_1} = 0.036350306 * 0.241300709 * 0.05 = 0.000438568$$

The Backprogation Pass

We can now update w_1:

$$w_1^+ = w_1 - \eta * \frac{\partial E_{total}}{\partial w_1} = 0.15 - 0.5 * 0.000438568 = 0.149780716$$

Repeating this for w_2, w_3, and w_4

$$w_2^+ = 0.19956143$$

$$w_3^+ = 0.24975114$$

$$w_4^+ = 0.29950229$$

Finally, we've updated all of our weights! When we fed forward the 0.05 and 0.1 inputs originally, the error on the network was 0.298371109. After this first round of backpropagation, the total error is now down to 0.291027924. It might not seem like much, but after repeating this process 10,000 times, for example, the error plummets to 0.0000351085. At this point, when we feed forward 0.05 and 0.1, the two outputs neurons generate 0.015912196 (vs 0.01 target) and 0.984065734 (vs 0.99 target).

CHAPTER 3

Improving the way neural networks learn

When a golf player is first learning to play golf, they usually spend most of their time developing a basic swing. Only gradually do they develop other shots, learning to chip, draw and fade the ball, building on and modifying their basic swing. In a similar way, up to now we've focused on understanding the backpropagation algorithm. It's our "basic swing", the foundation for learning in most work on neural networks. In this chapter I explain a suite of techniques which can be used to improve on our vanilla implementation of backpropagation, and so improve the way our networks learn.

The techniques we'll develop in this chapter include: a better choice of cost function, known as the cross-entropy cost function; four so-called "regularization" methods (L1 and L2 regularization, dropout, and artificial expansion of the training data), which make our networks better at generalizing beyond the training data; a better method for initializing the weights in the network; and a set of heuristics to help choose good hyper-parameters for the network. I'll also overview several other techniques in less depth

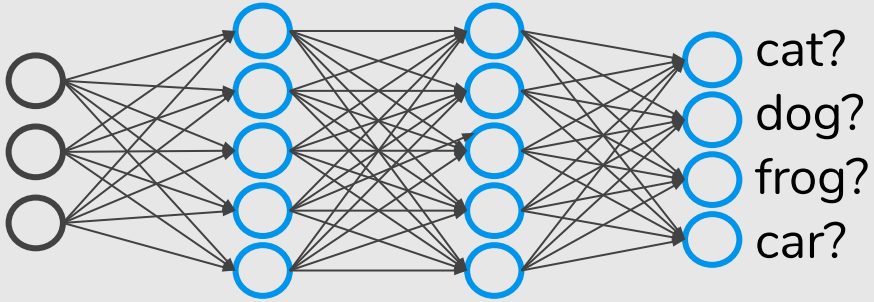
Multi-class Classification

Cat

Dog

Frog

Car

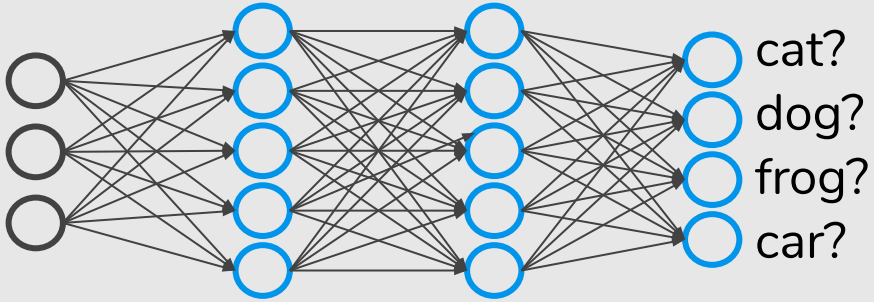


Cat

Dog

Frog

Car



Want $h_\Theta(x) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, when cat

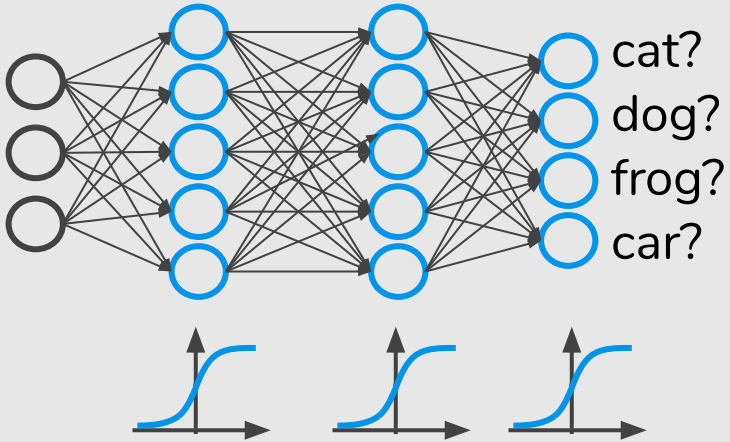
$h_\Theta(x) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, when dog

$h_\Theta(x) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, when frog

$h_\Theta(x) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$ when car

Softmax Classification

The **output layer** is typically modified **by replacing** the individual activation functions **by a shared softmax** function.



Softmax Classification

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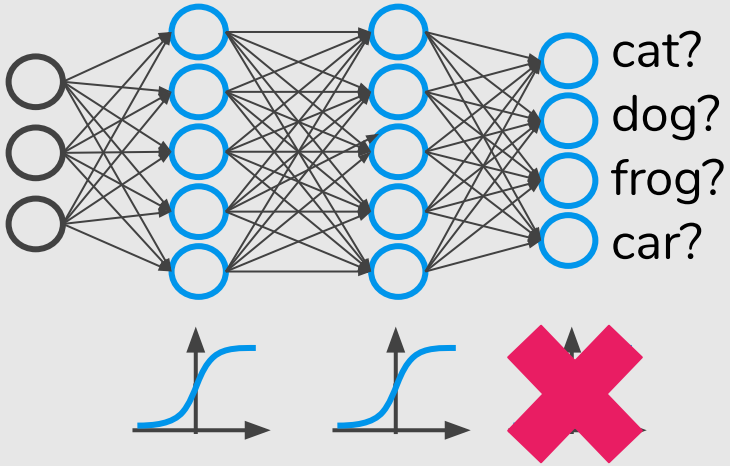

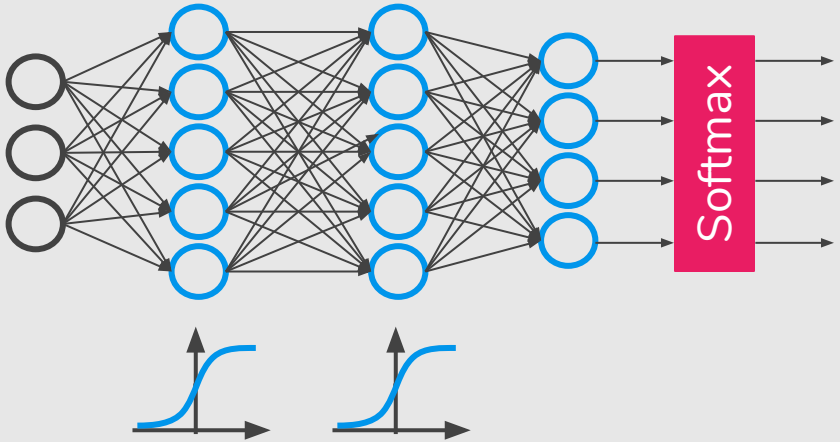

Softmax Classification

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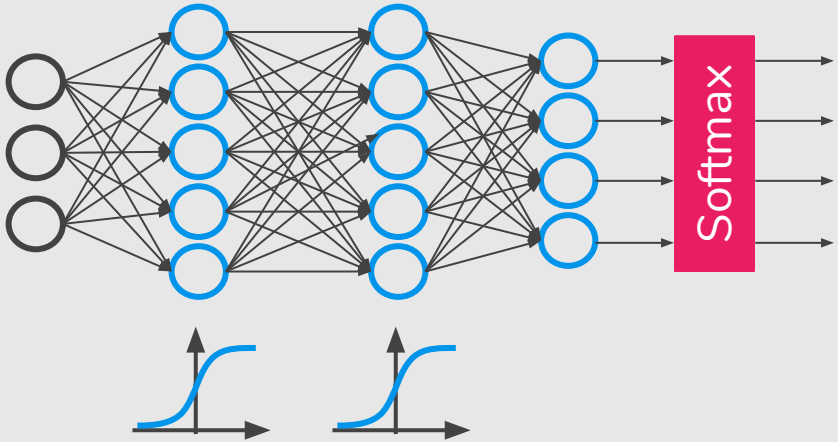
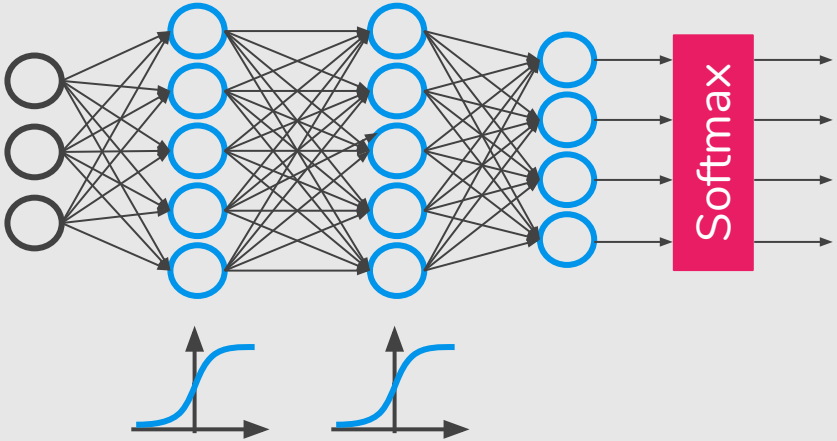


$$f(\mathbf{z})_k = \frac{e^{z_k}}{\sum_{j=1}^{K} e^{z_j}}$$

Softmax Classification



Cat	5.1	164.0	0.87
Dog	3.2	24.5	0.13
Frog	-1.7	0.18	0.00
Car	-2.0	0.13	0.00

$$f(\mathbf{z})_k = \frac{e^{z_k}}{\sum_{j=1}^{K} e^{z_j}}$$

References

Machine Learning Books

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 10
- Pattern Recognition and Machine Learning, Chap. 5
- Pattern Classification, Chap. 6
- Free online book: **http://neuralnetworksanddeeplearning.com**

Machine Learning Courses

- https://www.coursera.org/learn/machine-learning, Week 4 & 5
- https://www.coursera.org/learn/neural-networks