Neural Networks

- What is a neural network?
- Predicting with a neural network
- Training neural networks
- Practical concerns

This lecture

- What is a neural network?
- Predicting with a neural network
- Training neural networks
  - Backpropagation
- Practical concerns

Training a neural network

- Given
  - A network architecture (layout of neurons, their connectivity and activations)
  - A dataset of labeled examples
    - $S = \{(\mathbf{x}_i, y_i)\}$
- The goal: Learn the weights of the neural network
- *Remember*: For a fixed architecture, a neural network is a function parameterized by its weights
  - Prediction: $y = NN(\boldsymbol{x}, \boldsymbol{w})$

Recall: Learning as loss minimization

We have a classifier *NN* that is completely defined by its weights

Learn the weights by minimizing a loss L

$$\min_{\boldsymbol{w}} \sum_i L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i)$$

Perhaps with a *regularizer*

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So far, we saw that this strategy worked for:

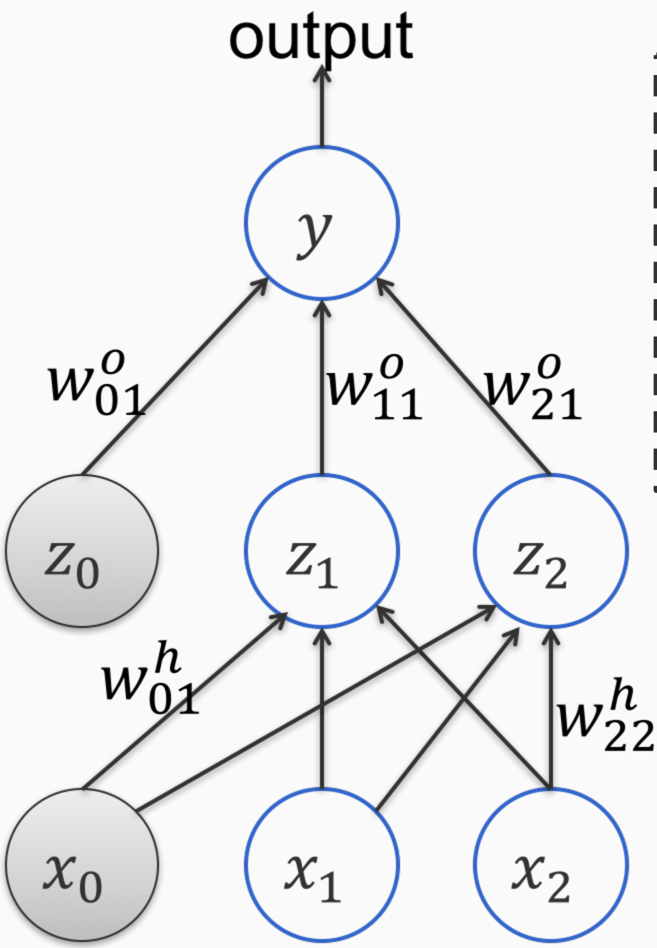
1. Logistic Regression
2. Support Vector Machines
3. Perceptron
4. LMS regression

Each minimizes a different loss function

All of these are linear models

Same idea for non-linear models too!

Back to our running example



Given an input **x**, how is the output predicted

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

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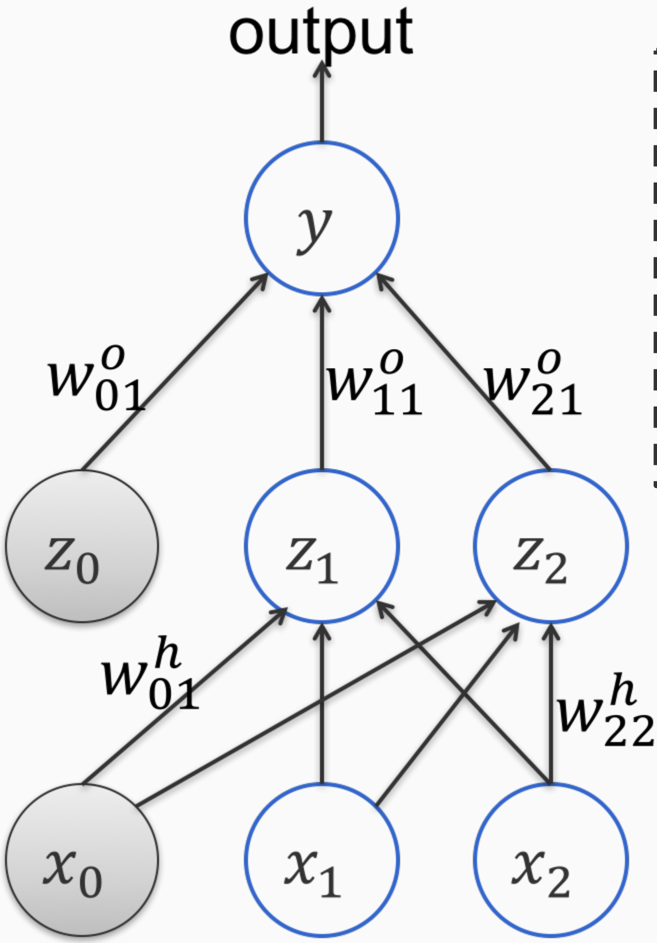

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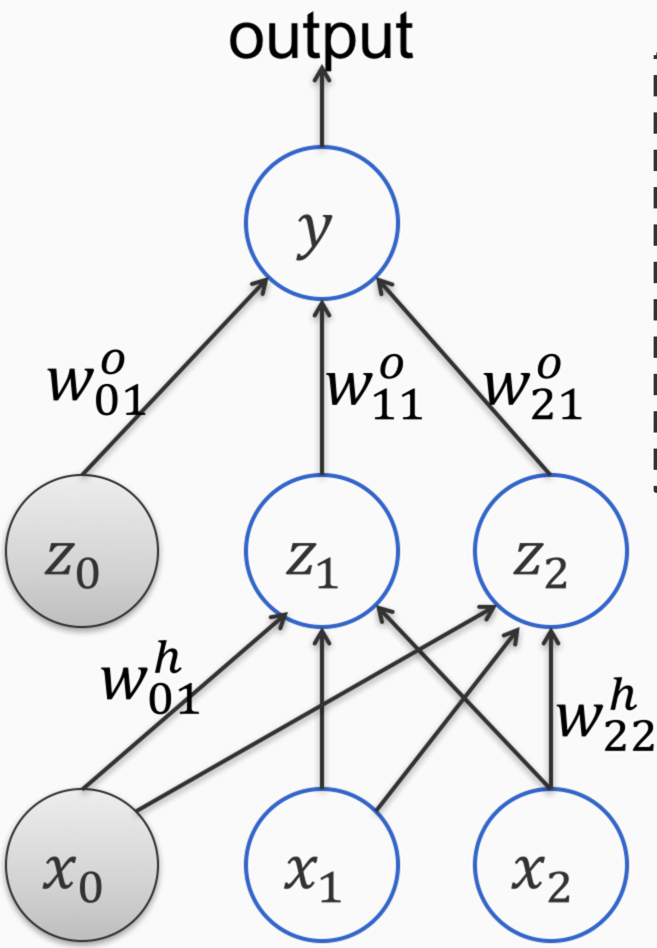

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We can write the *square loss* for this example as:

$$L = \frac{1}{2}(y - y_i)^2$$

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Learn the weights by minimizing a loss L

$$\min_{\boldsymbol{w}} \sum_i L(NN(x_i, w), y_i)$$

Perhaps with a *regularizer*

How do we solve the optimization problem?

$$\min_{\boldsymbol{w}} \sum_i L(NN(x_i, w), y_i)$$

Stochastic gradient descent

Given a training set $S = \{(\mathbf{x}_i, y_i)\}, \mathbf{x} \in \Re^d$

1. Initialize parameters w
2. For epoch = 1 … T:

3. Return w

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Have we solved everything?

The derivative of the loss function?

$\nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i)$

If the neural network is a differentiable function, we can find the gradient

- Or maybe its sub-gradient
- This is decided by the activation functions and the loss function

It was easy for SVMs and logistic regression

- Only one layer

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We need an efficient algorithm: Backpropagation

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Let's look at some simple expressions

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Useful to keep in mind what these derivatives represent In these (and all other) cases:

$$\frac{\partial f}{\partial x}$$

Represents the rate of change of the function f with respect to a small change in x

More complicated cases?

$$f(x, y, z) = x(y^2 + z)$$

This is still simple enough to manually take derivatives, but let us work through this in a slightly different way.

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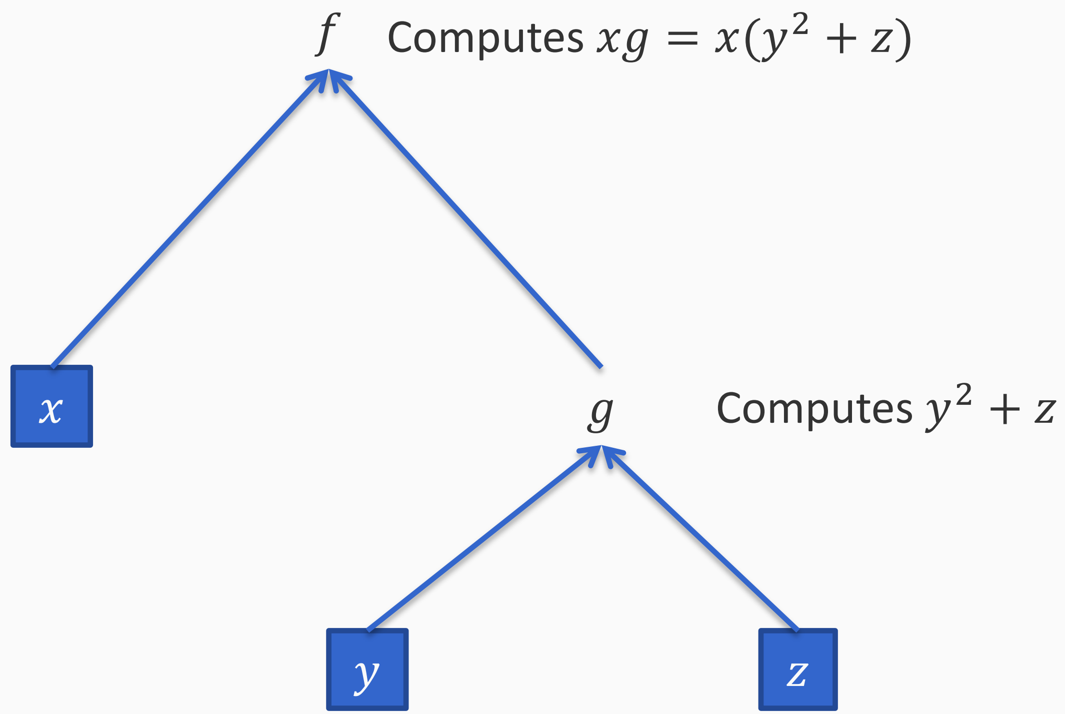
Key idea: Build up derivatives of compound expressions by breaking it down into simpler pieces, and applying the **chain rule**

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial y} = x \cdot 2y = 2xy$$

In terms of “computation graphs”

$$f(x, y, z) = x(y^2 + z)$$



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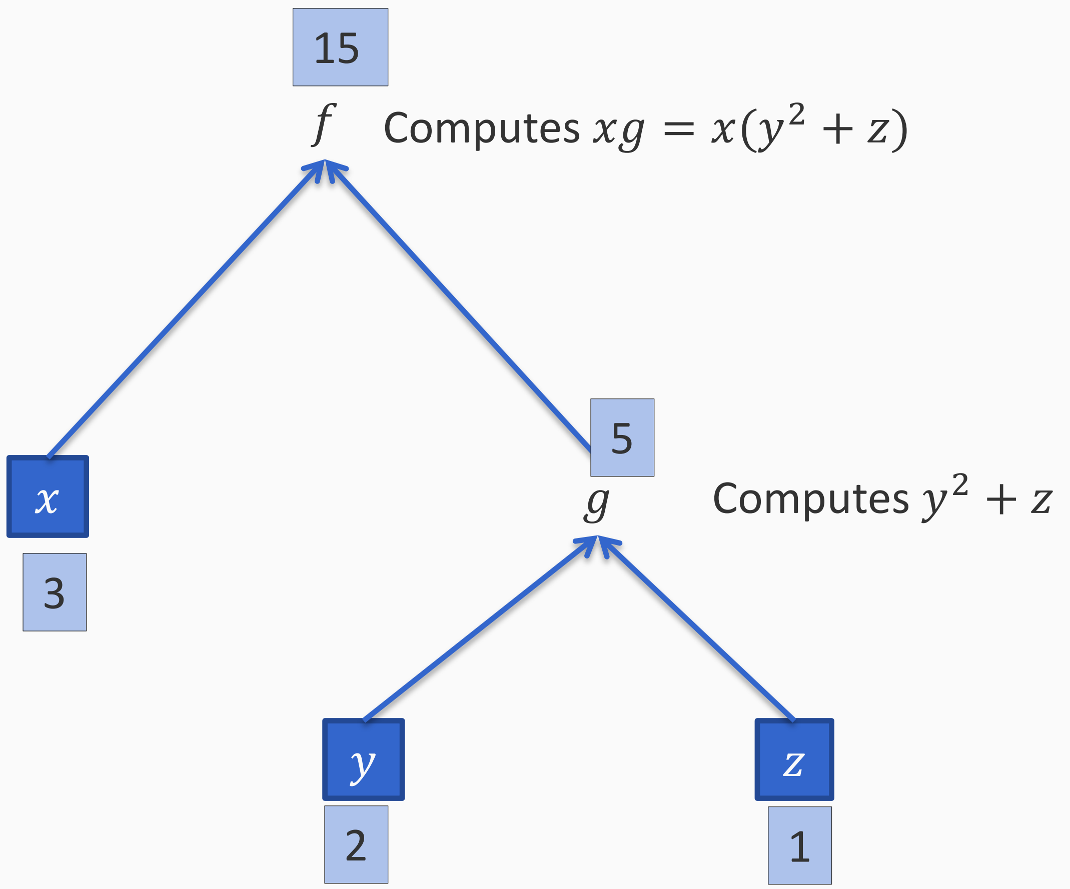
The forward pass: Computes function values for specific inputs



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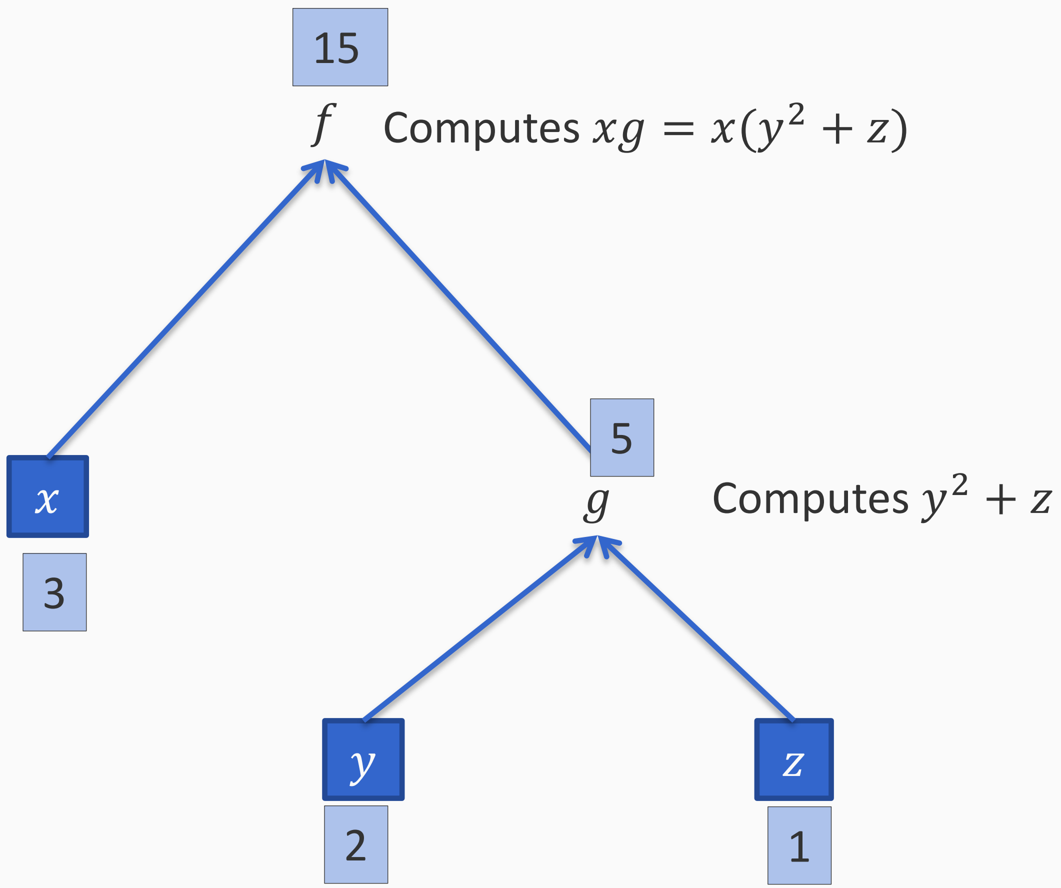
The backward pass: Computes derivatives of each intermediate node



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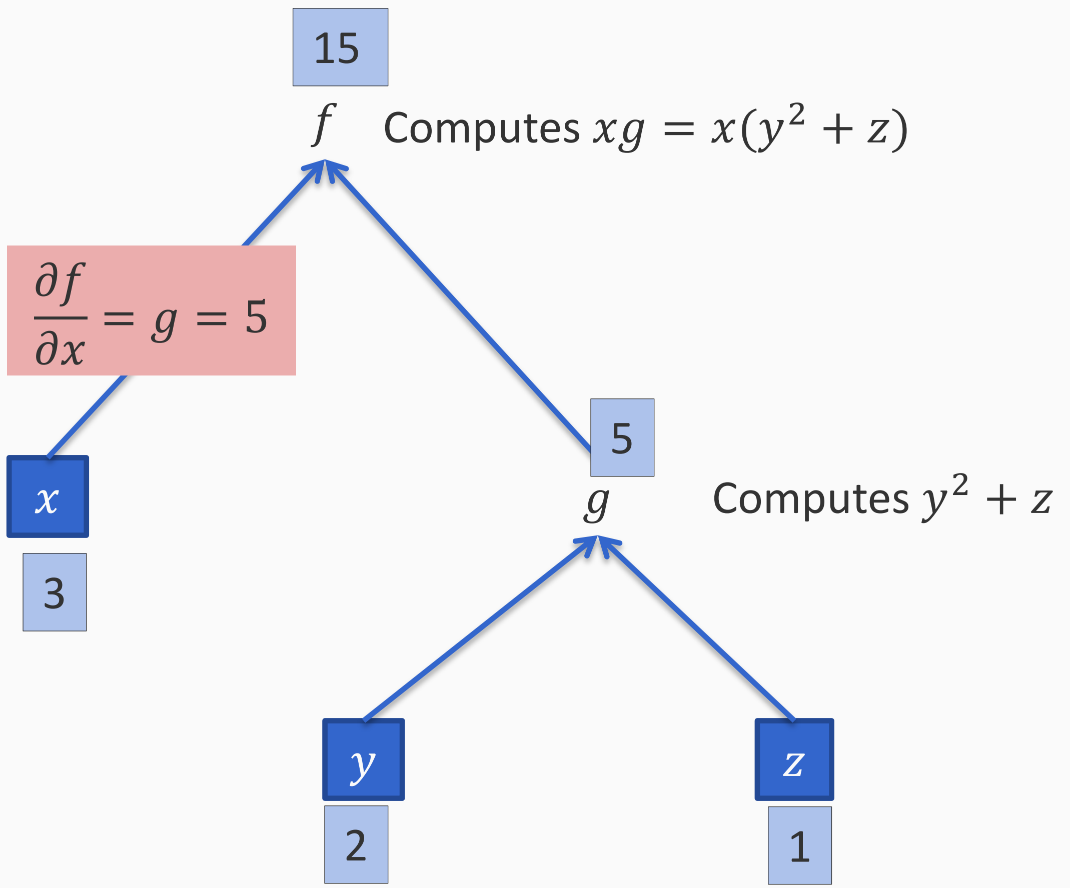

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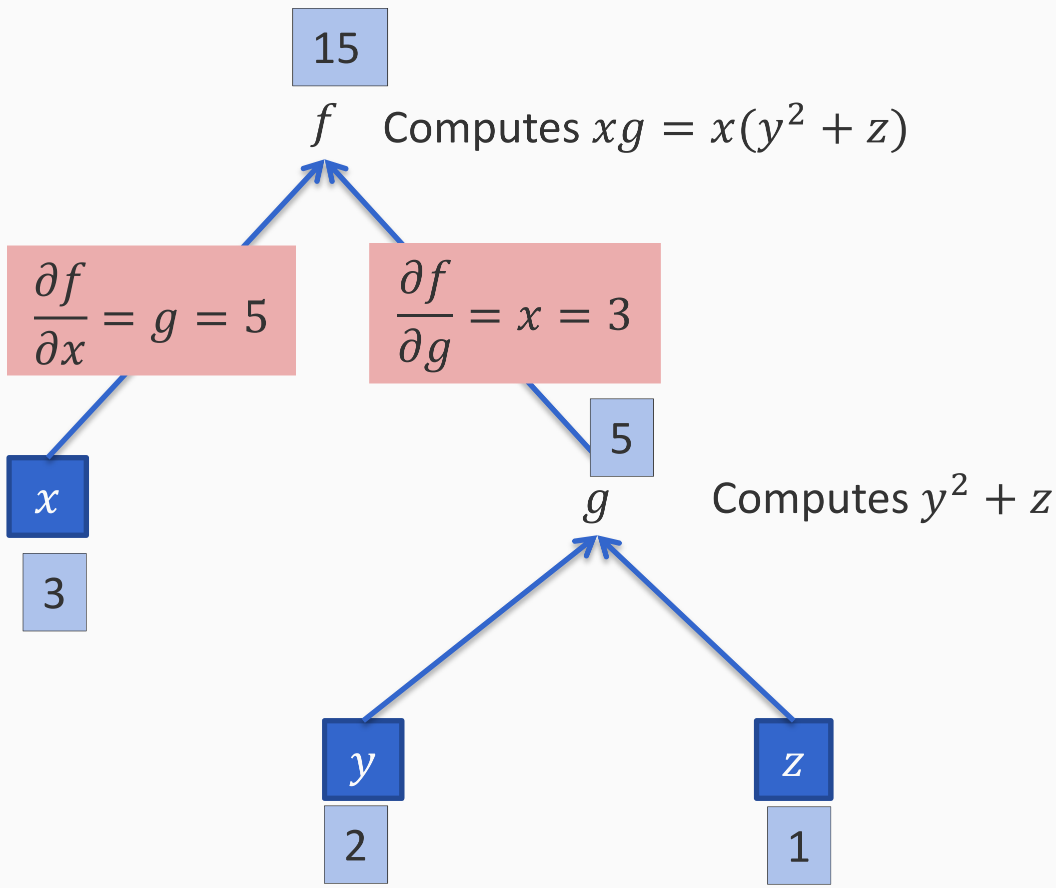

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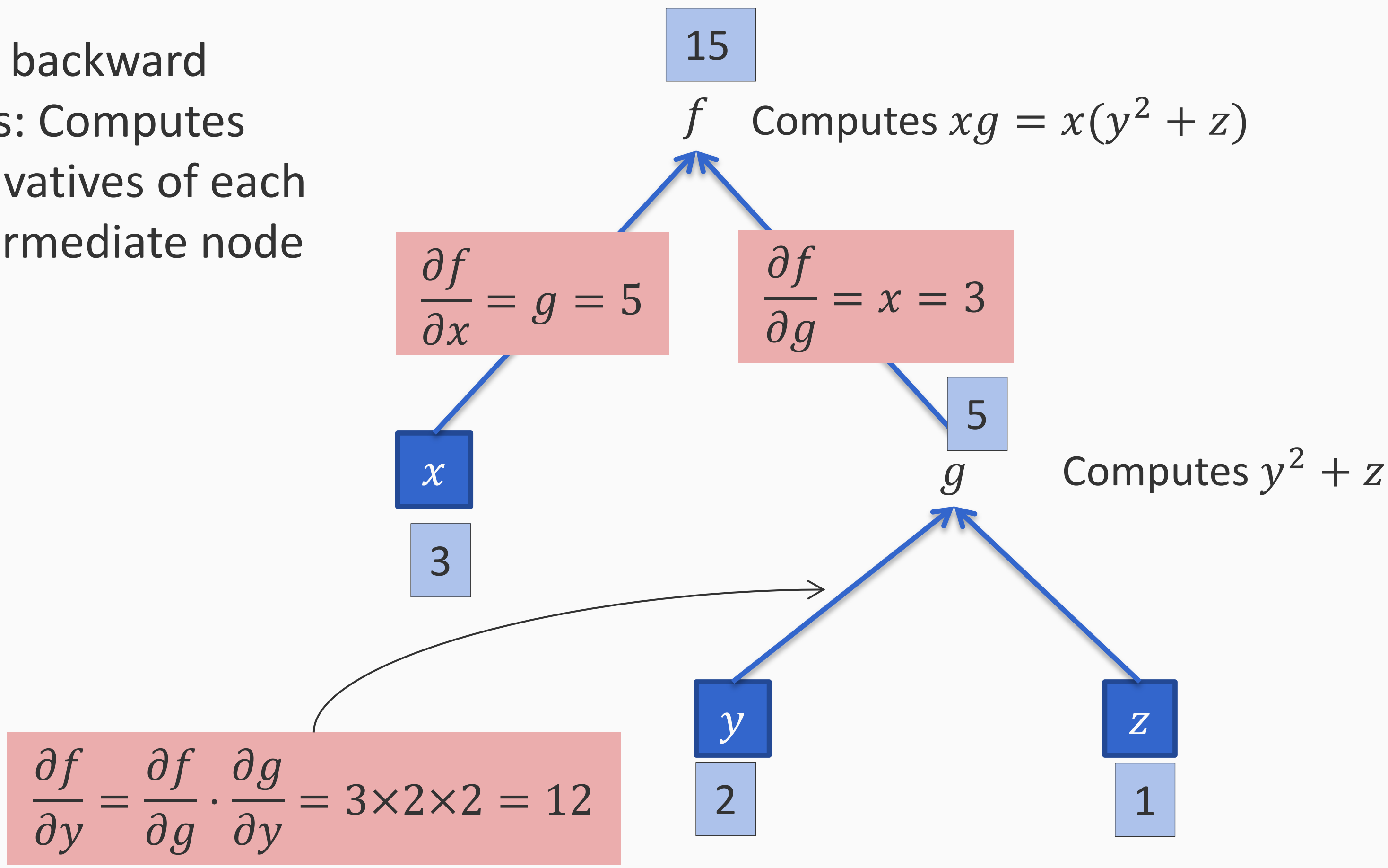

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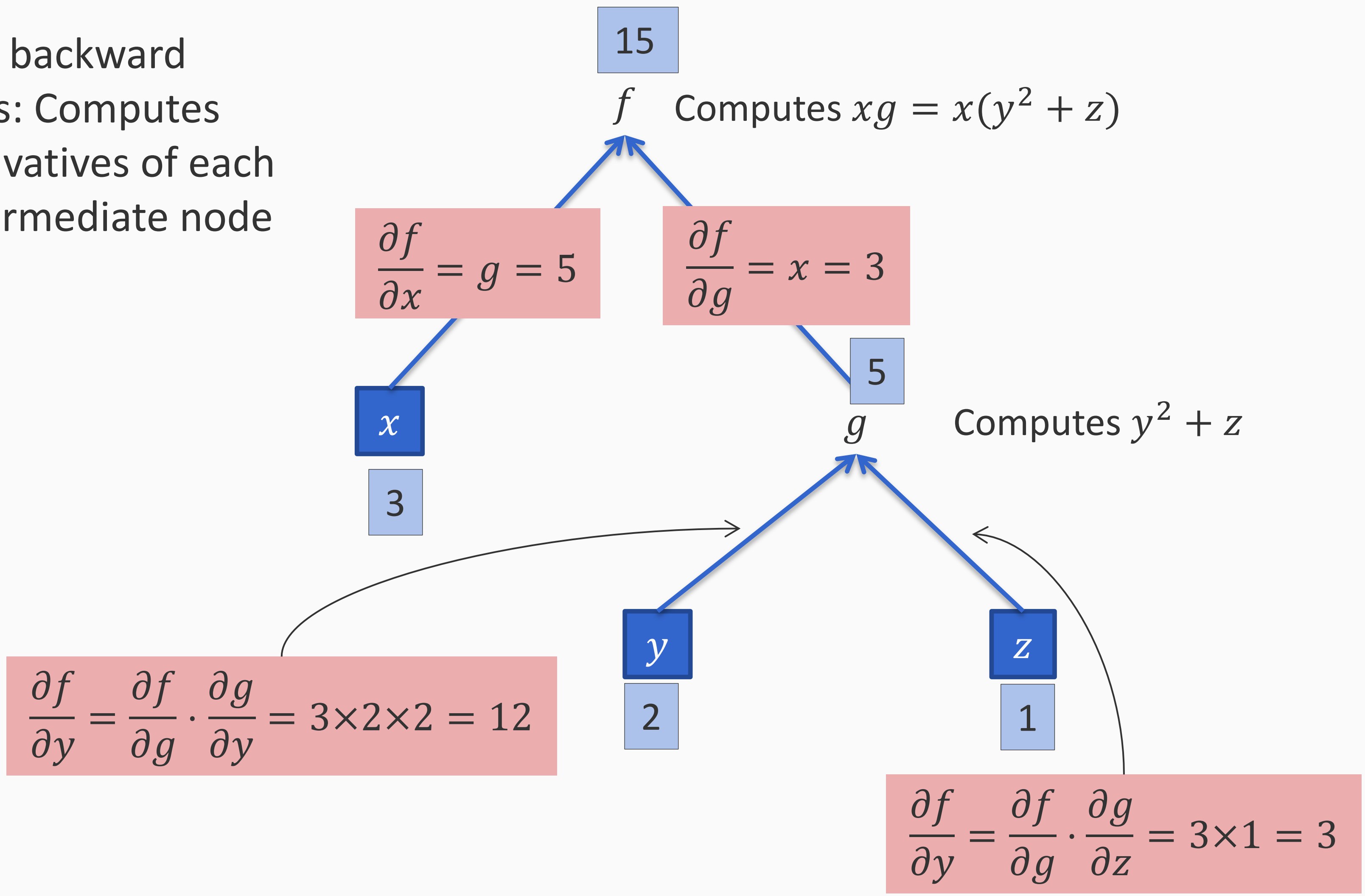

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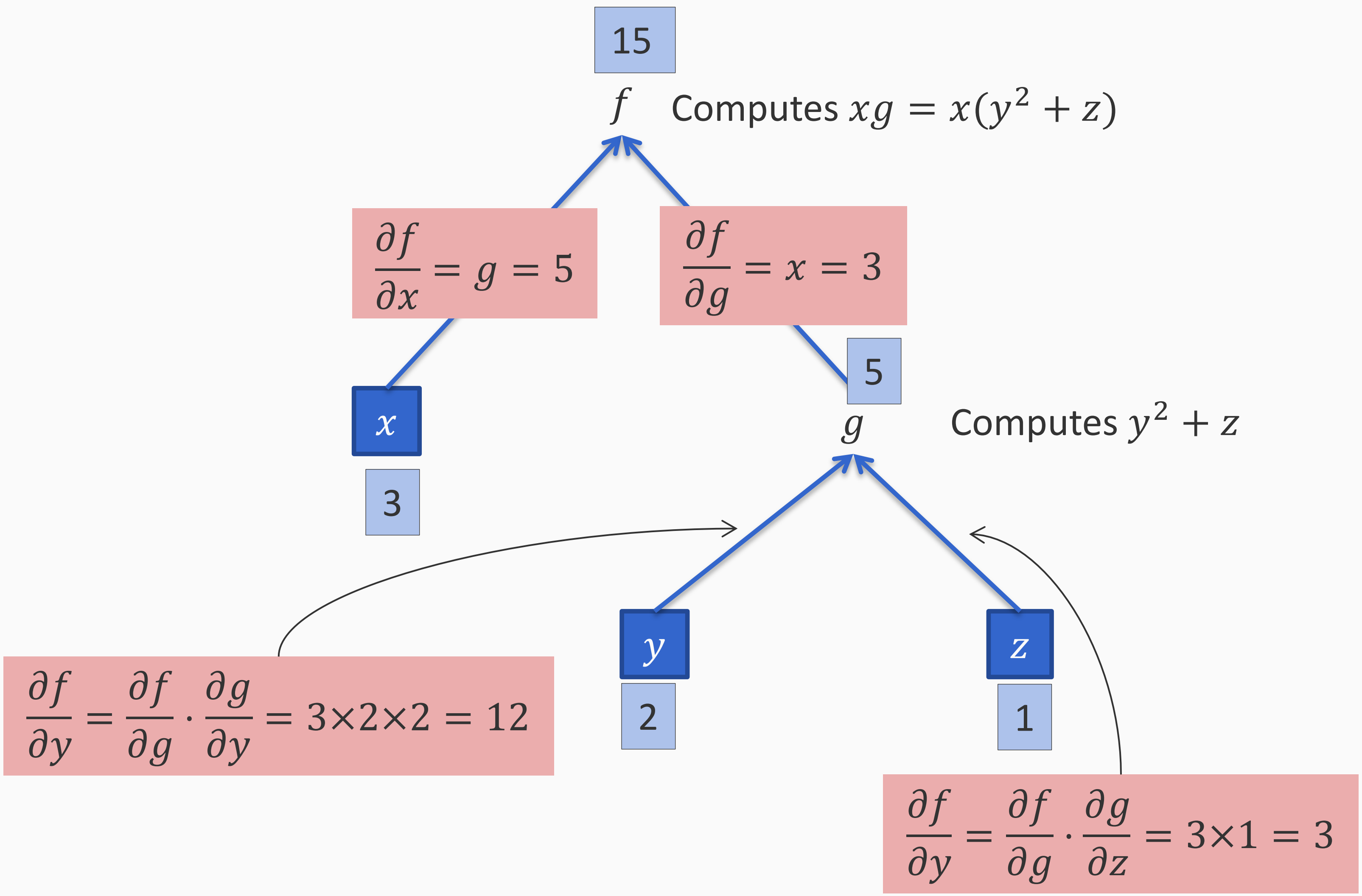


The abstraction

- Each node in the graph knows two things:
  1. How to compute the value of a function with respect to its inputs (forward)

  2. How to compute the partial derivative of its output with respect to each of its inputs (backward)

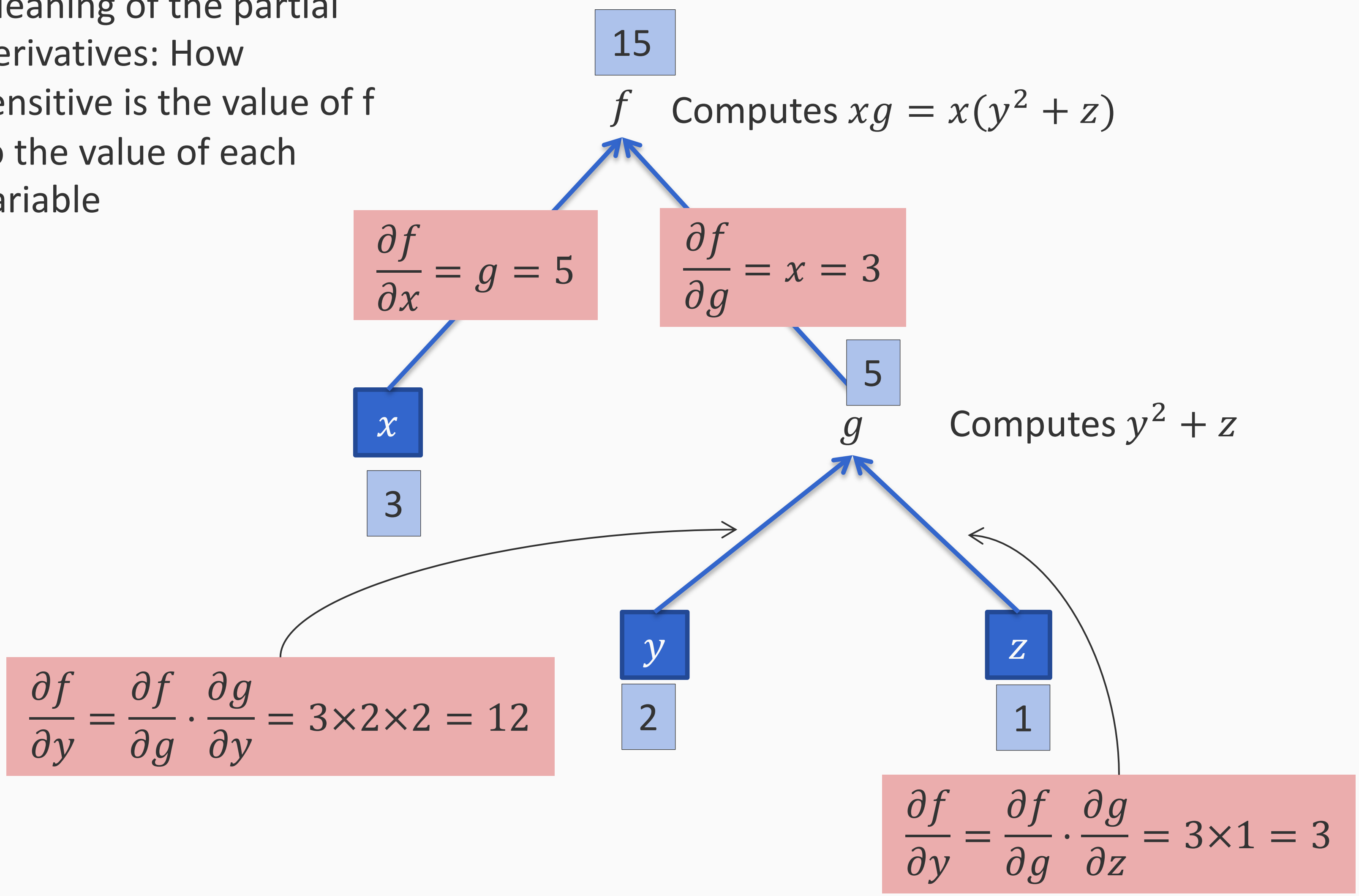
- These can be defined independently of what happens in the rest of the graph

- We can build up complicated functions using simple nodes, and compute values and partial derivatives of these as well

In terms of “computation graphs”

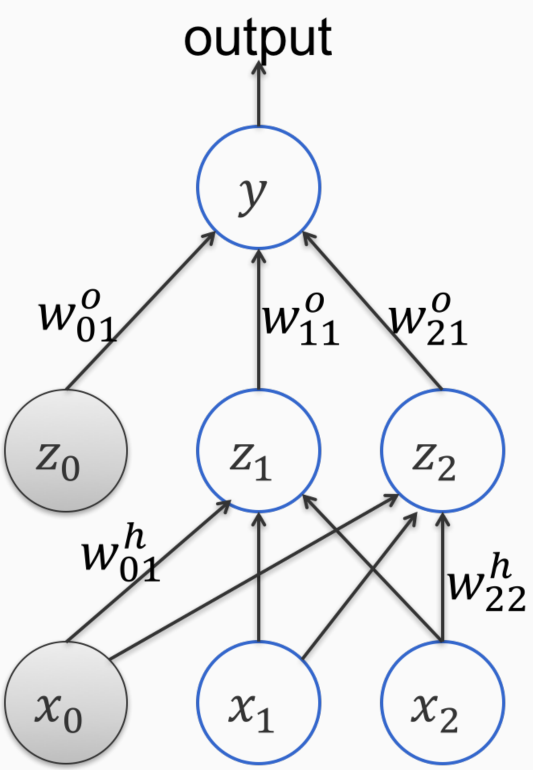
$$f(x, y, z) = x(y^2 + z)$$

Meaning of the partial derivatives: How sensitive is the value of f to the value of each variable



A notational convenience

Commonly nodes in the networks represent not only single numbers (e.g. features, outputs) but also entire *vectors* (an array of numbers), *matrices* (a 2d array of numbers) or *tensors* (an n-dimensional array of numbers).



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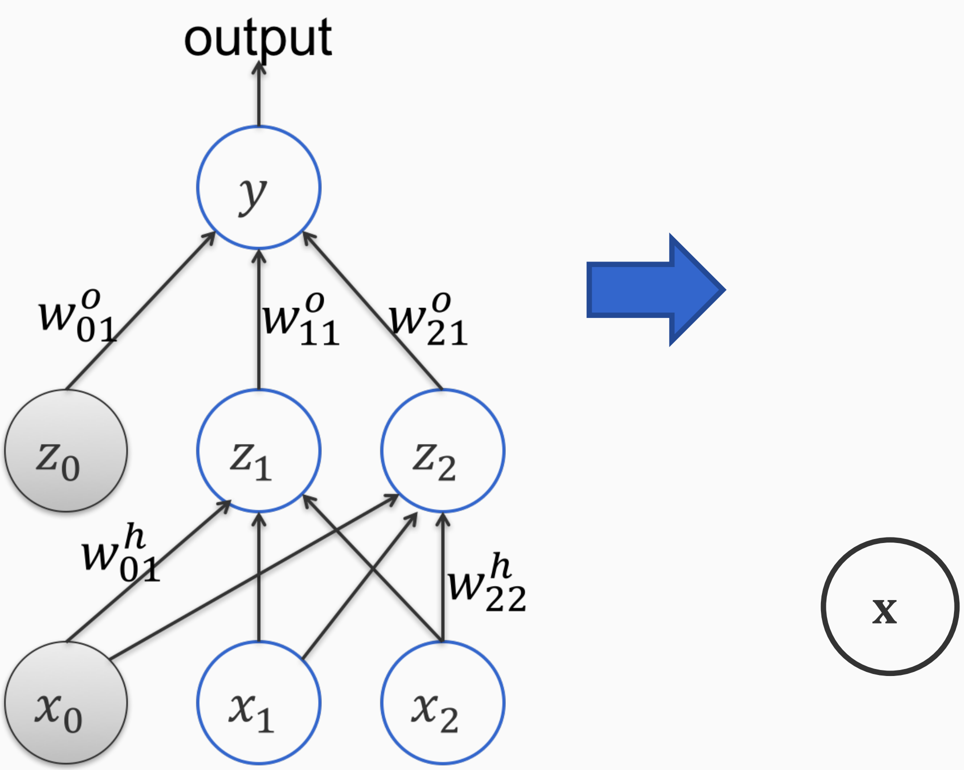

Represents $[x_0, x_1, x_2]$

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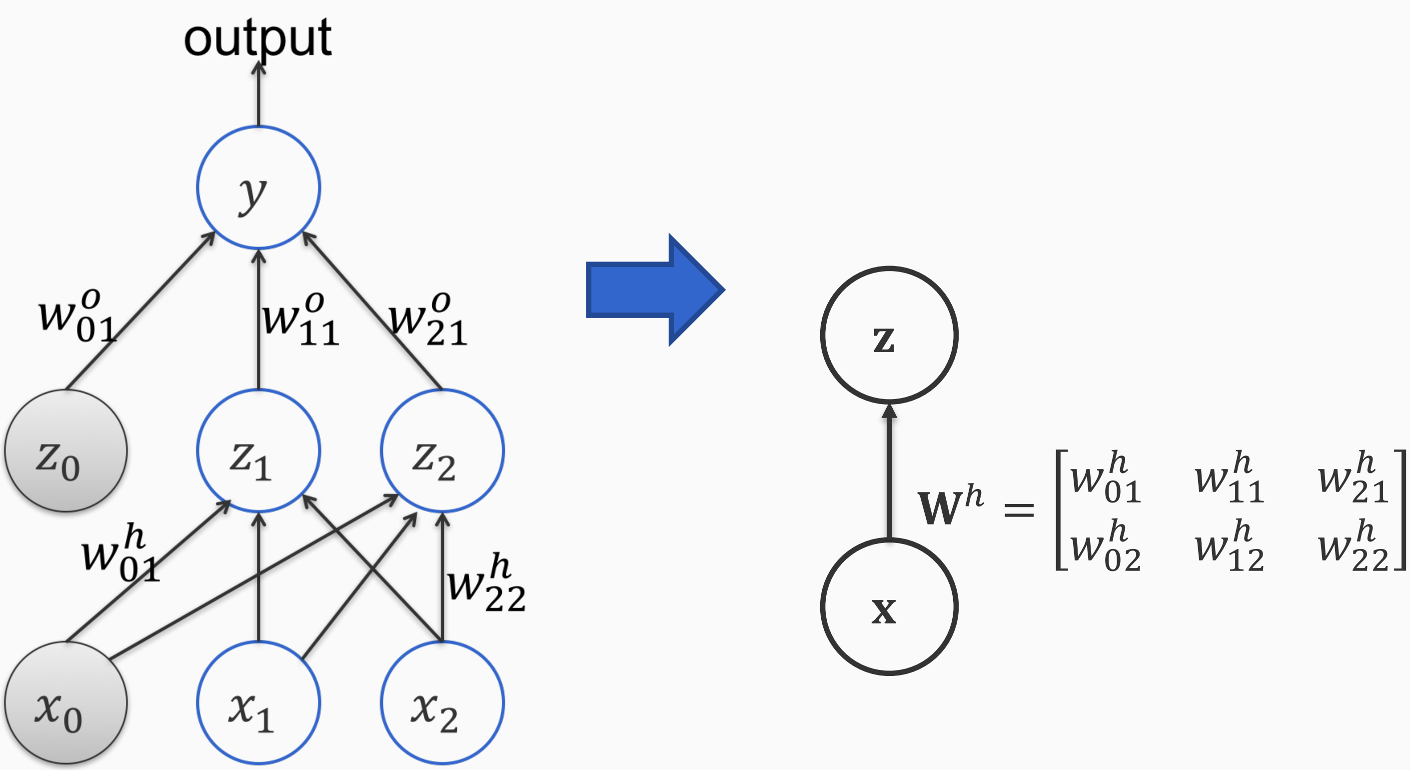

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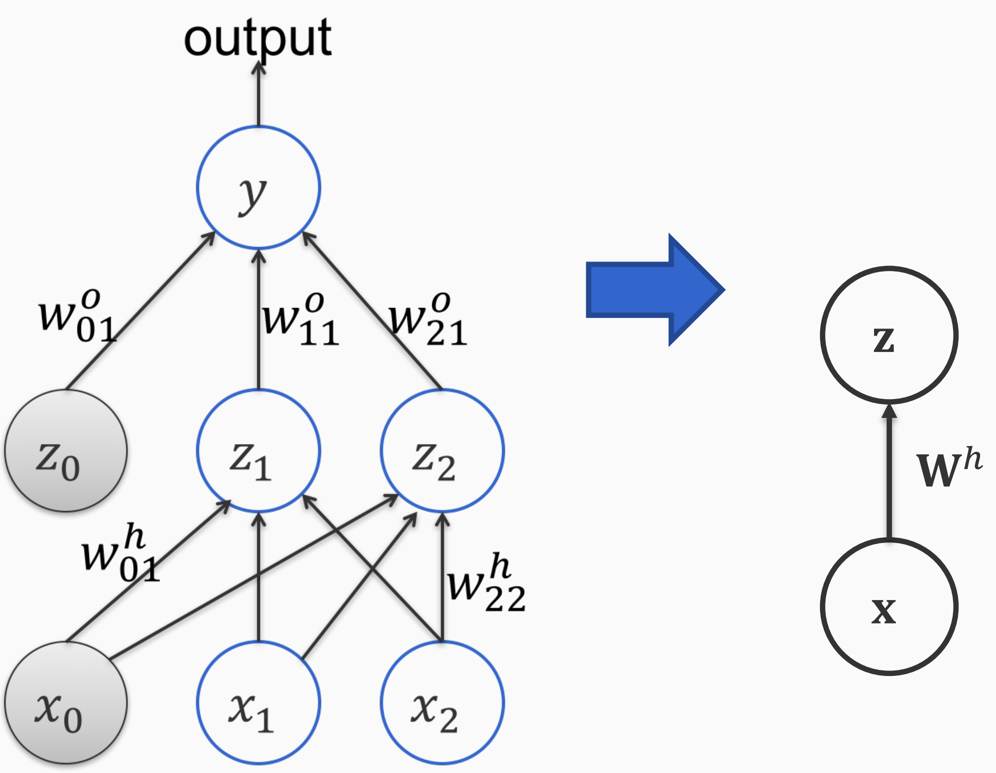

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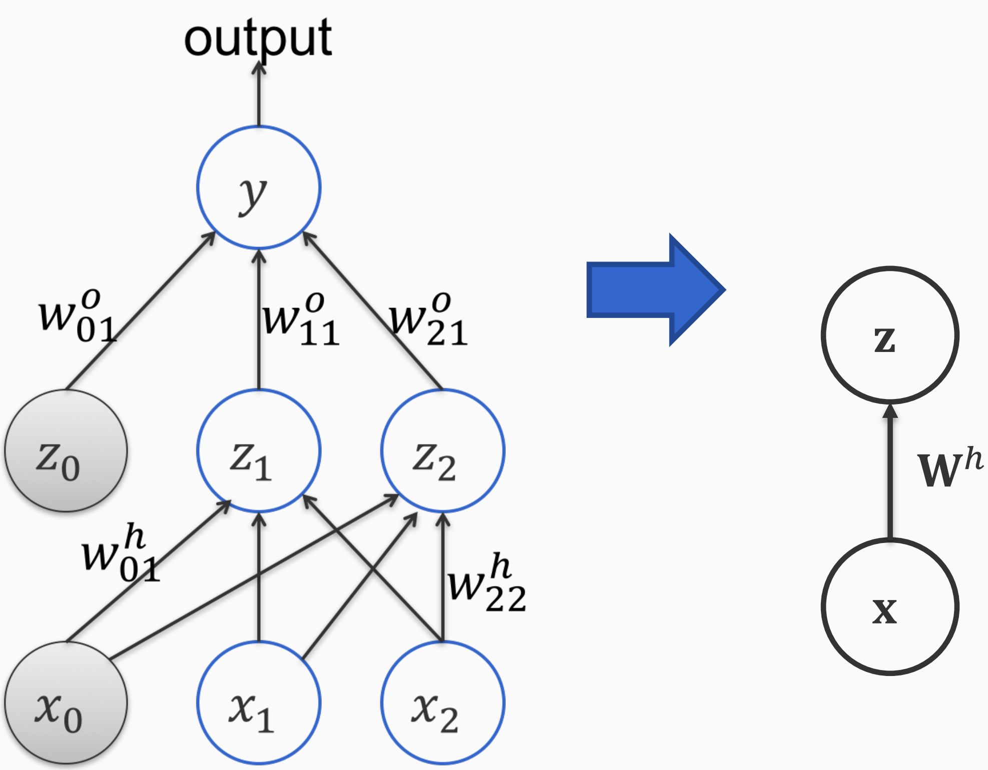

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Each element of $\mathbf{z}$ is z_i, and is generated by the sigmoid activation to each element of $\mathbf{W}^h\mathbf{x}$.

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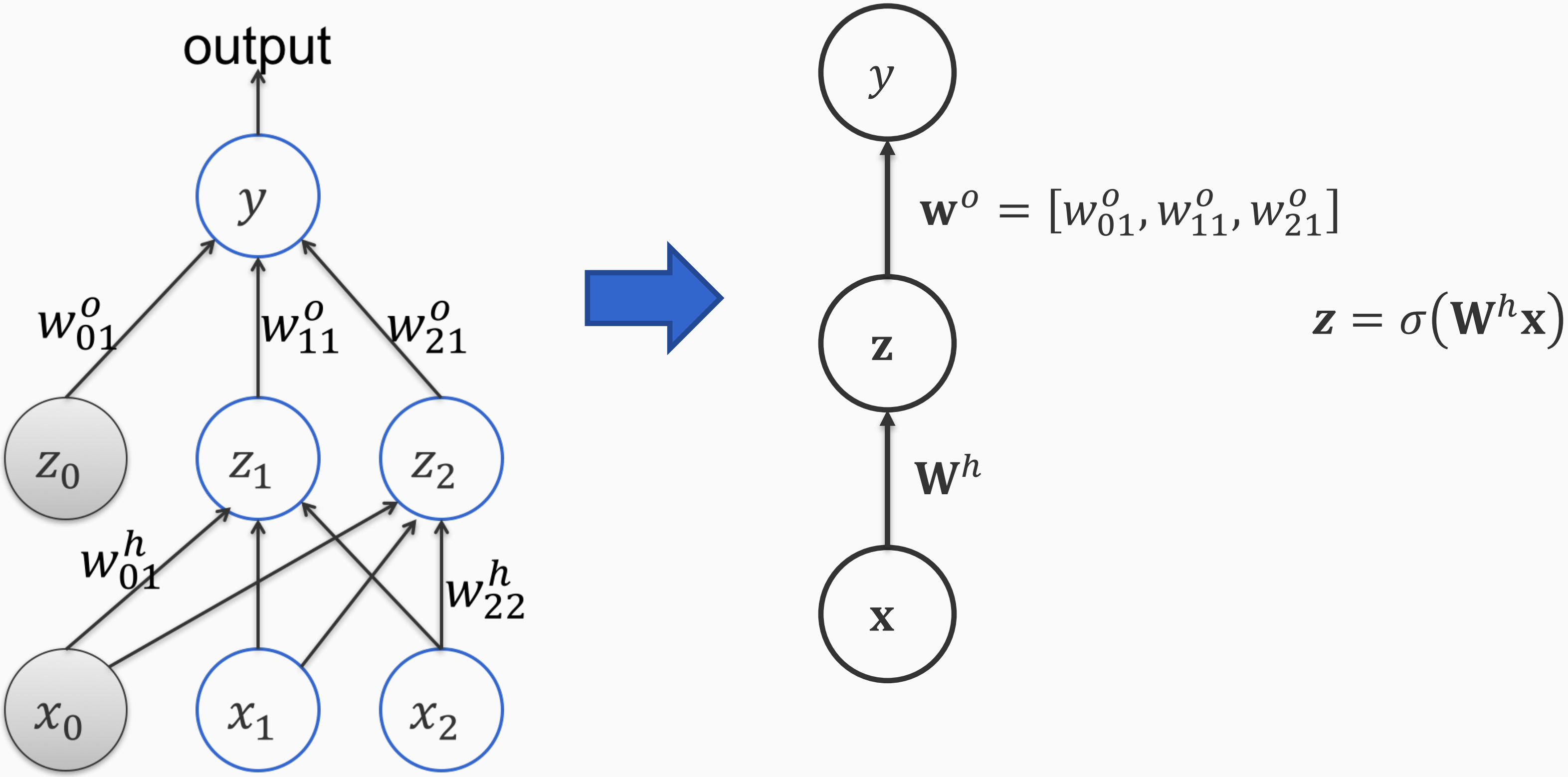

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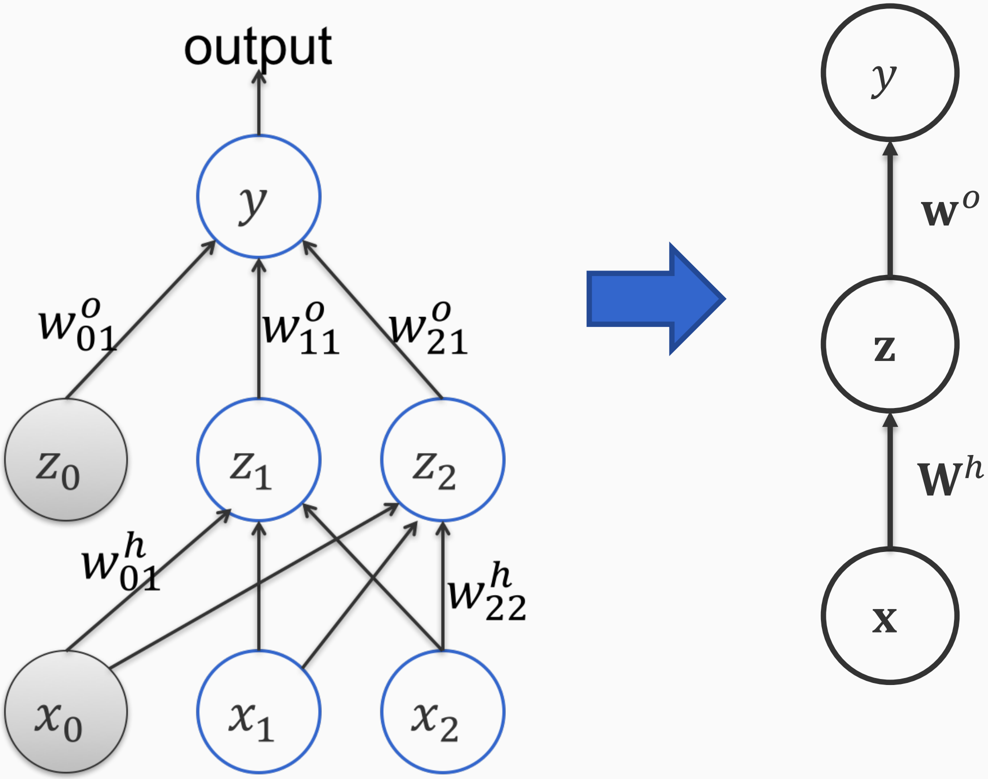

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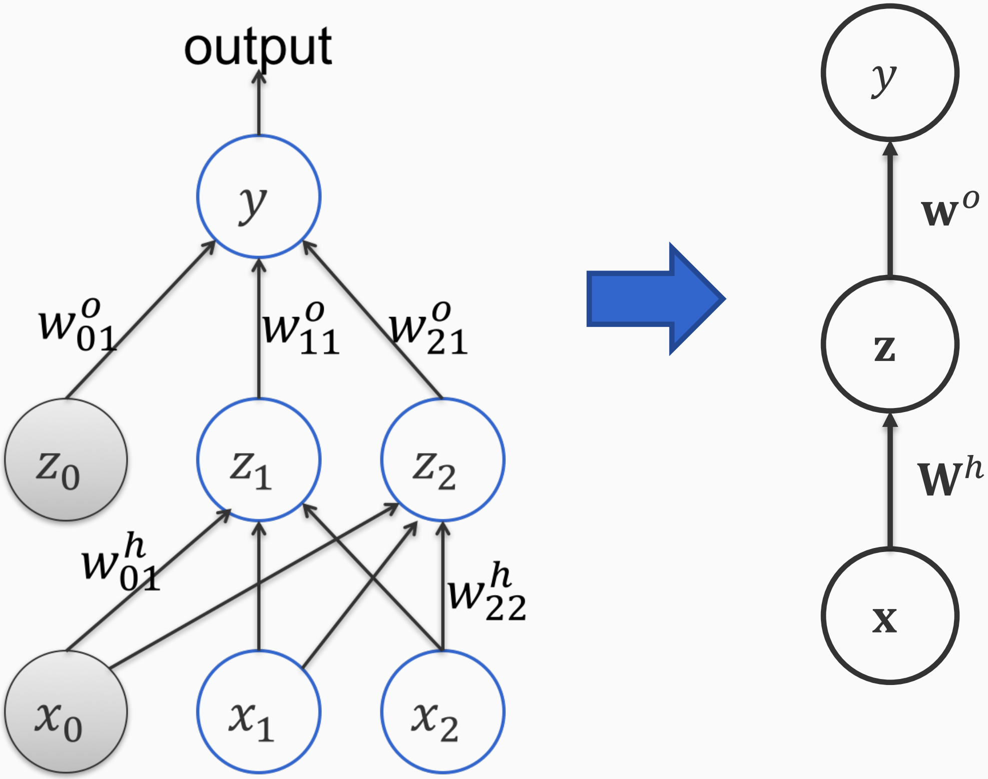


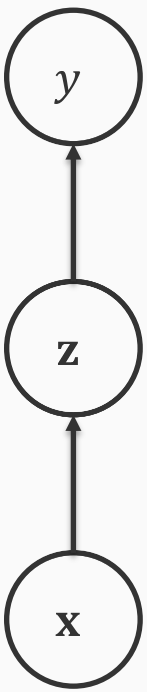
$$y = \mathbf{w}^{o}\mathbf{z}$$

No activation because the output is defined to be linear

$$\mathbf{z} = \sigma(\mathbf{W}^{h}\mathbf{x})$$

Reminder: Chain rule for derivatives

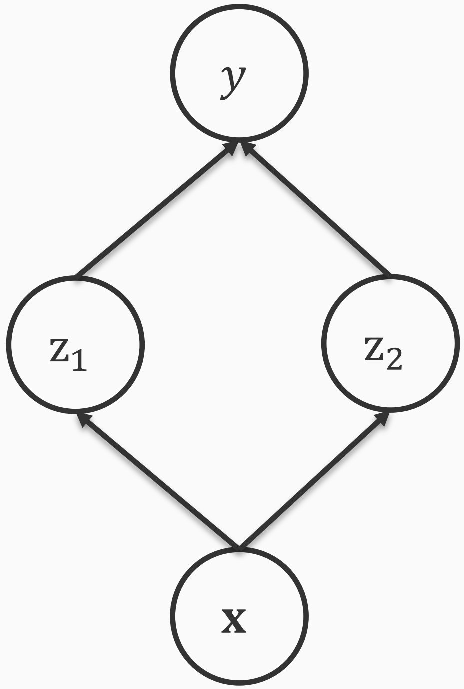
- If y is a function of $\mathbf{z}$ and $\mathbf{z}$ is a function of $\mathbf{x}$
  - Then y is a function of $\mathbf{x}$, as well
- Question: how to find $\frac{\partial y}{\partial \mathbf{x}}$



$$\frac{\partial y}{\partial \mathbf{x}} = \frac{\partial y}{\partial \mathbf{z}} \cdot \frac{\partial \mathbf{z}}{\partial \mathbf{x}}$$

Reminder: Chain rule for derivatives

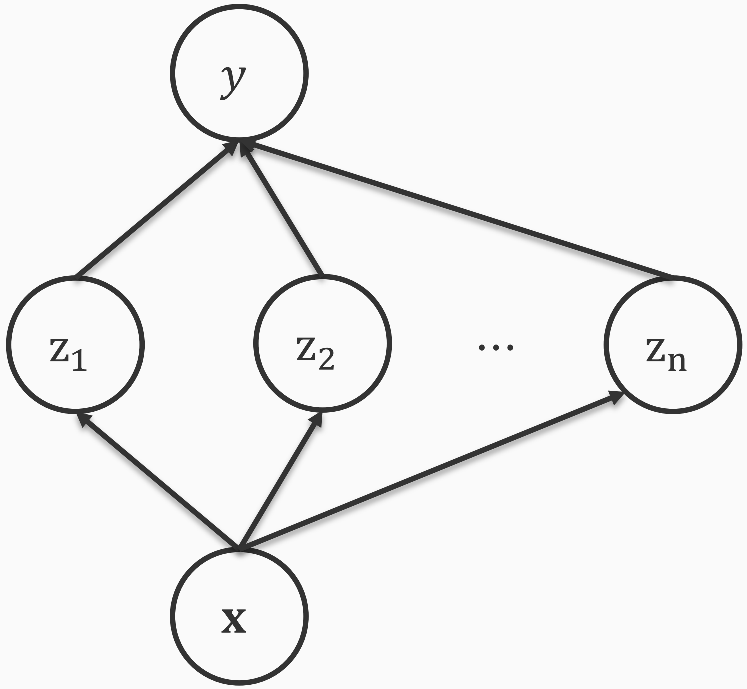
- If $y =$ a function of z_1 + a function of z_2, and the z_i's are functions of x
  - Then y is a function of x, as well
- Question: how to find $\frac{\partial y}{\partial x}$



$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial z_1} \cdot \frac{\partial z_1}{\partial x} + \frac{\partial y}{\partial z_2} \cdot \frac{\partial 2}{\partial x}$$

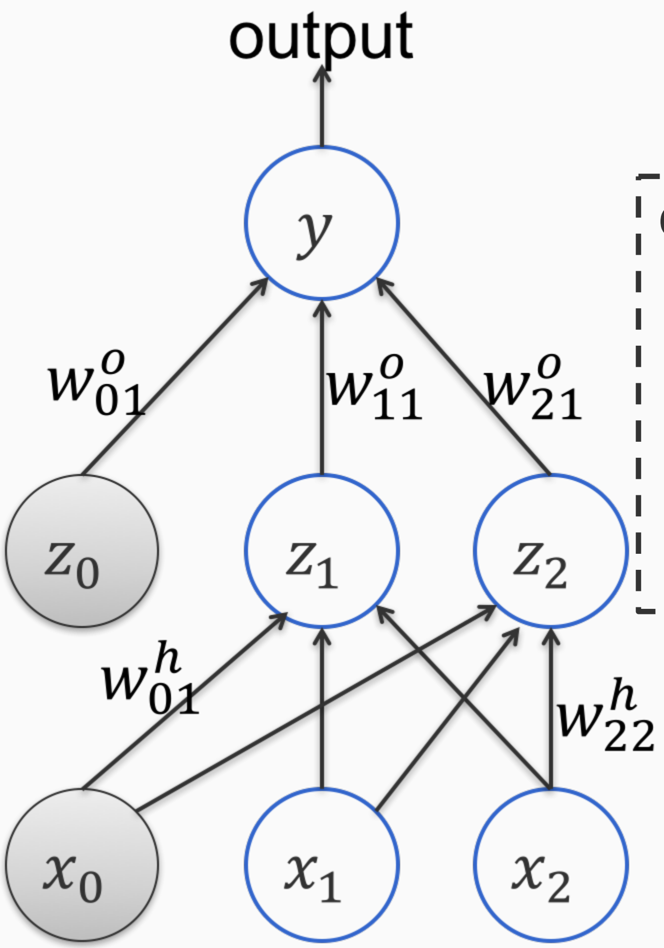
Reminder: Chain rule for derivatives

- If $y =$ sum of functions of x
  - Then y is a function of x, as well
- Question: how to find $\frac{\partial y}{\partial x}$



$$\frac{\partial y}{\partial x} = \sum_{i=1}^{n} \frac{\partial y}{\partial z_i} \cdot \frac{\partial z_i}{\partial x}$$

Backpropagation



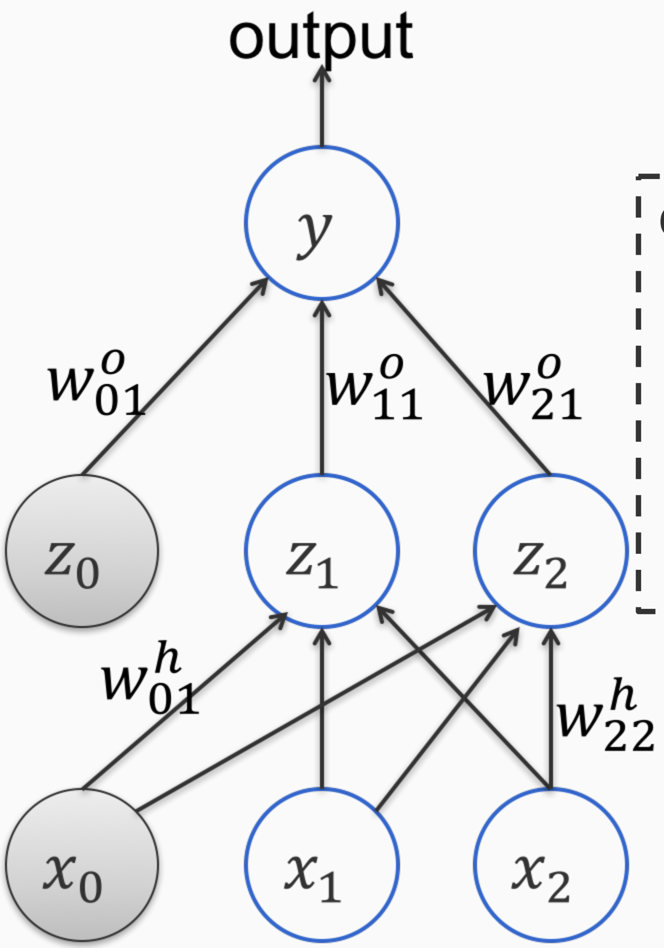
$$L = \frac{1}{2}(y - y^*)^2$$

output $\mathrm{y} = w^o_{01} + w^o_{11} z_1 + w^o_{21} z_2$

$$z_2 = \sigma(w^h_{02} + w^h_{12} x_1 + w^h_{22} x_2)$$

$$\mathrm{z}_1 = \sigma(w^h_{01} + w^h_{11} x_1 + w^h_{21} x_2)$$

Backpropagation



$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

$$z_1 = \sigma(w_{01}^h + w_{11}^h x_1 + w_{21}^h x_2)$$

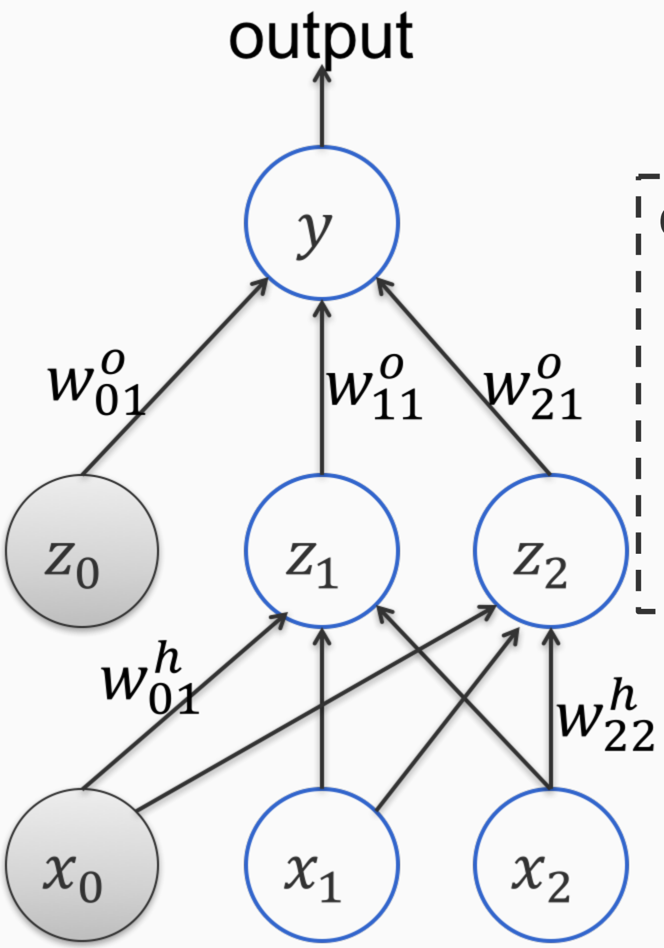
We want to compute

$\frac{\partial L}{\partial w_{ij}^o}$ and $\frac{\partial L}{\partial w_{ij}^h}$

Important: L is a differentiable function of all the weights

Backpropagation

Applying the chain rule to compute the gradient
(And remembering partial computations along the way to speed up things)



$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w^o_{01} + w^o_{11} z_1 + w^o_{21} z_2$

$$z_2 = \sigma(w^h_{02} + w^h_{12} x_1 + w^h_{22} x_2)$$

$$z_1 = \sigma(w^h_{01} + w^h_{11} x_1 + w^h_{21} x_2)$$

We want to compute

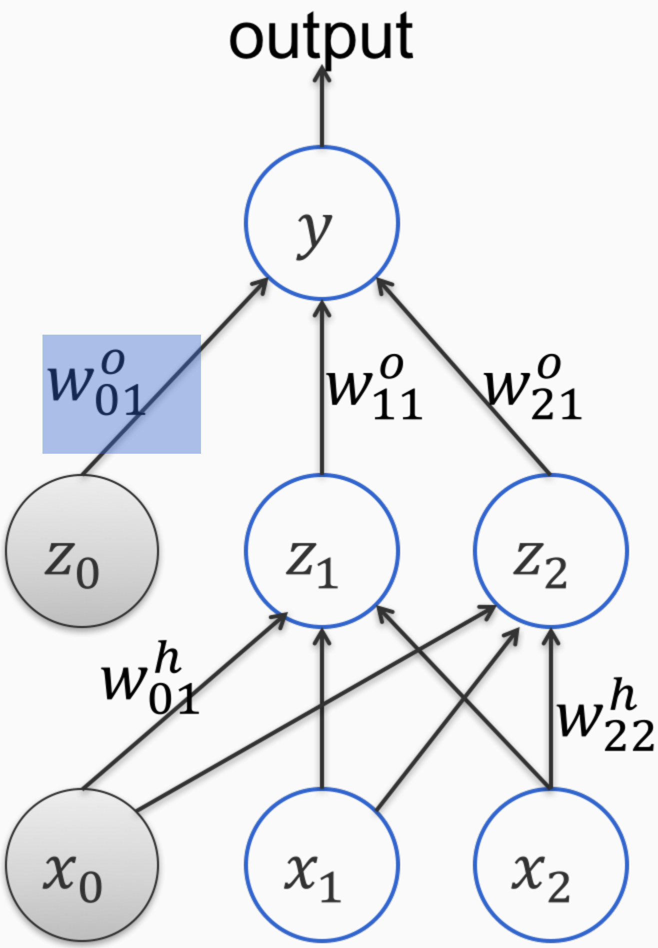
$\frac{\partial L}{\partial w^o_{ij}}$ and $\frac{\partial L}{\partial w^h_{ij}}$

Important: L is a differentiable function of all the weights

Output layer

$$L = \frac{1}{2}(y - y^*)^2$$

output $\quad y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

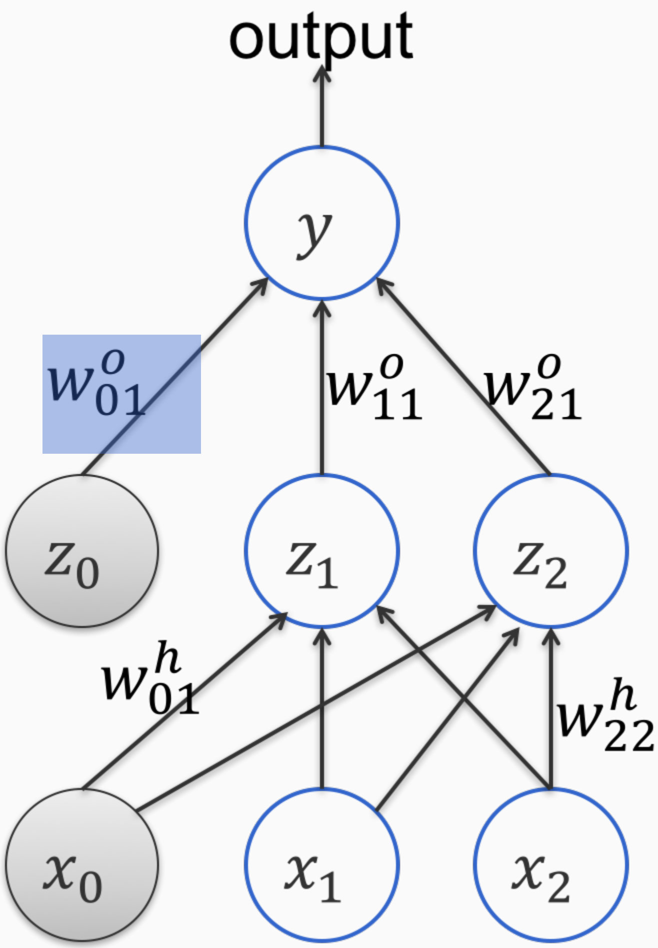


$$\frac{\partial L}{\partial w_{01}^o}$$

Output layer

$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

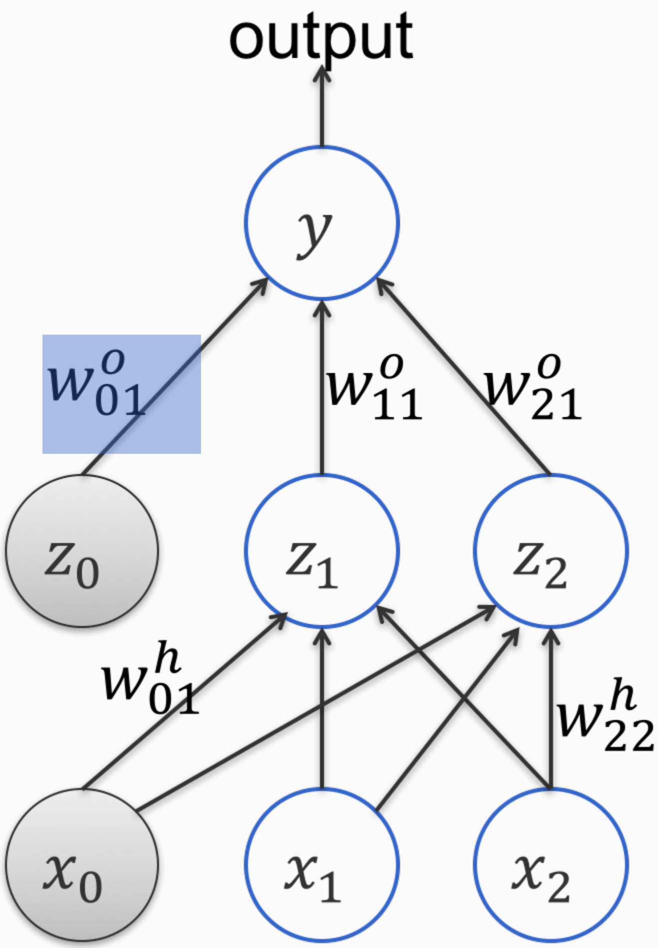


$$\frac{\partial L}{\partial w_{01}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{01}^o}$$

Output layer

$$L = \frac{1}{2}(y - y^*)^2$$

output $\quad y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$



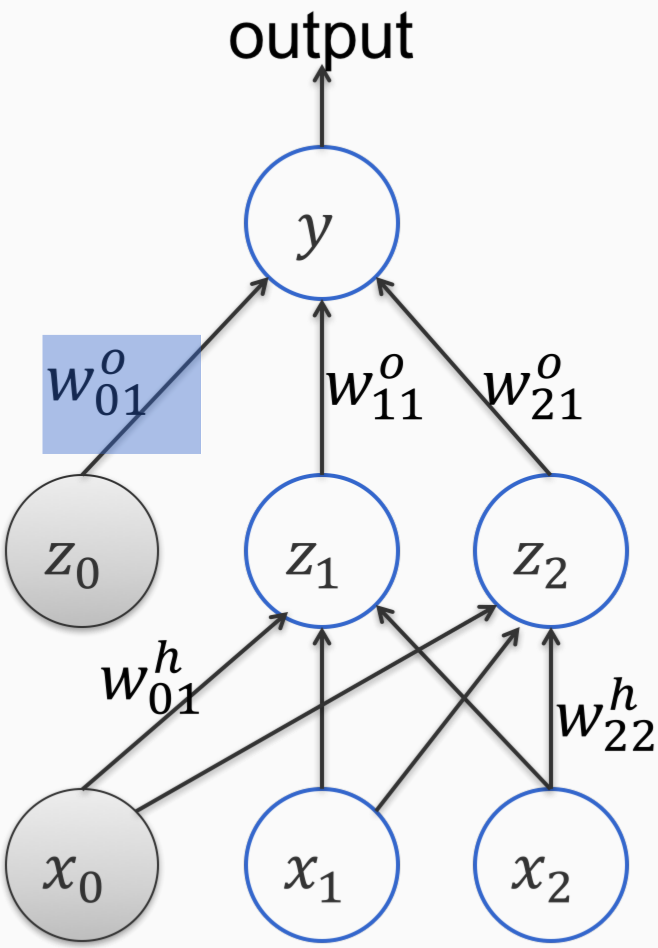
$$\frac{\partial L}{\partial w_{01}^o} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial w_{01}^o}$$

$$\frac{\partial L}{\partial y} = y - y^*$$

Output layer

$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$



$$\frac{\partial L}{\partial w_{01}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{01}^o}$$

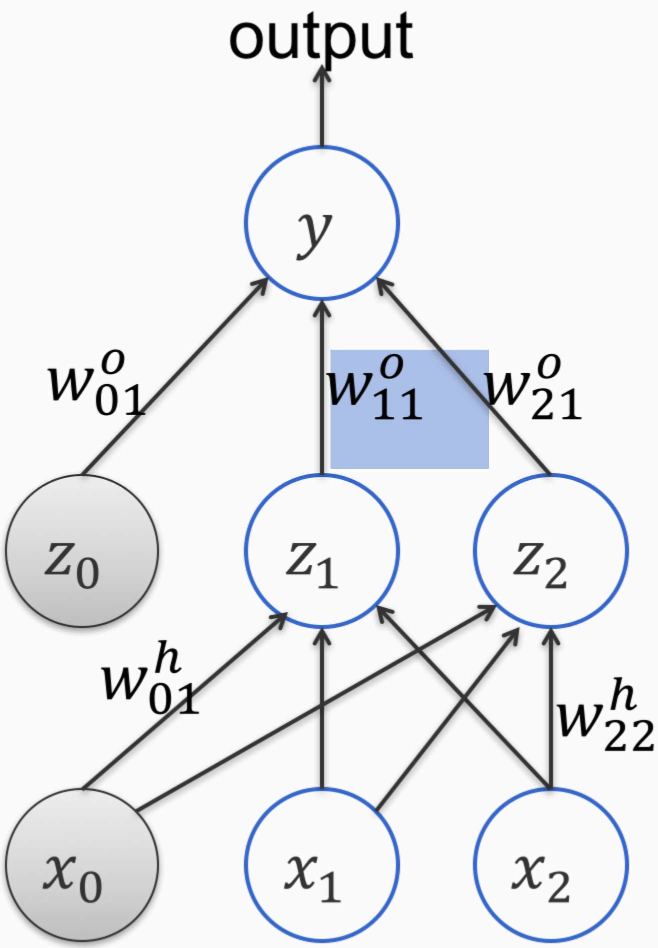
$$\frac{\partial L}{\partial y} = y - y^*$$

$$\frac{\partial y}{\partial w_{01}^o} = 1$$

Output layer

$$L = \frac{1}{2}(y - y^*)^2$$

output $\quad y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

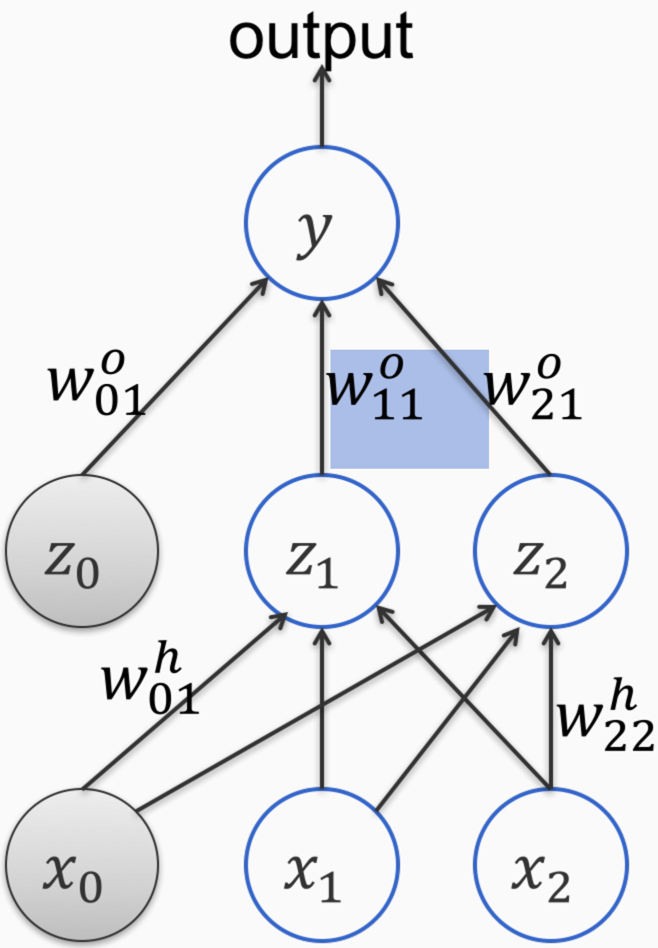


$$\frac{\partial L}{\partial w_{11}^o}$$

$$L = \frac{1}{2}(y - y^*)^2$$

Output layer

output $\quad y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

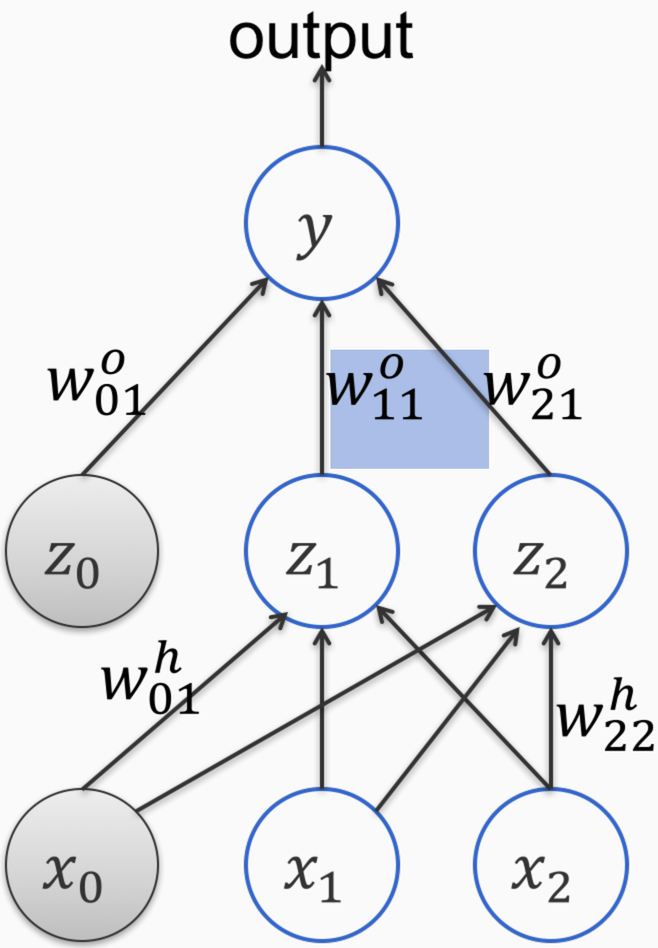


$$\frac{\partial L}{\partial w_{11}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{11}^o}$$

Output layer

$$L = \frac{1}{2}(y - y^*)^2$$

output $\quad y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$



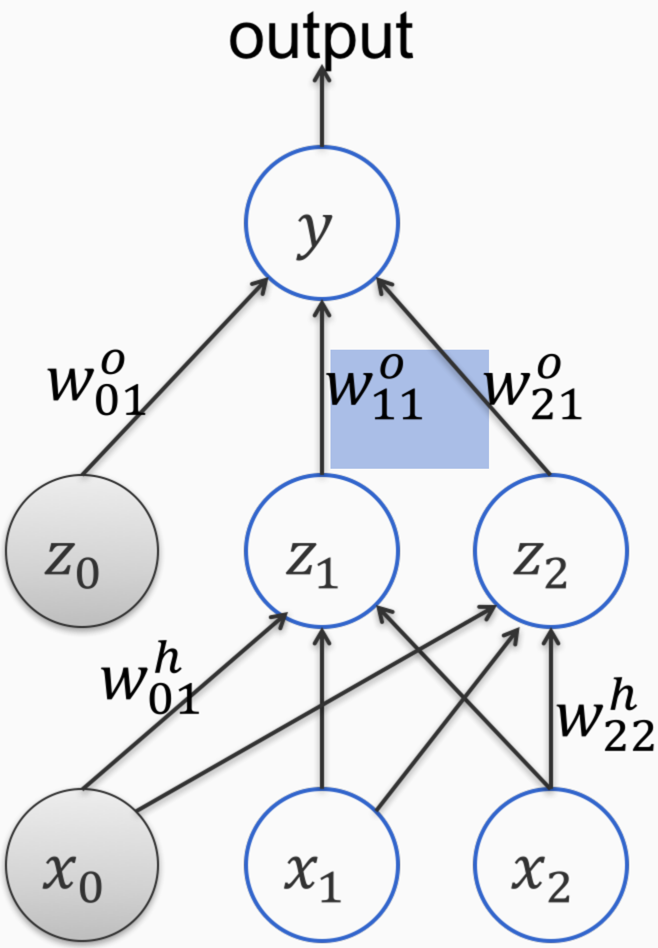
$$\frac{\partial L}{\partial w_{11}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{11}^o}$$

$$\frac{\partial L}{\partial y} = y - y^*$$

Output layer

$$L = \frac{1}{2}(y - y^*)^2$$

output $\quad y = w^o_{01} + w^o_{11} z_1 + w^o_{21} z_2$



$$\frac{\partial L}{\partial w^o_{11}} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial w^o_{11}}$$

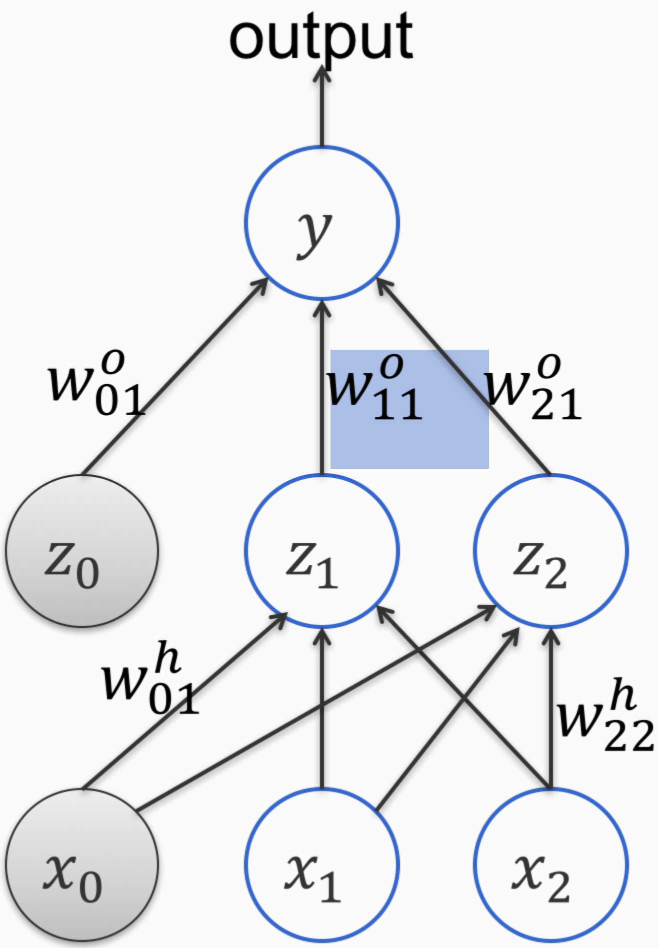
$$\frac{\partial L}{\partial y} = y - y^*$$

$$\frac{\partial y}{\partial w^o_{01}} = z_1$$

Output layer

$$L = \frac{1}{2}(y - y^*)^2$$

output $\quad y = w^o_{01} + w^o_{11} z_1 + w^o_{21} z_2$



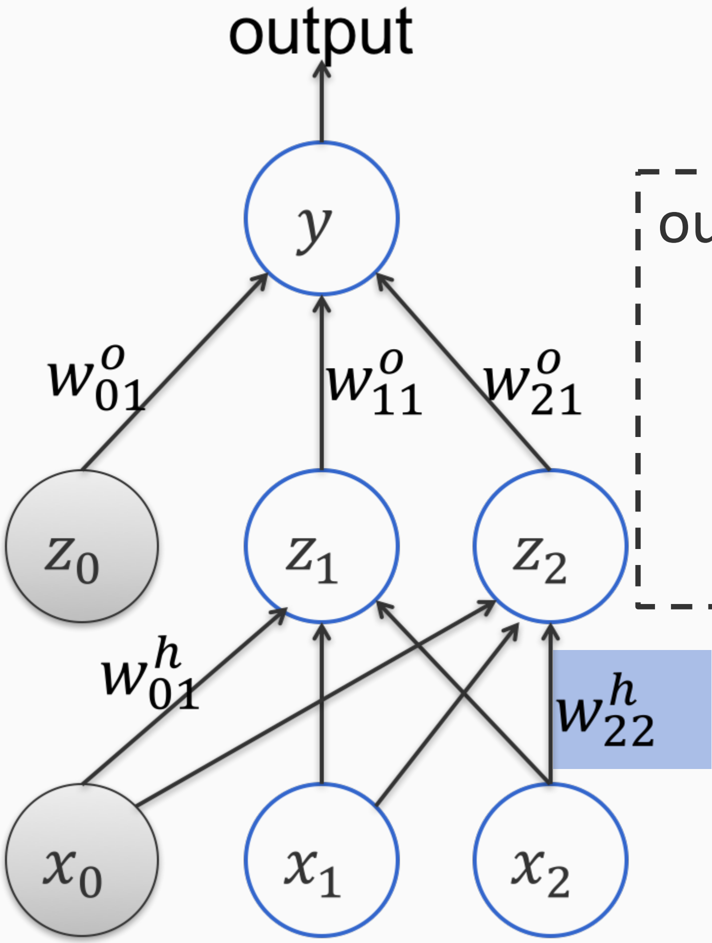
$$\frac{\partial L}{\partial w^o_{11}} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w^o_{11}}$$

$$\frac{\partial L}{\partial y} = y - y^* \qquad \frac{\partial y}{\partial w^o_{01}} = z_1$$

We have already computed this partial derivative for the previous case

Cache to speed up!

Hidden layer derivatives



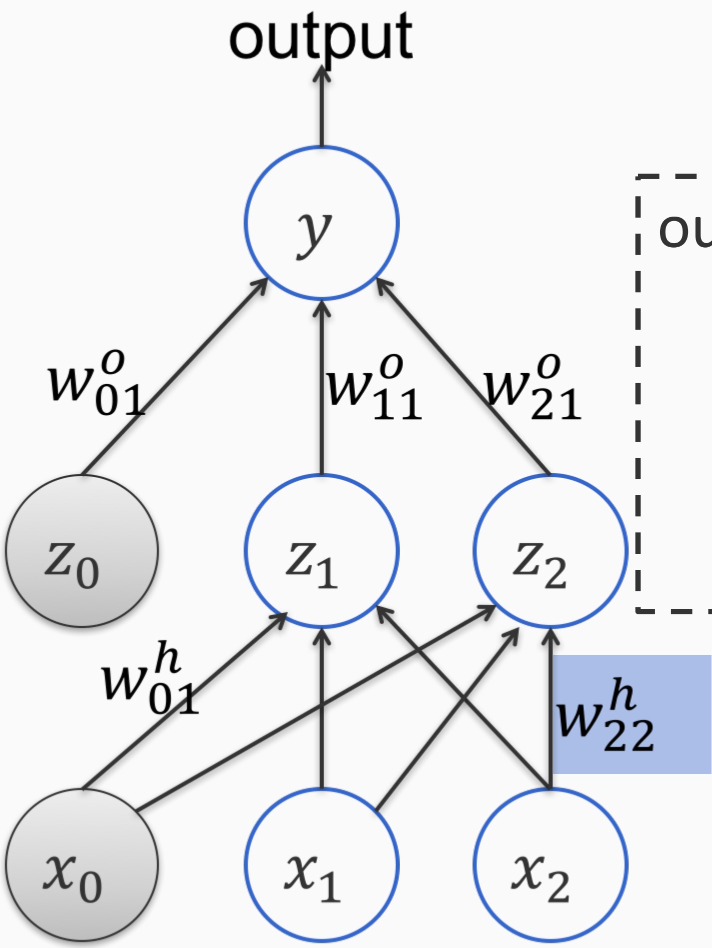
$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$

$$z_2 = \sigma(w_{02}^{h} + w_{12}^{h} x_1 + w_{22}^{h} x_2)$$

$$z_1 = \sigma(w_{01}^{h} + w_{11}^{h} x_1 + w_{21}^{h} x_2)$$

Hidden layer derivatives



$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

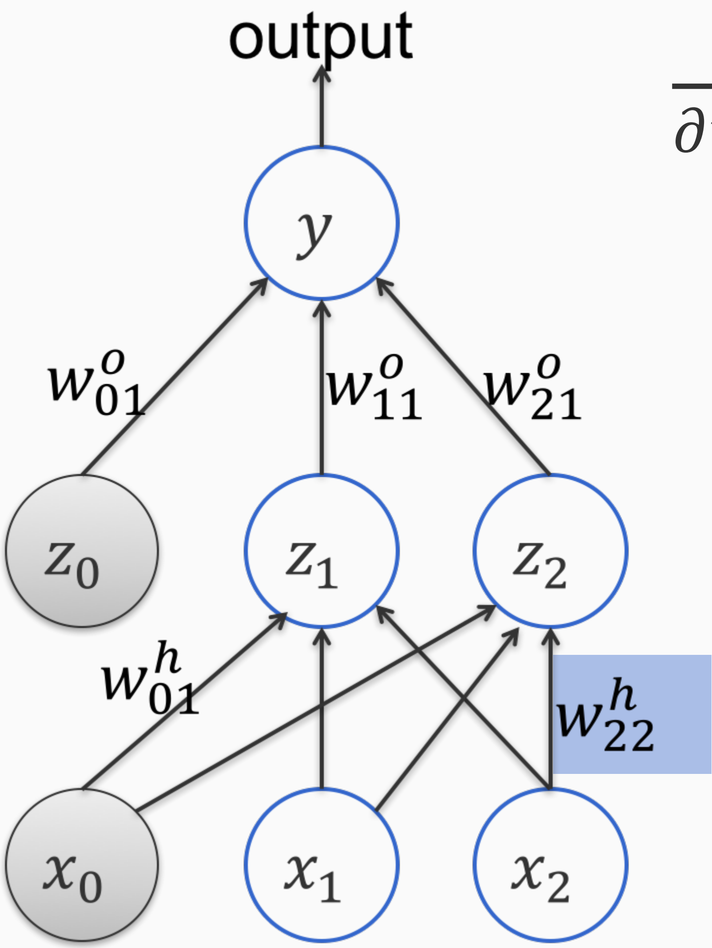
$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

$$z_1 = \sigma(w_{01}^h + w_{11}^h x_1 + w_{21}^h x_2)$$

We want $\dfrac{\partial L}{\partial w_{22}^h}$

$$L = \frac{1}{2}(y - y^*)^2$$

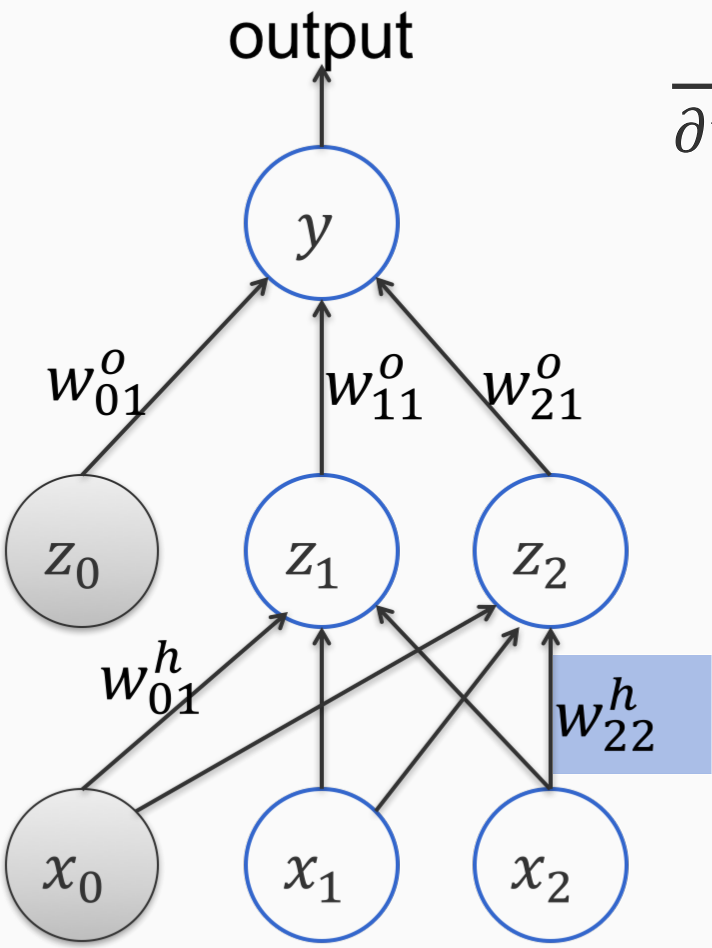
Hidden layer derivatives



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^h}$$

Hidden layer

$$y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$$

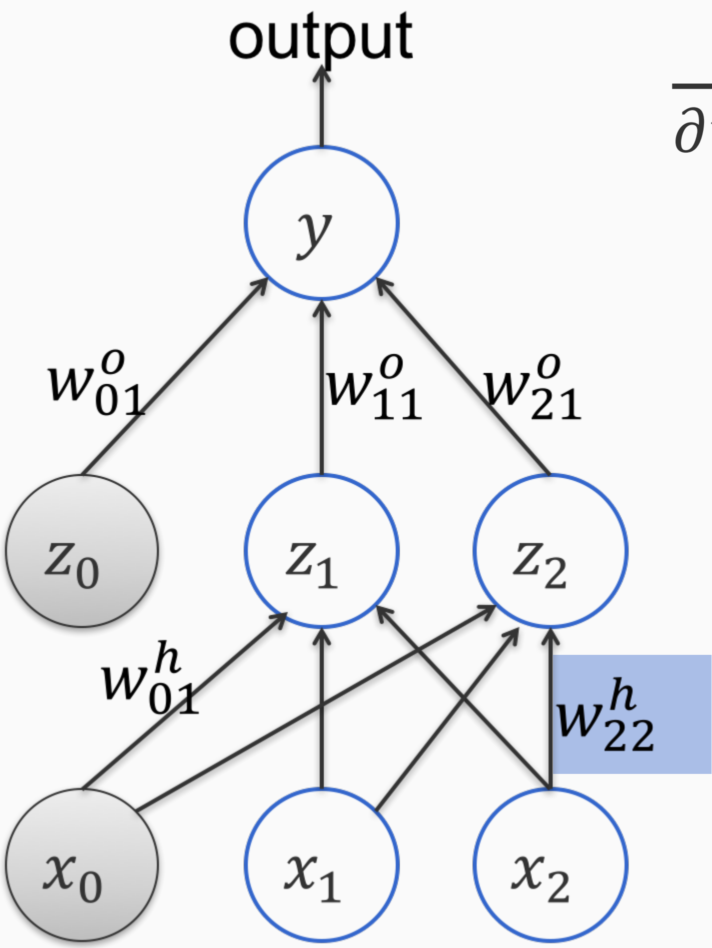


$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial w_{22}^h}$$

$$= \frac{\partial L}{\partial y} \frac{\partial}{\partial w_{22}^h} (w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2)$$

Hidden layer

$$y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$$



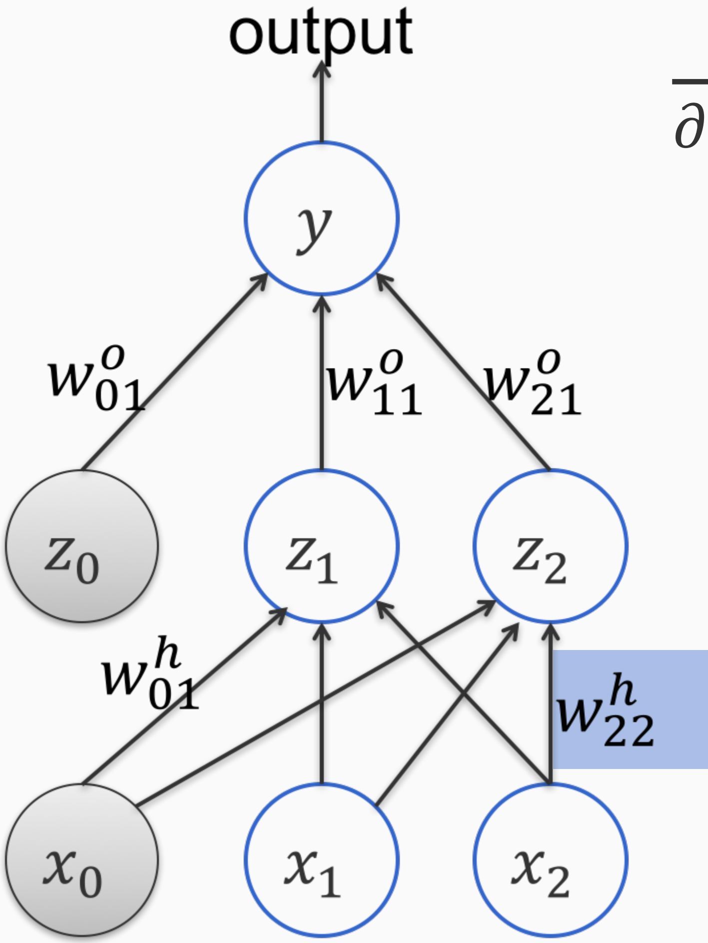
$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^h}$$

$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^h}(w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2)$$

$$= \frac{\partial L}{\partial y}(w_{11}^o \frac{\partial}{\partial w_{22}^h} z_1 + w_{21}^o \frac{\partial}{\partial w_{22}^h} z_2)$$

Hidden layer

$$y = w^o_{01} + w^o_{11} z_1 + w^o_{21} z_2$$

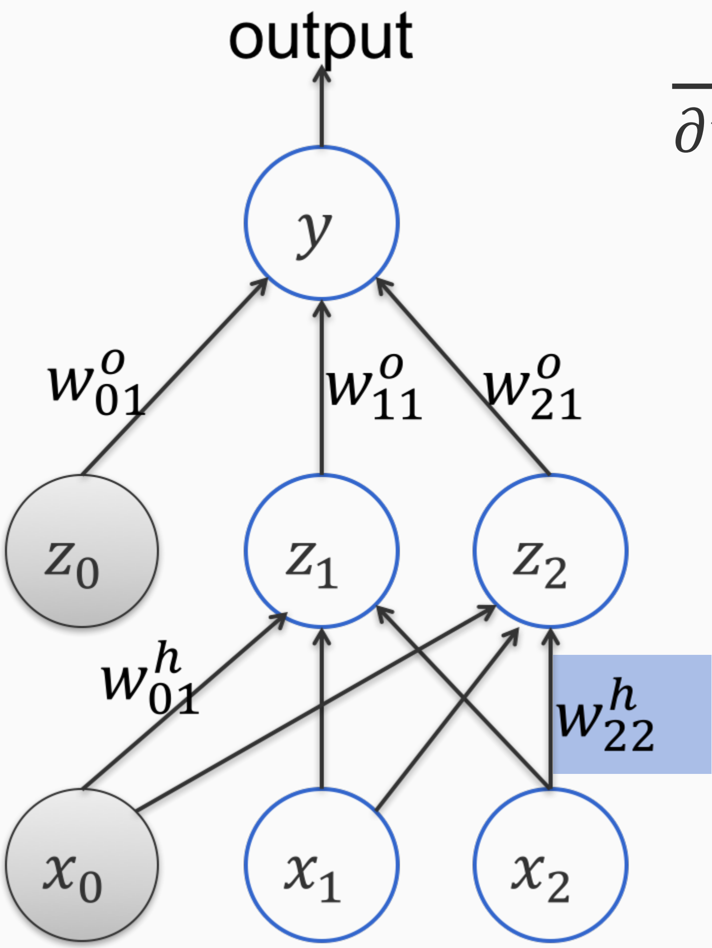


$$\begin{aligned}
\frac{\partial L}{\partial w^h_{22}} &= \frac{\partial L}{\partial y}\frac{\partial y}{\partial w^h_{22}} \\
&= \frac{\partial L}{\partial y}\frac{\partial}{\partial w^h_{22}}\left(w^o_{01} + w^o_{11} z_1 + w^o_{21} z_2\right) \\
&= \frac{\partial L}{\partial y}\left(w^o_{11}\underbrace{\frac{\partial}{\partial w^h_{22}} z_1}_{0} + w^o_{21}\frac{\partial}{\partial w^h_{22}} z_2\right)
\end{aligned}$$

z_1 is not a function of w^h_{22}

Hidden layer

$$y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$$



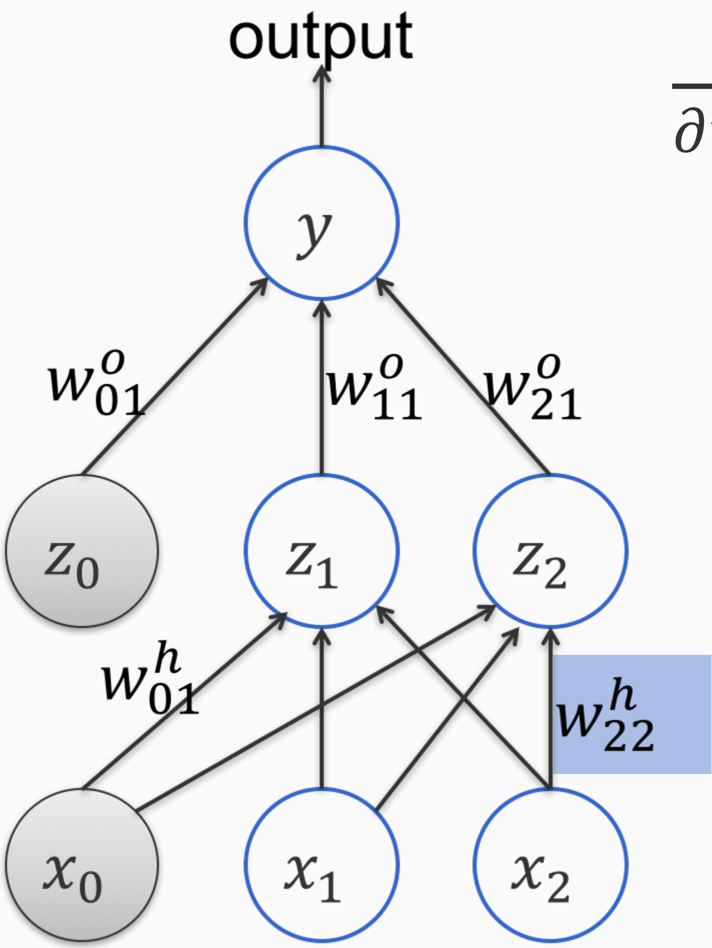
$$\frac{\partial L}{\partial w_{22}^{h}} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial w_{22}^{h}}$$

$$= \frac{\partial L}{\partial y} \frac{\partial}{\partial w_{22}^{h}} (w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2)$$

$$= \frac{\partial L}{\partial y} w_{21}^{o} \frac{\partial z_2}{\partial w_{22}^{h}}$$

Hidden layer

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^h}$$

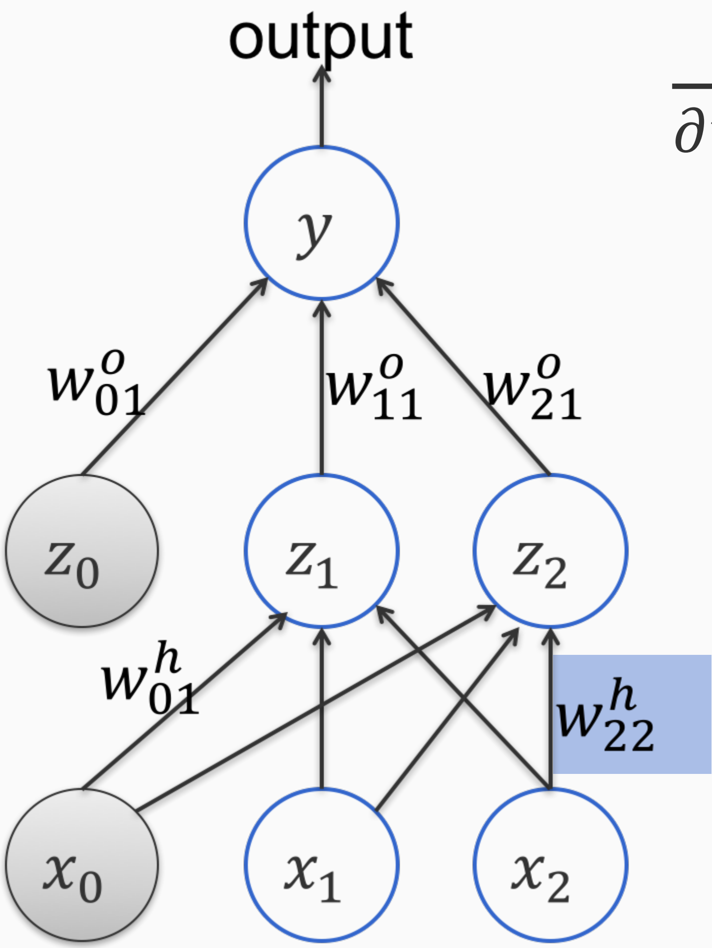
$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^h}(w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2)$$

$$= \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial w_{22}^h}$$

Hidden layer

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s



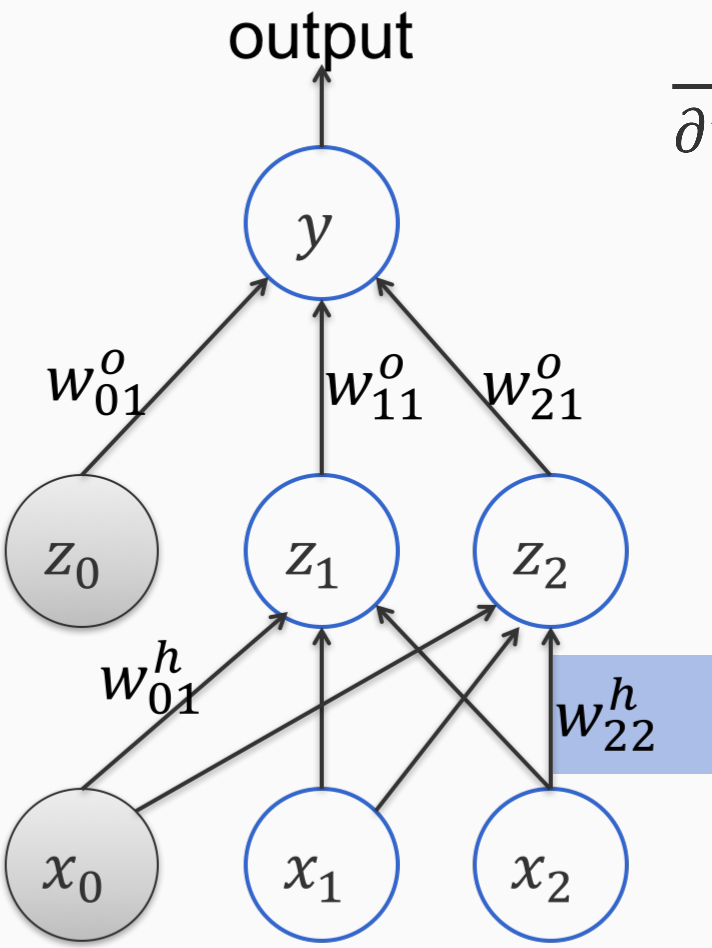
$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^h}$$

$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^h}(w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2)$$

$$= \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial w_{22}^h}$$

Hidden layer

$$z_2 = \sigma(\underbrace{w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2}_{\text{Call this s}})$$



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^h}$$

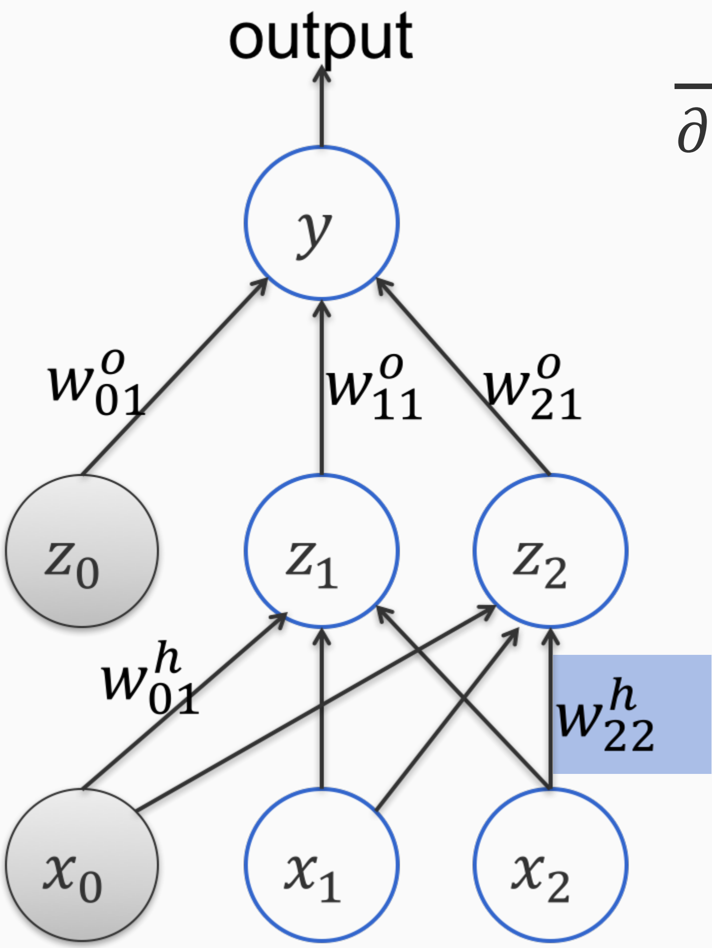
$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^h}(w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2)$$

$$= \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial w_{22}^h}$$

$$= \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s}\frac{\partial s}{\partial w_{22}^h}$$

Hidden layer

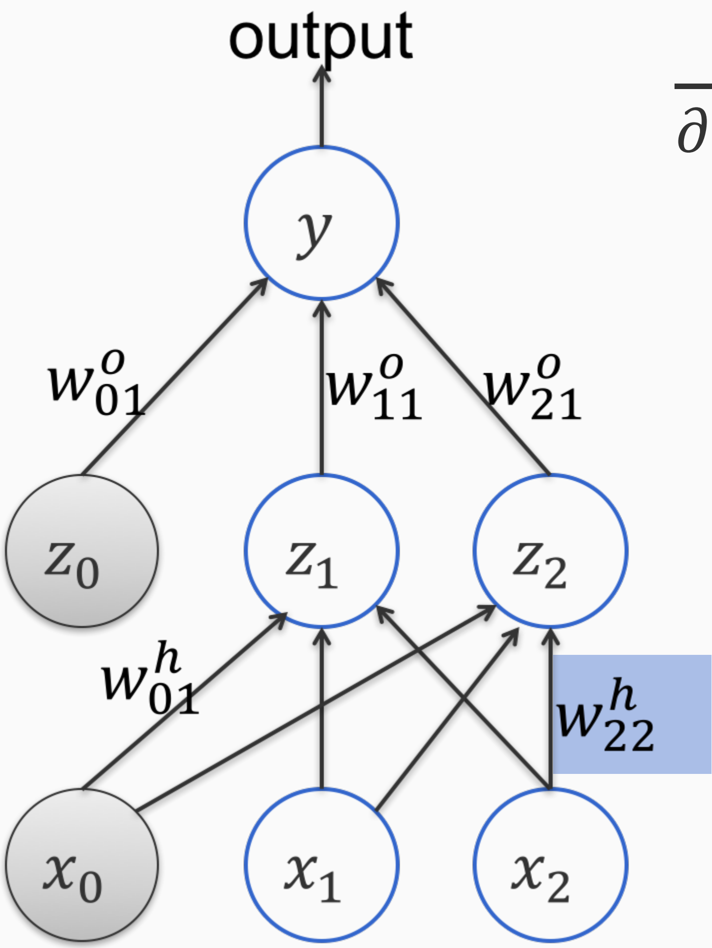
$$z_2 = \sigma(\underbrace{w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2}_{\text{Call this s}})$$



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$ (From previous slide)

Hidden layer

$$z_2 = \sigma(\underbrace{w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2}_{\text{Call this } s})$$

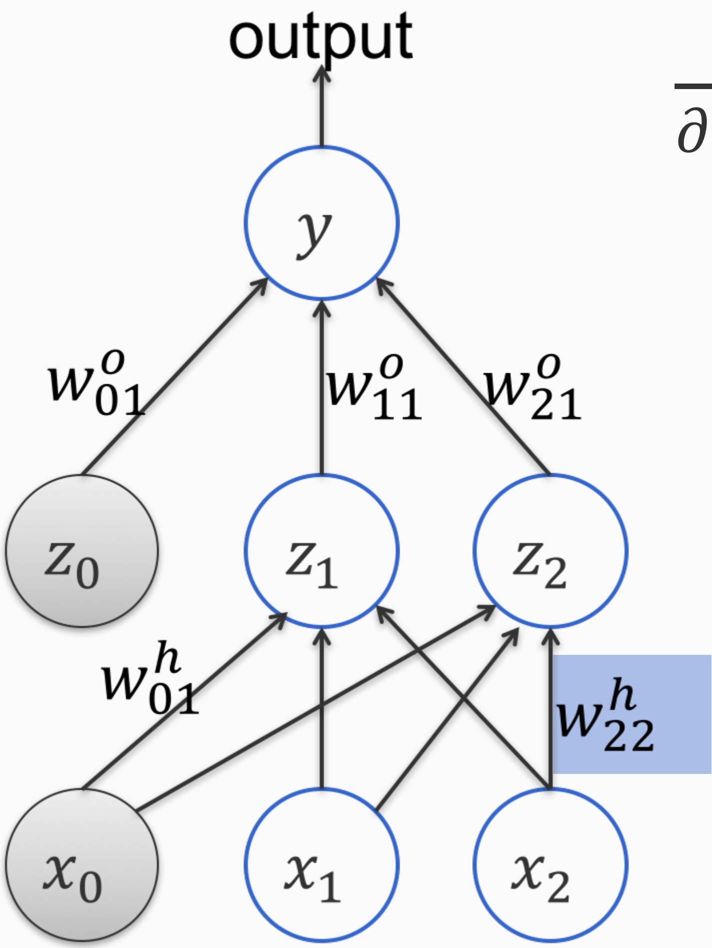


$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$

Each of these partial derivatives is easy

Hidden layer

$$z_2 = \sigma(\underbrace{w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2}_{\text{Call this s}})$$



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$

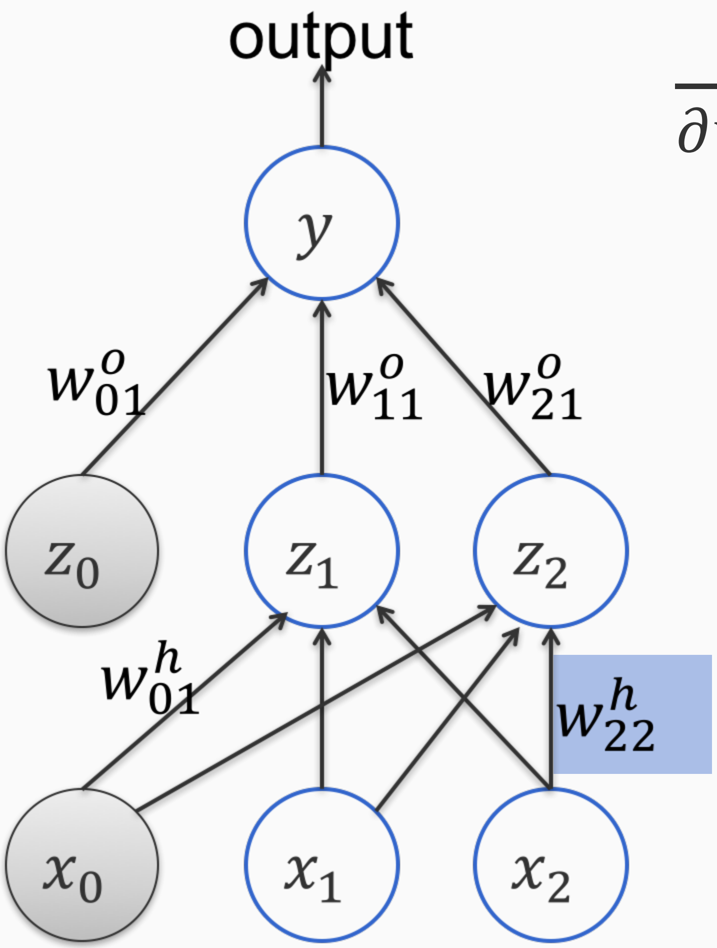
Each of these partial derivatives is easy

$$\frac{\partial L}{\partial y} = y - y^*$$

Hidden layer

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$

Each of these partial derivatives is easy

$$\frac{\partial L}{\partial y} = y - y^*$$

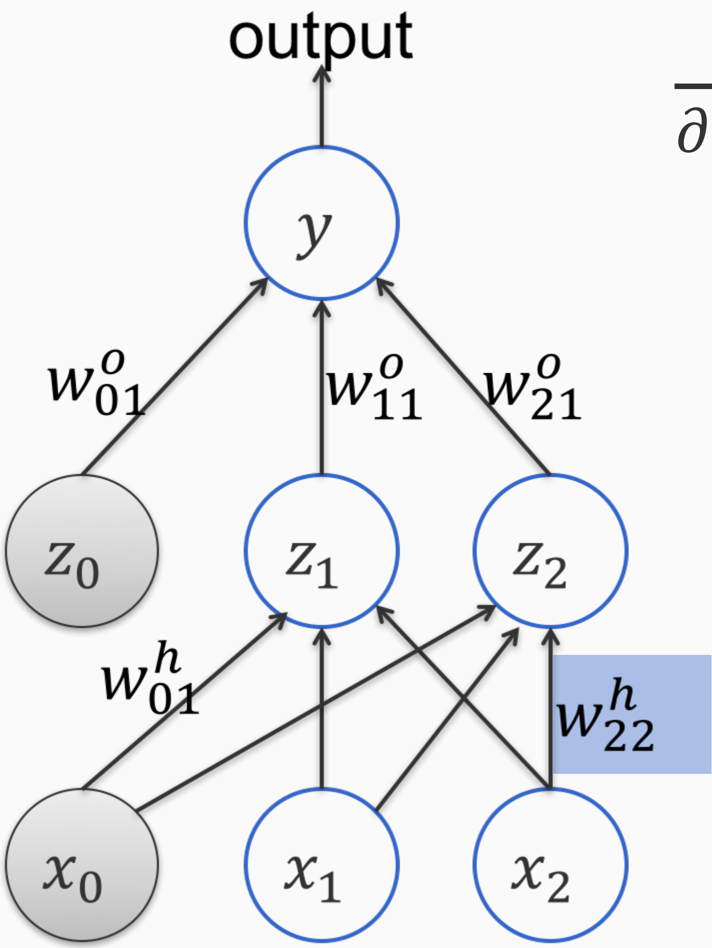
$$\frac{\partial z_2}{\partial s} = z_2(1 - z_2)$$

Why? Because $z_2(s)$ is the logistic function we have already seen

Hidden layer

$$z_2 = \sigma(w^h_{02} + w^h_{12}x_1 + w^h_{22}x_2)$$

Call this s



$$\frac{\partial L}{\partial w^h_{22}} = \frac{\partial L}{\partial y} w^o_{21} \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w^h_{22}}$$

Each of these partial derivatives is easy

$$\frac{\partial L}{\partial y} = y - y^*$$

$$\frac{\partial z_2}{\partial s} = z_2(1 - z_2)$$

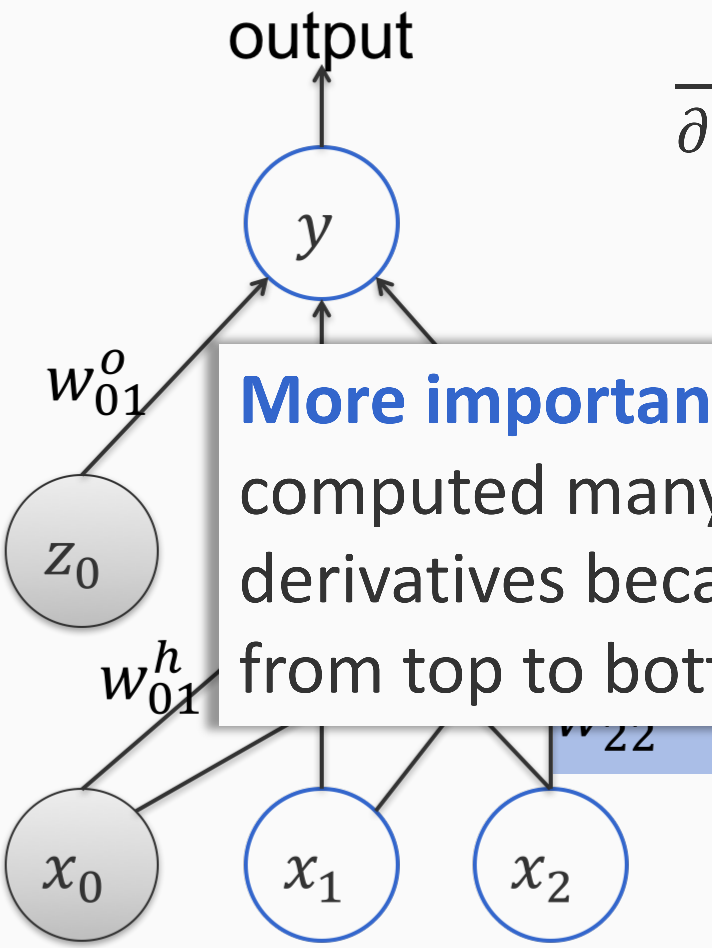
$$\frac{\partial s}{\partial w^h_{22}} = x_2$$

Why? Because $z_2(s)$ is the logistic function we have already seen

Hidden layer

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$

Each of these partial derivatives is easy

More important: We have already computed many of these partial derivatives because we are proceeding from top to bottom (i.e. backwards)

cause $z_2(s)$
istic
we have
een

$$\frac{\partial s}{\partial w_{22}^h} = x_2$$

The Backpropagation Algorithm

The same algorithm works for multiple layers, and more complicated architectures

Repeated application of the chain rule for partial derivatives

- First perform forward pass from inputs to the output
- Compute loss

- From the loss, proceed backwards to compute partial derivatives using the chain rule
- Cache partial derivatives as you compute them
  - Will be used for lower layers

Mechanizing learning

- Backpropagation gives you the gradient that will be used for gradient descent
  - SGD gives us a generic learning algorithm
  - Backpropagation is a generic method for computing partial derivatives

- A recursive algorithm that proceeds from the top of the network to the bottom

- Modern neural network libraries implement automatic differentiation using backpropagation
  - Allows easy exploration of network architectures
  - Don’t have to keep deriving the gradients by hand each time

$$\min_{w} \sum_{i} L(NN(x_i, w), y_i)$$

Stochastic gradient descent

Given a training set $S = \{(\mathbf{x}_i, y_i)\}, \mathbf{x} \in \Re^d$

1. Initialize parameters w
2. For epoch = 1 … T:
   1. Shuffle the training set
   2. For each training example $(\mathbf{x}_i, y_i) \in S$:
      - Treat this example as the entire dataset
      - Compute the gradient of the loss $\nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i)$ using backpropagation
      - Update: $\boldsymbol{w} \leftarrow \boldsymbol{w} - \gamma_t \nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i))$
3. Return w

The objective is not convex.
Initialization can be important

γ_t: learning rate,
many tweaks possible