

# Lecture 12: Learning Parameters of Multi-layer Perceptrons with Backpropagation

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**COMP90049**

**Introduction to Machine Learning**

Semester 1, 2021

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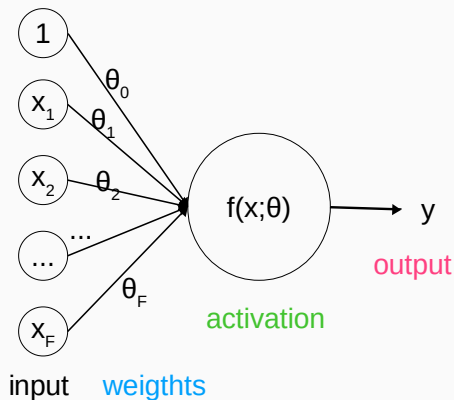
## Last lecture

- From perceptrons to neural networks
- multilayer perceptron
- some examples
- features and limitations

## Today

- Learning parameters of neural networks
- The Backpropagation algorithm

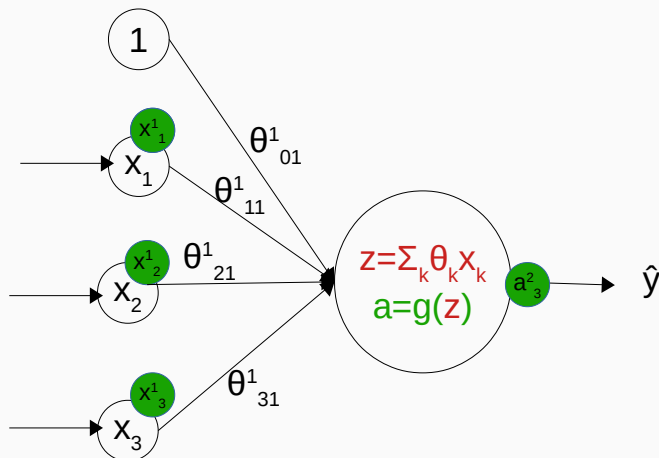
## Recap: Multi-layer perceptrons



$$y = f(\theta^T x)$$

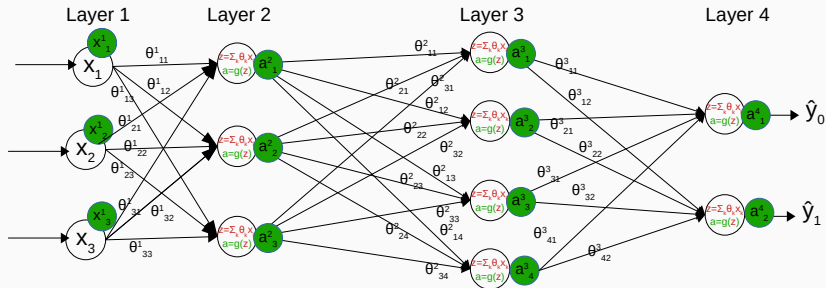
- Linearly separable data
- Perceptron learning rule

## Recap: Multi-layer perceptrons

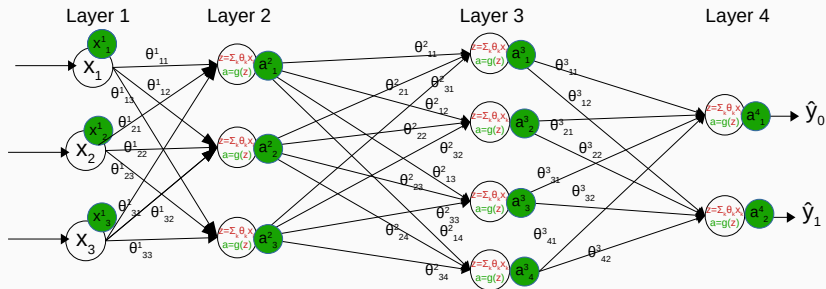


- Linearly separable data
- Perceptron learning rule

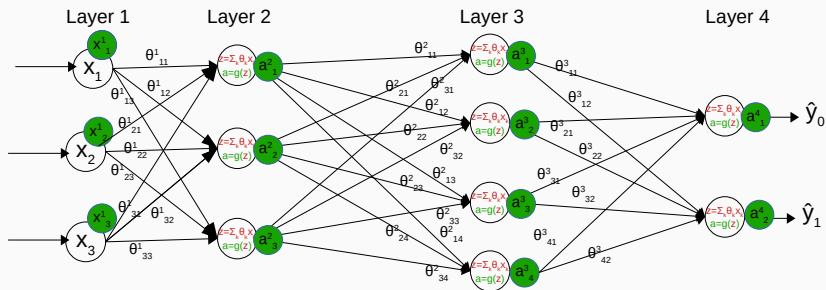
# Recap: Multi-layer perceptrons



# Recall: Supervised learning



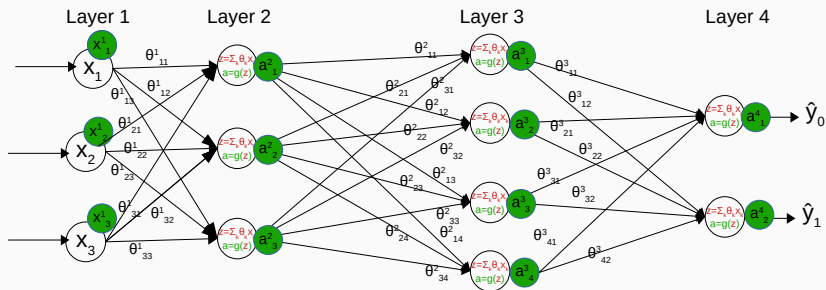
# Recall: Supervised learning



## Recipe

1. Forward propagate an input  $x$  from the **training set**
2. Compute the output  $\hat{y}$  with the MLP

# Recall: Supervised learning

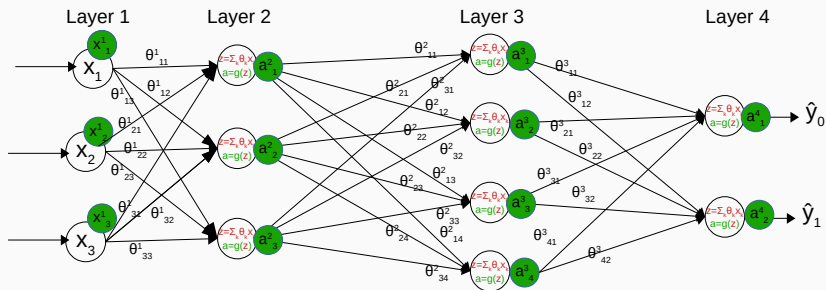


## Recipe

1. Forward propagate an input  $x$  from the **training set**
2. Compute the output  $\hat{y}$  with the MLP
3. Compare predicted output  $\hat{y}$  against true output  $y$ ; compute the **error**



# Recall: Supervised learning

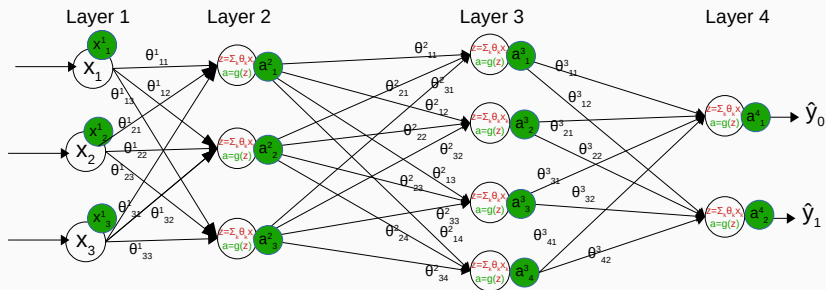


## Recipe

1. Forward propagate an input  $x$  from the **training set**
2. Compute the output  $\hat{y}$  with the MLP
3. Compare predicted output  $\hat{y}$  against true output  $y$ ; compute the **error**
4. **Modify each weight** such that the error decreases in future predictions (e.g., by applying **gradient descent**)



# Recall: Supervised learning

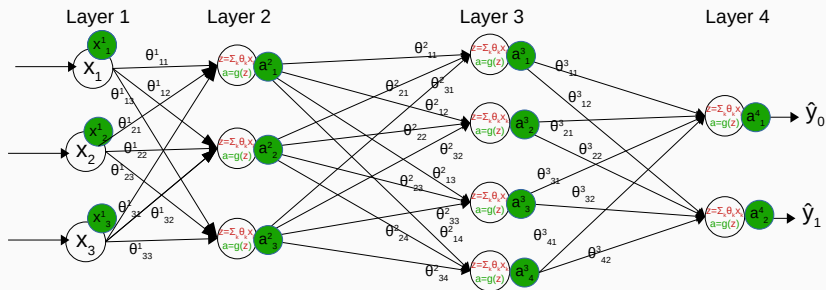


## Recipe

1. Forward propagate an input  $x$  from the **training set**
2. Compute the output  $\hat{y}$  with the MLP
3. Compare predicted output  $\hat{y}$  against true output  $y$ ; compute the **error**
4. **Modify each weight** such that the error decreases in future predictions (e.g., by applying **gradient descent**)
5. Repeat.



# Recall: Optimization with Gradient Descent



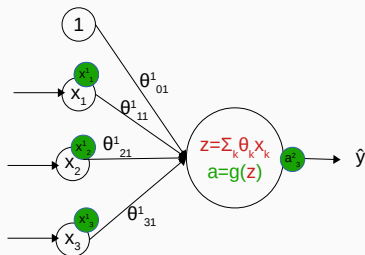
We want to

1. Find the best parameters, which lead to the smallest error  $E$
2. Optimize each model parameter  $\theta_{ij}^l$
3. We will use **gradient descent** to achieve that
4.  $\theta_{ij}^{l,(t+1)} \leftarrow \theta_{ij}^{l,(t)} + \Delta \theta_{ij}^l$



## Recall Perceptron learning:

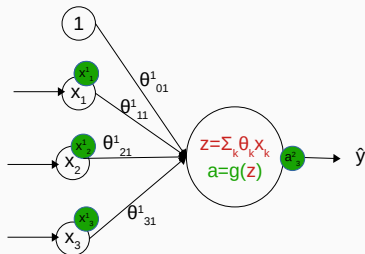
- Pass an input through and compute  $\hat{y}$
- Compare  $\hat{y}$  against  $y$
- Weight update  $\theta_i \leftarrow \theta_i + \eta(y - \hat{y})x_i$



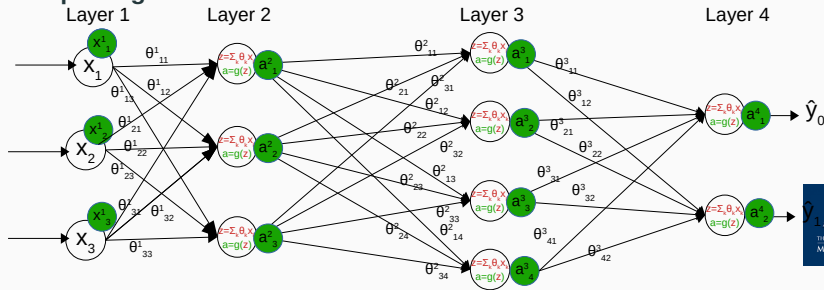
# Towards Backpropagation

## Recall Perceptron learning:

- Pass an input through and compute  $\hat{y}$
- Compare  $\hat{y}$  against  $y$
- Weight update  $\theta_i \leftarrow \theta_i + \eta(y - \hat{y})x_i$

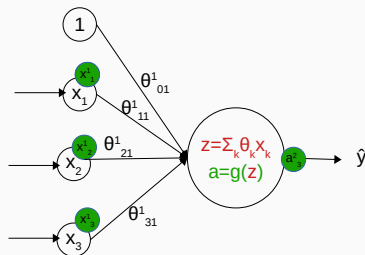


## Compare against the MLP:



## Recall Perceptron learning:

- Pass an input through and compute  $\hat{y}$
- Compare  $\hat{y}$  against  $y$
- Weight update  $\theta_i \leftarrow \theta_i + \eta(y - \hat{y})x_i$



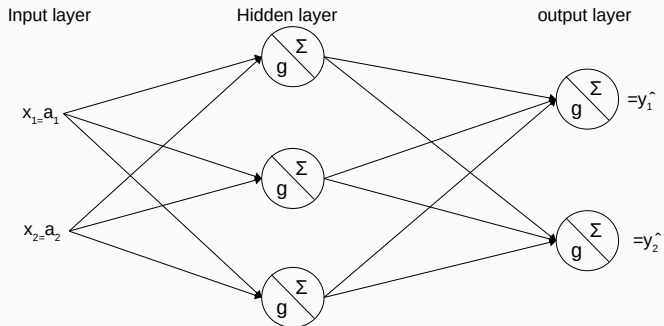
## Problems

- This update rule depends on **true target outputs**  $y$
- We only have access to true outputs for the **final layer**
- We do not know the **true activations** for the **hidden layers**. Can we **generalize** the above rule to also update the hidden layers?

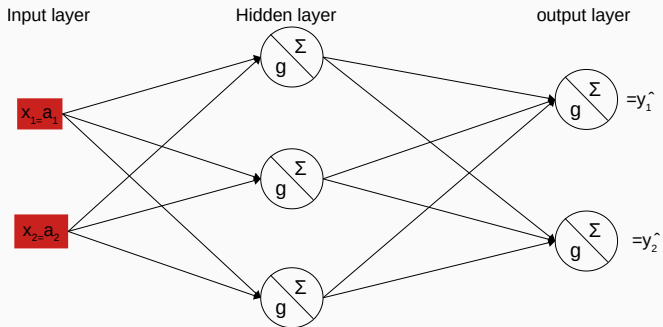
**Backpropagation provides us with an efficient way of computing partial derivatives of the error of an MLP wrt. each individual weight.**



# Backpropagation: Demo



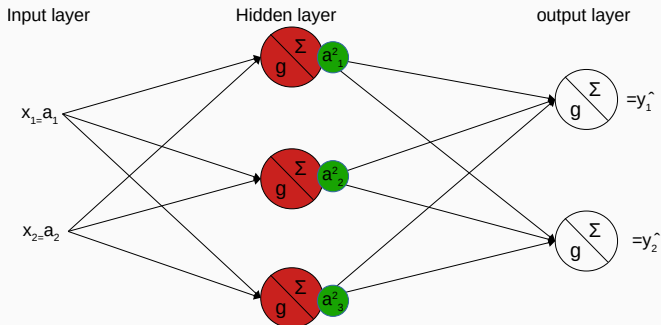
# Backpropagation: Demo



- Receive input

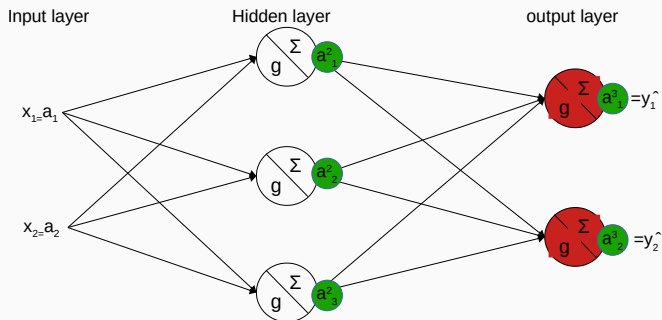


# Backpropagation: Demo



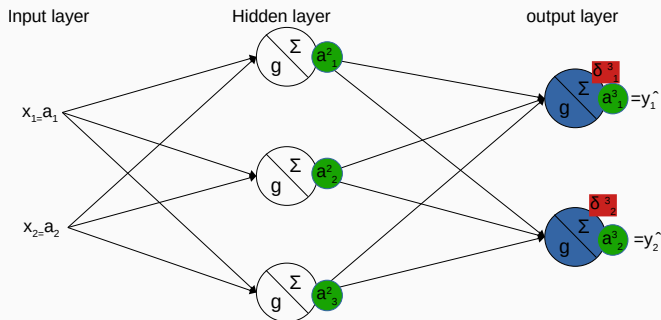
- Receive input
- Forward pass: propagate activations through the network

# Backpropagation: Demo



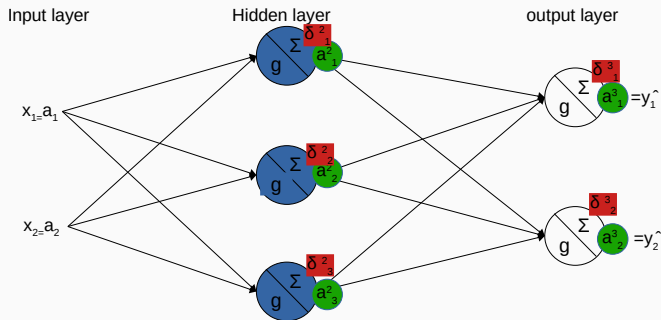
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# Backpropagation: Demo



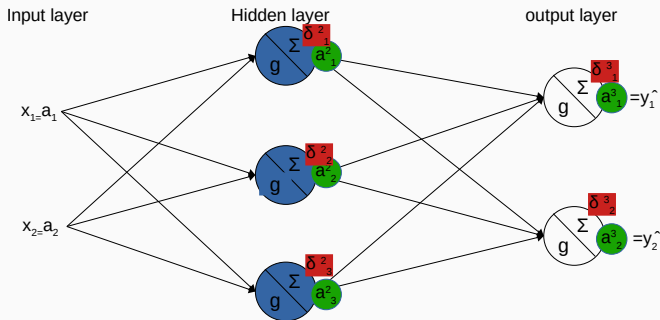
- Receive input
- Forward pass: propagate activations through the network
- Compute Error : compare output  $\hat{y}$  against true  $y$

# Backpropagation: Demo



- Receive input
- Forward pass: propagate activations through the network
- Compute Error : compare output  $\hat{y}$  against true  $y$
- Backward pass: propagate **error terms** through the network

# Backpropagation: Demo



- Receive input
- Forward pass: propagate activations through the network
- Compute Error : compare output  $\hat{y}$  against true  $y$
- Backward pass: propagate **error terms** through the network
- Calculate  $\Delta\theta_{ij}^l$  for all  $\theta_{ij}^l$
- Update weights  $\theta_{ij}^l \leftarrow \theta_{ij}^l + \Delta\theta_{ij}^l$

- We recall what a MLP is
- We recall that we want to learn its parameters such that our prediction error is minimized
- We recall that gradient descent gives us a rule for updating the weights

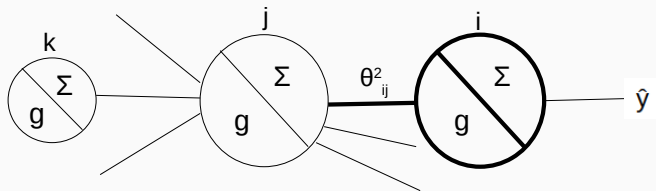
$$\theta_i \leftarrow \theta_i + \Delta\theta_i \text{ with } \Delta\theta_i = -\eta \frac{\partial E}{\partial \theta_i}$$

- But how do we compute  $\frac{\partial E}{\partial \theta_i}$ ?
- **Backpropagation** provides us with an **efficient way** of computing partial derivatives of the error of an MLP wrt. each individual weight.

## The (Generalized) Delta Rule

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## Backpropagation 1: Model definition



- Assuming a sigmoid activation function, the output of neuron  $i$  (or its activation  $a_i$ ) is

$$a_i = g(z_i) = \frac{1}{1 + e^{-z_i}}$$

- And  $z_i$  is the input of all incoming activations into neuron  $i$

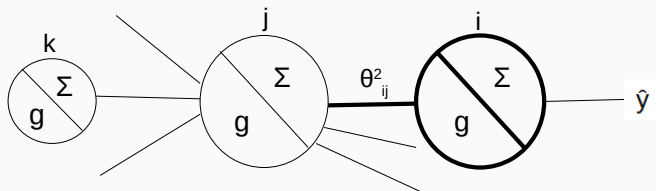
$$z_i = \sum_j \theta_{ij} a_j$$

- And Mean Squared Error (MSE) as **error function**  $E$

$$E = \frac{1}{2N} \sum_{i=1}^N (y^i - \hat{y}^i)^2$$



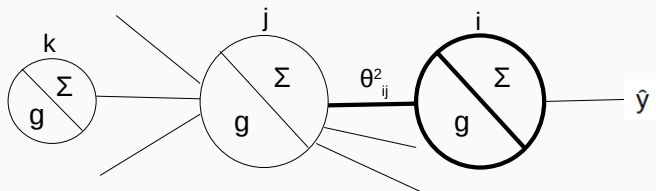
## Backpropagation 2: Error of the final layer



- Apply gradient descent for input  $p$  and weight  $\theta_{ij}^2$  connecting node  $j$  with node  $i$

$$\Delta \theta_{ij}^2 = -\eta \frac{\partial E}{\partial \theta_{ij}^2} = \eta (y^p - \hat{y}^p) g'(z_i) a_j$$

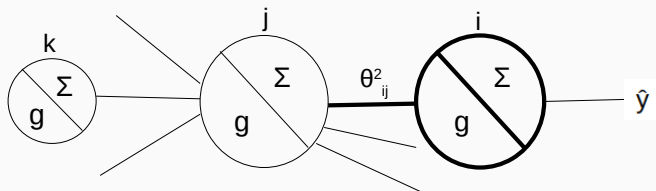
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## Backpropagation 2: Error of the final layer

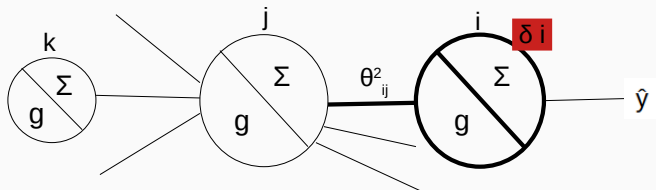


- Apply gradient descent for input  $p$  and weight  $\theta_{ij}^2$  connecting node  $j$  with node  $i$

$$\begin{aligned}\Delta \theta_{ij}^2 &= -\eta \frac{\partial E}{\partial \theta_{ij}^2} = \eta (y^p - \hat{y}^p) g'(z_i) a_j \\ &= \eta \delta_i a_j\end{aligned}$$

- The weight update corresponds to an error term ( $\delta_i$ ) scaled by the incoming activation
- We attach a  $\delta$  to **node**  $i$

# Backpropagation: The Generalized Delta Rule



- The Generalized Delta Rule

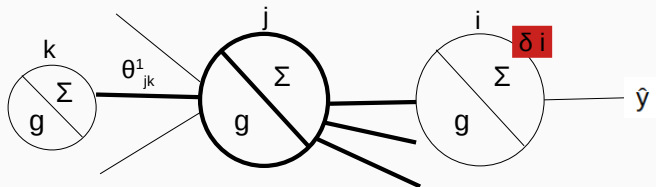
$$\Delta \theta_{ij}^2 = -\eta \frac{\partial E}{\partial \theta_{ij}^2} = \eta (y^p - \hat{y}^p) g'(z_i) a_j = \eta \delta_i a_j$$

$$\delta_i = (y^p - \hat{y}^p) g'(z_i)$$

- The above  $\delta_i$  can only be applied to output units, because it relies on the **target outputs**  $y^p$ .
- We do not have target outputs  $y$  for the intermediate layers



# Backpropagation: The Generalized Delta Rule

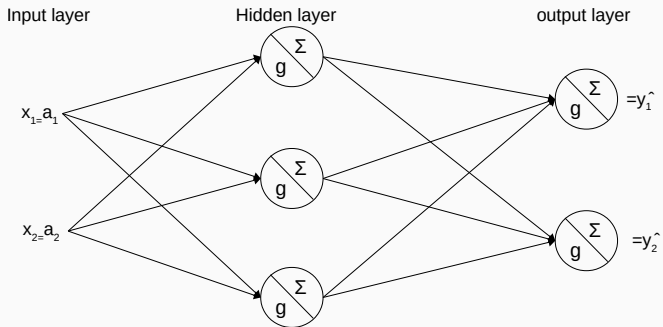


- Instead, we **backpropagate** the errors ( $\delta$ s) from right to left through the network

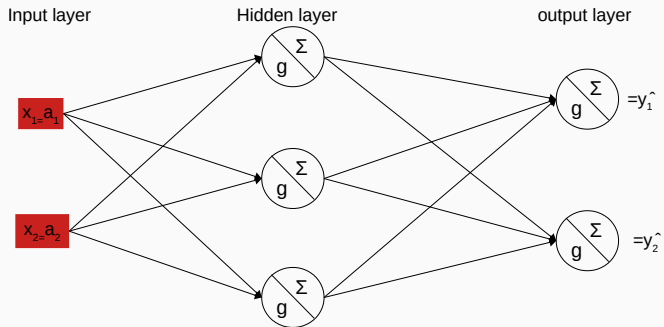
$$\Delta\theta_{jk}^1 = \eta \delta_j a_k$$

$$\delta_j = \sum_i \theta_{ij}^1 \delta_i g'(z_j)$$

# Backpropagation: Demo

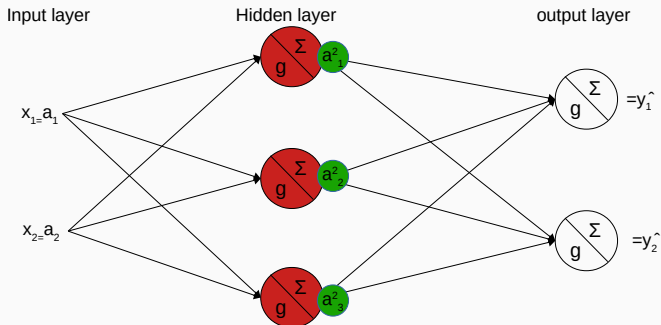


# Backpropagation: Demo



- Receive input

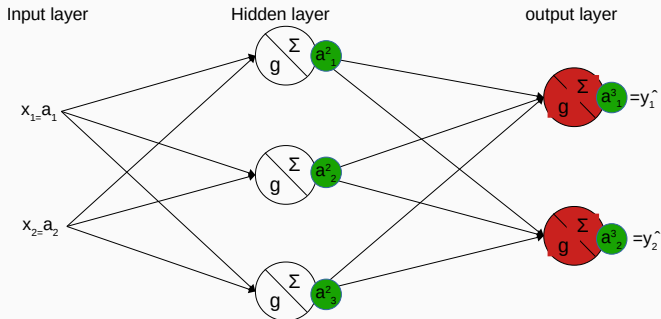
# Backpropagation: Demo



- Receive input
- Forward pass: propagate activations through the network

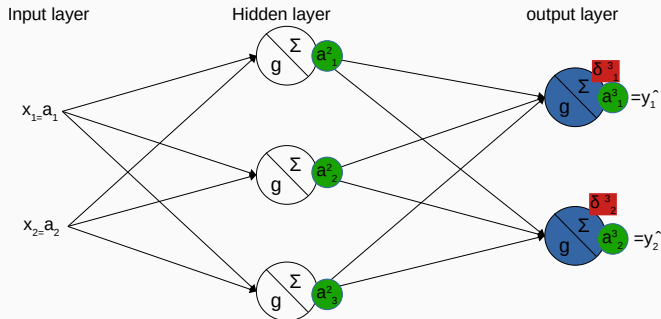


# Backpropagation: Demo



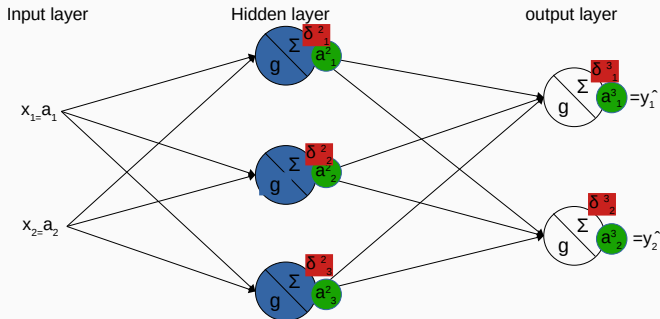
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# Backpropagation: Demo



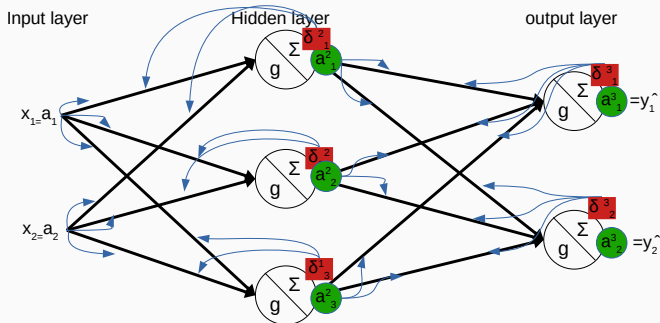
- Receive input
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# Backpropagation: Demo



- Receive input
- Forward pass: propagate activations through the network
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# Backpropagation: Demo



- Receive input
- Forward pass: propagate activations through the network
- Compute Error : compare output  $\hat{y}$  against true  $y$
- Backward pass: propagate error terms through the network
- Calculate  $\frac{\partial E}{\partial \theta^l_{ij}}$  for all  $\theta^l_{ij}$
- Update weights  $\theta^l_{ij} \leftarrow \theta^l_{ij} + \Delta \theta^l_{ij}$

# Backpropagation Algorithm

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Design your neural network

Initialize parameters  $\theta$

**repeat**

**for** training instance  $x_i$  **do**

1. **Forward pass** the instance through the network, compute activations, determine output
2. Compute the **error**
3. Propagate error **back** through the network, and compute for all weights between nodes  $ij$  in all layers  $l$

$$\Delta\theta_{ij}^l = -\eta \frac{\partial E}{\partial \theta_{ij}^l} = \eta \delta_i a_j$$

4. Update **all** parameters **at once**

$$\theta_{ij}^l \leftarrow \theta_{ij}^l + \Delta\theta_{ij}^l$$

**until** stopping criteria reached.

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## Derivation of the update rules

... optional slides after the next (summary) slide, for those who are interested!

## After this lecture, you be able to understand

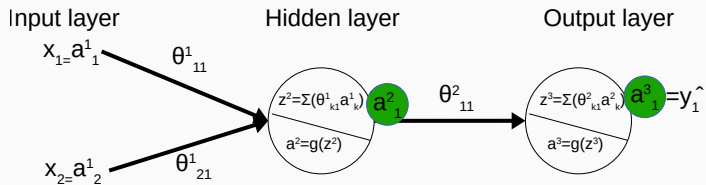
- Why estimation of the MLP parameters is difficult
- How and why we use Gradient Descent to optimize the parameters
- How Backpropagation is a special instance of gradient descent, which allows us to efficiently compute the gradients of all weights wrt. the error
- The mechanism behind gradient descent
- The mathematical justification of gradient descent

## Good job, everyone!

- You now know what (feed forward) neural networks are
- You now know what to consider when designing neural networks
- You now know how to estimate their parameters
- That's more than the average 'data scientist' out there!

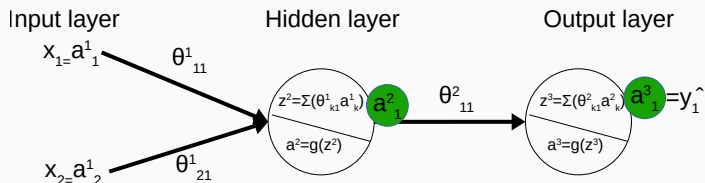


# Backpropagation: Derivation





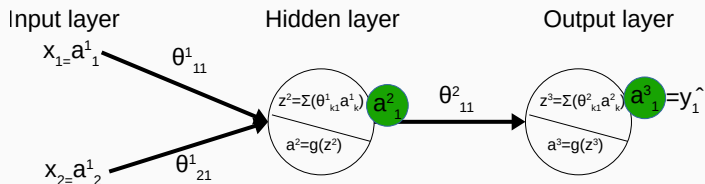
# Backpropagation: Derivation



**Chain of reactions** in the forward pass, focussing on the **output layer**

- varying  $a^2$  causes a change in  $z^3$
- varying  $z^3$  causes a change in  $a^3_1 = g(z^3)$
- varying  $a^3_1 = \hat{y}$  causes a change in  $E(y, \hat{y})$

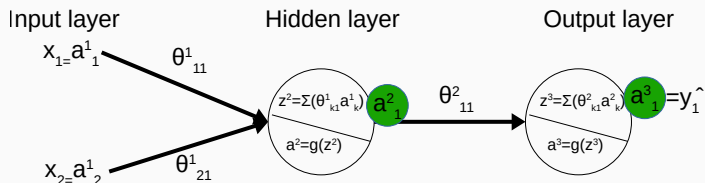
# Backpropagation: Derivation



We can use the **chain rule** to capture the behavior of  $\theta^2_{11}$  wrt  $E$

$$\Delta\theta^2 = -\eta \frac{\partial E}{\partial \theta^2} = -\eta \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial \theta^2} \right) =$$

# Backpropagation: Derivation



We can use the **chain rule** to capture the behavior of  $\theta^2_{11}$  wrt  $E$

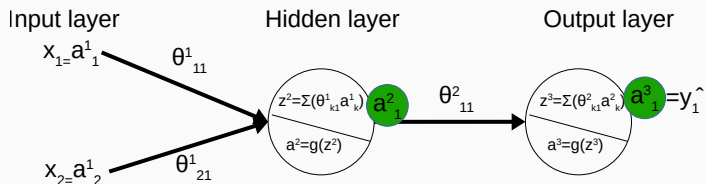
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Let's look at each term individually

$$\frac{\partial E}{\partial a_i} = -(y_i - a_i) \quad \text{recall that } E = \sum_i^N \frac{1}{2} (y_i - a_i)^2$$



# Backpropagation: Derivation



We can use the **chain rule** to capture the behavior of  $\theta^2_{11}$  wrt  $E$

$$\Delta\theta^2 = -\eta \frac{\partial E}{\partial \theta^2} = -\eta \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial \theta^2} \right) =$$

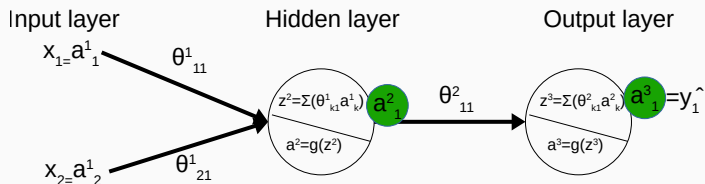
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$$\frac{\partial a}{\partial z} = \frac{\partial g(z)}{\partial z} = g'(z)$$



# Backpropagation: Derivation



We can use the **chain rule** to capture the behavior of  $\theta^2_{11}$  wrt  $E$

$$\Delta\theta^2 = -\eta \frac{\partial E}{\partial \theta^2} = -\eta \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial \theta^2} \right) =$$

Let's look at each term individually

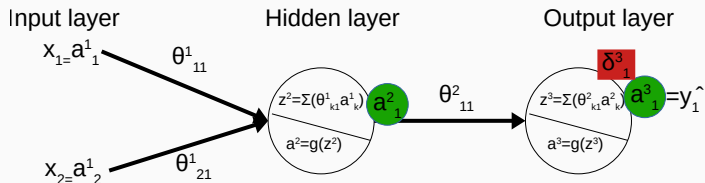
$$\frac{\partial E}{\partial a_i} = -(y_i - a_i) \quad \text{recall that } E = \sum_i^N \frac{1}{2} (y_i - a_i)^2$$

$$\frac{\partial a}{\partial z} = \frac{\partial g(z)}{\partial z} = g'(z)$$

$$\frac{\partial z}{\partial \theta_{ij}} = \frac{\partial}{\partial \theta_{ij}} \sum_{i'} \theta_{i'j} a_{i'} = \sum_{i'} \frac{\partial}{\partial \theta_{ij}} \theta_{i'j} a_{i'} = a_i$$



# Backpropagation: Derivation



We can use the **chain rule** to capture the behavior of  $\theta^2_{11}$  wrt  $E$

$$\Delta \theta^2 = -\eta \frac{\partial E}{\partial \theta^2} = -\eta \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial \theta^2} \right) = \underbrace{\eta (y - a^3_1) (g'(z^3))}_{= \delta^3_1} (a^2_1) = \eta \delta^3_1 a^2_1$$

Let's look at each term individually

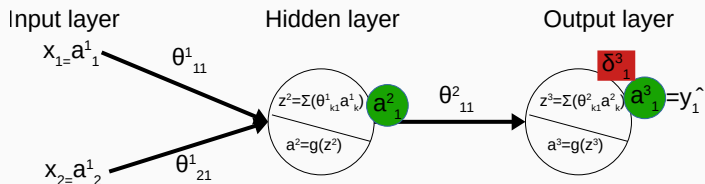
$$\frac{\partial E}{\partial a_i} = -(y_i - a_i) \quad \text{recall that } E = \sum_i^N \frac{1}{2} (y_i - a_i)^2$$

$$\frac{\partial a}{\partial z} = \frac{\partial g(z)}{\partial z} = g'(z)$$

$$\frac{\partial z}{\partial \theta_{ij}} = \frac{\partial}{\partial \theta_{ij}} \sum_{i'} \theta_{i'j} a_{i'} = \sum_{i'} \frac{\partial}{\partial \theta_{ij}} \theta_{i'j} a_{i'} = a_i$$



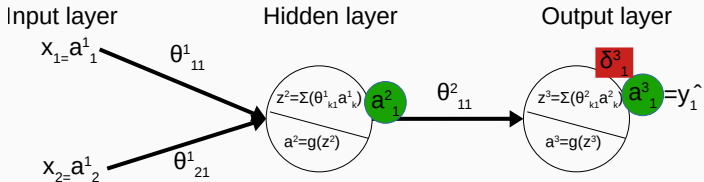
# Backpropagation: Derivation



We have another **chain reaction**. Let's consider **layer 2**

- varying any  $\theta^1_{k1}$  causes a change in  $z^2$
- varying  $z^2$  causes a change in  $a^2_1 = g(z^2)$
- varying  $a^2_1$  causes a change in  $z^3$  (we consider  $\theta^2$  fixed for the moment)
- varying  $z^3$  causes a change in  $a^3_1 = g(z^3)$
- varying  $a^3_1 = \hat{y}$  causes a change in  $E(y, \hat{y})$

## Backpropagation: Derivation



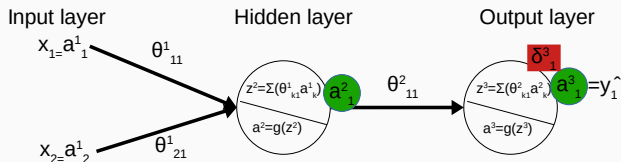
Formulating this again as the chain rule

$$\Delta\theta_{k1}^1 = -\eta \frac{\partial E}{\partial \theta_{k1}^1} = -\eta \left( \left( \frac{\partial E}{\partial \mathbf{a}_1^3} \right) \left( \frac{\partial \mathbf{a}_1^3}{\partial \mathbf{z}^3} \right) \left( \frac{\partial \mathbf{z}^3}{\partial \mathbf{a}_1^2} \right) \right) \left( \frac{\partial \mathbf{a}_1^2}{\partial \mathbf{z}^2} \right) \left( \frac{\partial \mathbf{z}^2}{\partial \theta_{k1}^1} \right)$$





# Backpropagation: Derivation



Formulating this again as the chain rule

$$\Delta\theta^1_{k1} = -\eta \frac{\partial E}{\partial \theta^1_{k1}} = -\eta \left( \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial a^2_1} \right) \right) \left( \frac{\partial a^2_1}{\partial z^2} \right) \left( \frac{\partial z^2}{\partial \theta^1_{k1}} \right)$$

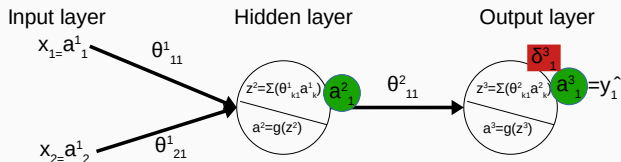
We already know that

$$\frac{\partial E}{\partial a^3_1} = -(y - a^3_1)$$

$$\frac{\partial a^3_1}{\partial z^3} = g'(z^3)$$



# Backpropagation: Derivation



Formulating this again as the chain rule

$$\Delta\theta^1_{k1} = -\eta \frac{\partial E}{\partial \theta^1_{k1}} = -\eta \left( \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial a^2_1} \right) \right) \left( \frac{\partial a^2_1}{\partial z^2} \right) \left( \frac{\partial z^2}{\partial \theta^1_{k1}} \right)$$

And following the previous logic, we can calculate that

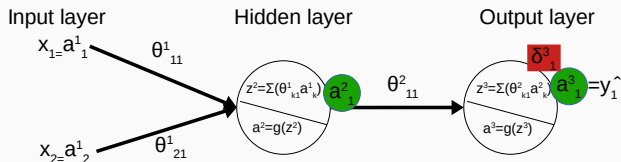
$$\frac{\partial z^3}{\partial a^2_1} = \frac{\partial \theta^2_{11} a^2_1}{\partial a^2_1} = \theta^2_{11}$$

$$\frac{\partial a^2_1}{\partial z^2} = \frac{\partial g(z^2)}{\partial z^2} = g'(z^2)$$

$$\frac{\partial z^2}{\partial \theta^1_{k1}} = a_k$$



# Backpropagation: Derivation



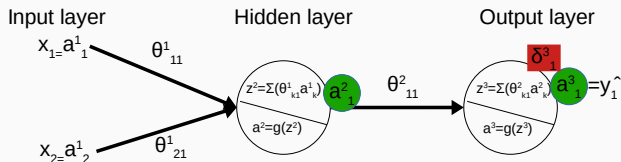
Formulating this again as the chain rule

$$\Delta\theta^1_{k1} = -\eta \frac{\partial E}{\partial \theta^1_{k1}} = -\eta \left( \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial a^2_1} \right) \right) \left( \frac{\partial a^2_1}{\partial z^2} \right) \left( \frac{\partial z^2}{\partial \theta^1_{k1}} \right)$$

Plugging these into the above we get

$$-\eta \frac{\partial E}{\partial \theta^1_{k1}} = -\eta \left( - (y - a^3_1) g'(z^3) \theta^2_{11} \right) g'(z^2) a_k$$

# Backpropagation: Derivation



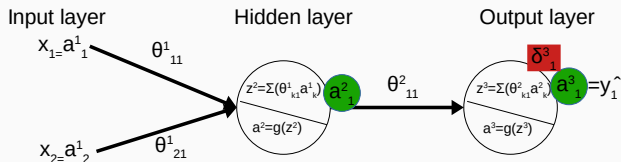
Formulating this again as the chain rule

$$\Delta\theta^1_{k1} = -\eta \frac{\partial E}{\partial \theta^1_{k1}} = -\eta \left( \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial a^2_1} \right) \right) \left( \frac{\partial a^2_1}{\partial z^2} \right) \left( \frac{\partial z^2}{\partial \theta^1_{k1}} \right)$$

Plugging these into the above we get

$$\begin{aligned} -\eta \frac{\partial E}{\partial \theta^1_{k1}} &= -\eta \left( - (y - a^3_1) g'(z^3) \theta^2 \right) g'(z^2) a_k \\ &= \eta \left( (y - a^3_1) g'(z^3) \theta^2 \right) g'(z^2) a_k \end{aligned}$$

# Backpropagation: Derivation



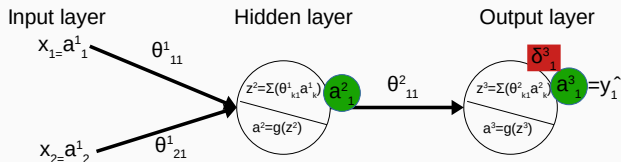
Formulating this again as the chain rule

$$\Delta\theta^1_{k1} = -\eta \frac{\partial E}{\partial \theta^1_{k1}} = -\eta \left( \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial a^2_1} \right) \right) \left( \frac{\partial a^2_1}{\partial z^2} \right) \left( \frac{\partial z^2}{\partial \theta^1_{k1}} \right)$$

Plugging these into the above we get

$$\begin{aligned} -\eta \frac{\partial E}{\partial \theta^1_{k1}} &= -\eta \left( - (y - a^3_1) g'(z^3) \theta^2 \right) g'(z^2) a_k \\ &= \eta \left( \underbrace{(y - a^3_1) g'(z^3) \theta^2}_{=\delta^3_1} \right) g'(z^2) a_k \\ &= \delta^3_1 \end{aligned}$$

# Backpropagation: Derivation



Formulating this again as the chain rule

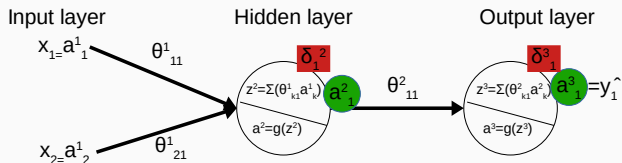
$$\Delta\theta^1_{k1} = -\eta \frac{\partial E}{\partial \theta^1_{k1}} = -\eta \left( \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial a^2_1} \right) \right) \left( \frac{\partial a^2_1}{\partial z^2} \right) \left( \frac{\partial z^2}{\partial \theta^1_{k1}} \right)$$

Plugging these into the above we get

$$\begin{aligned} -\eta \frac{\partial E}{\partial \theta^1_{k1}} &= -\eta \left( - (y - a^3_1) g'(z^3) \theta^2 \right) g'(z^2) a_k \\ &= \eta \left( \underbrace{(y - a^3_1) g'(z^3) \theta^2}_{=\delta^3_1} \right) g'(z^2) a_k = \eta \left( \delta^3_1 \theta^2 \right) g'(z^2) a_k \end{aligned}$$



# Backpropagation: Derivation



Formulating this again as the chain rule

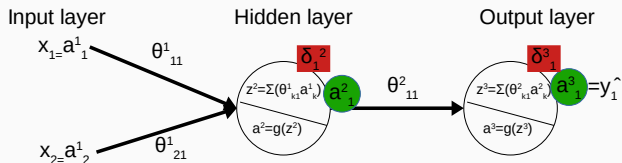
$$\Delta\theta_{k1}^1 = -\eta \frac{\partial E}{\partial \theta_{k1}^1} = -\eta \left( \left( \frac{\partial E}{\partial a_1^3} \right) \left( \frac{\partial a_1^3}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial a_1^2} \right) \right) \left( \frac{\partial a_1^2}{\partial z^2} \right) \left( \frac{\partial z^2}{\partial \theta_{k1}^1} \right)$$

Plugging these into the above we get

$$\begin{aligned} -\eta \frac{\partial E}{\partial \theta_{k1}^1} &= -\eta \left( - (y - a_1^3) g'(z^3) \theta^2 \right) g'(z^2) a_k \\ &= \eta \left( \underbrace{(y - a_1^3) g'(z^3) \theta^2}_{= \delta_1^3} \right) g'(z^2) a_k = \eta \left( \underbrace{\delta_1^3 \theta^2}_{= \delta_1^2} \right) g'(z^2) a_k \end{aligned}$$



# Backpropagation: Derivation



Formulating this again as the chain rule

$$\Delta\theta_{k1}^1 = -\eta \frac{\partial E}{\partial \theta_{k1}^1} = -\eta \left( \left( \frac{\partial E}{\partial a_1^3} \right) \left( \frac{\partial a_1^3}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial a_1^2} \right) \right) \left( \frac{\partial a_1^2}{\partial z^2} \right) \left( \frac{\partial z^2}{\partial \theta_{k1}^1} \right)$$

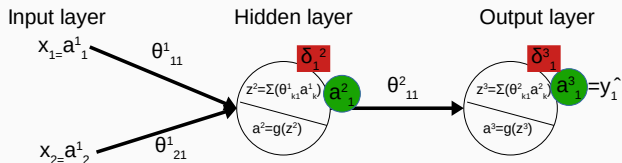
Plugging these into the above we get

$$\begin{aligned} -\eta \frac{\partial E}{\partial \theta_{k1}^1} &= -\eta \left( - (y - a_1^3) g'(z^3) \theta^2 \right) g'(z^2) a_k \\ &= \eta \left( \underbrace{(y - a_1^3) g'(z^3) \theta^2}_{= \delta_1^3} \right) g'(z^2) a_k = \eta \left( \underbrace{\delta_1^3 \theta^2}_{= \delta_1^2} \right) g'(z^2) a_k = \eta \delta_1^2 a_k \end{aligned}$$





# Backpropagation: Derivation



Formulating this again as the chain rule

$$-\eta \frac{\partial E}{\partial \theta^1_{k1}} = -\eta \left( \left( \frac{\partial E}{\partial a^3_1} \right) \left( \frac{\partial a^3_1}{\partial z^3} \right) \left( \frac{\partial z^3}{\partial a^2_1} \right) \right) \left( \frac{\partial a^2_1}{\partial z^2} \right) \left( \frac{\partial z^2}{\partial \theta^1_{k1}} \right)$$

If we had more than one weight  $\theta^2$

$$\begin{aligned} -\eta \frac{\partial E}{\partial \theta^1_{k1}} &= \eta \left( \sum_j \underbrace{(y_j - a^3_j) g'(z^3_j) \theta^2_{1j}}_{= \delta^3_j} \right) g'(z^2) a_k \\ &= \eta \left( \underbrace{\sum_j \delta^3_j \theta^2_{1j}}_{= \delta^2_1} \right) g'(z^2) a_k = \eta \delta^2_1 a_k \end{aligned}$$

