Neural Networks

A basic and intuitive introduction to “shallow” fully-connected feed-forward networks

Lion Krischer

Goal for Now + First Part of the Afternoon

- Fully understand and implement a simple feed-forward neural network from scratch.
- Little math (and probably slightly wrong notation).
- Go slow and step by step.

A bit tedious at times but not very hard.

Modern and deep networks are a bit more complicated but not fundamentally different.

Machine Learning

Input $\longrightarrow$ f(x) $\longrightarrow$ Output

Input ⟶ **f(x)** ⟶ **Output**

Physical Model

Source Parameters
Earth Model

F(Earth Model, Source Parameters)

Seismograms

Input $\longrightarrow$ f(x) $\longrightarrow$ Output

Anything | Machine Learning Model | Anything

In a way we replace our knowledge of the physics or the logic of a problem with an arbitrary “learned” function.

Input → **f(x)** → **Output**

Input	f(x)	Output
Anything	Machine Learning Model	Anything

Input → **f(x)** → **Output**

Anything | Machine Learning Model | Anything

Data Driven

Input → f(x) → Output

Anything

Supervised Machine Learning Model
Neural Network

Anything

Data Driven

When is this a good idea/useful?

- If it is very hard to make a physical or logical model.
    - Image and speech recognition, self-driving cars, language translation, …
    - Phase detection and recognition (see Thursday), signal classification (see Wednesday), …
- If the physical model is very expensive to compute but the result is somehow “simple”.
- And: One has a LOT of data.

Neural Networks

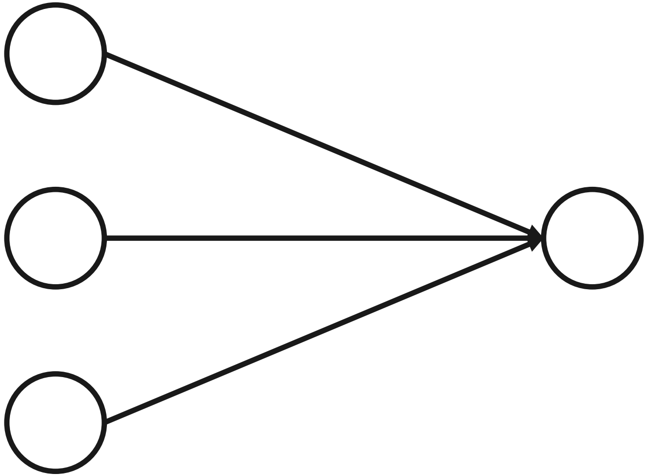
Universal Function Approximators

- **Universal approximation theorem**: Feed-forward networks of finite size with a single hidden layer and non-linear activation functions can approximate any continuous function (under some mathematical restrictions).
- Newer results reduce the necessary width of the networks under some conditions.
- Only a statement that one could always create a neural network to perform a certain action. Not if it is actually learnable.

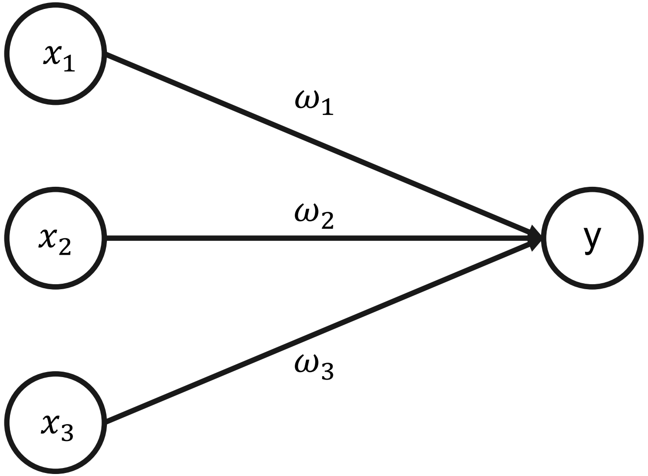
Thus the questions is not “Can a neural network do this?” but “Can I make it learn what I want it to do?”.

Neural Networks Step by Step

Weighted Sum

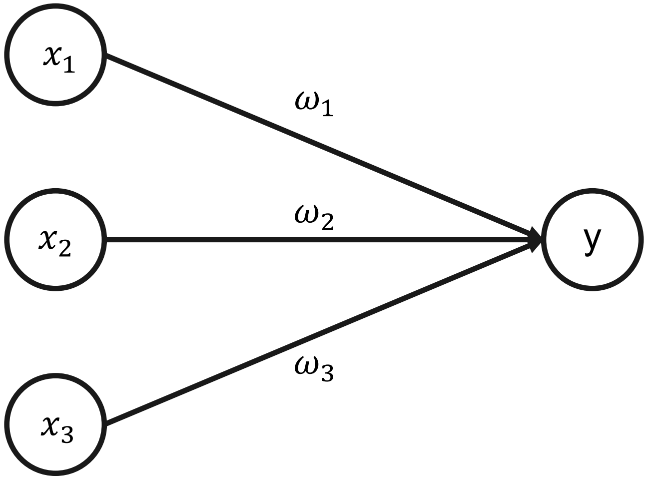


Weighted Sum



Weighted Sum

$$y = \omega_1 * x_1 + \omega_2 * x_2 + \omega_3 * x_3 = \sum_i \omega_i x_i$$



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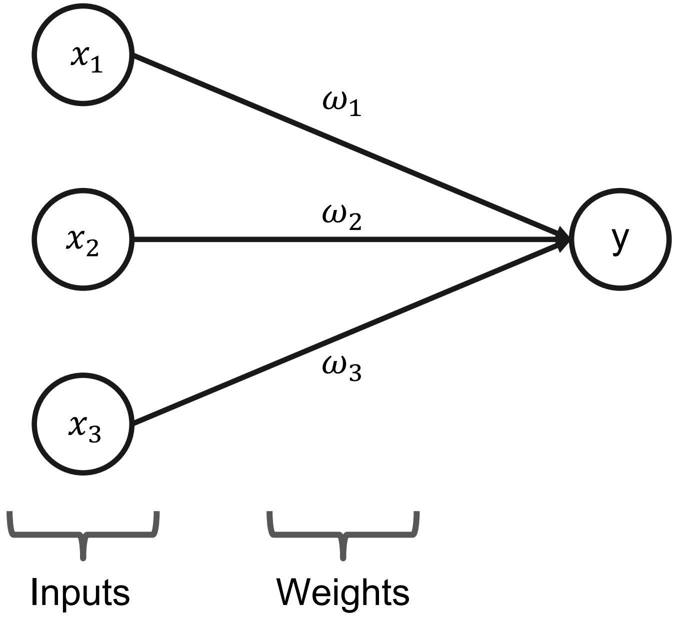
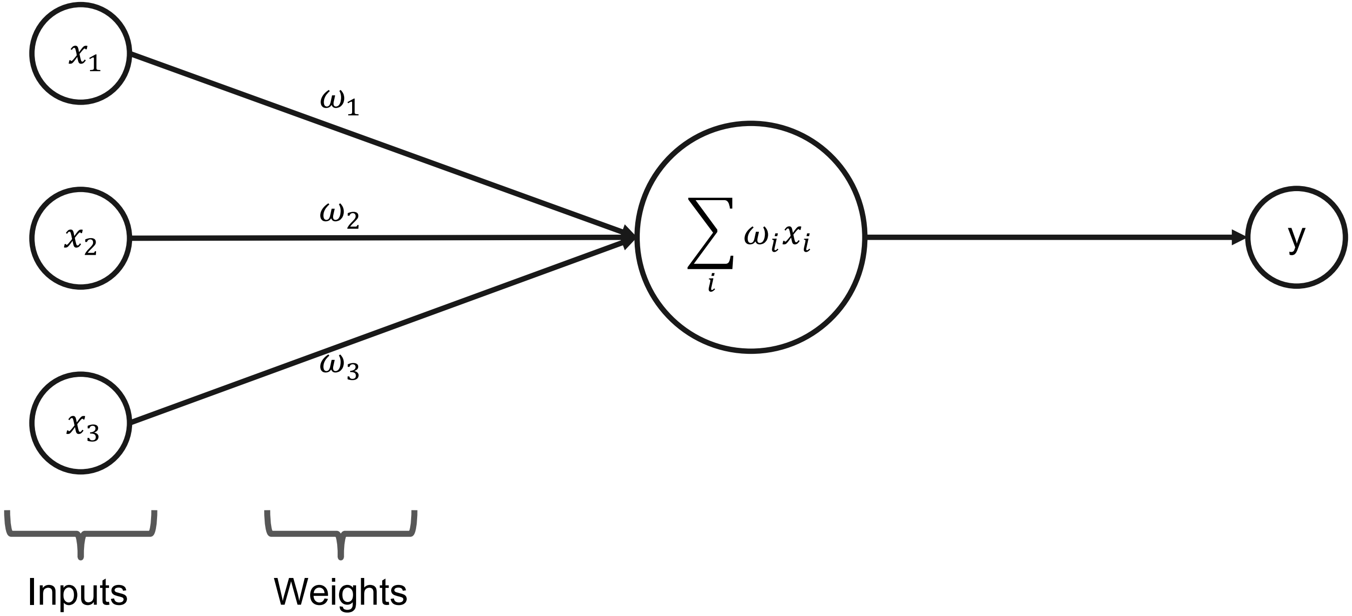


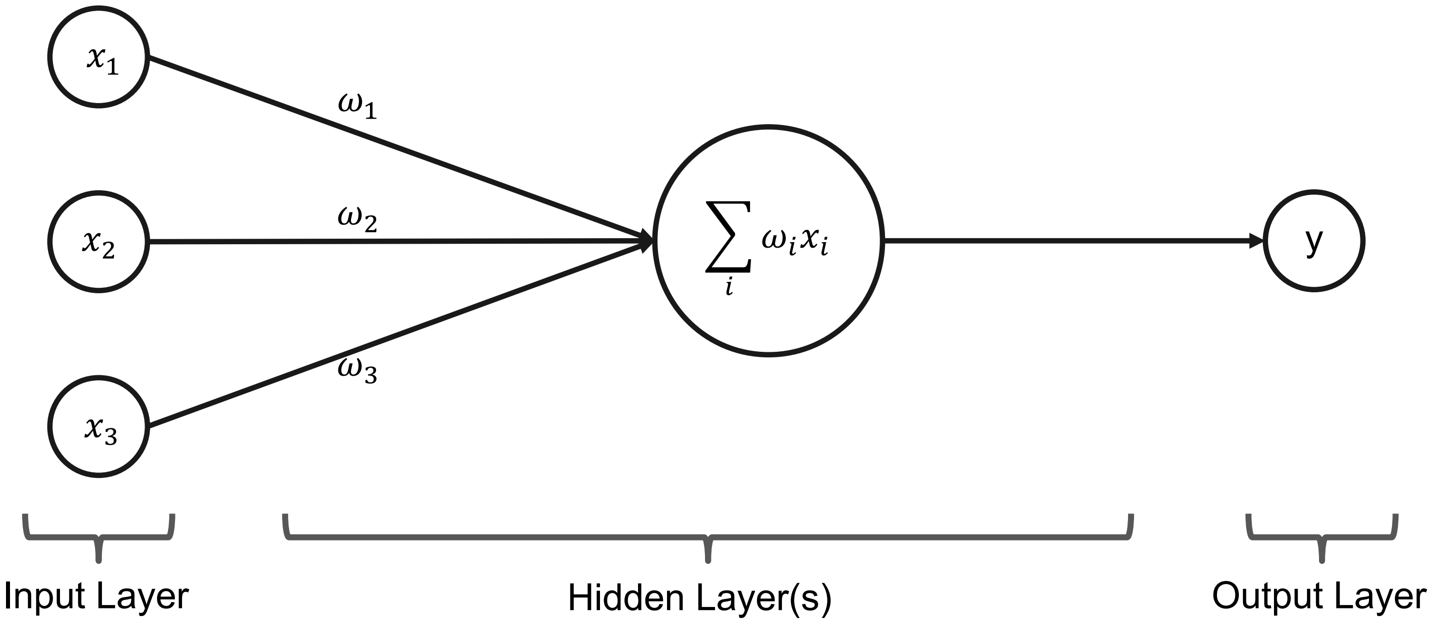
Weighted Sum

Not too useful yet – basically a dot product

Weighted Sum

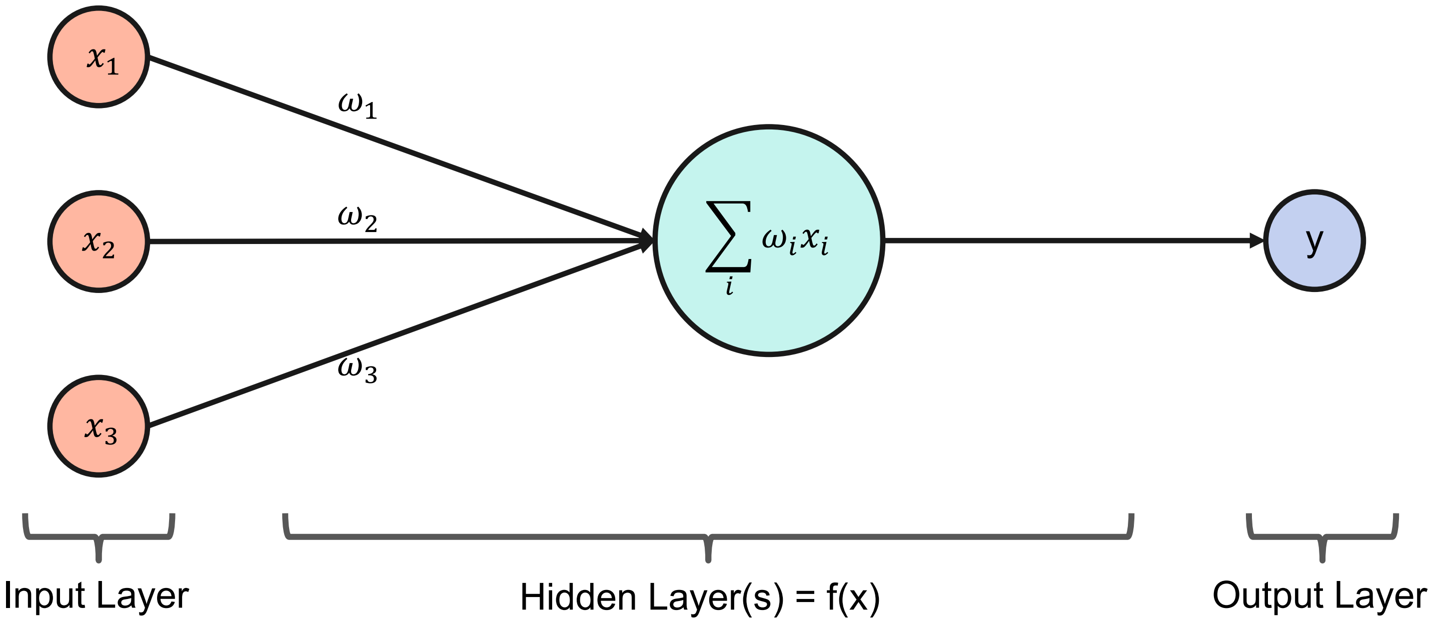


Weighted Sum



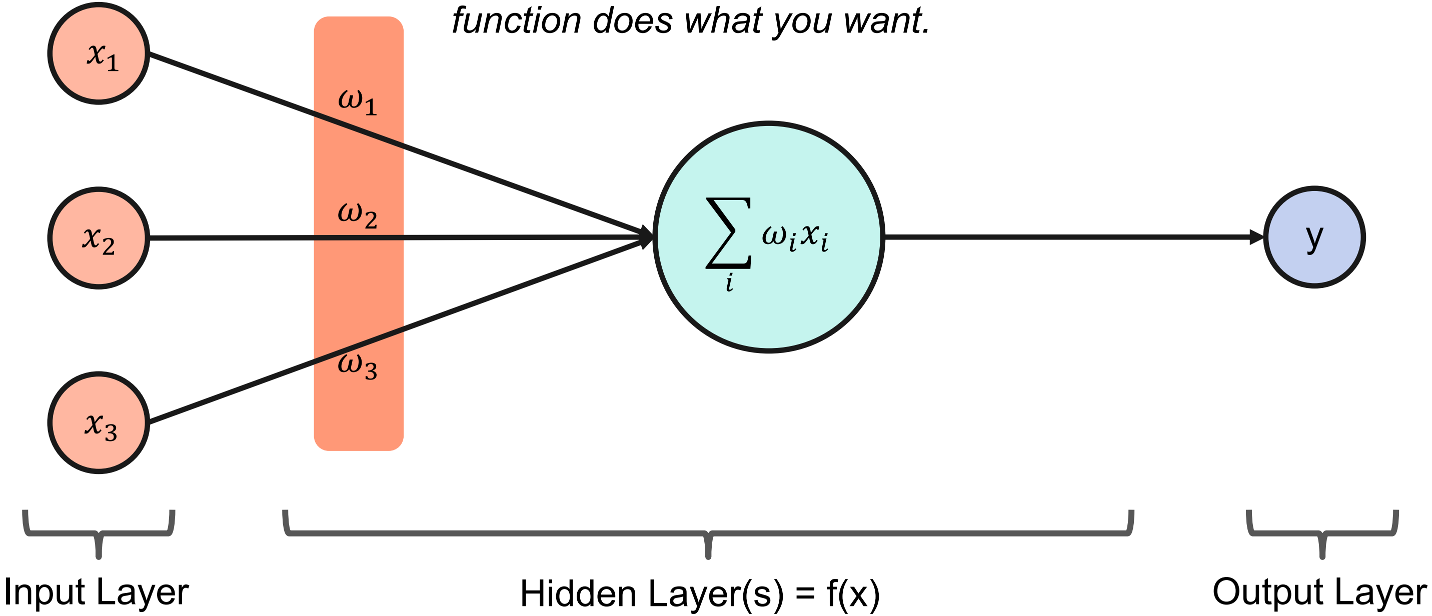
$$\text{Input} \longrightarrow f(x) \longrightarrow \text{Output}$$

Weighted Sum



Weighted Sum

Change weights to change the behavior of the function. "Learning" would thus be to find better weights so the function does what you want.



Weighted Sum

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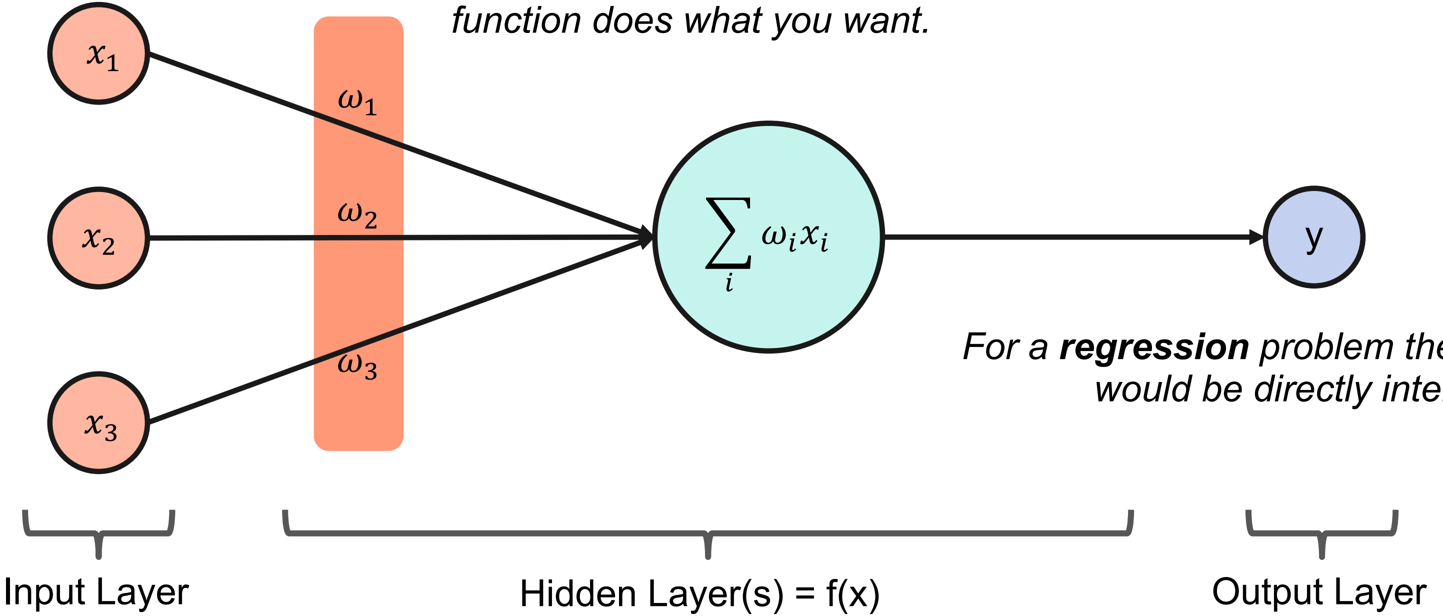
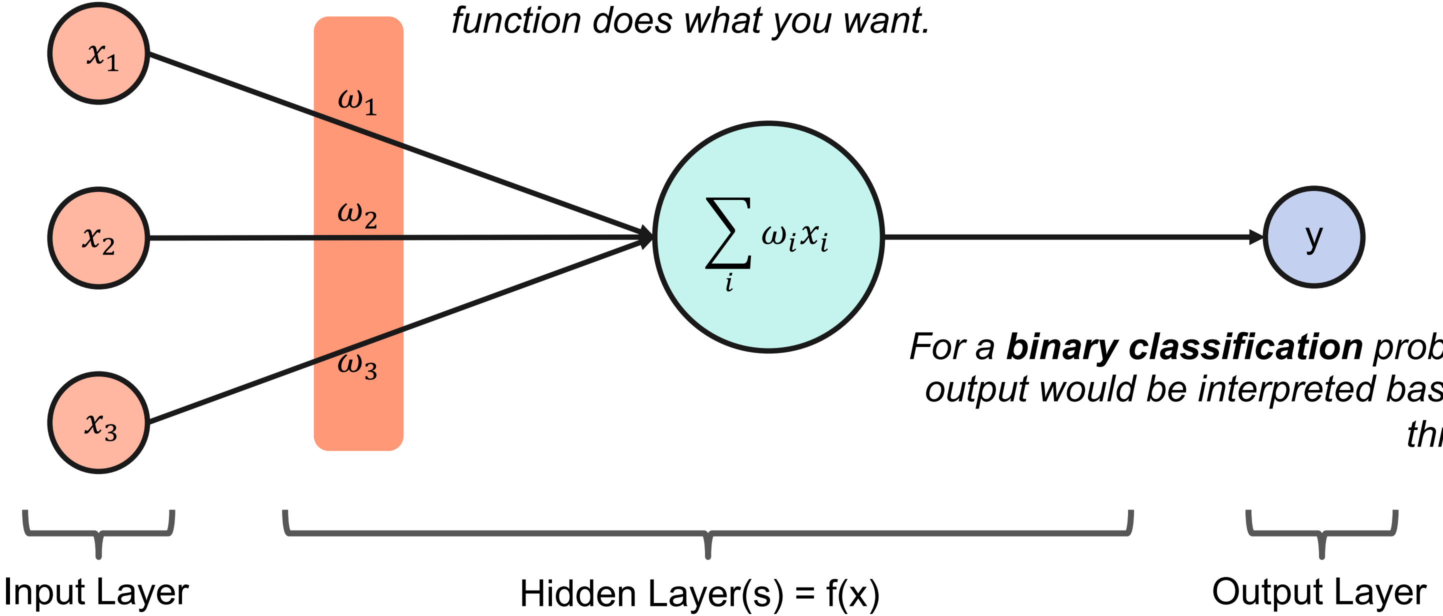


*For a **regression** problem the output would be directly interpreted.*

Weighted Sum

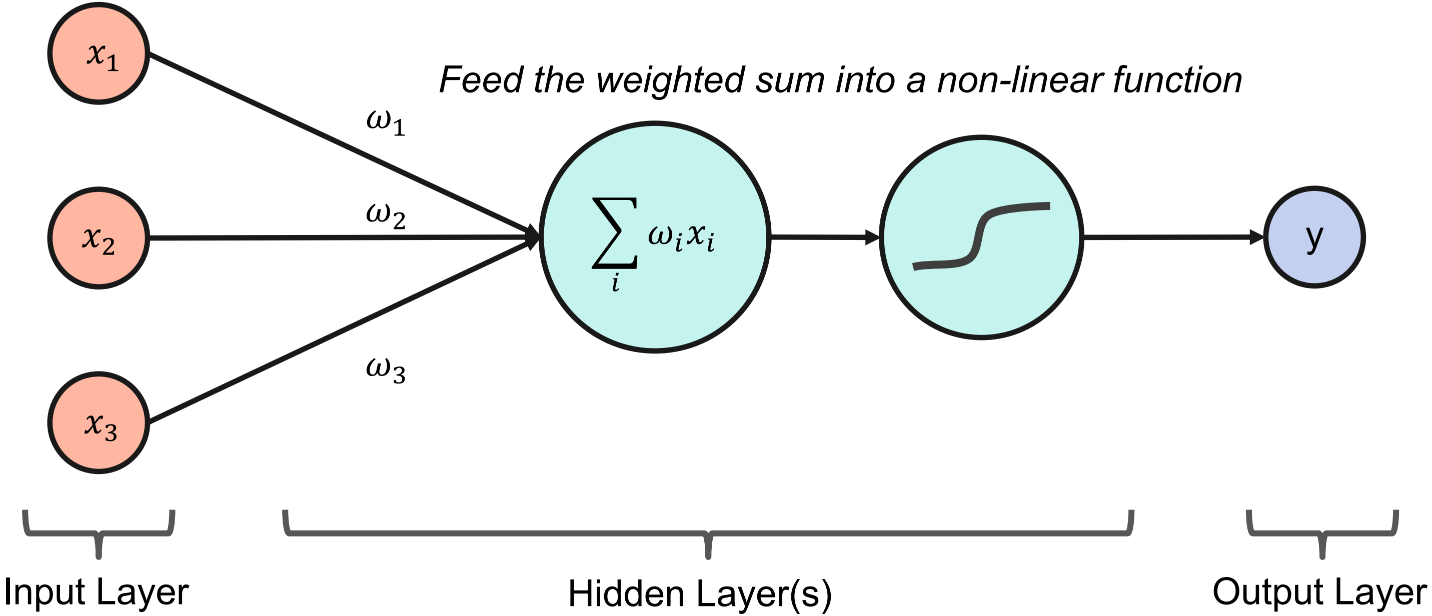
Change weights to change the behavior of the function. "Learning" would thus be to find better weights so the function does what you want.



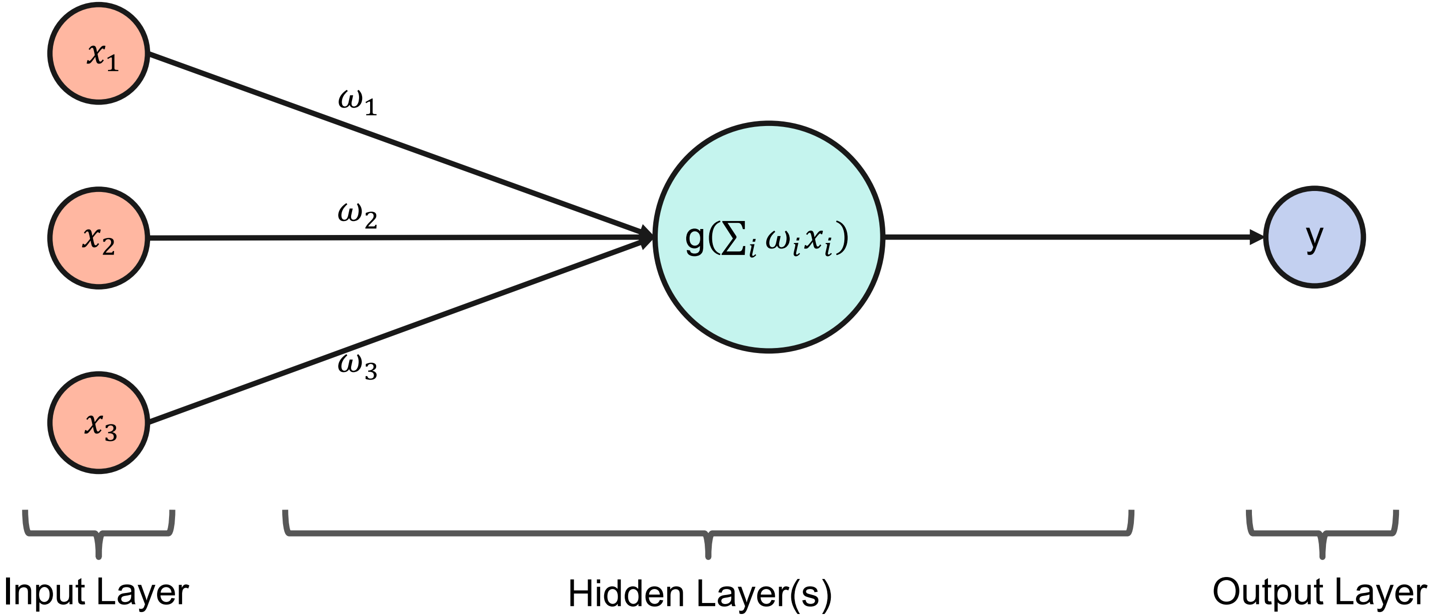
*For a **binary classification** problem the output would be interpreted based on a threshold.*

Computing something non-linear might be useful.

Activation Function



Activation Function



Why do we need an activation function?

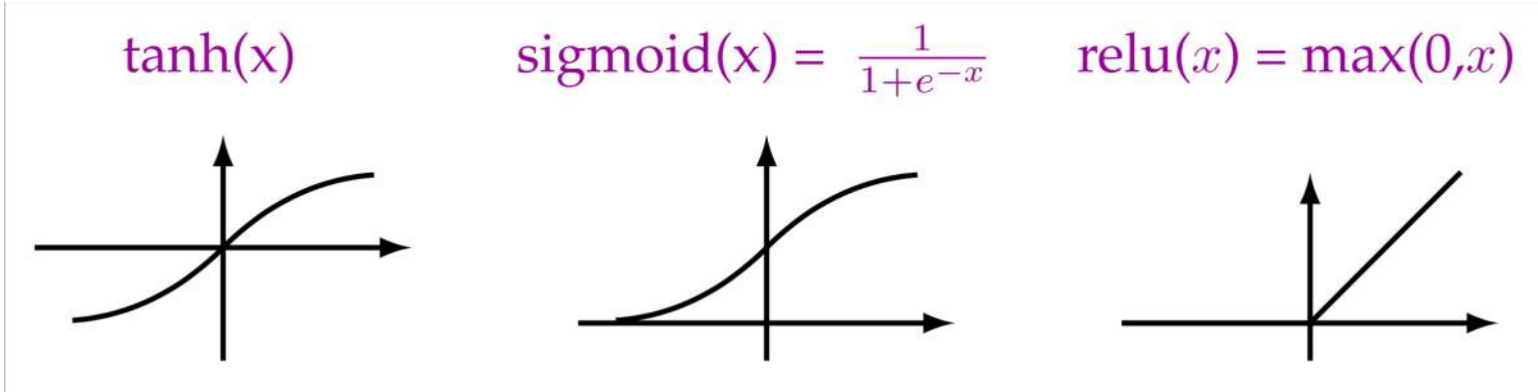
- Some non-linearity is needed to compute anything non-linear.

- More complex relationships between inputs and outputs cannot be represented by something purley linear.

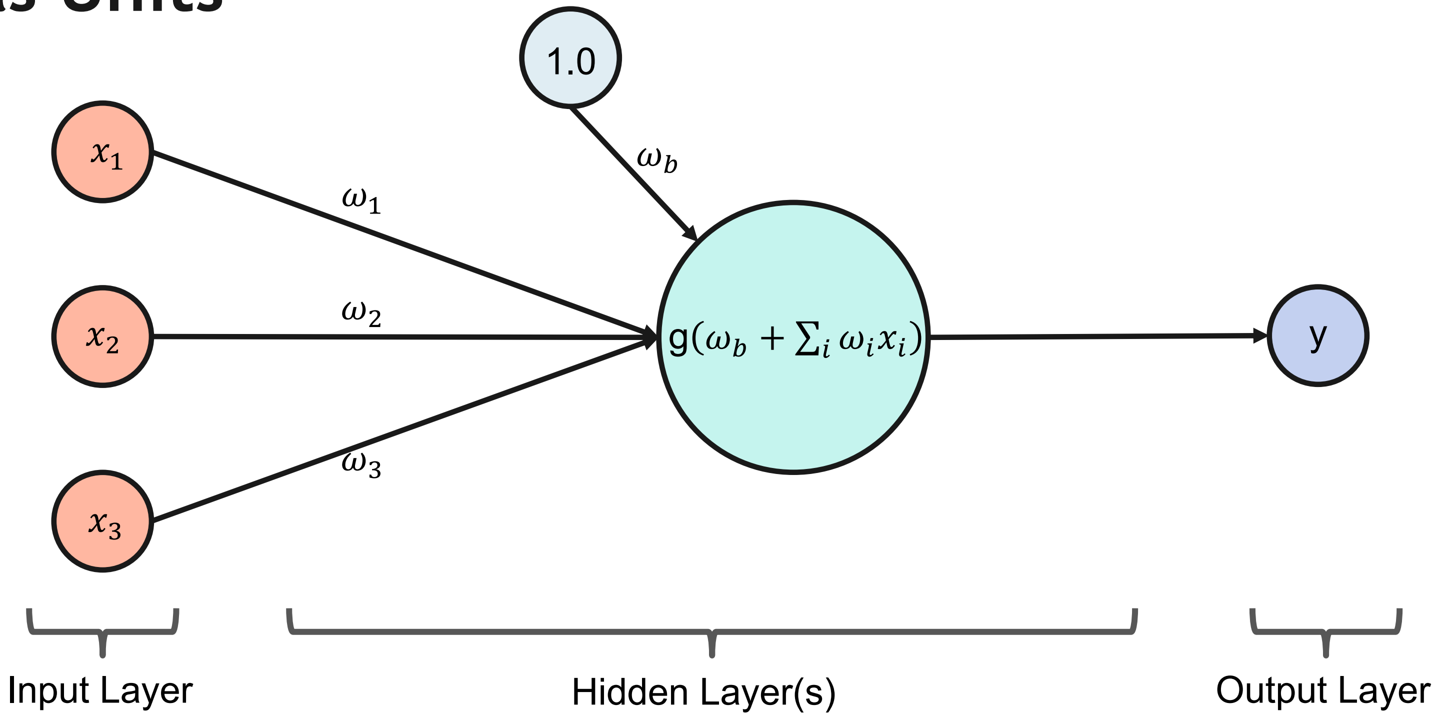
- (I think) they are called activation functions because the first one used was a Heaviside function and thus either “activated” a neuron or not for a given set of inputs.

Popular Choices

- Features people are looking for in activation function:
  - At least piecewise differentiable for reasons we'll elaborate upon later
  - Monotonous
  - Helpful if they bound the output (but not all modern choices do that)
  - Computationally cheap

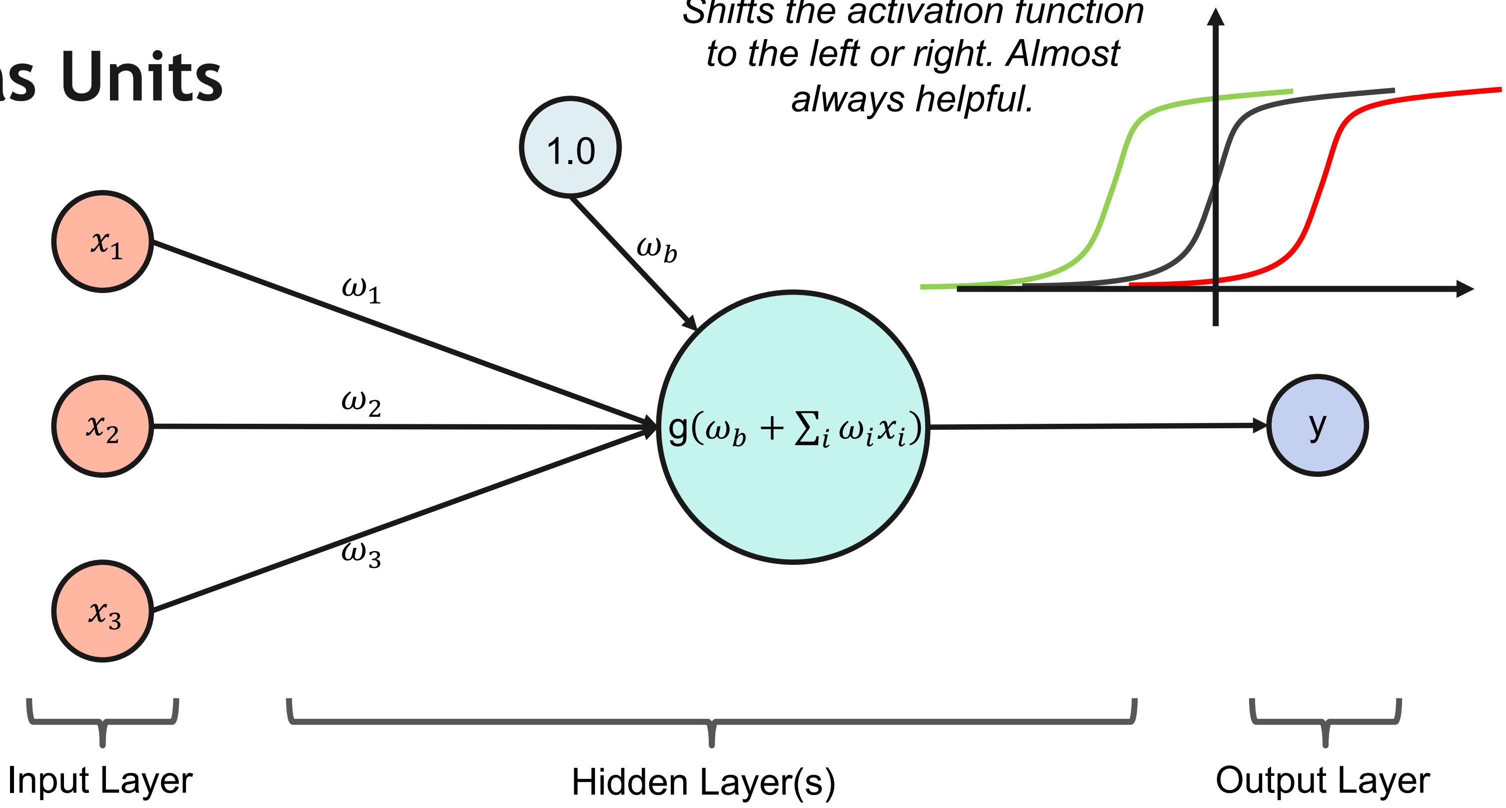


Bias Units


1.0
x_1
x_2
x_3
ω_b
ω_1
ω_2
ω_3
$g(\omega_b + \sum_i \omega_i x_i)$
y
Input Layer
Hidden Layer(s)
Output Layer

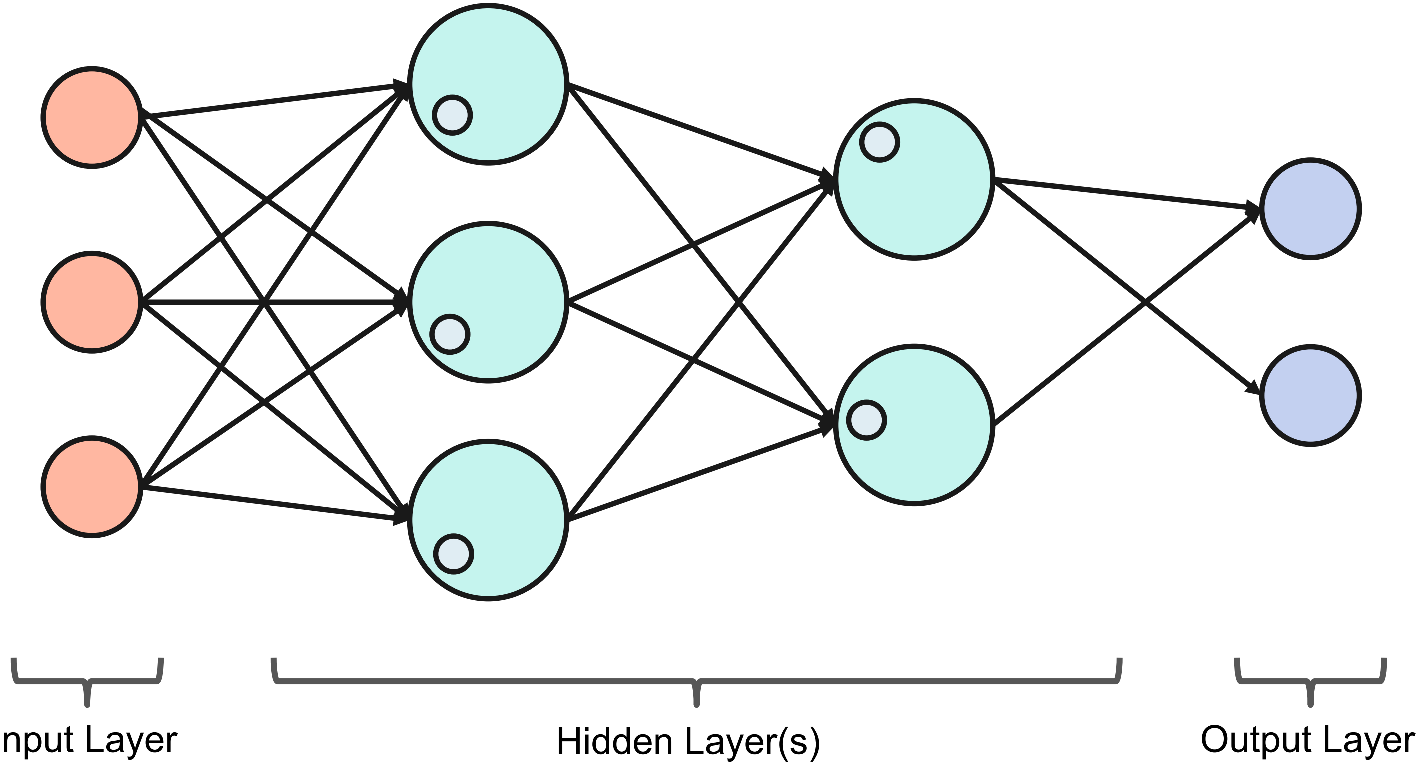
Bias Units

Shifts the activation function to the left or right. Almost always helpful.



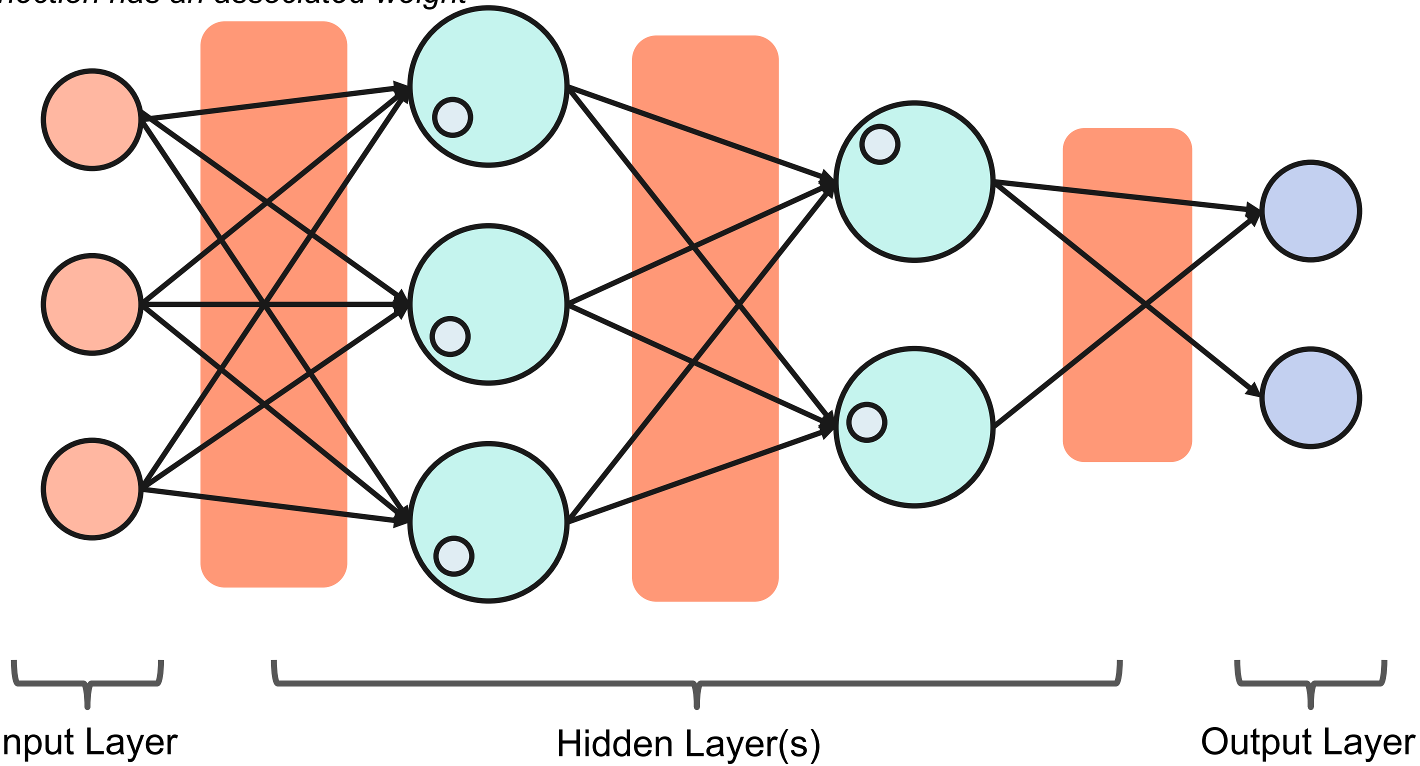
Now let’s start to build a proper network.

Fully-connected Feed-forward Neural Network

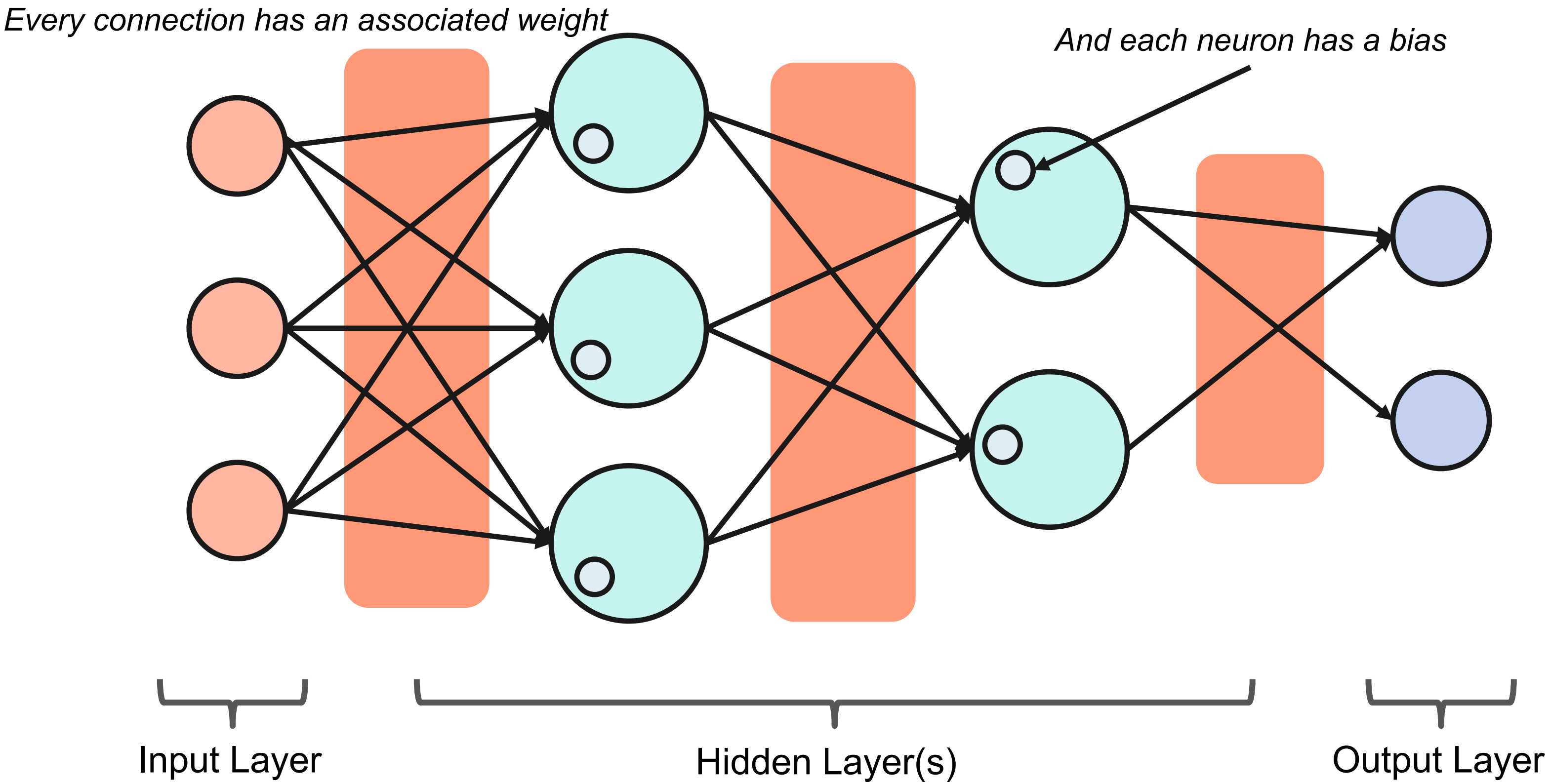


Fully-connected Feed-forward Neural Network

Every connection has an associated weight



Fully-connected Feed-forward Neural Network



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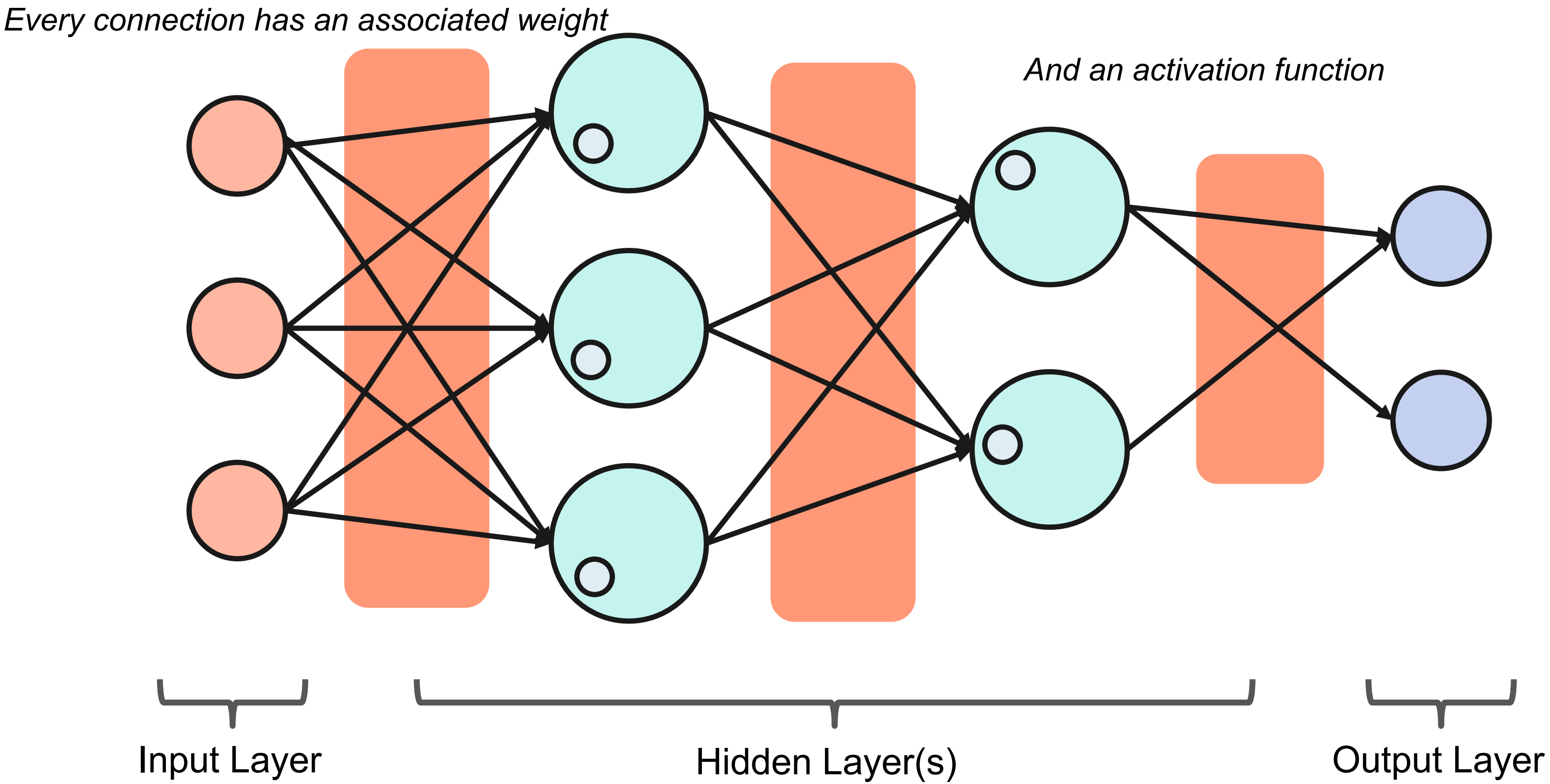

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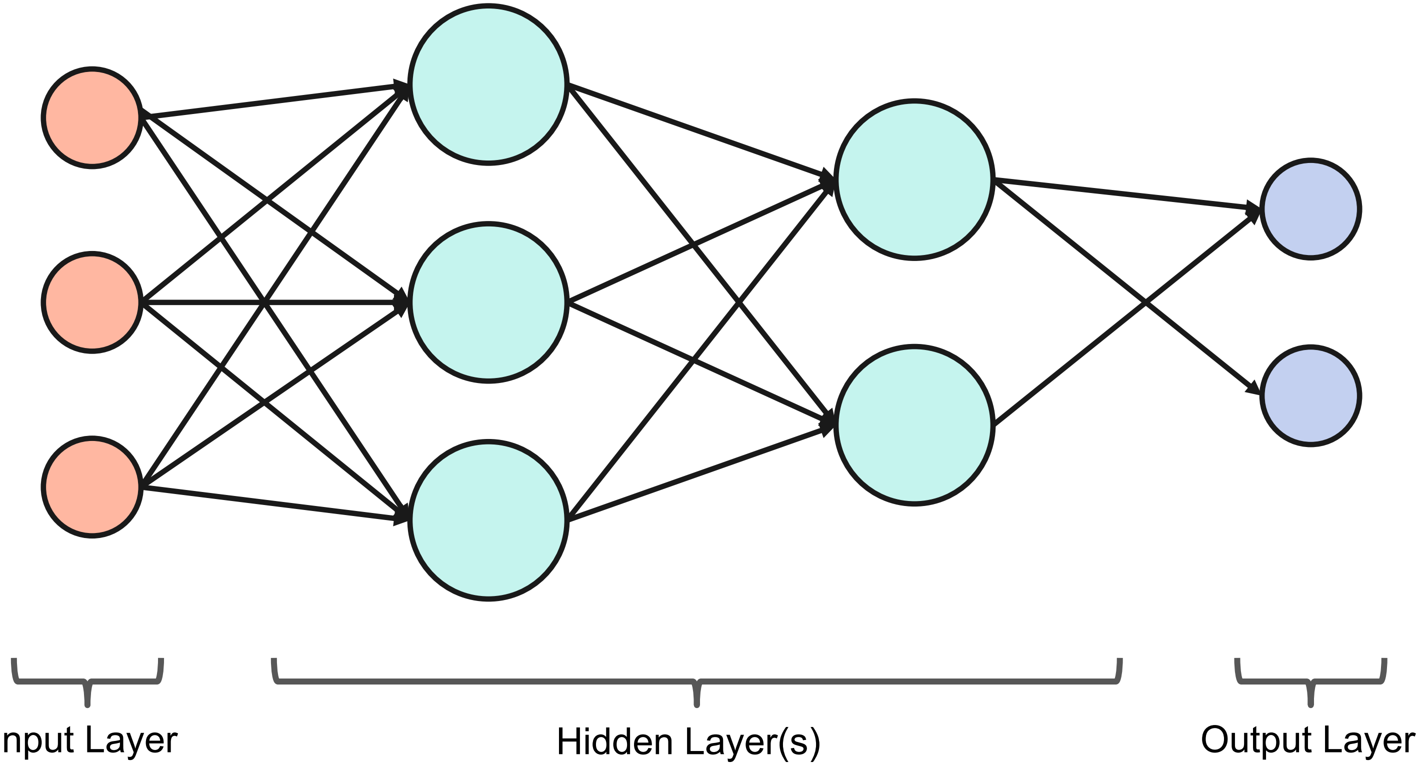


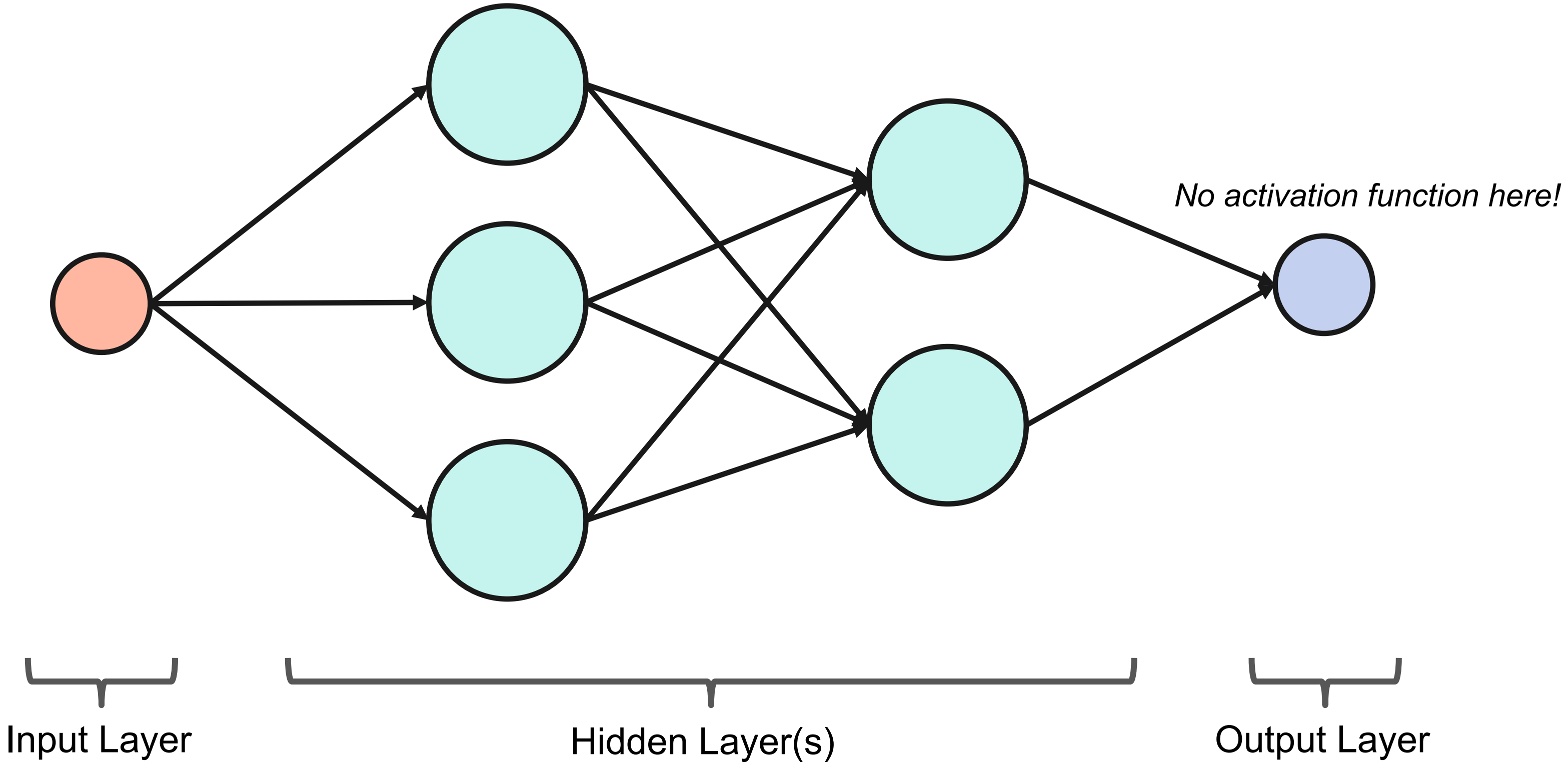
What is gained by adding more “depth”?

- Remember that everything can also be done with a single layer but this layer might get very large.
- If done properly the hope is to decompose a problem in many separate processing or computation steps.
- More layers thus means more steps which allows more complicated functions.
- This generalizes better and also requires fewer parameters.
- Deep networks are discussed in depth on Thursday.

Now we know how a neural network computes something.

Let’s implement this!

Exercise: Forward Pass of this Network



Open the Neural Networks from Scratch Notebook.

How to make it do what we want?

So far we just multiplying numbers together…

$$\text{Input} \longrightarrow f(x) \longrightarrow \text{Output}$$

Input $\longrightarrow$ f(x) $\longrightarrow$ Output

Known input data

Known output data

Input ⟶ f(x) ⟶ Output

Known input data

Optimize for the parameters of f(x)

Known output data

Known input data

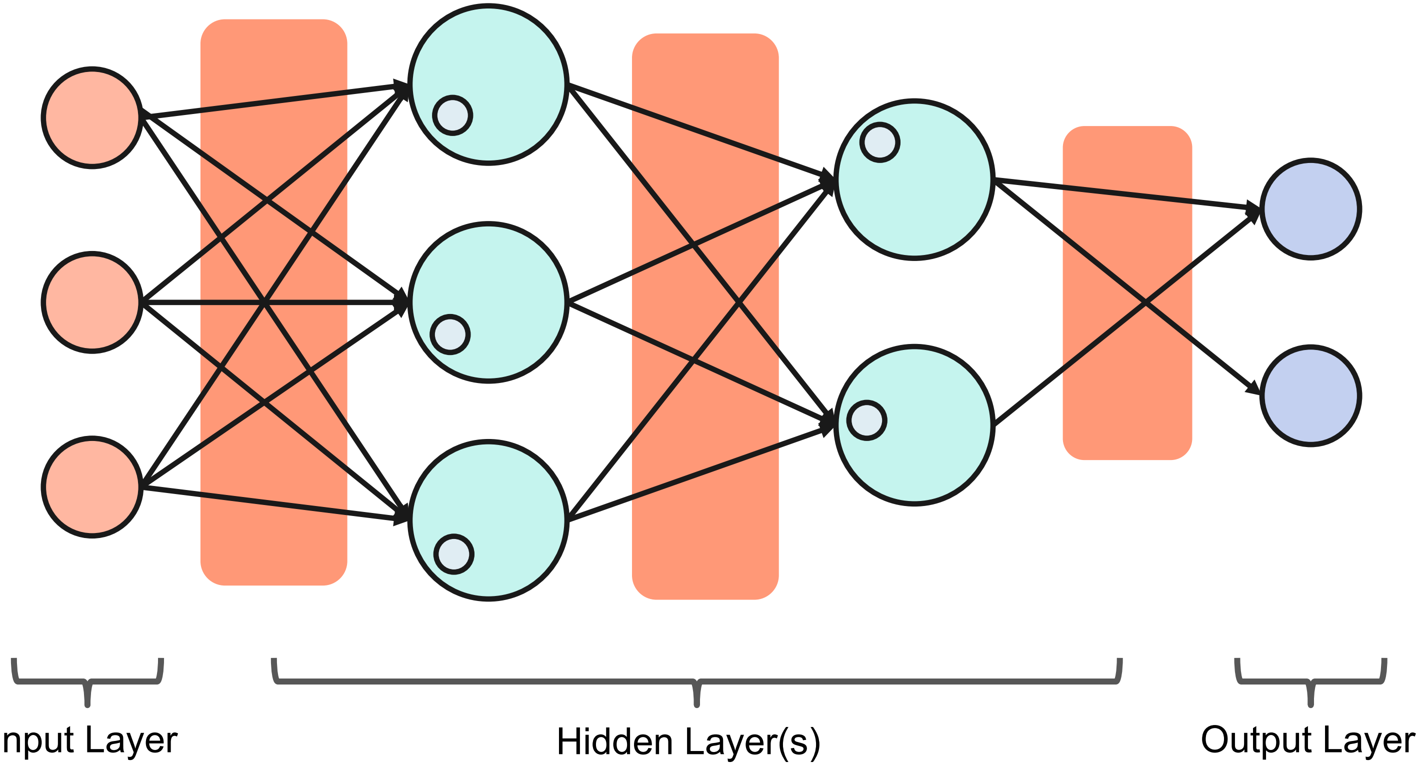
Optimize for the parameters of f(x)

Known output data

Objective for neural networks: Find a set of weights so that it can convert the inputs to output with as little error as possible.

The actual network layout is fixed.

Fully-connected Feed-forward Neural Network



Numerical Optimization Problem

- These networks can have a lot of parameters => Global search methods infeasible
- Derivatives can be computed analytically
    - => Local gradient based optimization

We require two ingredients:

- A way to compute derivatives (back-propagation)
- A way to perform the actual optimization (here we use simple gradient descent)

Back-Propagation with Pen & Paper

What is Back-Propagation?

- Returns the analytic gradients of some objective function/misfit measurement/loss function with respect to the weights of a neural network
- Thus tells us how we have to change the network parameters to increase that loss function. We of course go the other way.
- It is really just the repeated application of the chain rule.
- Works just the same as auto-differentiation does.

Simple Example

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

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Goal:

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

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Goal:

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

Chain rule:

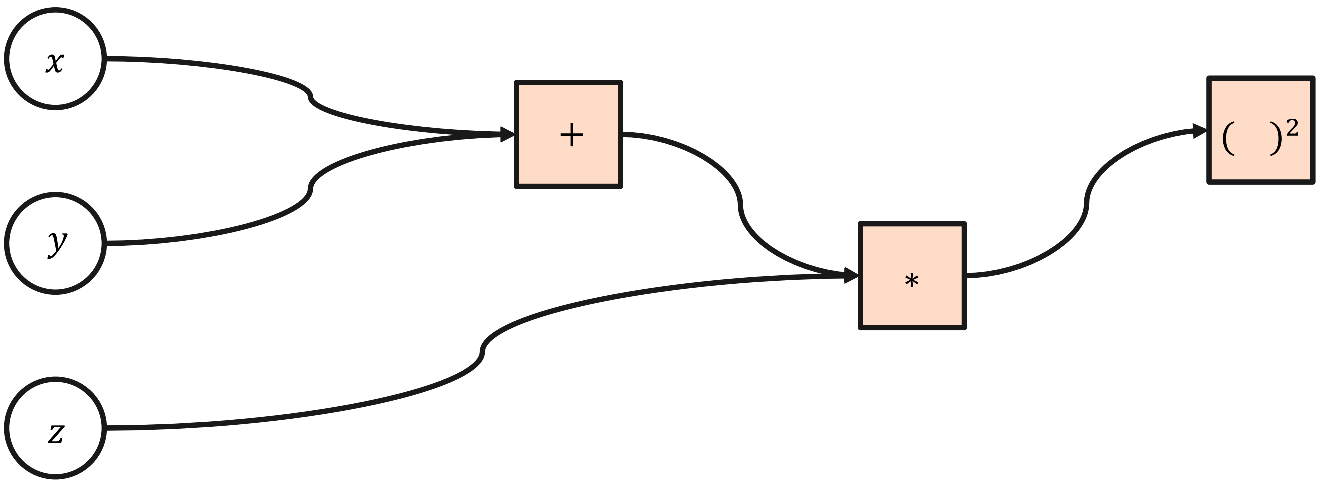
$$\frac{\partial f}{\partial z} = 2\,\big((x + y)z\big)(x + y)$$

of course works, but tedious for deeply nested computations.

And inefficient, assuming that we already calculated for example $(x + y)$ if we evaluated the function once.

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

Simple Example



Simple Example

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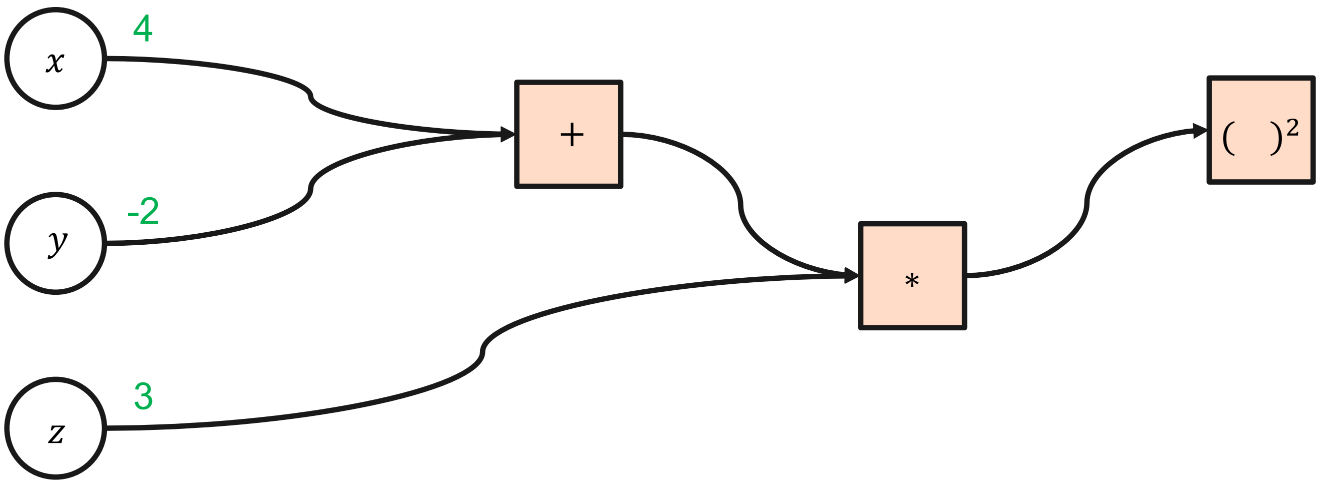
Forward Pass



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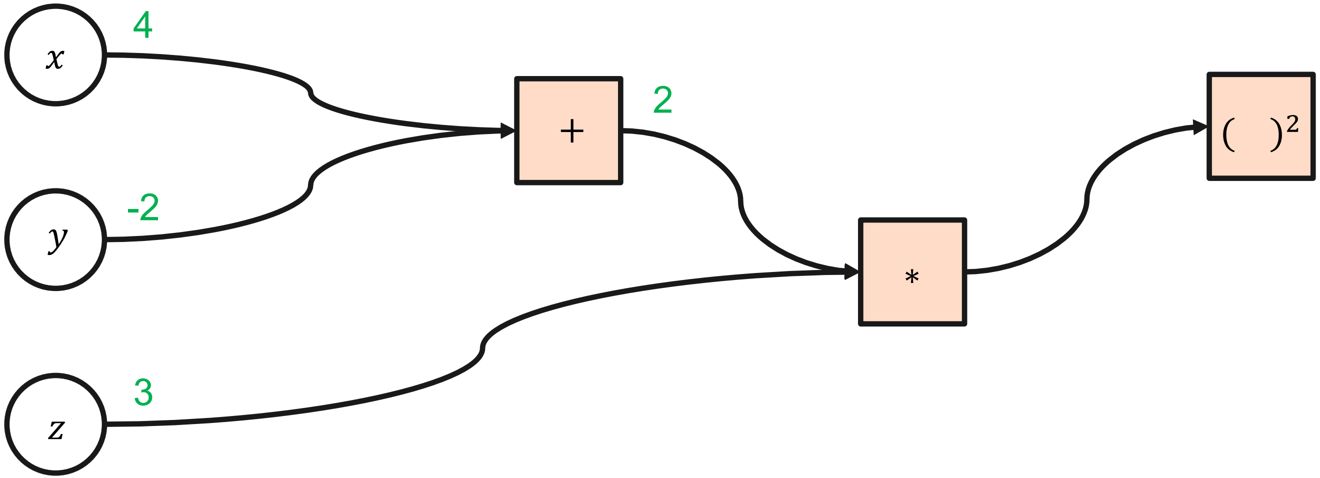
Simple Example

Forward Pass



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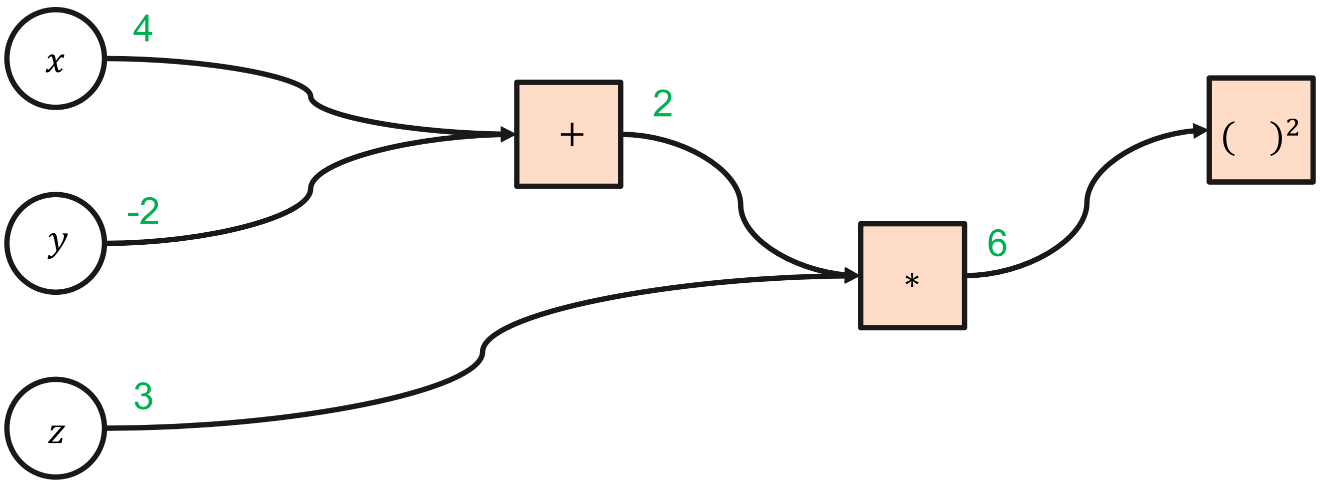
Simple Example

Forward Pass



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Simple Example

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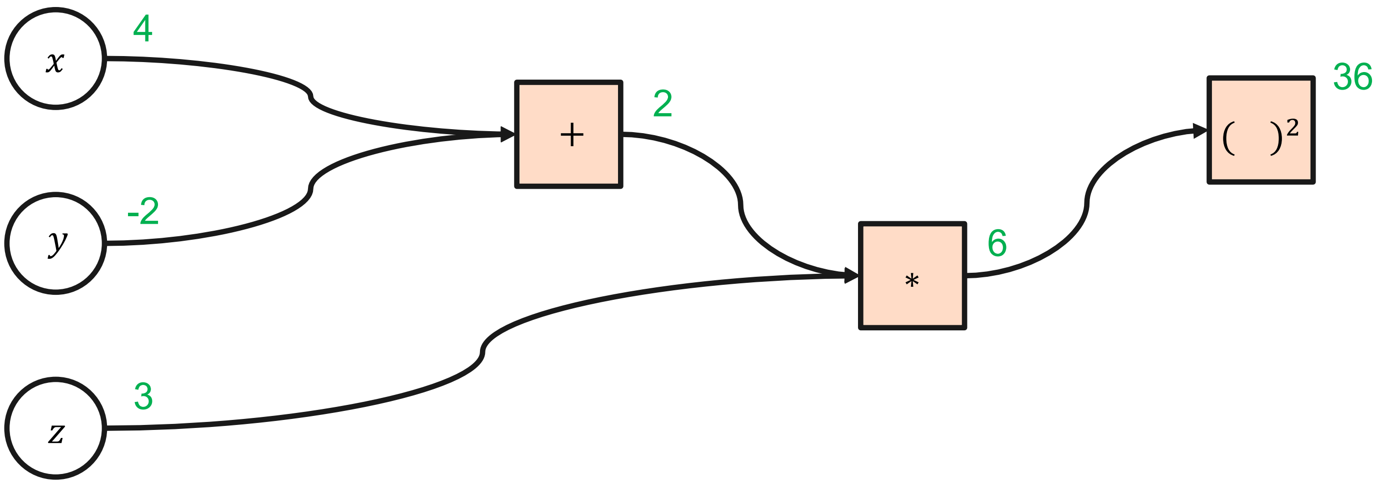

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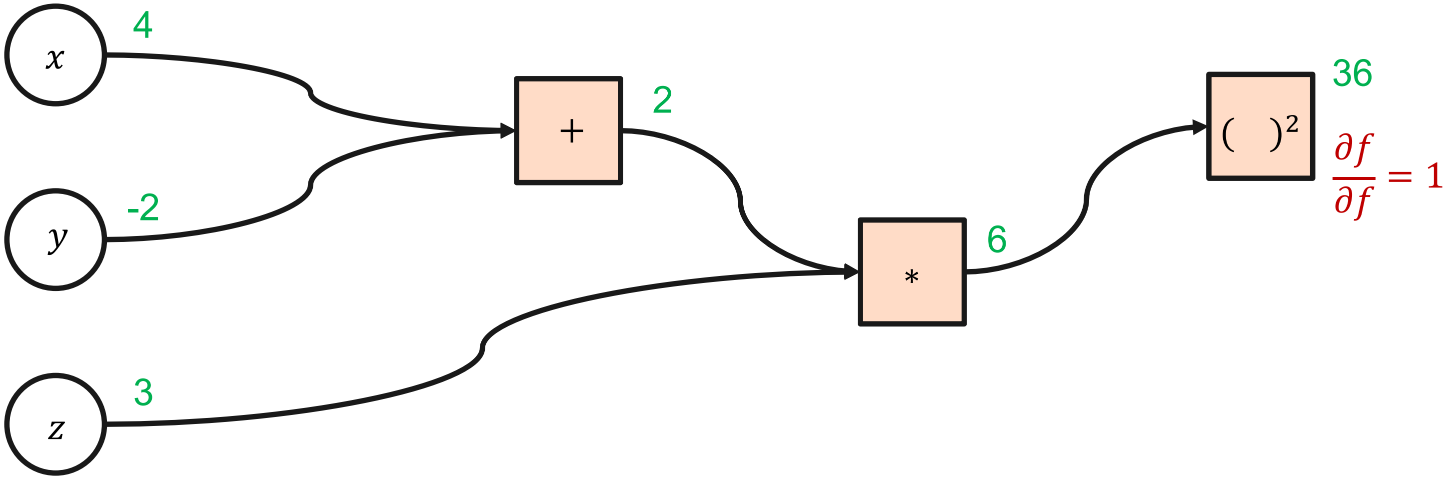
Simple Example

Forward Pass
Backward Pass



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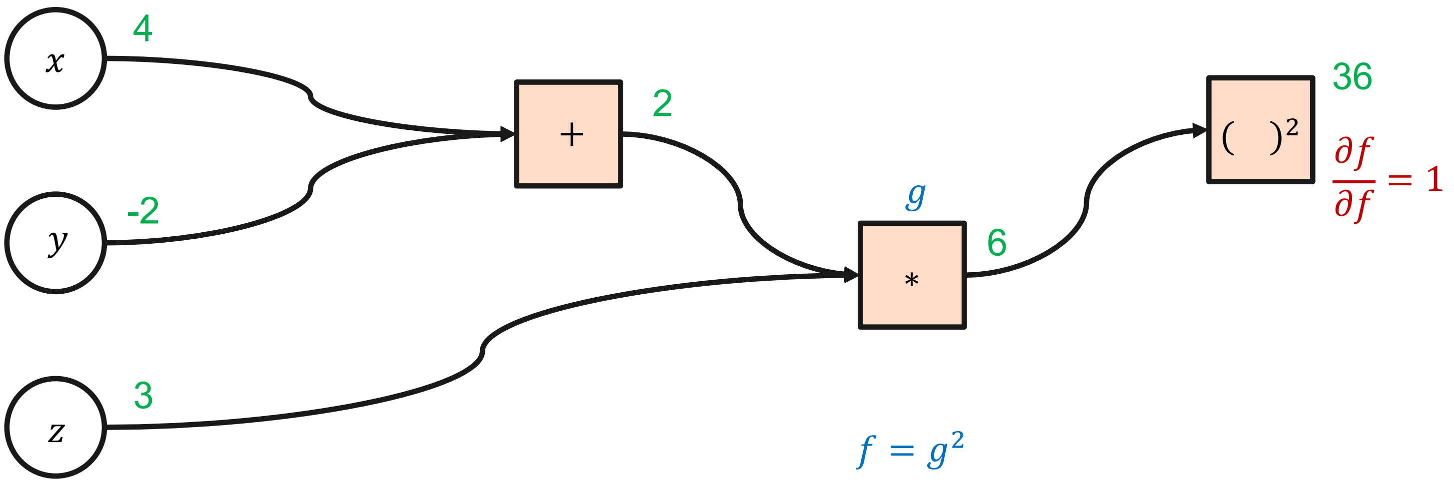
Simple Example

Forward Pass
Backward Pass



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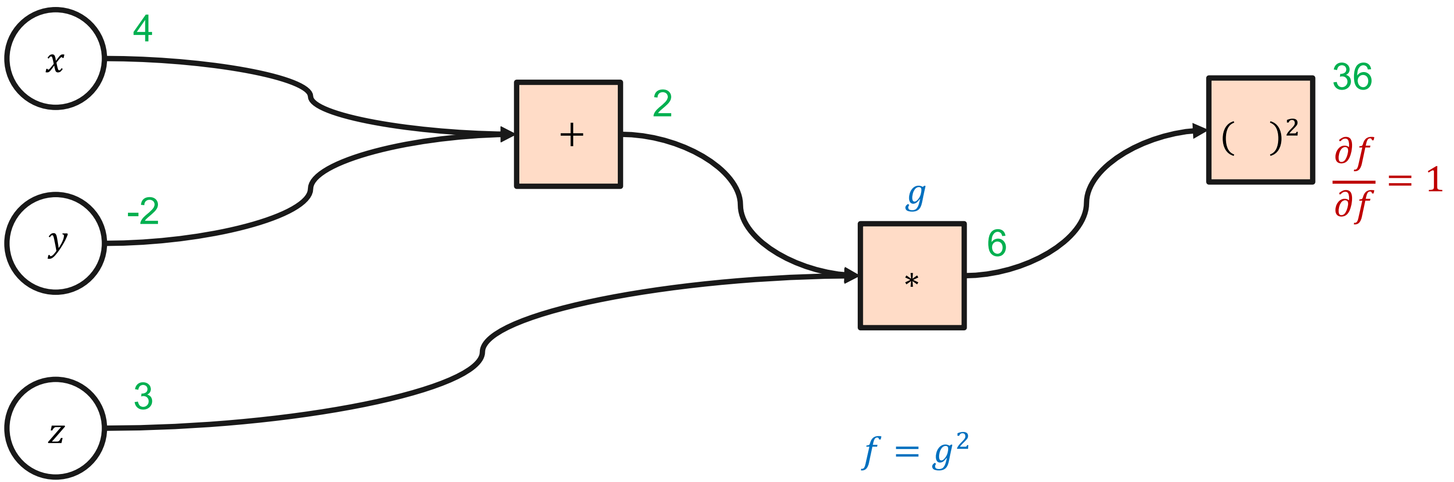
Simple Example

Forward Pass
Backward Pass



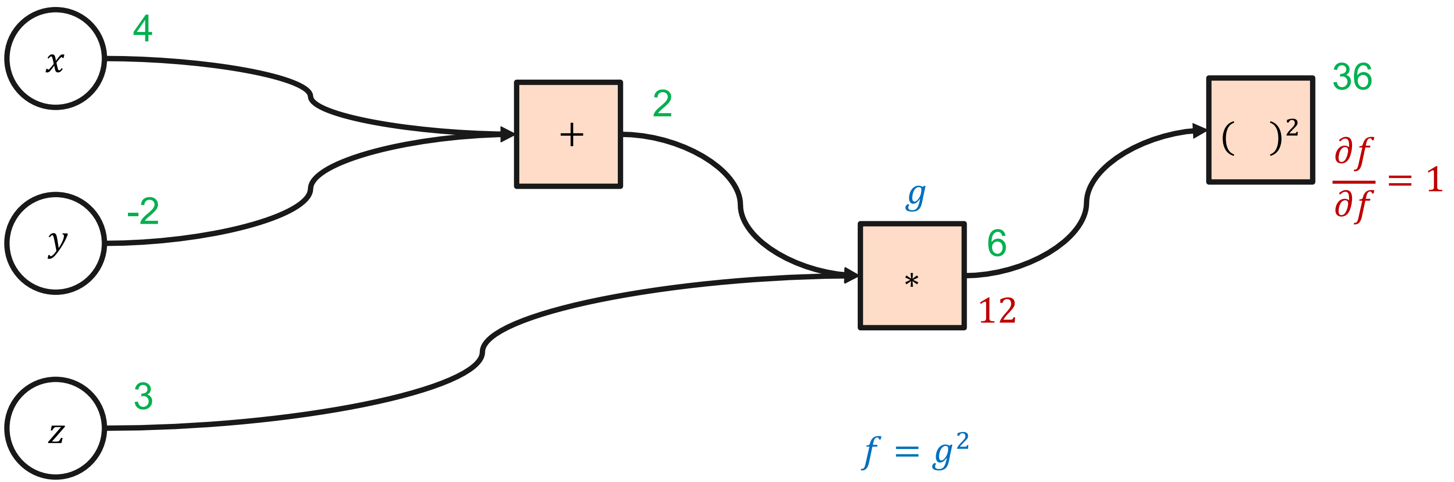
$$f = g^2$$

$$\frac{\partial f}{\partial g} = 2g$$

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

Simple Example

Forward Pass
Backward Pass



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Forward Pass
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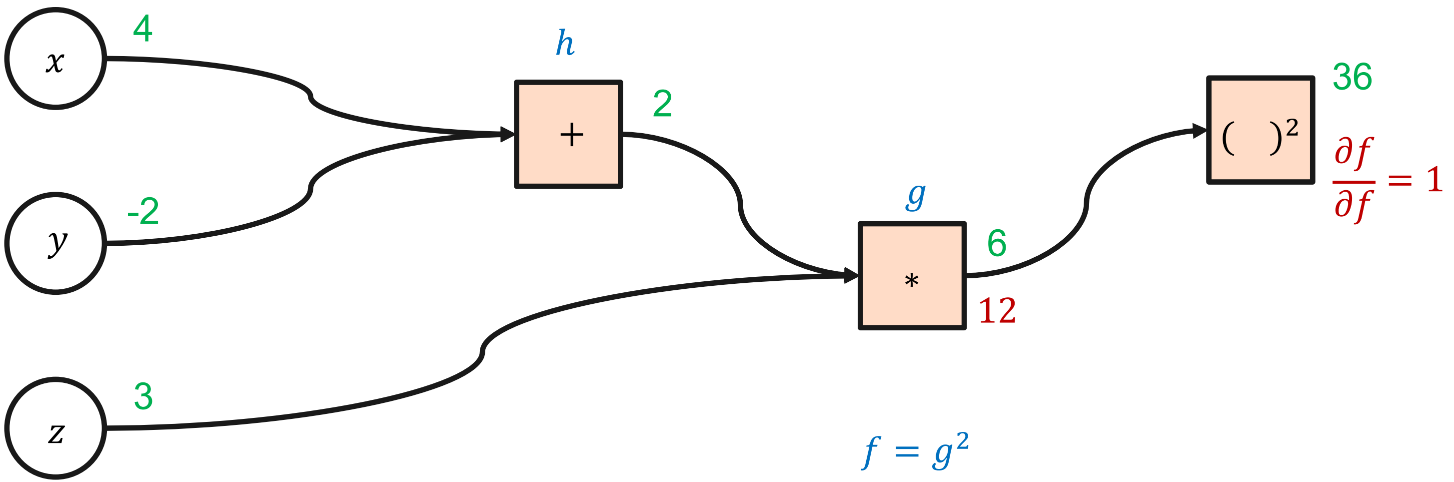


$$f = g^2$$

$$\frac{\partial f}{\partial g} = 2g$$

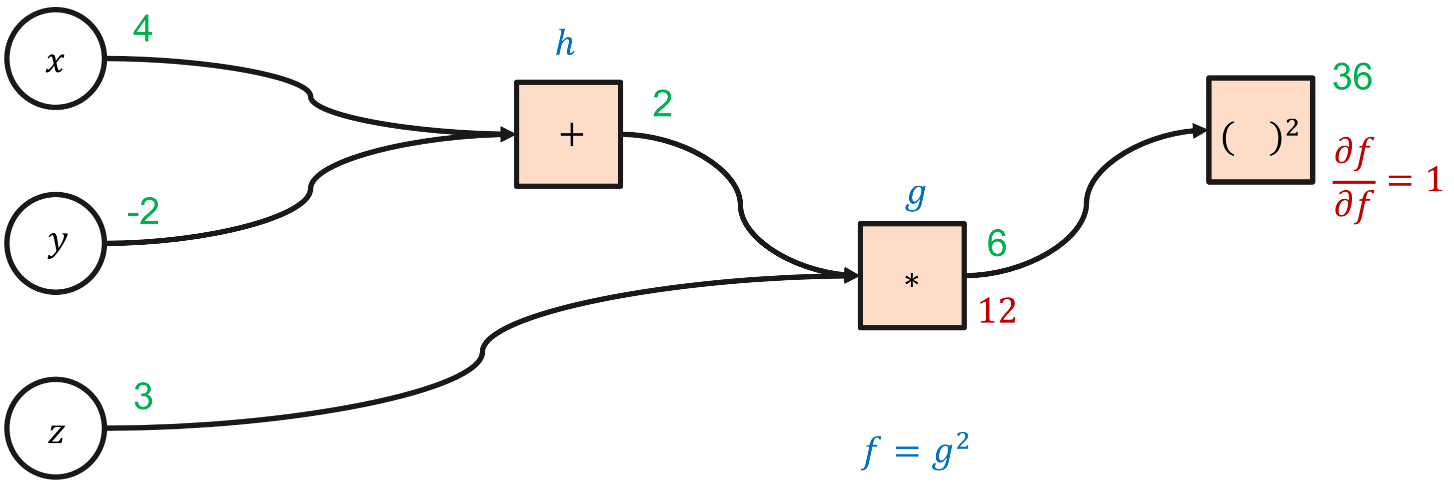
Simple Example

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

$$g = hz$$

$$\frac{\partial g}{\partial z} = h$$

Forward Pass
Backward Pass



$$f = g^2$$

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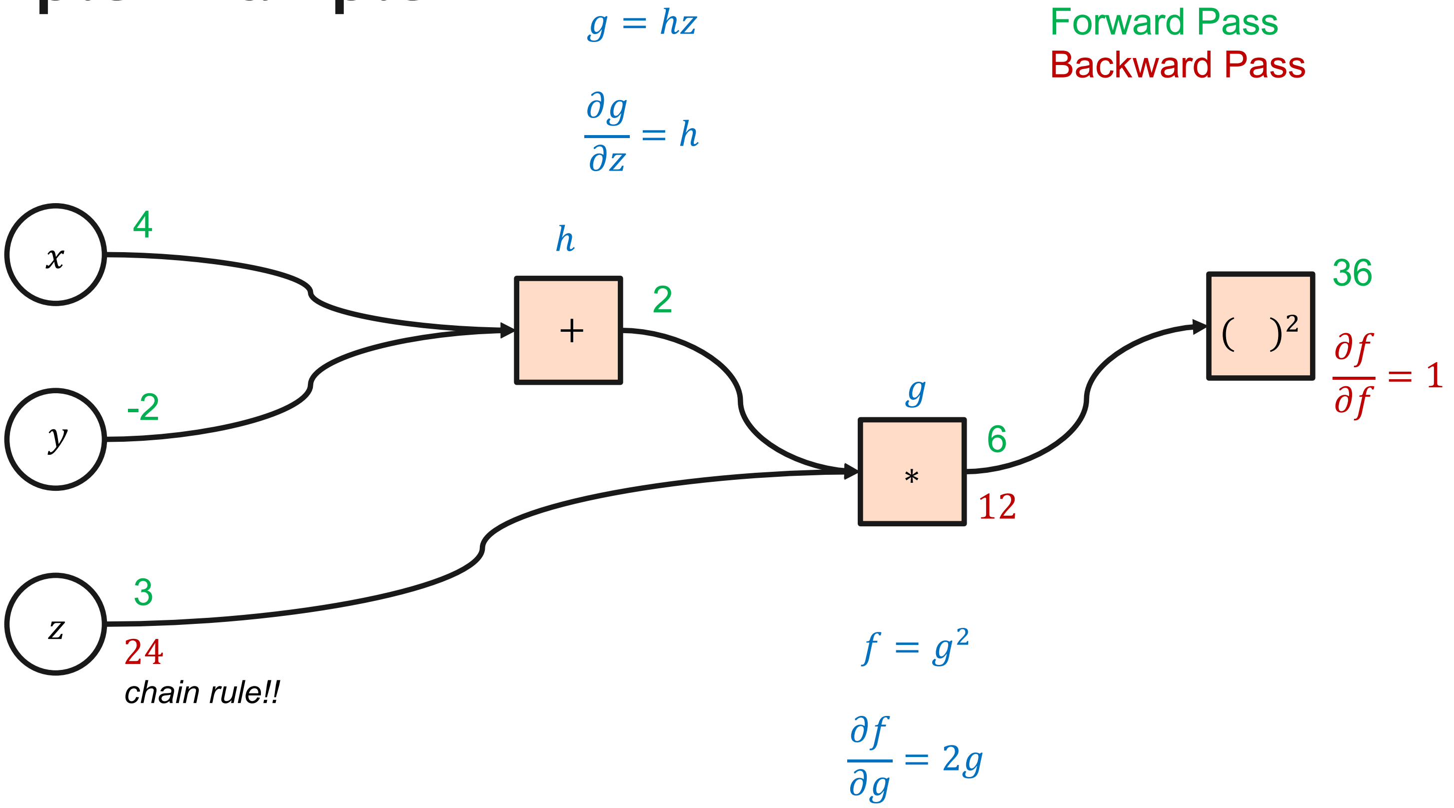
Simple Example

Forward Pass
Backward Pass



Simple Example

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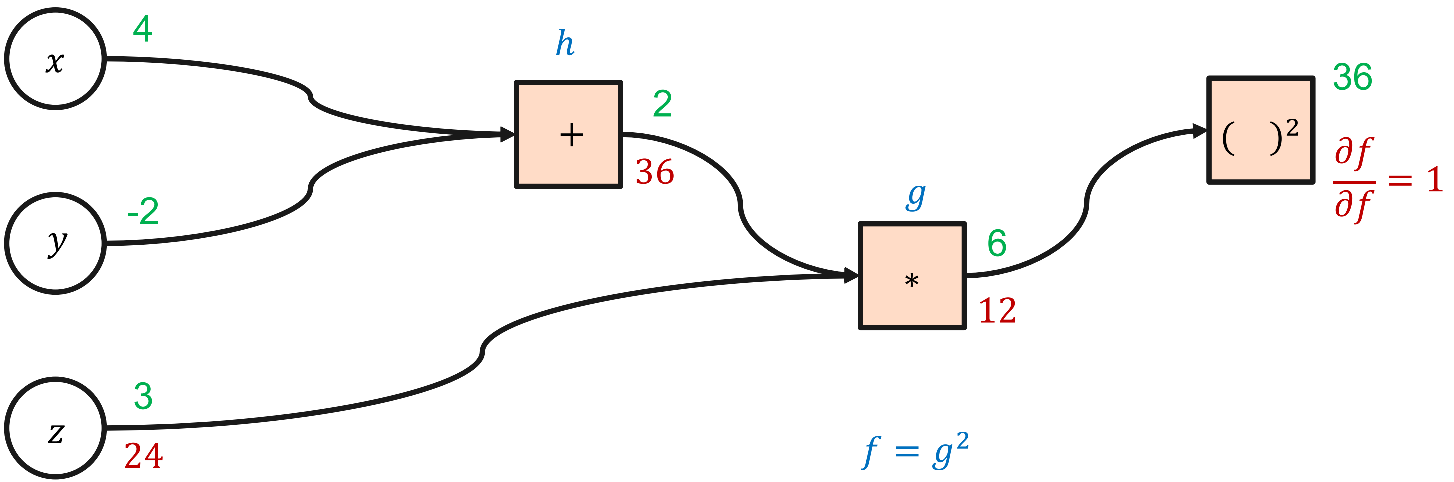
Forward Pass
Backward Pass

$$g = hz$$

$$\frac{\partial g}{\partial z} = h$$



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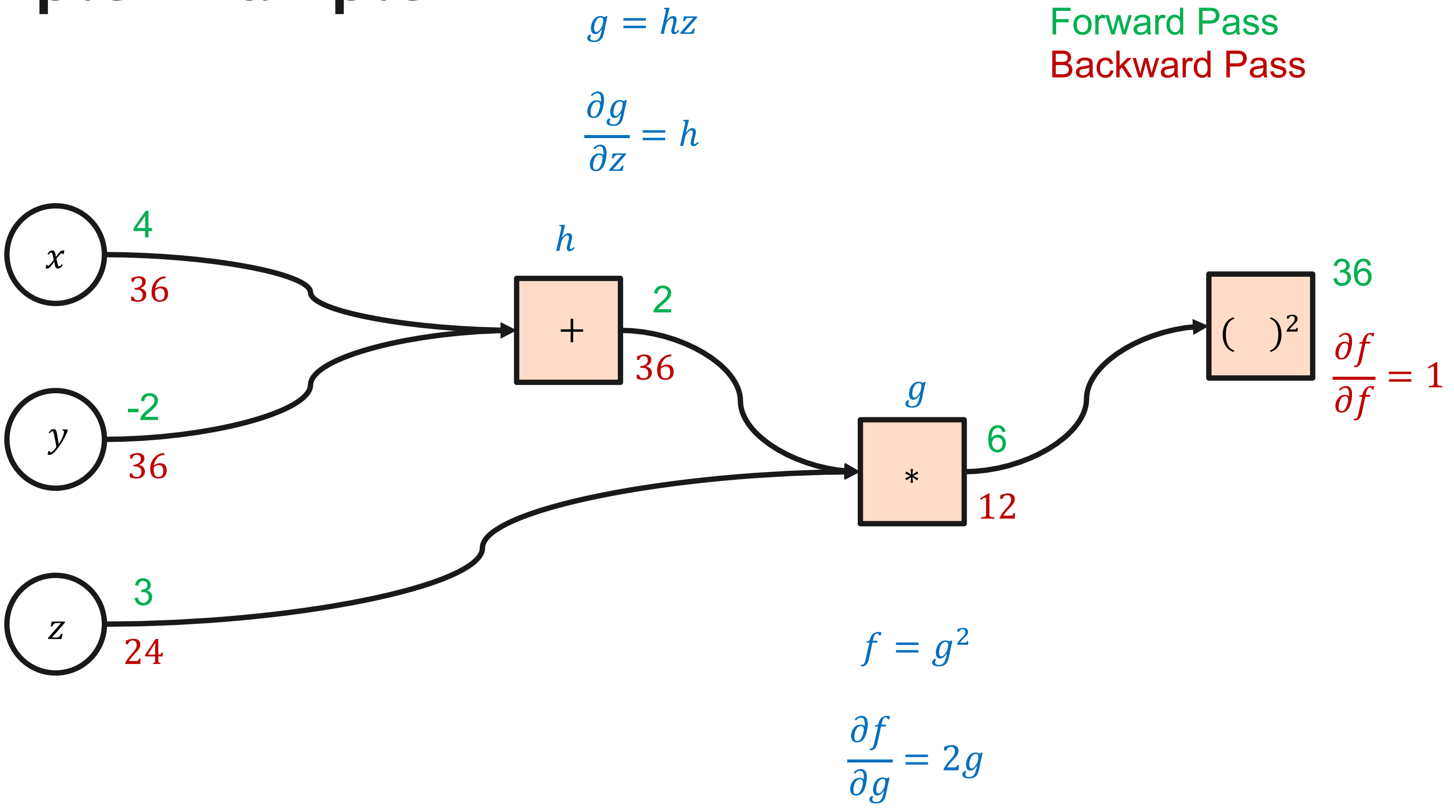
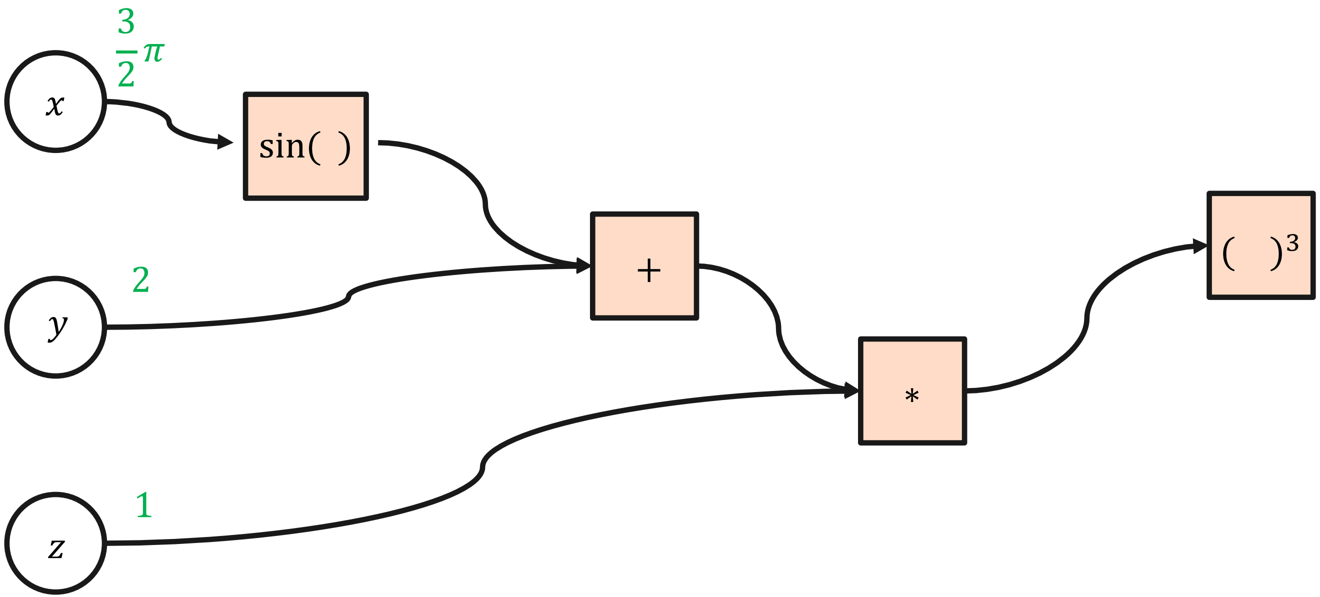


Exercise

$$f(x, y, z) = \left((\sin(x) + y)z\right)^3$$

Forward Pass



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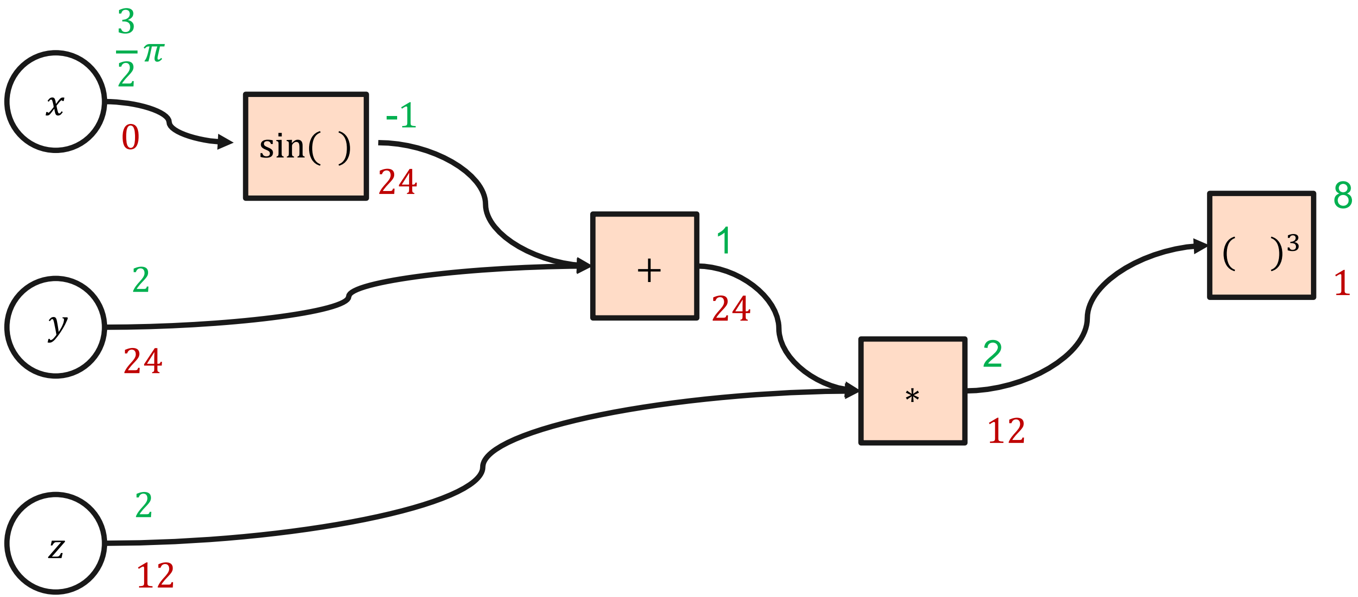
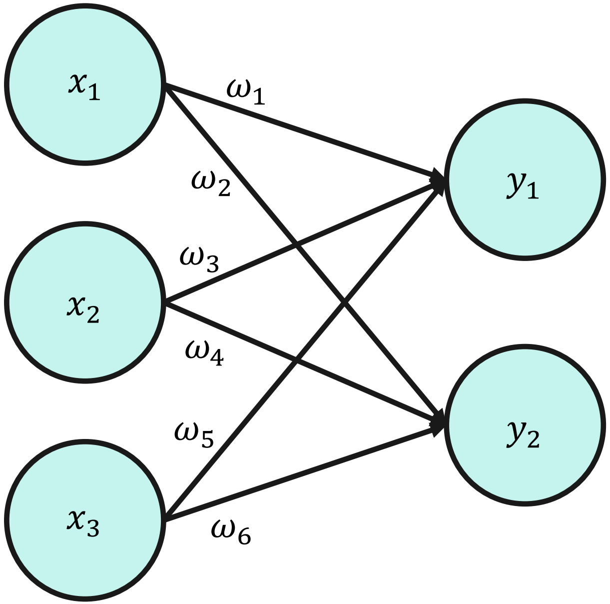
Exercise

Forward Pass
Backward Pass

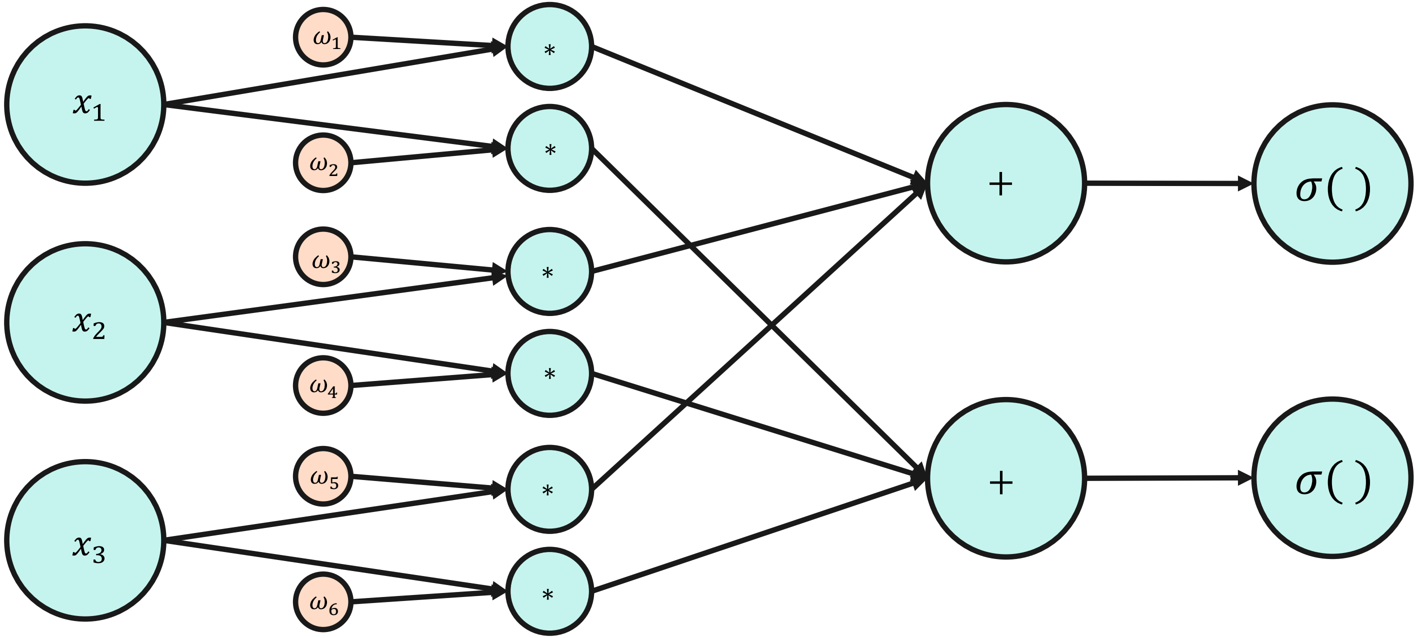


How to do Backpropagation Through This Layer?

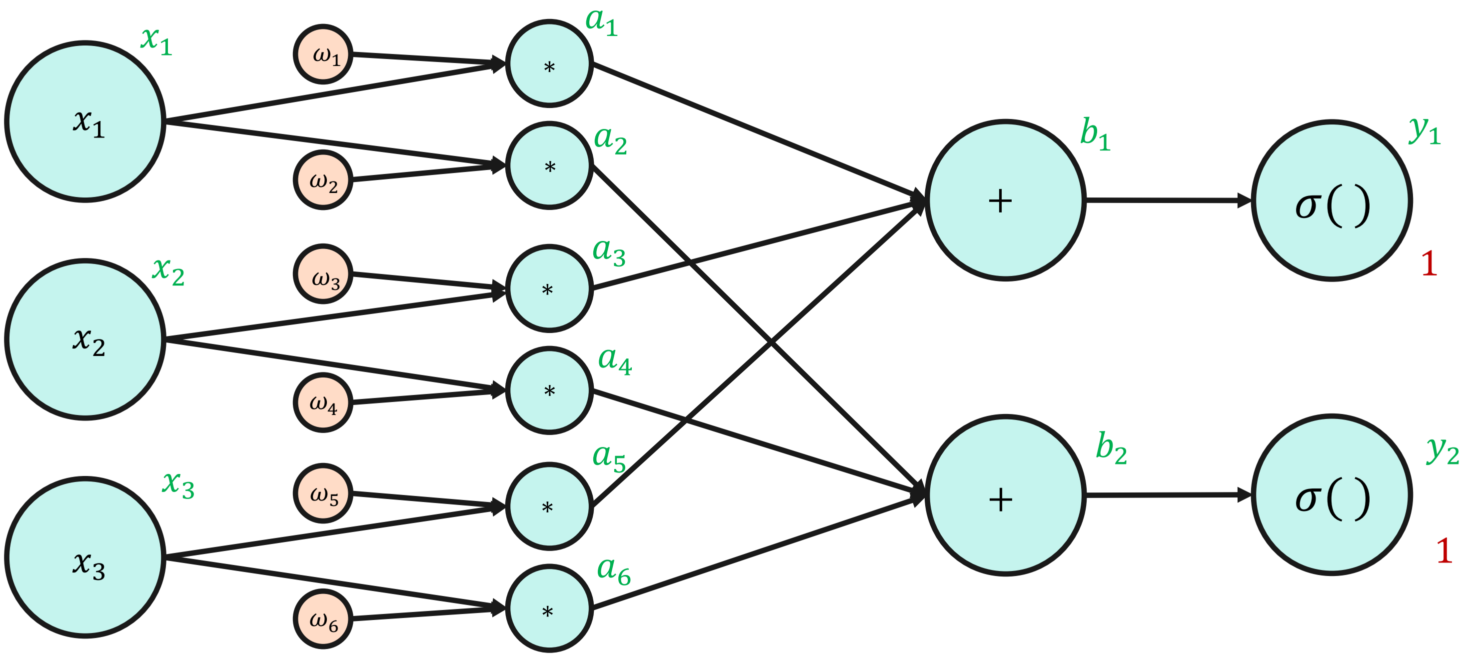
activation function already applied



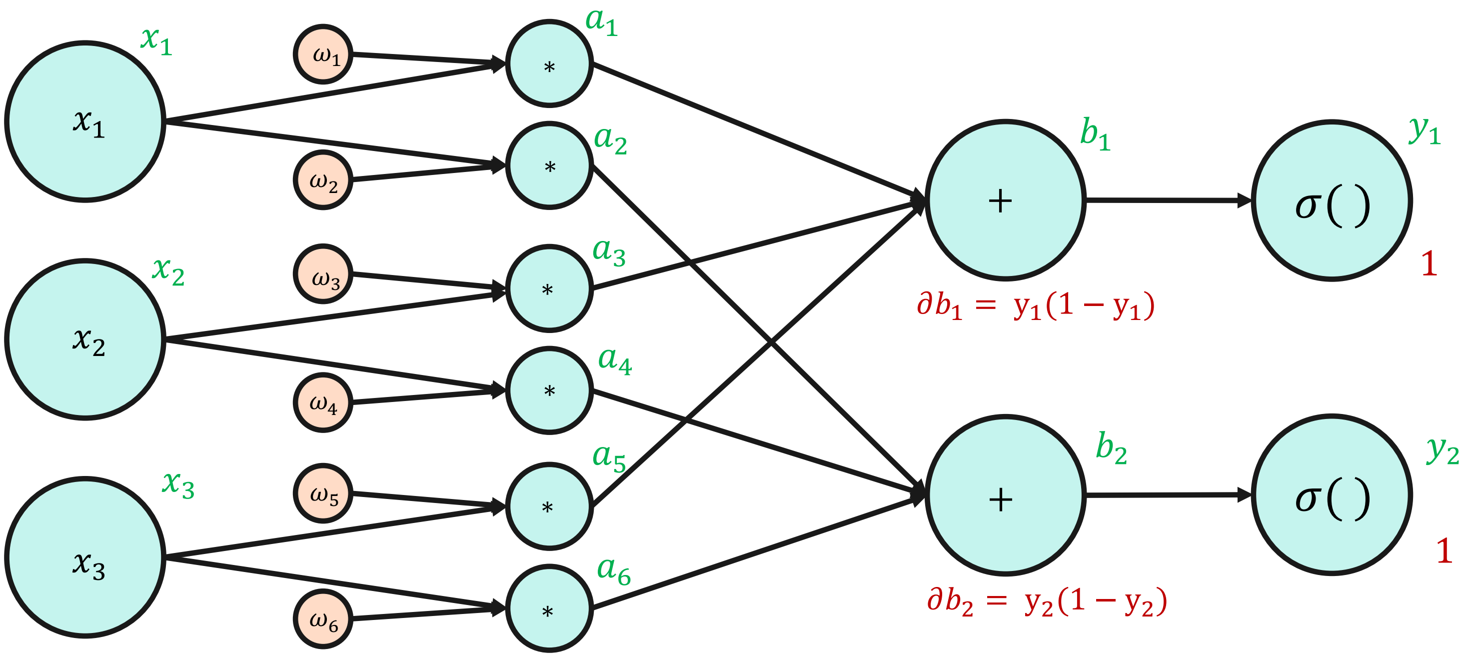
requires activation function



x_1
x_2
x_3
ω_1
ω_2
ω_3
ω_4
ω_5
ω_6
*
*
*
*
*
*
+
+
$\sigma(\,)$
$\sigma(\,)$

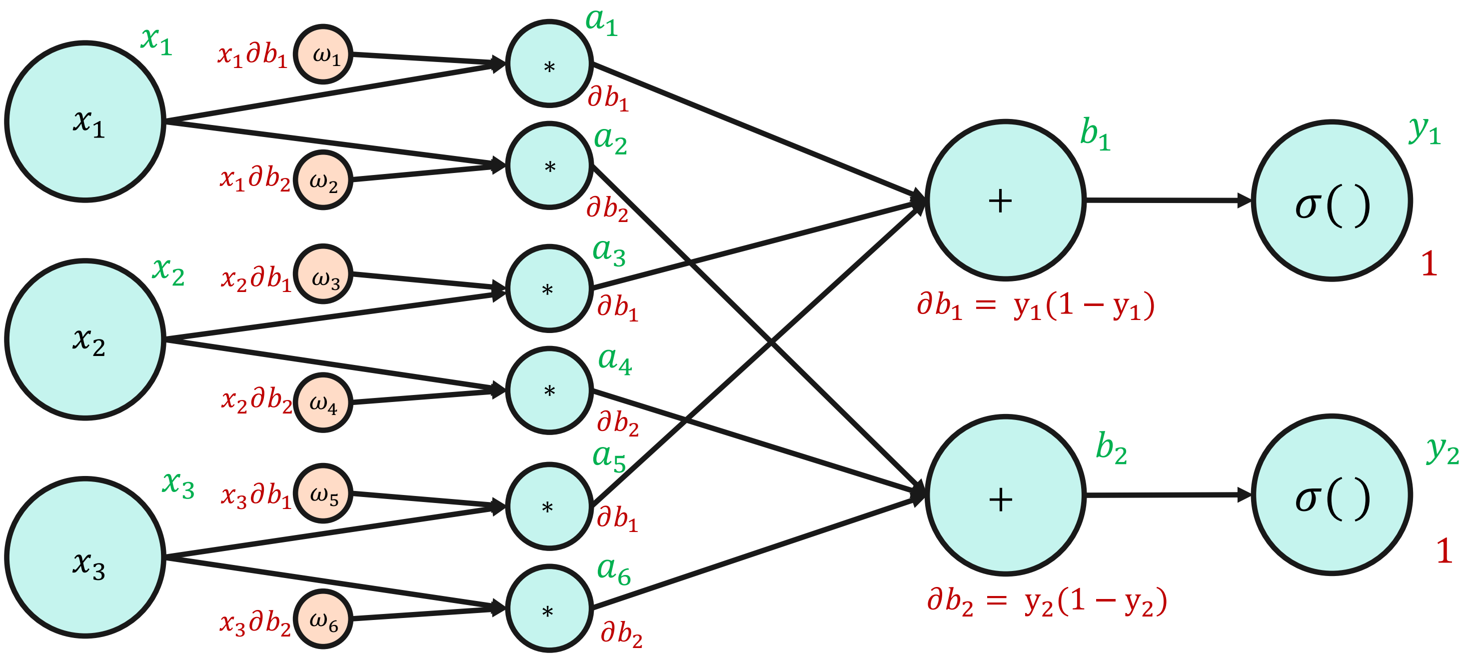

x_1
x_1
x_2
x_2
x_3
x_3
ω_1
ω_2
ω_3
ω_4
ω_5
ω_6
a_1
a_2
a_3
a_4
a_5
a_6
*
b_1
b_2
+
y_1
y_2
$\sigma(\,)$
1
1

$$\sigma(\mathrm{x}) = \frac{1}{1 + \mathrm{e}^{-\mathrm{x}}} \qquad \frac{\partial \sigma}{\partial x} = \sigma(x)(1 - \sigma(x))$$



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

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



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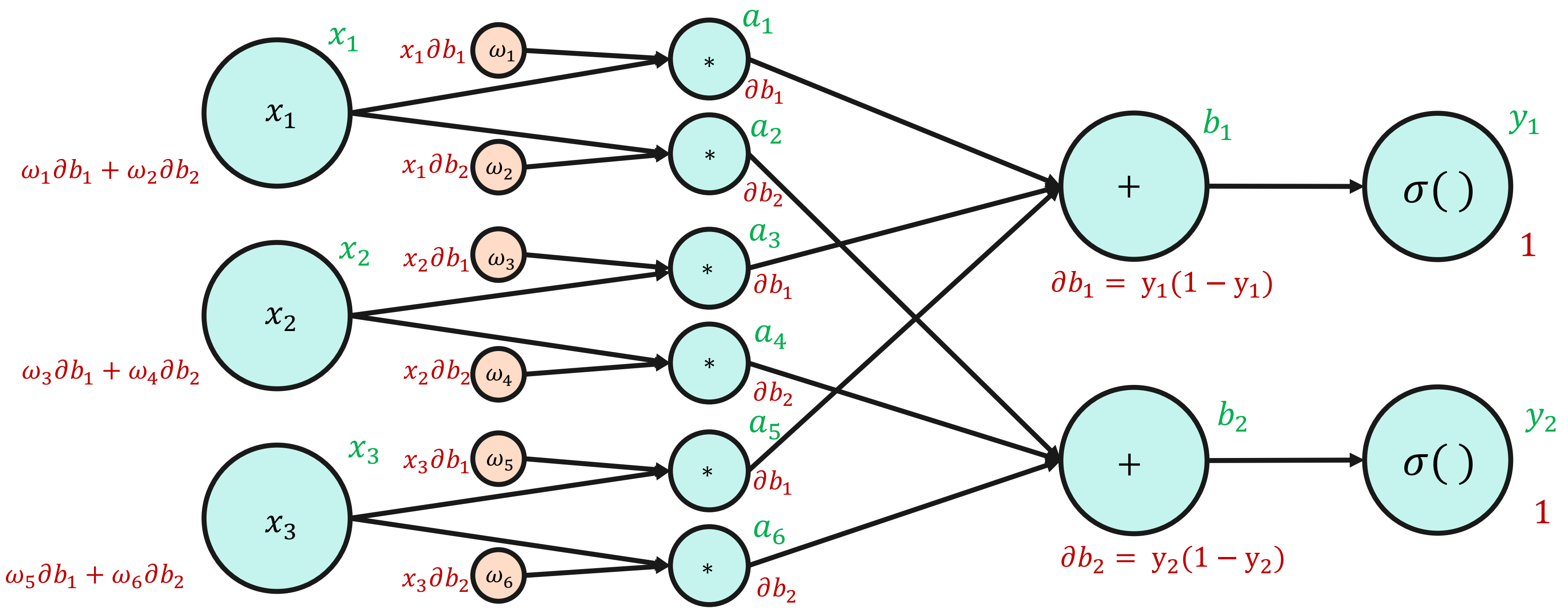
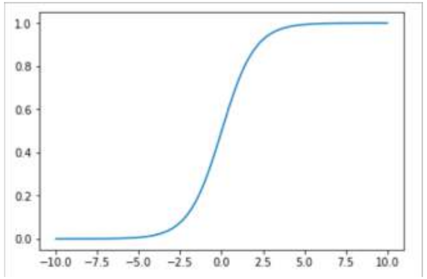


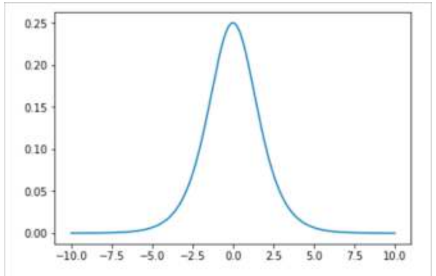
Everything can again be expressed using matrix multiplications.

Also note that we require all x and y values from the forwards pass!

Sigmoid Activation Function



$$\sigma(\mathrm{x}) = \frac{1}{1 + \mathrm{e}^{-\mathrm{x}}} \qquad \frac{\partial \sigma}{\partial x} = \sigma(x)(1 - \sigma(x))$$



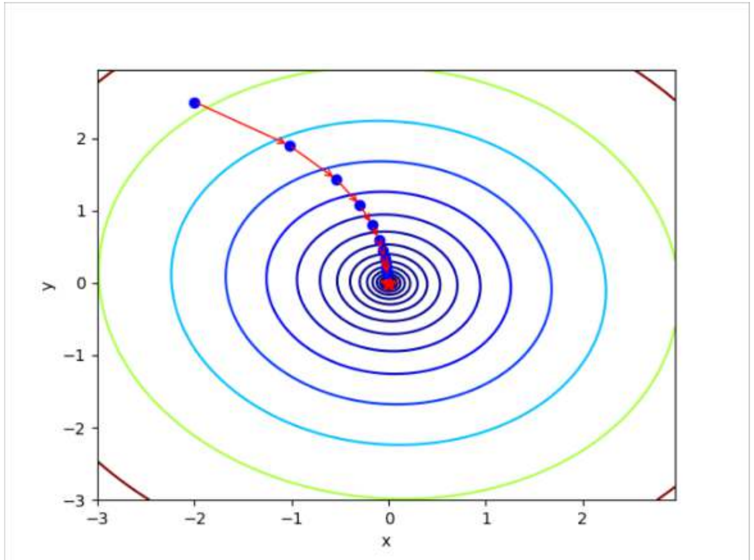
- Remember that back-propagation always multiplies with the previous gradients
- The maximum slop of the sigmoid function is 0.25 => very slow training for the first layers in deep network if sigmoid or similar activation functions are used.
- Gradients also very small for large absolute values
- Vanishing gradients
- Other activation functions are used for deep learning (see Thursday)

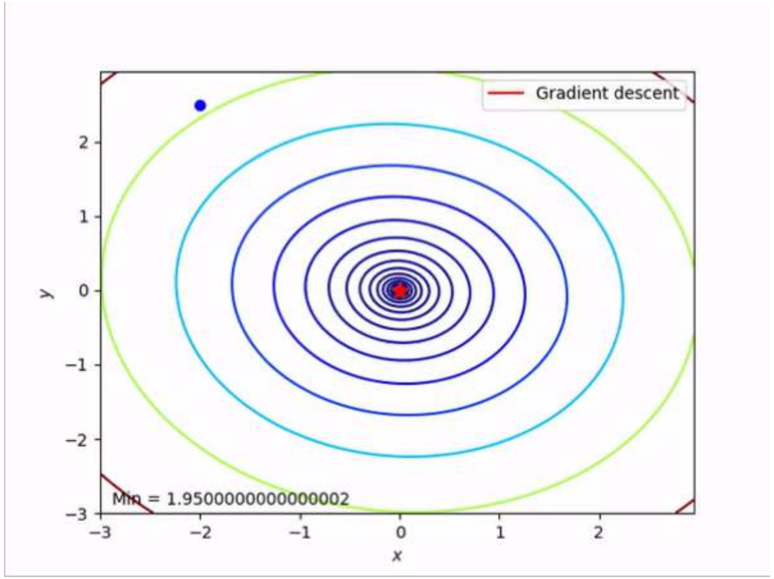
Let’s look at some code.

Gradient Descent

- Recall that we ruled out global optimization as there are just too many parameters in the network.
- And we have an analytic way to compute exact derivatives to all the parameters in our network.
- The most basic gradient based optimization algorithm is gradient descent:
    - Compute the gradient of the objective/loss function at the current point
    - Choose a step-length and walk in the direction of the negative gradient
    - Rinse and repeat

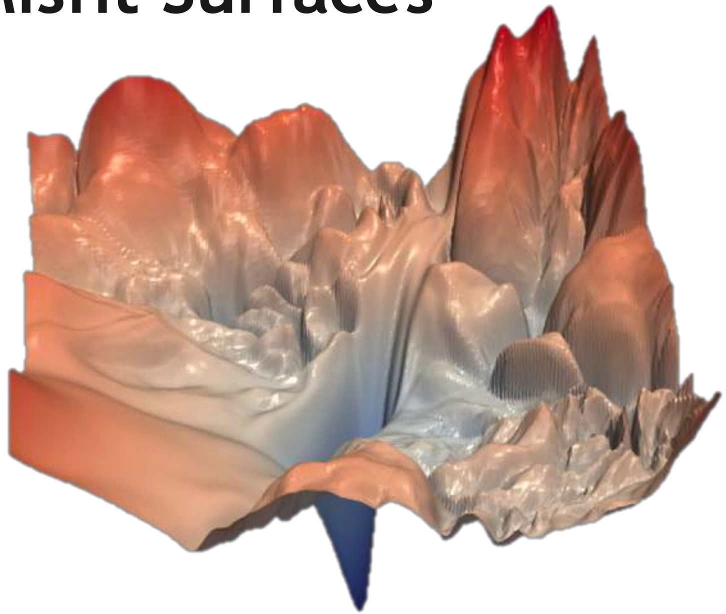
Gradient Descent Illustrations

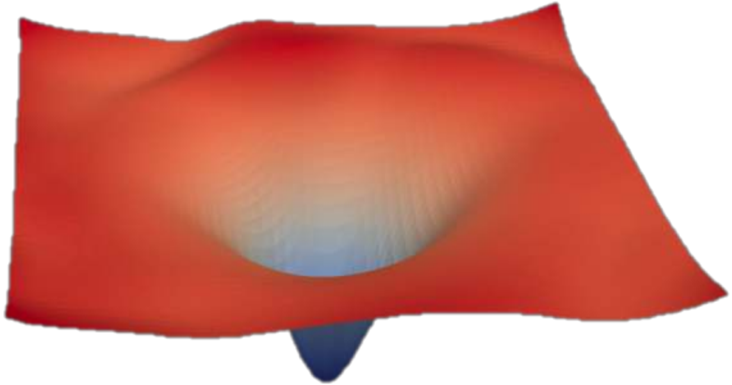




https://jed-ai.github.io/py1_gd_animation/

Misfit Surfaces





Li, Hao, et al. "Visualizing the loss landscape of neural nets." Advances in Neural Information Processing Systems. 2018.

Exercise: Implement Gradient Descent

How to Learn a Neural Network

- Design the network architecture (e.g number of inputs and outputs, number of layers, neurons in each layer, activation functions, ...).
- Loop until convergence:
    - Take a data sample, run a forward pass
    - Compute the loss of the result by comparing to the training data
    - Compute the gradient of the loss function with respect to the weights of the neural network via backpropagation
    - Update the weights with a chosen gradient based optimization algorithm

Have another look at the code.

Practicalities

- Straightforward gradient descent is rarely used. People instead use some for of stochastic gradient descent
- Higher-order methods like L-BFGS are also rarely used.
- The vanishing gradient problem needs to be dealt with.
- Regularization is important and all kinds of fancy tricks are done.
- Inputs and outputs are usually normalized in some fashion. Thus to actually use a neural network the outputs then have to be “denormalized” again.

Stochastic Gradient Descent

- Instead of computing the cumulative gradient of the whole training data set at once, compute it in so-called mini batches and update after each batch.
- This is called mini-batch gradient descent (stochastic gradient descent would be to update every time).
- Some momentum term is usually added to the optimization algorithm to deal with outliers in the gradients.

- Ends up being very fast (more efficient on GPUs to run many in parallel).
- Results in faster updates for highly redundant data.
- As the gradient is slightly different for each batch it can potentially get out of local minima again.

- State-of-the-art are adaptive mini-batched gradient descent methods like Adam, AdaGrad, RMSProb, …

http://ruder.io/optimizing-gradient-descent

Thank you.