COMP47750/COMP47990
Machine Learning with Python

Neural Networks

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Based on slides by Derek Greene

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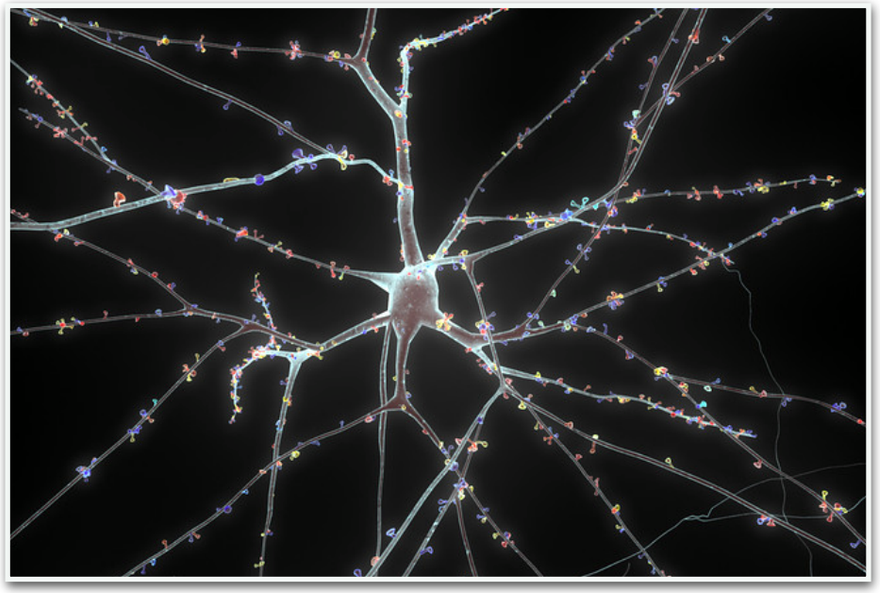
Motivation: Biological Inspiration

- Artificial Neural Networks (ANNs) are inspired by biological nervous systems, such as the brain, where large numbers of interconnected neurons work together to solve a problem.
- A neuron receives signals from other neurons through connections, called synapses.
- The combination of these signals, in excess of a certain activation level, will result in the neuron “firing” - i.e sending a signal on to other neurons connected to it.



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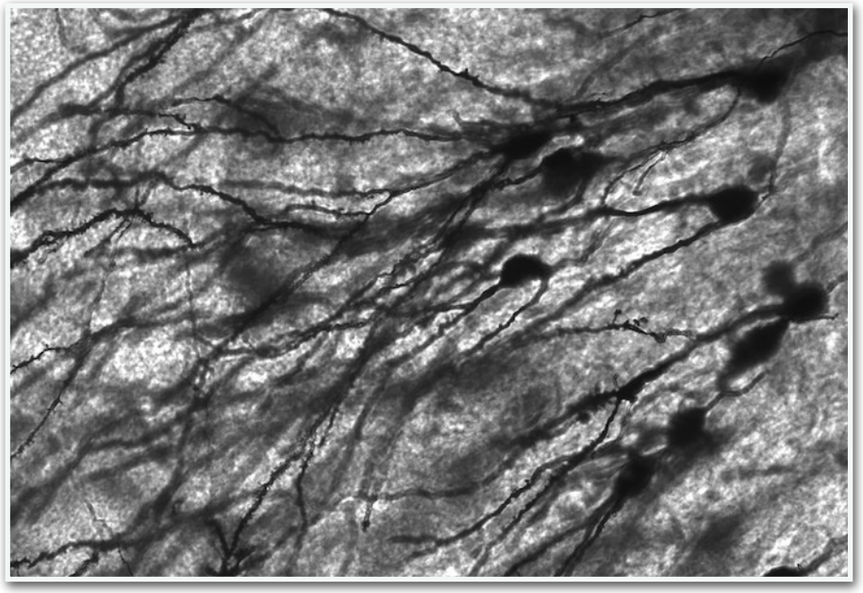
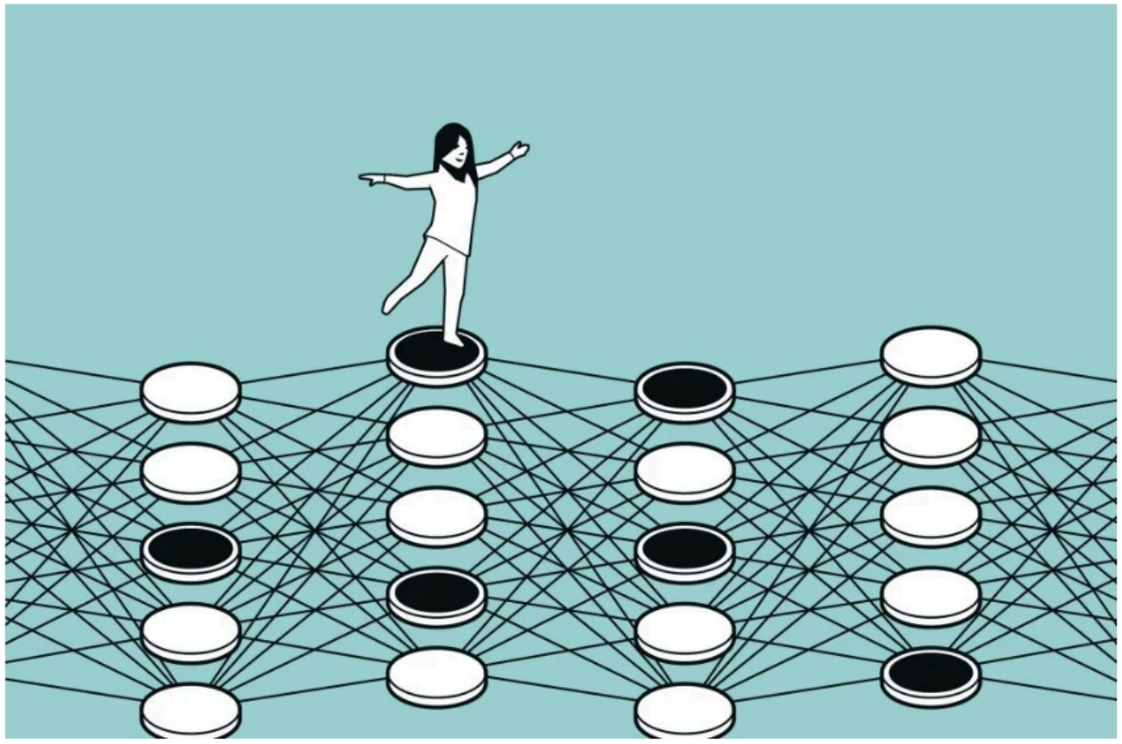


wikipedia.org

The Nobel Prize in Physics 2024

They used physics to find patterns in information

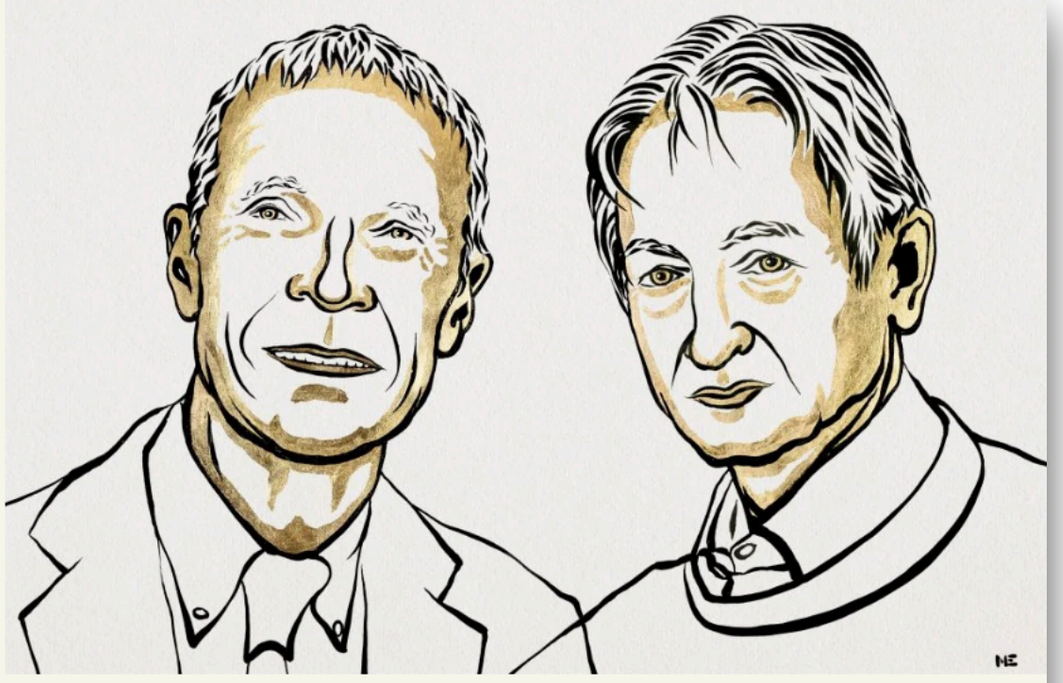
This year's laureates used tools from physics to construct methods that helped lay the foundation for today's powerful machine learning. John Hopfield created a structure that can store and reconstruct information. Geoffrey Hinton invented a method that can independently discover properties in data and which has become important for the large artificial neural networks now in use.



The 2024 physics laureates

The Nobel Prize in Physics 2024 was awarded to John J. Hopfield and Geoffrey E. Hinton "for foundational discoveries and inventions that enable machine learning with artificial neural networks."

John Hopfield created an associative memory that can store and reconstruct images and other types of patterns in data. Geoffrey Hinton invented a method that can autonomously find properties in data, and so perform tasks such as identifying specific elements in pictures.



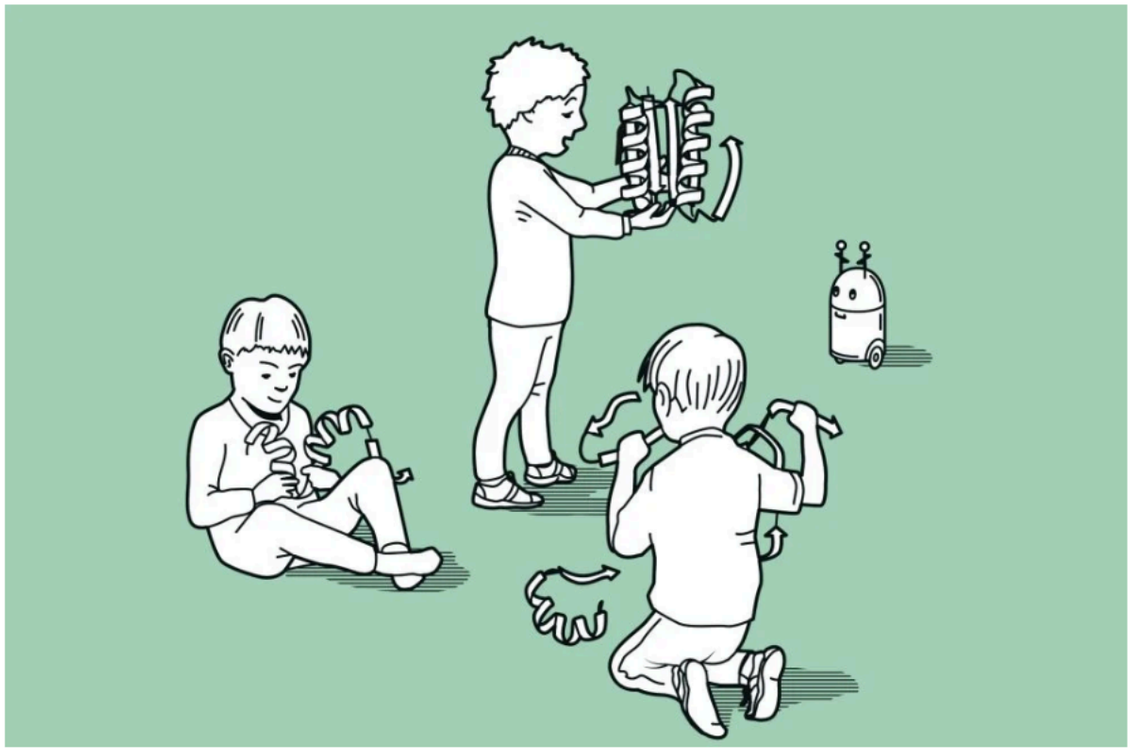
John Hopfield and Geoffrey Hinton. Ill. Niklas Elmehed © Nobel Prize Outreach

https://www.nobelprize.org/prizes/physics/

The Nobel Prize in Chemistry 2024

They cracked the code for proteins' amazing structures

The Nobel Prize in Chemistry 2024 is about proteins, life's ingenious chemical tools. David Baker has succeeded with the almost impossible feat of building entirely new kinds of proteins. Demis Hassabis and John Jumper have developed an AI model to solve a 50-year-old problem: predicting proteins' complex structures. These discoveries hold enormous potential.



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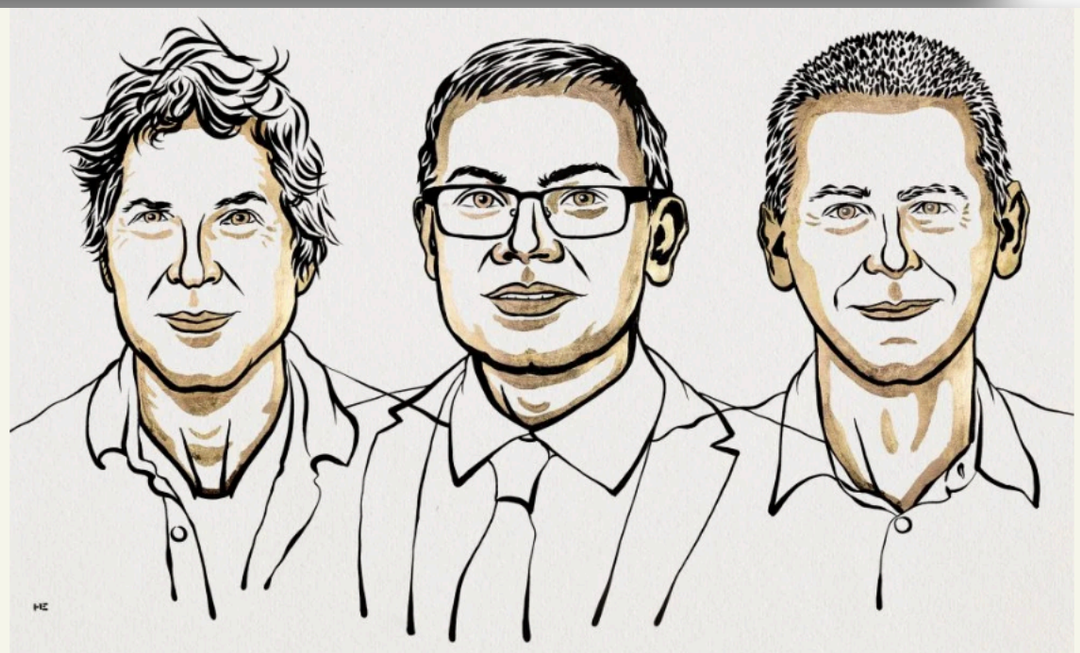
The 2024 chemistry laureates

The Nobel Prize in Chemistry 2024 was awarded with one half to David Baker "for computational protein design" and the other half jointly to Demis Hassabis and John M. Jumper "for protein structure prediction".

Demis Hassabis and John Jumper have successfully utilised artificial intelligence to predict the structure of almost all known proteins. David Baker has learned how to master life's building blocks and create entirely new proteins.



David Baker, Demis Hassabis and John Jumper. Ill. Niklas Elmehed
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https://www.nobelprize.org/prizes/chemistry/

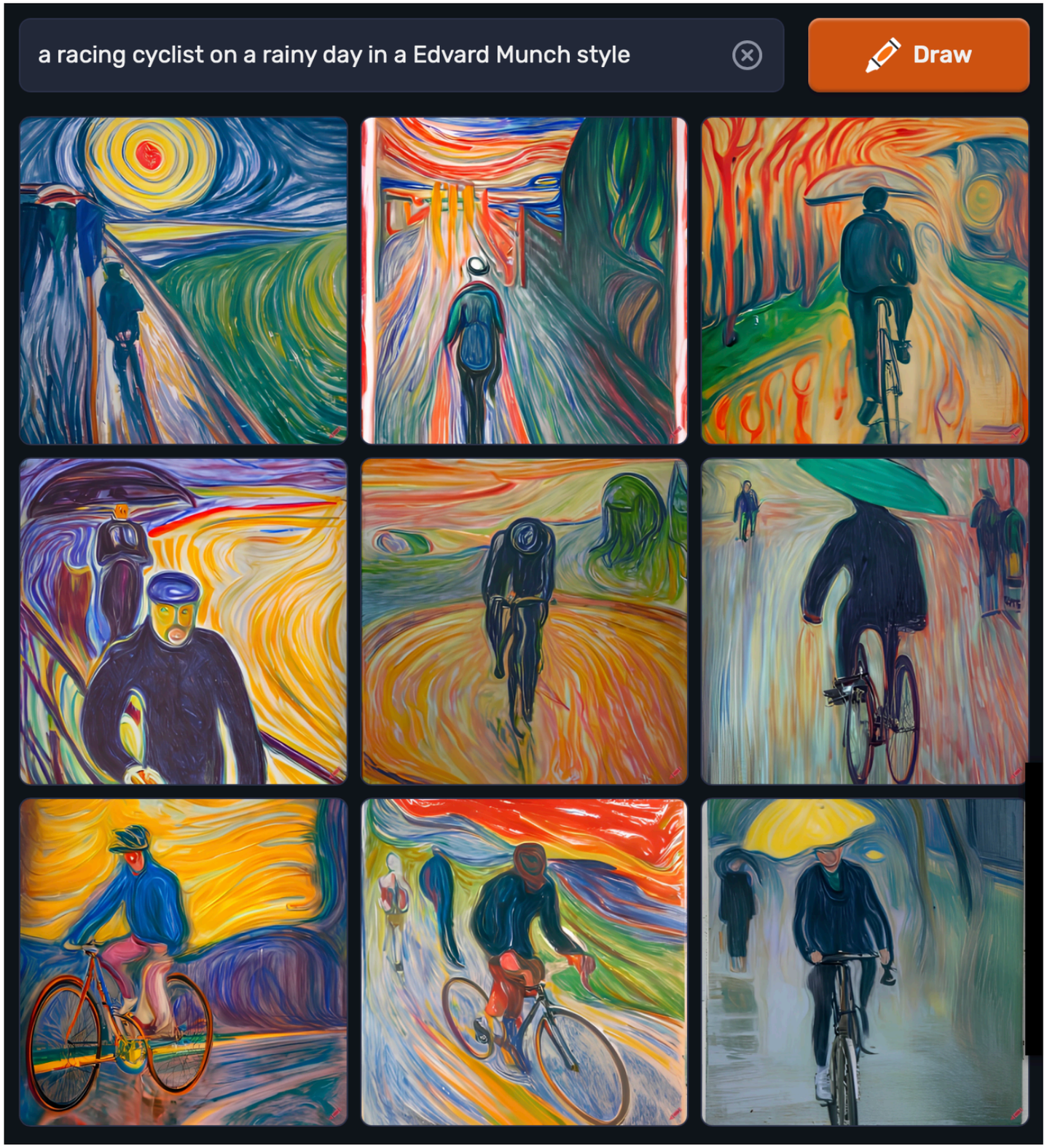
Why Neural Networks

- Transformer models are Deep NNs
  - Large Language Models (LLMs), e.g.
    - ChatGPT (generative pretrained transformer)
    - BERT
    - LaMDA - Google Bard
- Image Creation Tools
  - DALL-E
  -
- Deepfakes

"a racing cyclist on a rainy day in a Van Gogh style"

Algorithmic Bias

- BTW:
  - DALL-E seems to have a gender bias



COMP47750 Exam Aut 2023 Q1(f)

Why is it important for Neural Networks to have cost (loss) functions that are differentiable?

Cost functions, also known as loss functions, are used to quantify how well a neural network is performing on a particular task. They measure the difference between the predicted output of the network and the actual output, and this difference is used to update the network's parameters through a process called backpropagation.

One key reason why it is important for cost functions to be differentiable is that this property allows for the use of gradient-based optimization algorithms such as stochastic gradient descent (SGD) to update the network's parameters. These algorithms work by com
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Can you give me a shorter answer, say 80 words?

Differentiability is crucial for cost functions in neural networks because it enables the use of gradient-based optimization algorithms and automatic differentiation. These techniques are essential for efficiently updating the network's parameters to minimize the cost function and train the network to perform complex tasks. Without differentiability, the gradients of the cost function cannot be computed, and it becomes difficult to optimize the network.

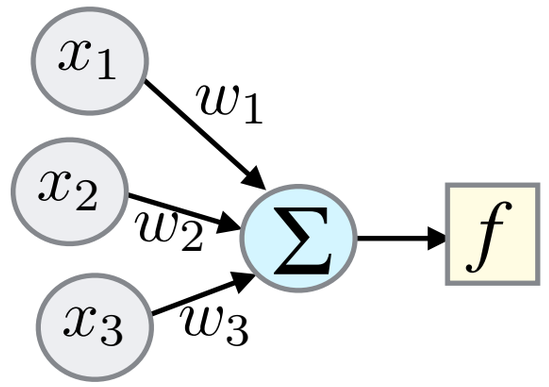
Motivation: Decision Making

Q. “Will a customer wait for a restaurant table?” - "Yes" or “No"
This decision might depend on a number of factors:

x_1 : Is the restaurant full? (0 or 1)

x_2 : Is the customer hungry? (0 or 1)

x_3 : Is a suitable alternative restaurant nearby? (0 or 1)



- We could determine weights w_i indicating how important each factor is in making the decision.
- For example, if x_2 is the most important factor, we might choose weights $w_1 = 0.2, w_2 = 0.6, w_3 = 0.2$
- If the weighted sum is greater than some predefined threshold, the customer might decide to move on to another restaurant ("No")

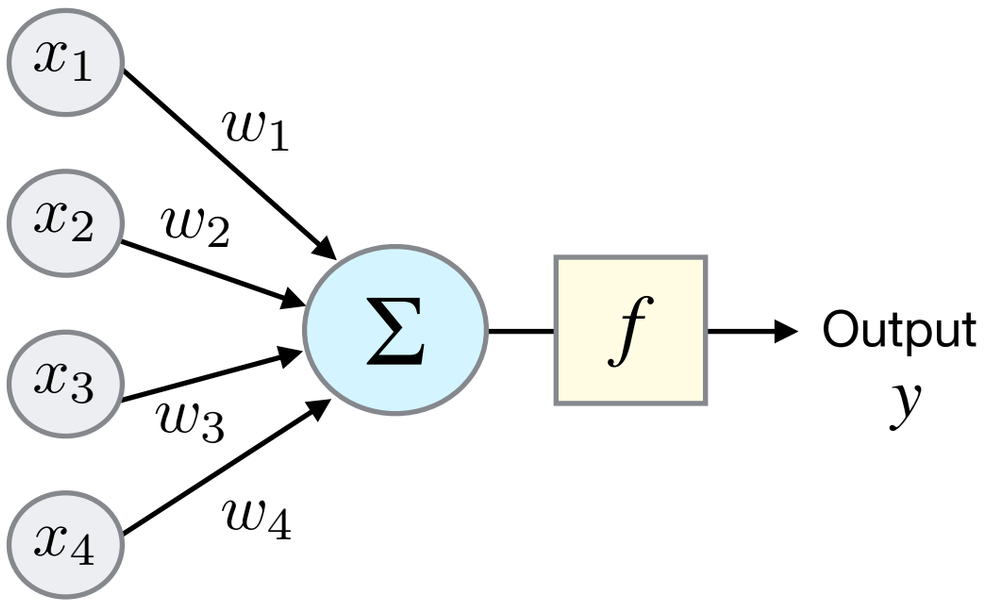
$$w_1 x_1 + w_2 x_2 + w_3 x_3 \geq \text{threshold}$$

$$\text{e.g. } (0.2 \times x_1) + (0.6 \times x_2) + (0.2 \times x_3) \geq 0.8$$

Modelling Neurons

- An artificial neuron makes decisions by weighing up evidence. It takes many input signals $\{x_1, x_2, \ldots\}$ and produces a single output.
- The inputs each have weights $\{w_1, w_2, \ldots\}$. These are real numbers which indicate the importance of the inputs to the output.
- The output y is computed by applying some function f to the weighted sum of the input signals $\{x_1, x_2, \ldots\}$. This is often called the activation function.

- **Example:** Neuron with 4 inputs and 4 corresponding weights.



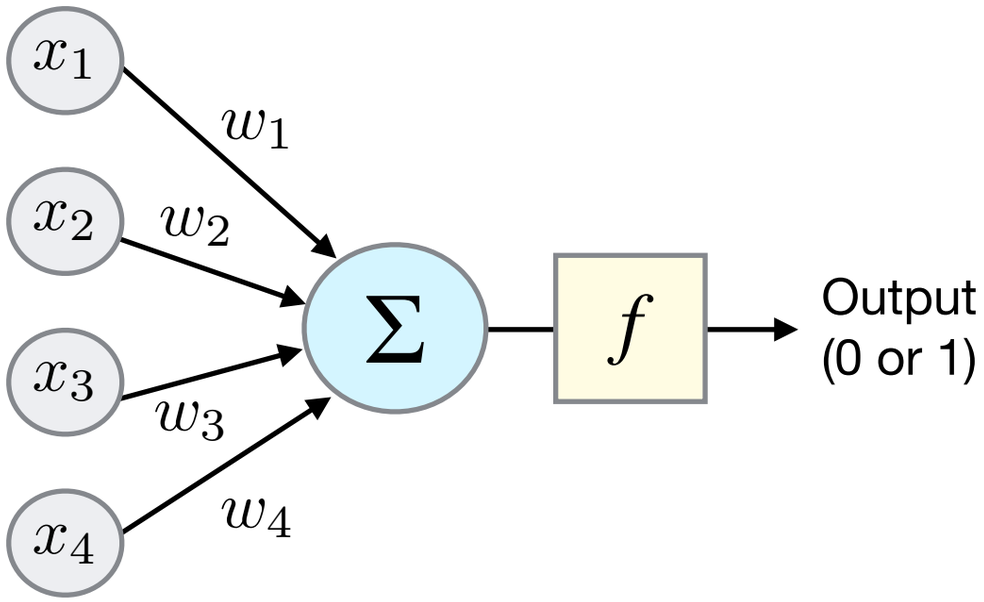
$$y = f(w_1x_1 + w_2x_2 + w_3x_3 + w_4x_4)$$

f : activation function

Note: neurons are sometimes called "units" or "nodes".

Perceptrons

- A perceptron is an artificial neuron which takes in many input signals and produces a single binary output signal (0 or 1). It can be used to solve simple binary classification problems.
- To produce a binary output (i.e. a classification decision), we apply a threshold function to the weighted sum of inputs $\{x_1, x_2, \ldots\}$
- This function determines if the perceptron activates ("fires").
- **Example:** Perceptron with 4 inputs and 4 corresponding weights.



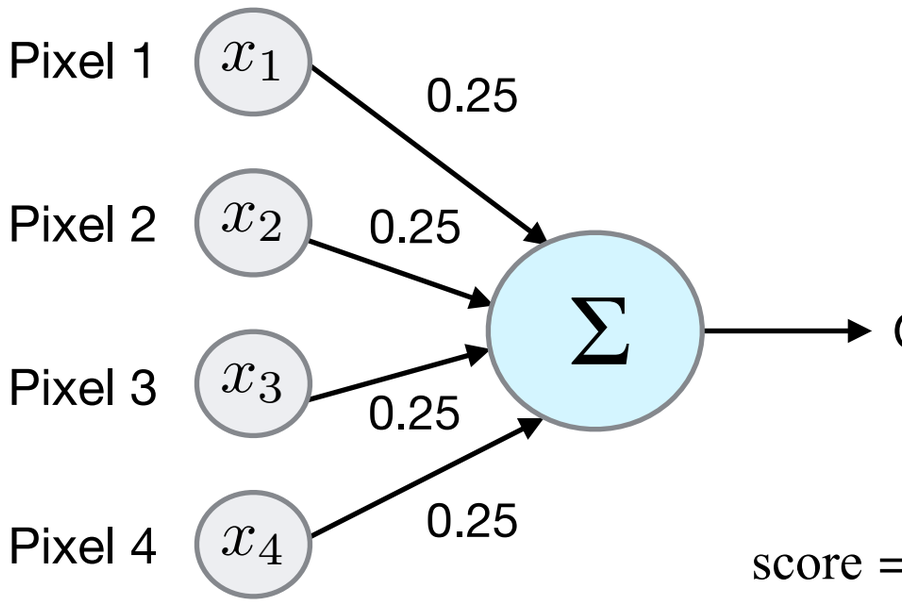
f : threshold function

$$\text{Output} = \begin{cases} 0 \text{ if } \sum_j w_j x_j < \text{ threshold} \\ 1 \text{ if } \sum_j w_j x_j \geq \text{ threshold} \end{cases}$$

Example: Perceptron

- Input is a 2x2 B&W image (i.e 4 pixels). Task is to classify the brightness of the image. All weights are equal (0.25) and using threshold value of 0.6. Output is "Dark" (0) or "Bright" (1).

x_1	x_2
x_3	x_4



Apply threshold function

$$\text{Output} = \begin{cases} 0 \text{ (Dark)} & \text{if score} < 0.6 \\ 1 \text{ (Bright)} & \text{if score} \geq 0.6 \end{cases}$$

$$\text{score} = (0.25 \times x_1) + (0.25 \times x_2) + (0.25 \times x_3) + (0.25 \times x_4)$$

1.0	1.0
1.0	1.0

score = 1.0

$\geq 0.6 \implies$ Bright

1.0	0.5
0.5	1.0

score = 0.75

$\geq 0.6 \implies$ Bright

1.0	0.5
0.5	0.0

score = 0.5

$< 0.6 \implies$ Dark

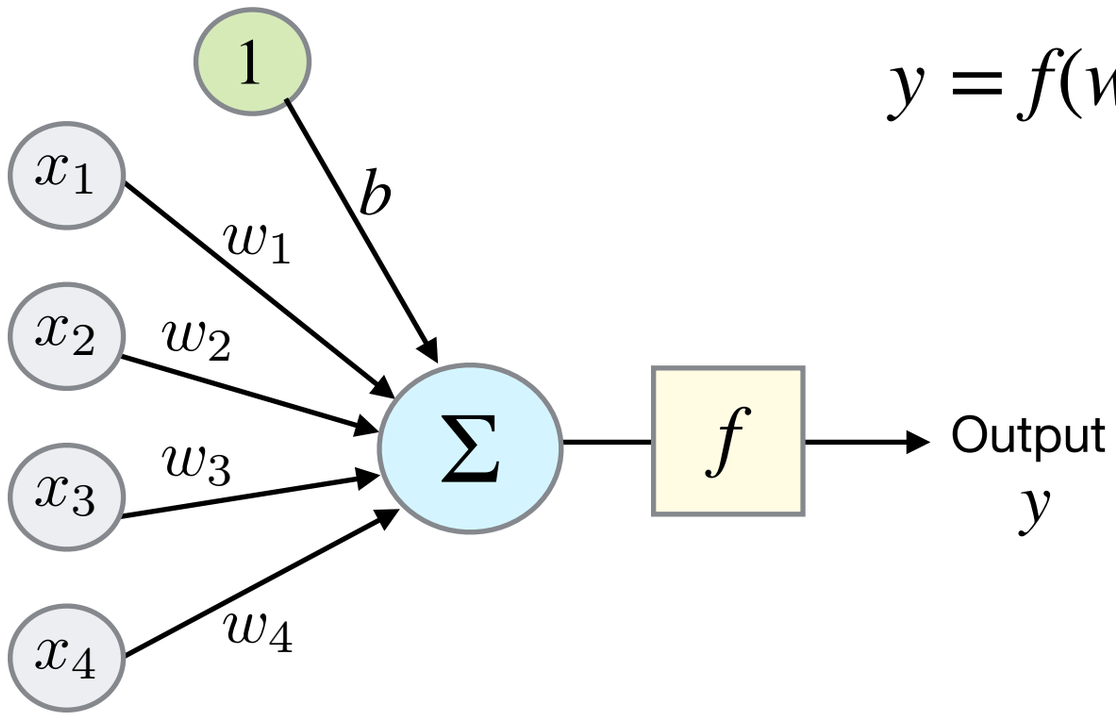
0.0	0.5
0.5	0.0

score = 0.25

$< 0.6 \implies$ Dark

Bias Term

- A bias term can be included in the network by adding an extra input with value $x_0 = 1$ to the inputs with weight b.
- Intuitively the bias represents how difficult it is for a particular neuron to send out a signal. It "shifts" the activation function.
- The bias term is treated like any other weight in the activation function. The main function of bias is to provide every neuron with a trainable constant value, in addition to the inputs.
- **Example:** Neuron with 4 inputs and a bias.



$$y = f(w_1x_1 + w_2x_2 + w_3x_3 + w_4x_4 + b)$$

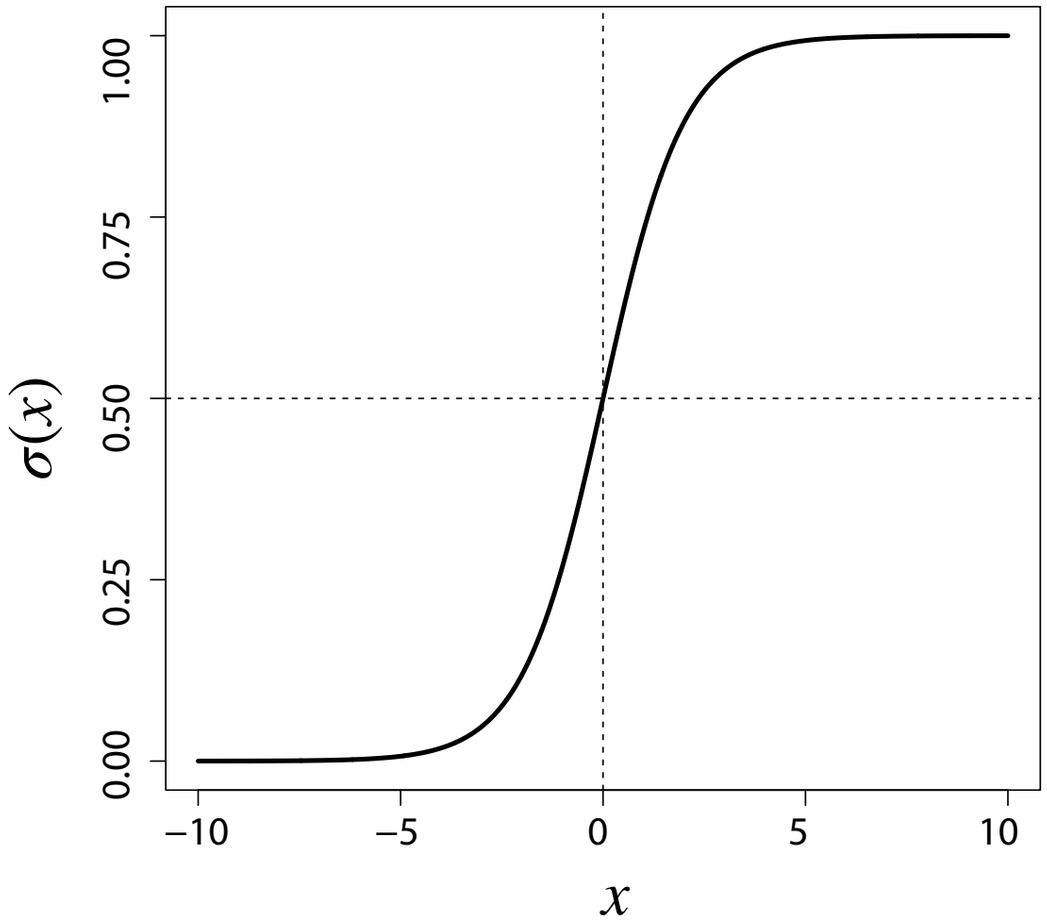
f : activation function

Now the weights and the bias impact on the output of the neuron.

Activation Functions

- An issue with a perceptron is that a small change in the input values can cause a large change in the output. This is because it has only two possible states: 0 or 1.
- Instead we can use alternative activation functions which produce a continuous output.
- The sigmoid function (also called logistic function) is a common example, which follows a S-shape.

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

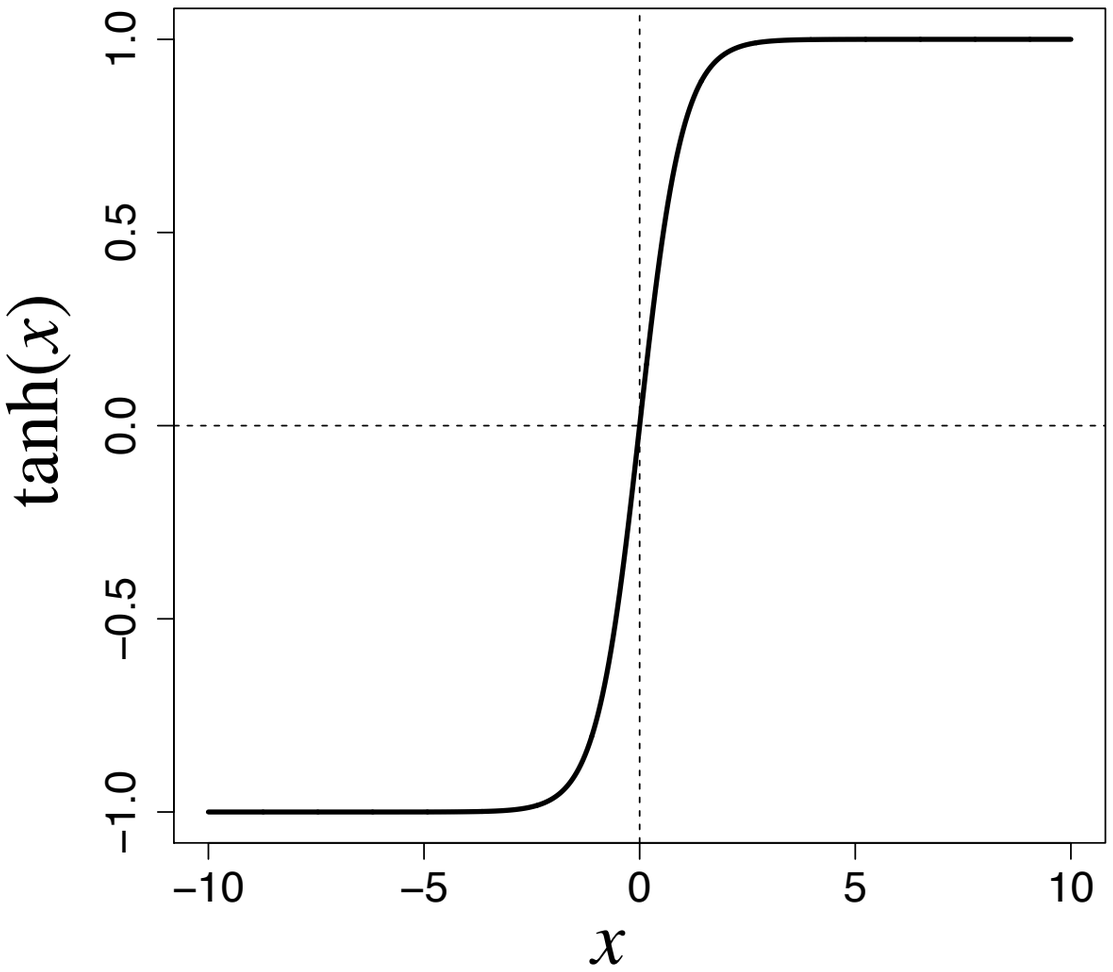


For a particularly positive or negative value of x, the output will be similar to a perceptron (0 or 1). For values closer to the boundary, the output will be near 0.5.

Activation Functions

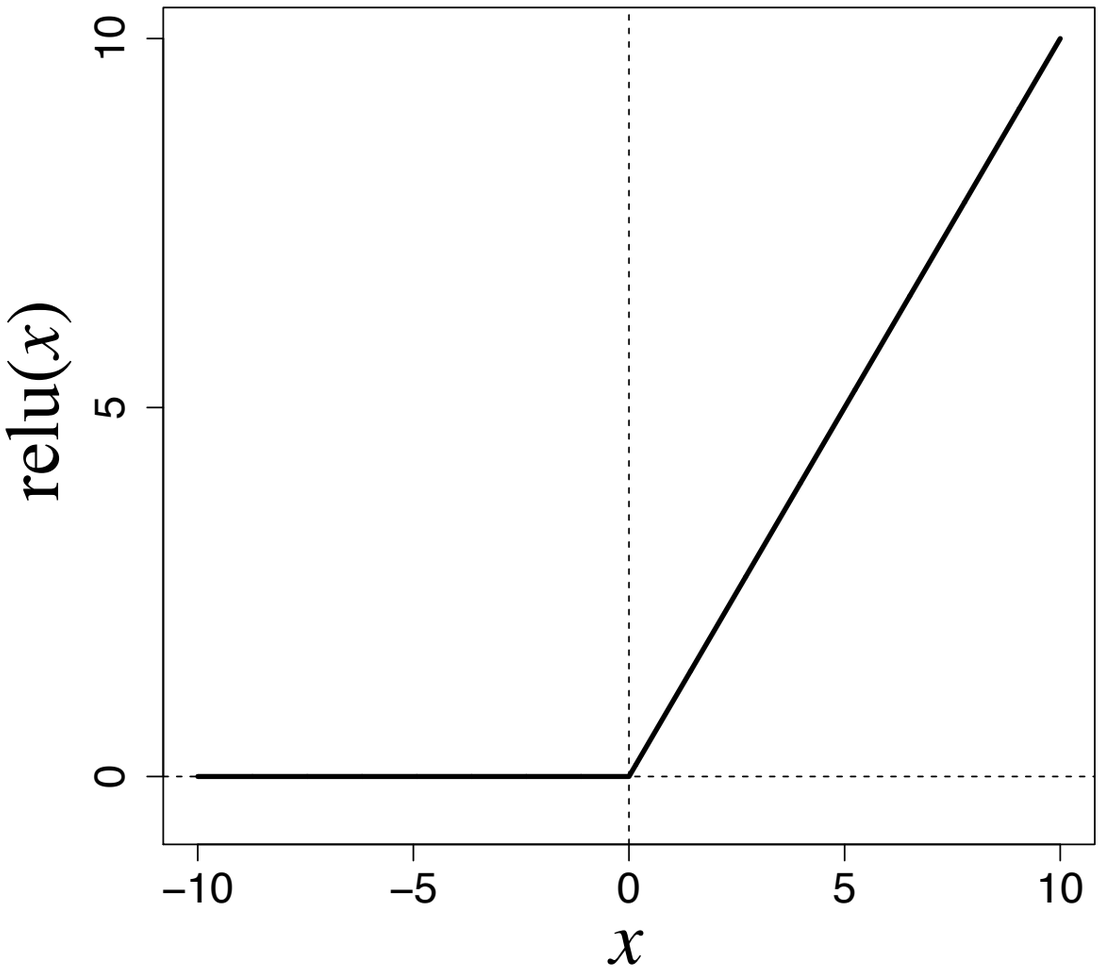
- Many other activation functions have been proposed...

Hyperbolic Tangent



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

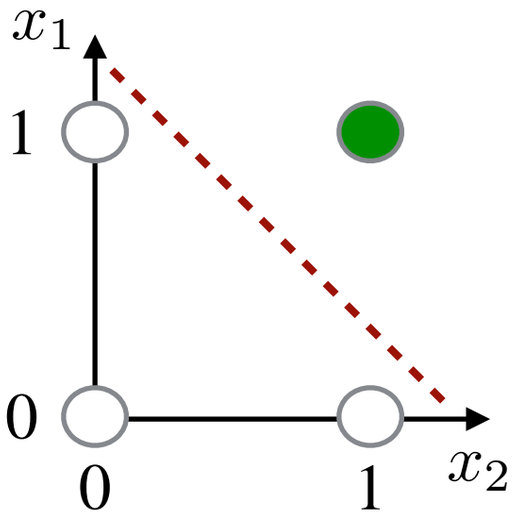
Rectifier ("Ramp")



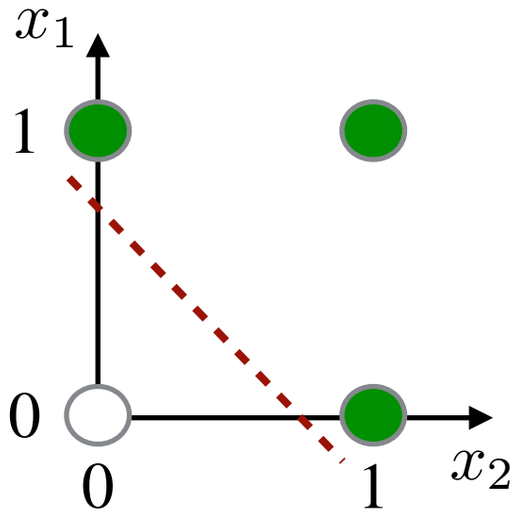
$$\text{relu}(x) = \max(0, x)$$

Perceptron Limitations

- A single perceptron can only handle linearly separable problems i.e. if there is a line that can divide the fires and the non-fires.
- **Example:** Boolean AND and OR functions are linearly separable.



x_1 **AND** x_2



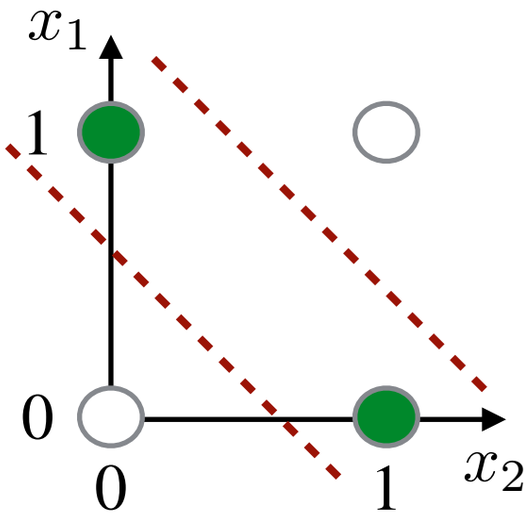
x_1 **OR** x_2

x_1	x_2	AND
0	0	0
0	1	0
1	0	0
1	1	1

x_1	x_2	OR
0	0	0
0	1	1
1	0	1
1	1	1

Perceptron Limitations

- A single perceptron can only handle linearly separable problems i.e. if there is a line that can divide the fires and the non-fires.
- **Example:** Boolean AND and OR functions are linearly separable. But the XOR ("Exclusive OR") function is not linearly separable.



x_1 **XOR** x_2

x_1	x_2	XOR
0	0	0
0	1	1
1	0	1
1	1	0

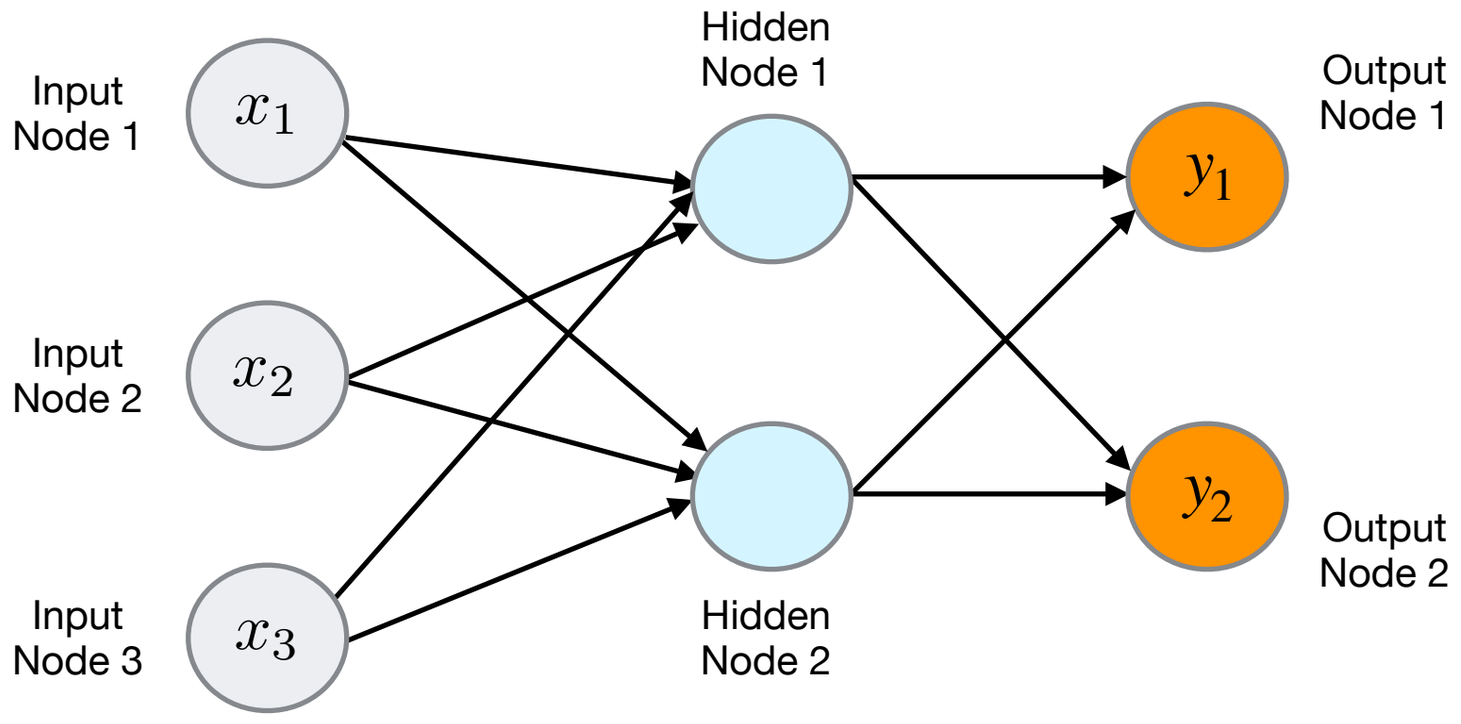
(Minsky & Papert, 1969)

Q. How can we solve non-linearly separable problems like this?

Multilayer Networks

- Depending on the problem, complex decisions may require long chains of computational stages.
- By building a slightly more complicated neural network with an intermediary layer, we can solve non-linear problems that cannot be solved using only a single layer of inputs and outputs.
- The inputs and outputs are typically represented as separate nodes. The network can have multiple outputs as well as inputs.

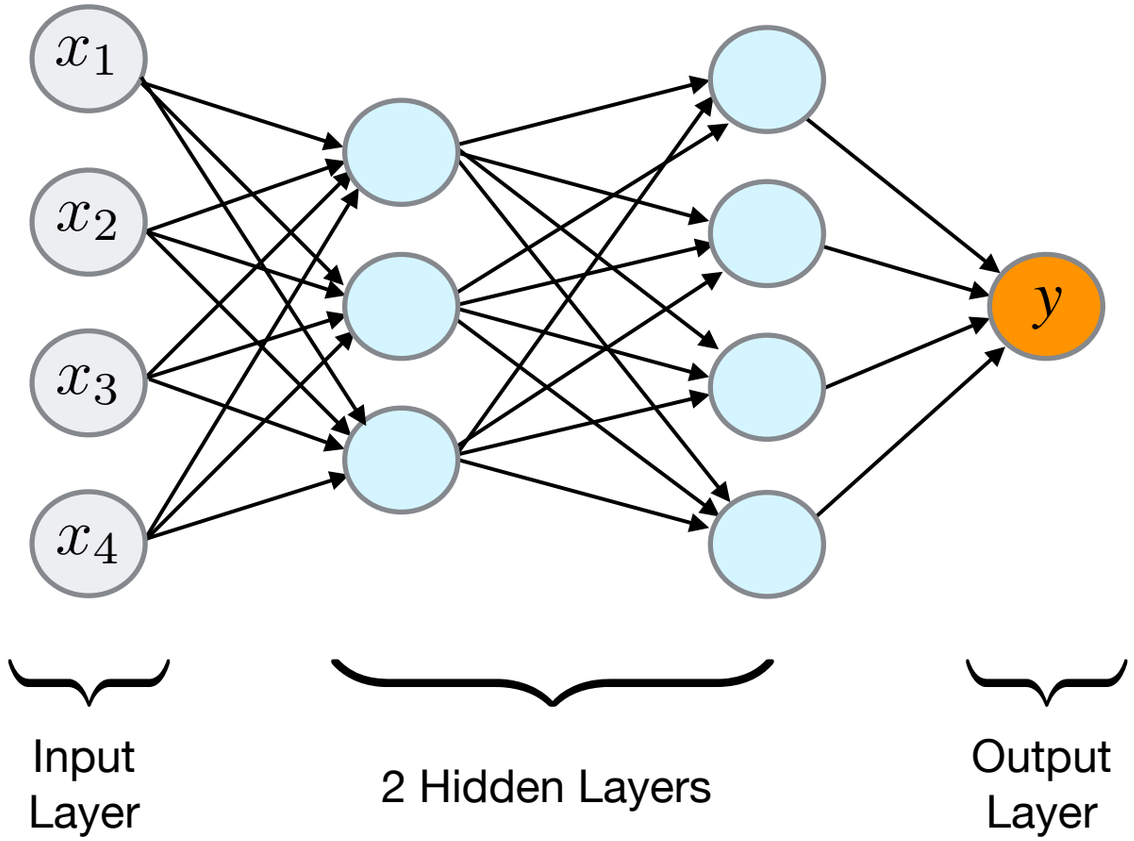
The nodes in between are "hidden".



Multilayer Networks

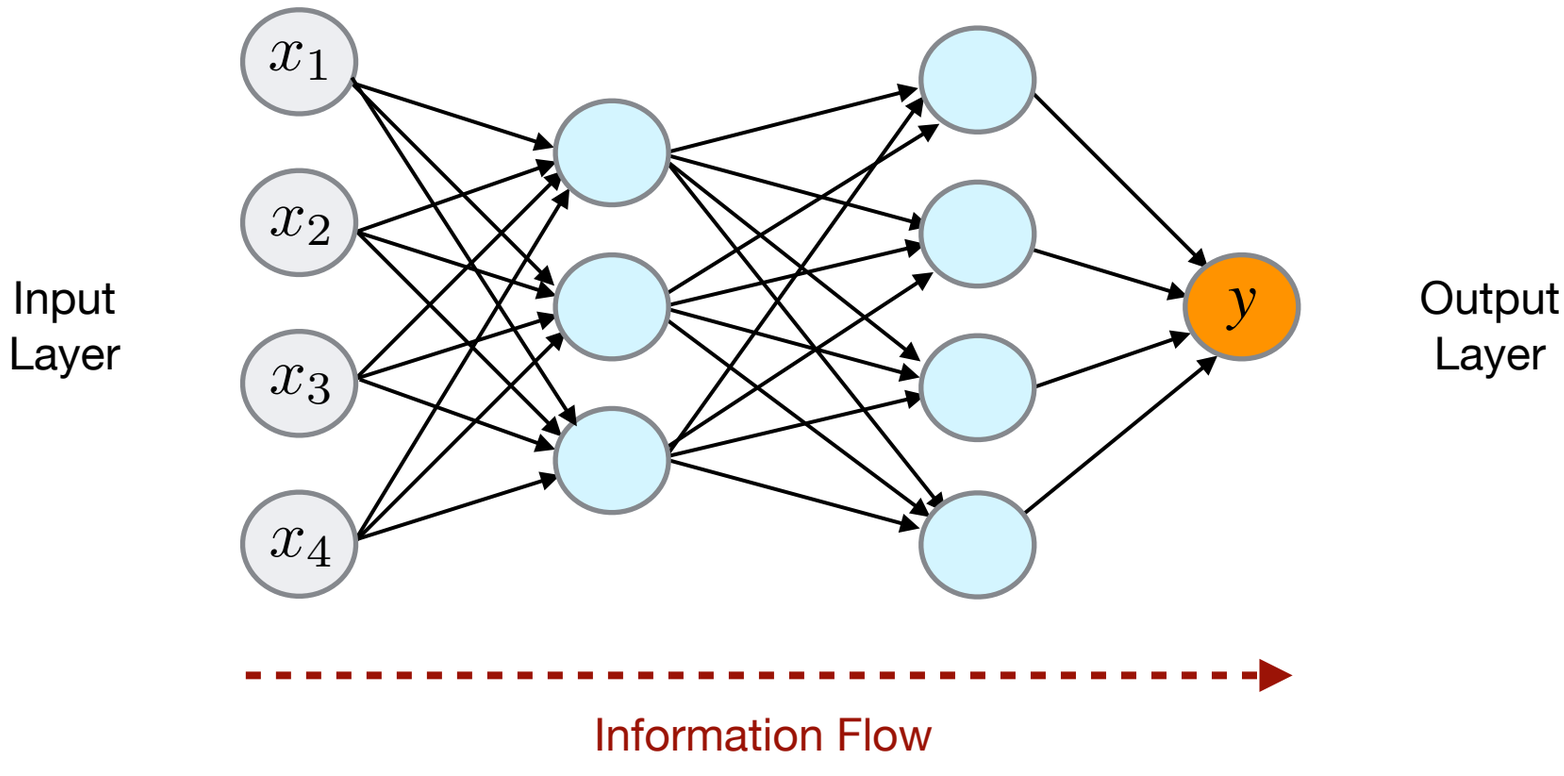
- We can build many different network configurations involving multiple layers of nodes (neurons):
  - 1st layer makes a decision based on the inputs.
  - 2nd layer makes a decision based on the decision from 1st layer.
  - 3rd layer can make an even more complex decision etc...

- The layers of nodes stacked between the inputs and outputs are called the hidden layers.
- Note nodes can feed into multiple new nodes in the next layer.



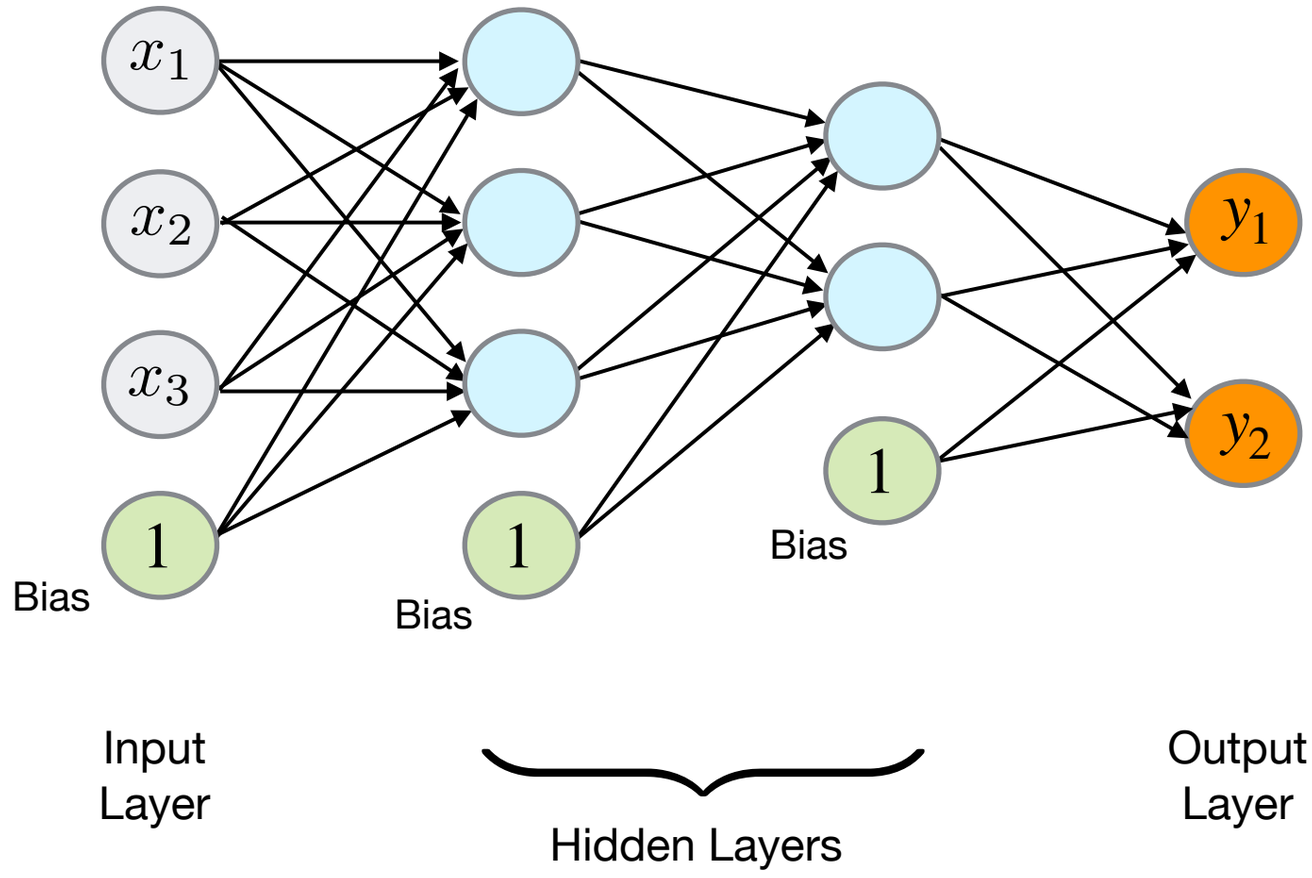
Feedforward Networks

- Since information flows in one direction and there are no cycles, this kind of network is often referred to as a feed-forward network.
- Each layer consists of nodes which receive their input from the previous layer directly above, and send their outputs to the next layer directly below. There are no connections within a layer.
- To compute the output of the network, we can successively compute all the activations in Layer 1, Layer 2, etc.



Bias in Multilayer Networks

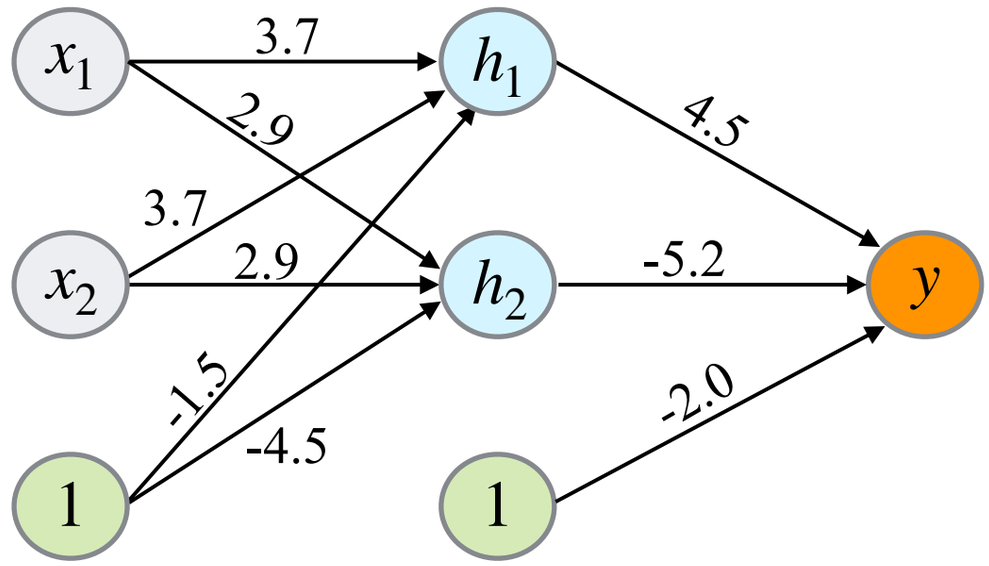
- In multi-layer networks we can add a bias term, with a constant value 1, as an extra node in each pre-output layer. In this case, the bias terms can all have different weights.
- These bias nodes are not connected to any nodes in the previous layer, so are not influenced by the outputs from previous layers.



Example: Multilayer Network

- **Configuration:** One input layer with 2 inputs. One hidden layer, one output. Using a sigmoid activation function.

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



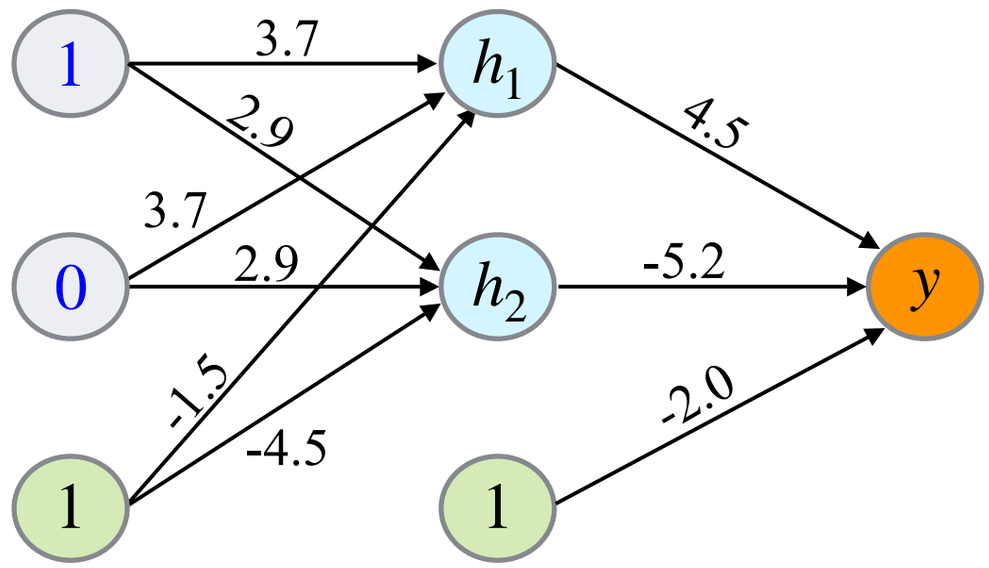
Example: Multilayer Network

- **Configuration:** One input layer with 2 inputs. One hidden layer, one output. Using a sigmoid activation function.

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

- Consider the case of the inputs:

$$x_1 = 1, x_2 = 0$$



- Compute values based on the inputs:

$$h_1 = \sigma((1 \times 3.7) + (0 \times 3.7) + (1 \times -1.5)) = \sigma(2.2) = \frac{1}{1 + e^{-2.2}} = 0.90$$

$$h_2 = \sigma((1 \times 2.9) + (0 \times 2.9) + (1 \times -4.5)) = \sigma(-1.6) = \frac{1}{1 + e^{1.6}} = 0.17$$

Example: Multilayer Network

- We now use these values as inputs to the output layer, in order to compute the output value of the network.

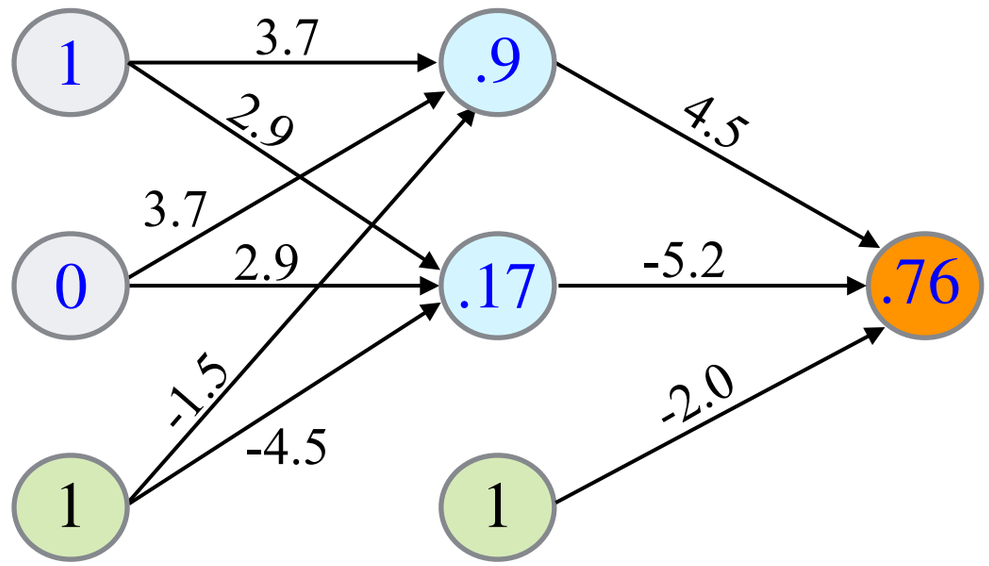
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

- Original inputs:

$$x_1 = 1, x_2 = 0$$

- Inputs to output layer:

$$h_1 = 0.9, h_2 = 0.17$$



- Compute output value:

$$y = \sigma((0.9 \times 4.5) + (0.17 \times -5.2) + (1 \times -2.0)) = \sigma(1.17)$$

$$= \frac{1}{1 + e^{-1.17}} = 0.76$$

Example: Multilayer Network

- We can compute other network outputs for different pairs of binary inputs in the same way:

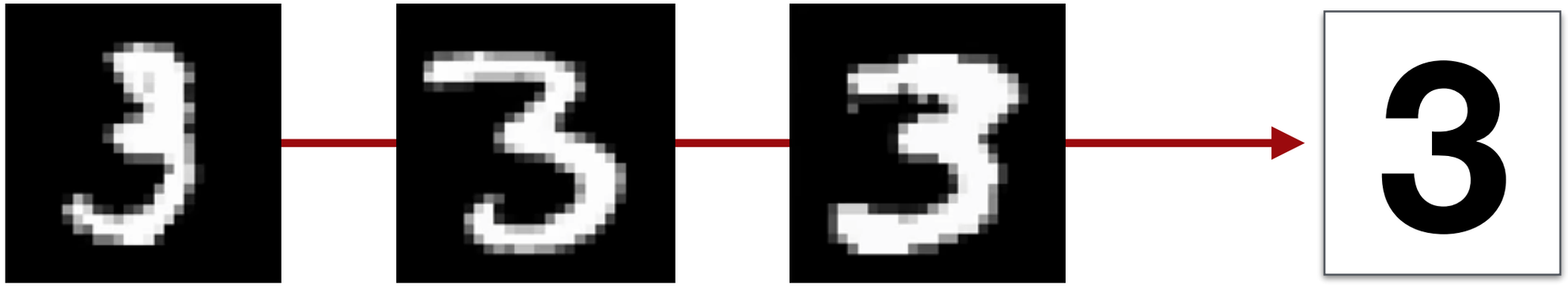
Input x_1	Input x_2	Hidden h_1	Hidden h_2	Output	Approx.
0	0	0.18	0.01	0.23	$\Longrightarrow 0$
0	1	0.90	0.17	0.76	$\Longrightarrow 1$
1	0	0.90	0.17	0.76	$\Longrightarrow 1$
1	1	1.00	0.79	0.17	$\Longrightarrow 0$

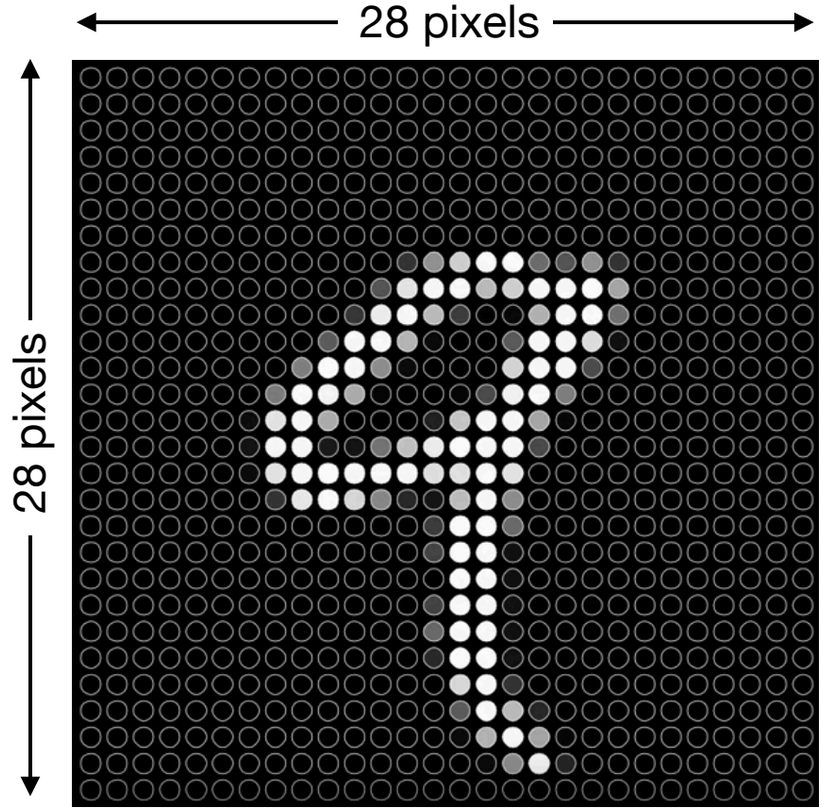
- Notice that this network roughly implements the XOR function.
- The hidden node h_1 implements the OR function.
- The hidden node h_2 implements the AND function.

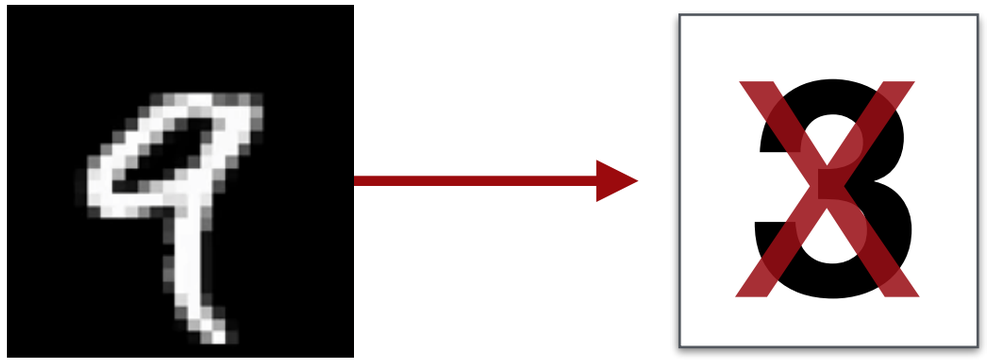
➡ By chaining these, we can solve a more complex problem.

Example: Handwritten Digits

- **Task:** How can we learn to automatically recognise hand written digits, based on their pixel representations?

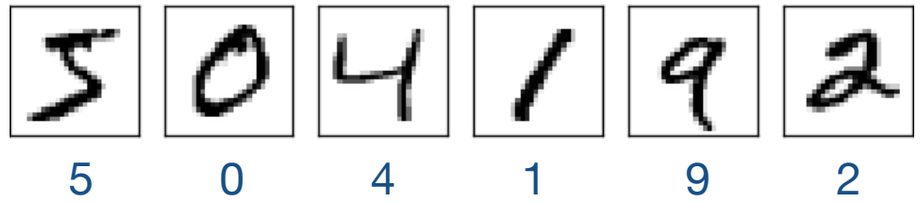






Example: Handwritten Digits

- **Goal:** Classify handwritten digit images into classes (0,1,…9)
- Input: Training set of many 28x28 pixel images labelled with correct digit.

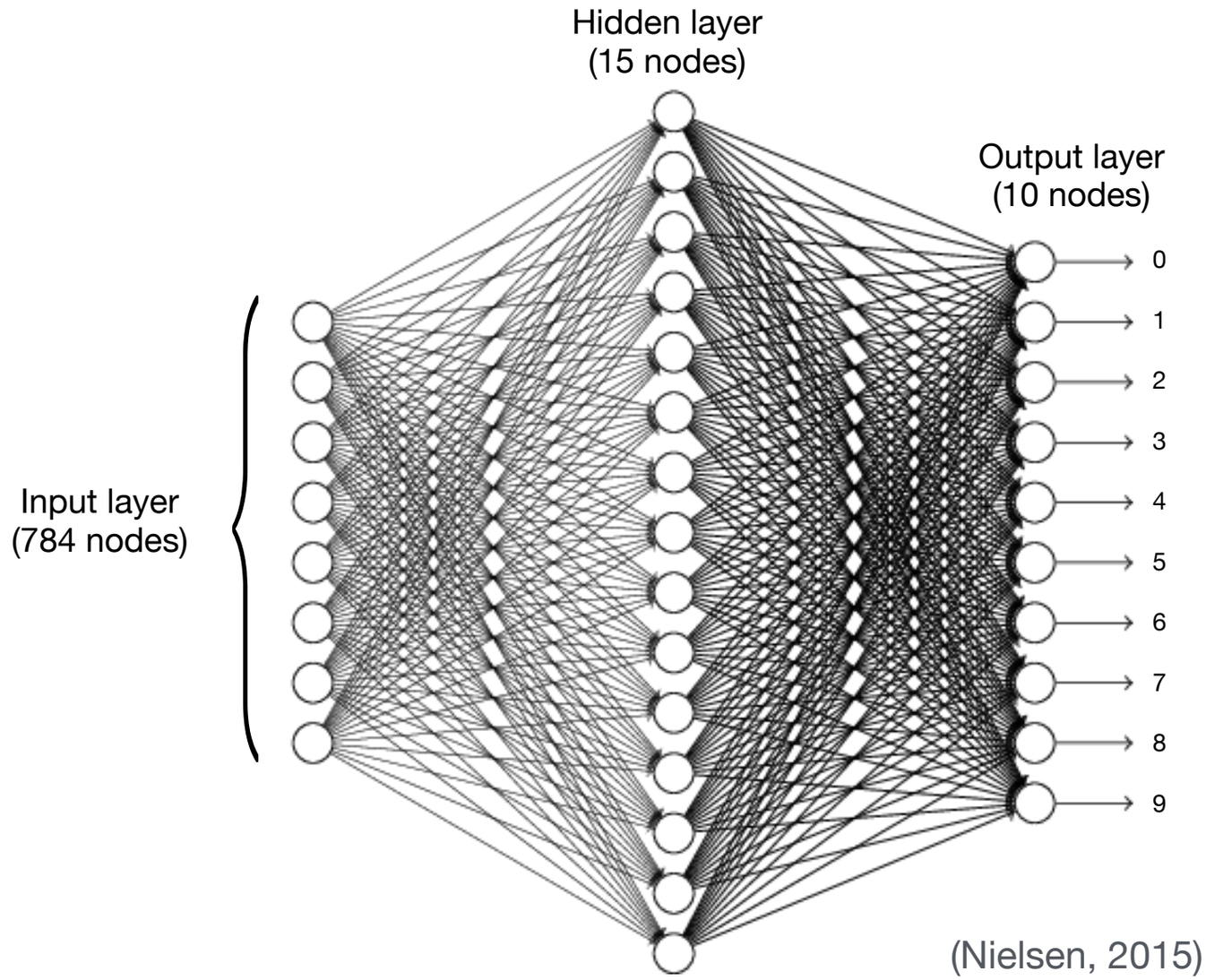


- Neural Network:

  Input layer:
  28x28 pixels=784 neurons

  Hidden layer:
  15 nodes

  Output layer:
  One output node per digit.
  To determine which class to to assign for an input, we look at which of the output nodes has the largest value.



(Nielsen, 2015)

COMP47490/COMP47990
Machine Learning with Python

Neural Networks

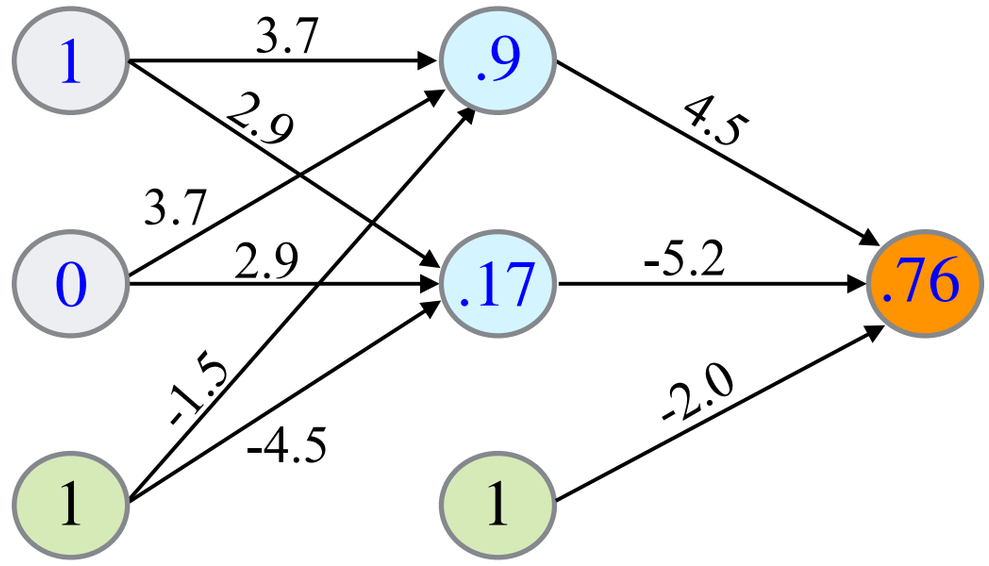
Part II
Errors, Cost Functions
Training

Pádraig Cunningham
Based on slides by Derek Greene

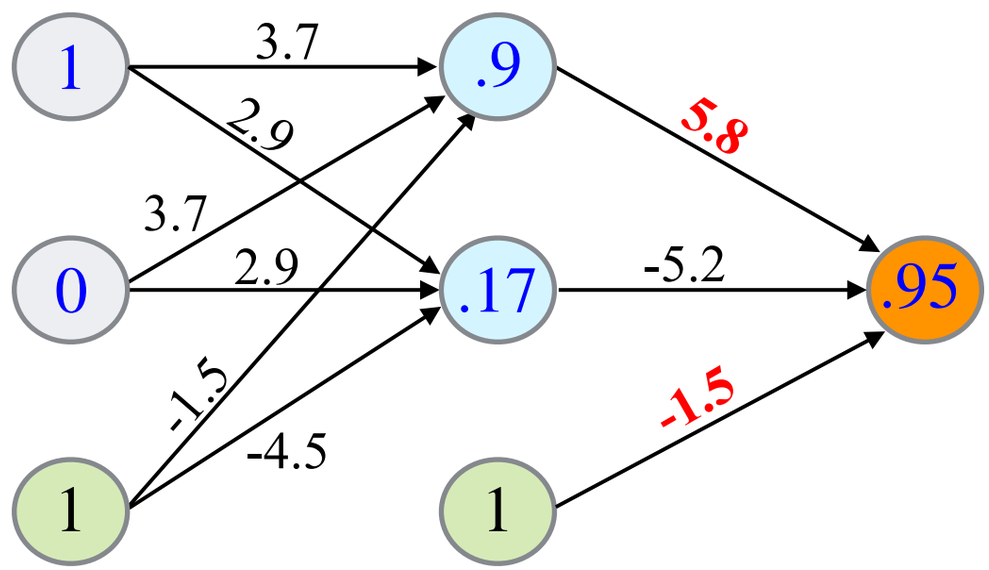
School of Computer Science

Error in Neural Networks

- Recall our previous network implementing the XOR function.
- Ideally the network's output for the inputs $x_1 = 1, x_2 = 0$ would have been 1.0, not 0.76



- We could adjust the weights in the network to reduce this error i.e the difference between the output values computed by the model and the correct values.
- Need to do this in a way that generalises to different inputs.



Cost Functions

- Once the architecture of the network has been chosen, its parameters (the weights w and biases b) need to be learned from the training data.
- Cost function: a function $C(w, b)$ is used in a neural network to quantify the inconsistency between predicted values and the corresponding correct values (also known as a loss function).
- The choice of cost function used in a network depends on the task being performed - e.g. regression, binary classification etc.
- Training a neural network involves applying an optimisation procedure to find weights and biases to minimise the cost function.
- The training algorithm has done a good job if it finds weights and biases so that the cost is low - i.e. $C(w, b) \approx 0$

Cost Functions

- A common cost function for regression is mean squared error. It is the average of the square of the difference between each predicted value $\hat{y}$ and the true value y:

$$C(w,b) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

w : All the weights in the network

b : All the biases in the network

n : Number of examples in the training set

- For binary classification, instead cross entropy (also called log loss) is often used. It measures the average uncertainty of the probabilities of the model p_i, compared to the true labels y:

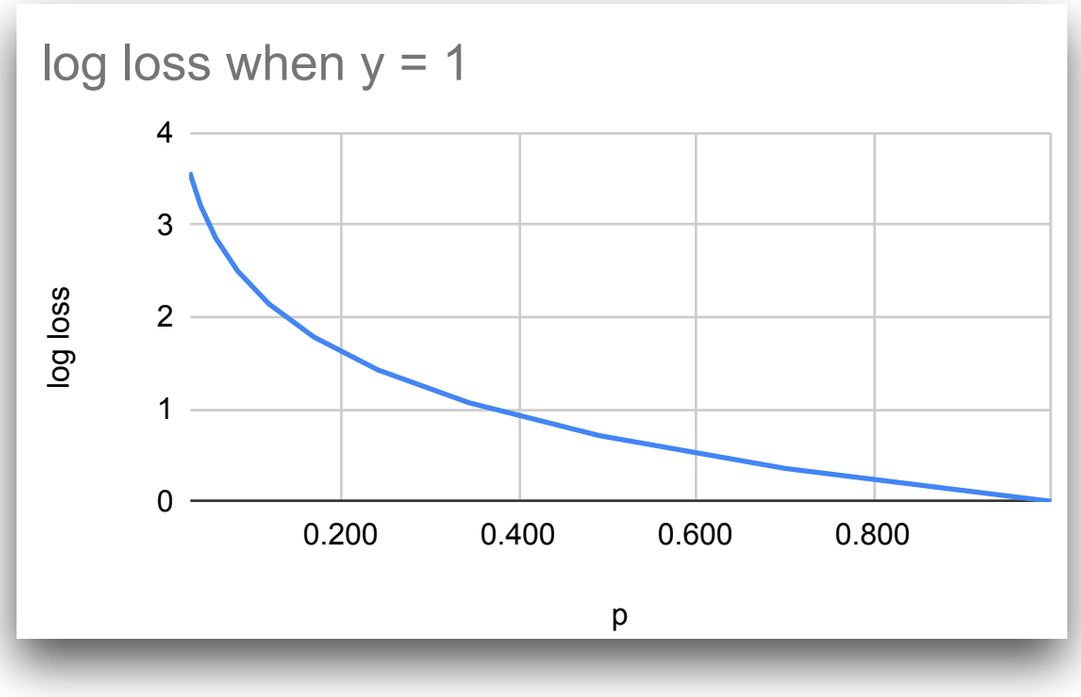
$$C(w,b) = -\frac{1}{n}\sum_{i=1}^{n}[y_i \log\, p_i + (1-y_i)\log\,(1-p_i)]$$

p_i : Predicted probability score from the model.

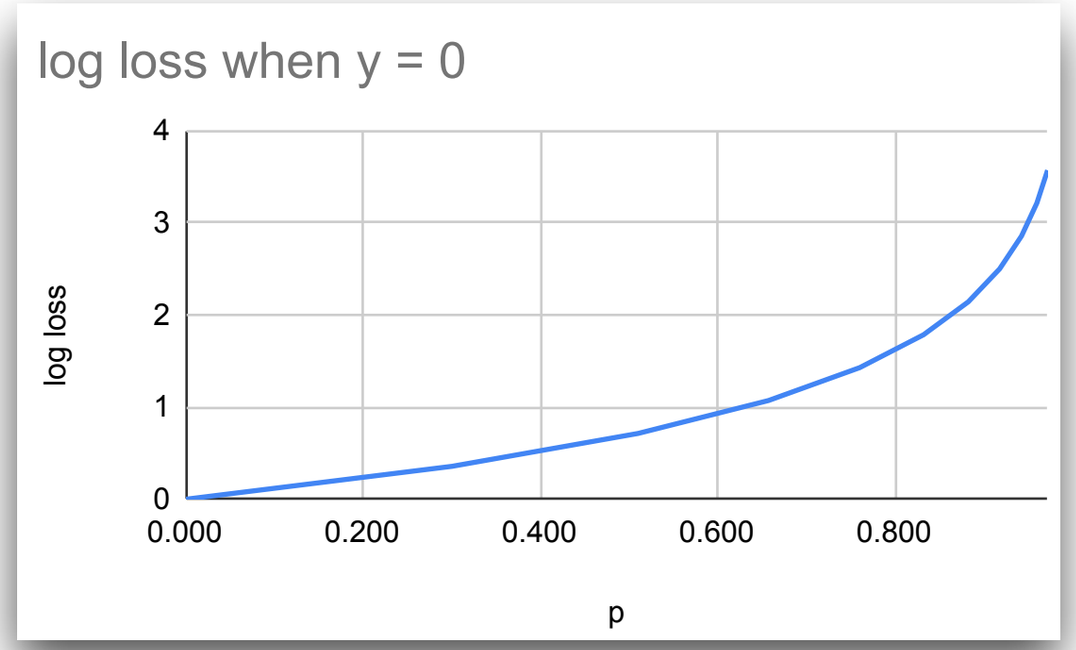
Q. How do we actually change the weights and biases in our neural network to minimise the value of a cost function $C(w,b)$?

Log loss = *- y log(p) - (1-y) log(1-p)*

When y = 1		
y	p	log loss
1	1.000	0
1	0.700	0.357
1	0.490	0.713
1	0.343	1.070
1	0.240	1.427
1	0.168	1.783
1	0.118	2.140
1	0.082	2.497
1	0.058	2.853
1	0.040	3.210
1	0.028	3.567

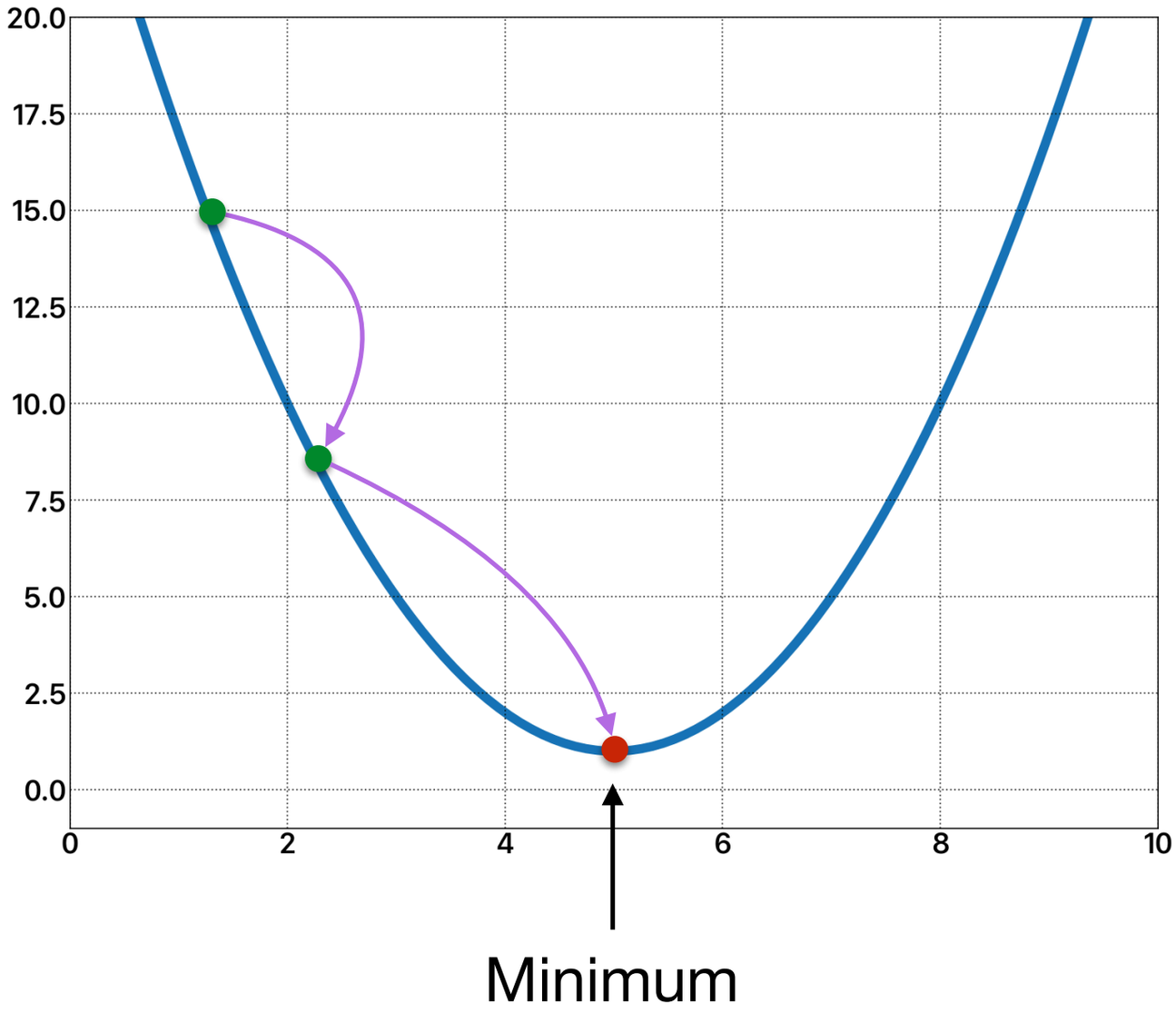


When y = 0		
y	p	log loss
0	0.000	0
0	0.300	0.357
0	0.510	0.713
0	0.657	1.070
0	0.760	1.427
0	0.832	1.783
0	0.882	2.140
0	0.918	2.497
0	0.942	2.853
0	0.960	3.210
0	0.972	3.567



Reminder: Gradient Descent

- Gradient descent is an algorithm that makes small steps along a function to find a local minimum.
- We start at some point and find the gradient (slope).
- We take a step in the opposite direction to the gradient (i.e. downhill). The size of the step is controlled by an adjustable parameter.
- This algorithm gets us closer and closer to the local minimum.

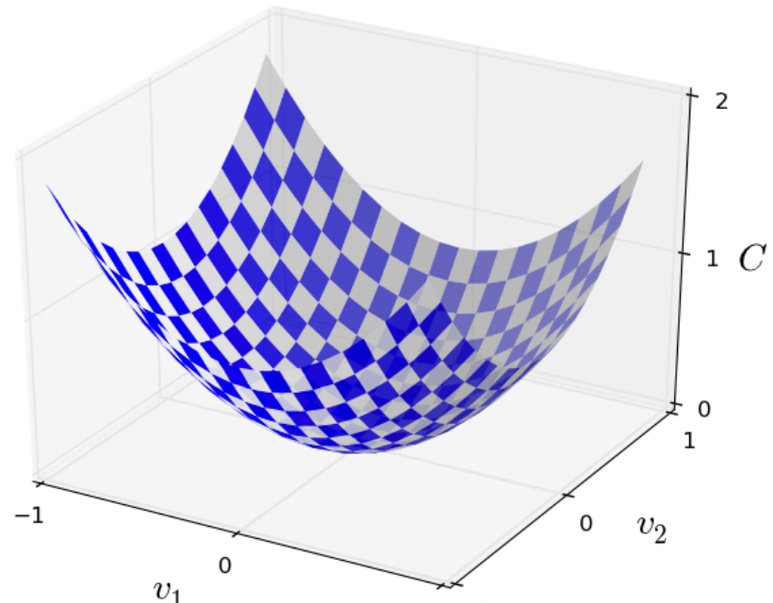


In a 3D space, it would be like rolling a ball down a hill to find the lowest point.

Training via Gradient Descent

- Neural networks generally apply the gradient descent algorithm to try to adjust all the weight and bias variables to find the minimum cost.
- This involves calculating the derivative of the cost function C.
- For the example with 2 variables, we can make a change Δv_1 and Δv_2 where the overall change in C is given by:

Example: 2 variables



(Nielsen, 2015)

$$\Delta C \approx \frac{\partial C}{\partial v_1}\Delta v_1 + \frac{\partial C}{\partial v_2}\Delta v_2$$

Partial derivatives

Δv_1 : Change to variable v_1

Δv_2 : Change to variable v_2

- We choose Δv_1 and Δv_2 so that the overall change ΔC is negative i.e. we want to get closer to the minimum.

Stochastic Gradient Descent

- In a neural network, rather than just two variables (v_1, v_2), we have many variables (the weights w and biases b), but the core optimisation strategy remains the same:

$$w_k \rightarrow w_k' = w_k - \eta \frac{\partial C}{\partial w_k} \qquad b_l \rightarrow b_l' = b_l - \eta \frac{\partial C}{\partial b_l}$$

η : Learning rate

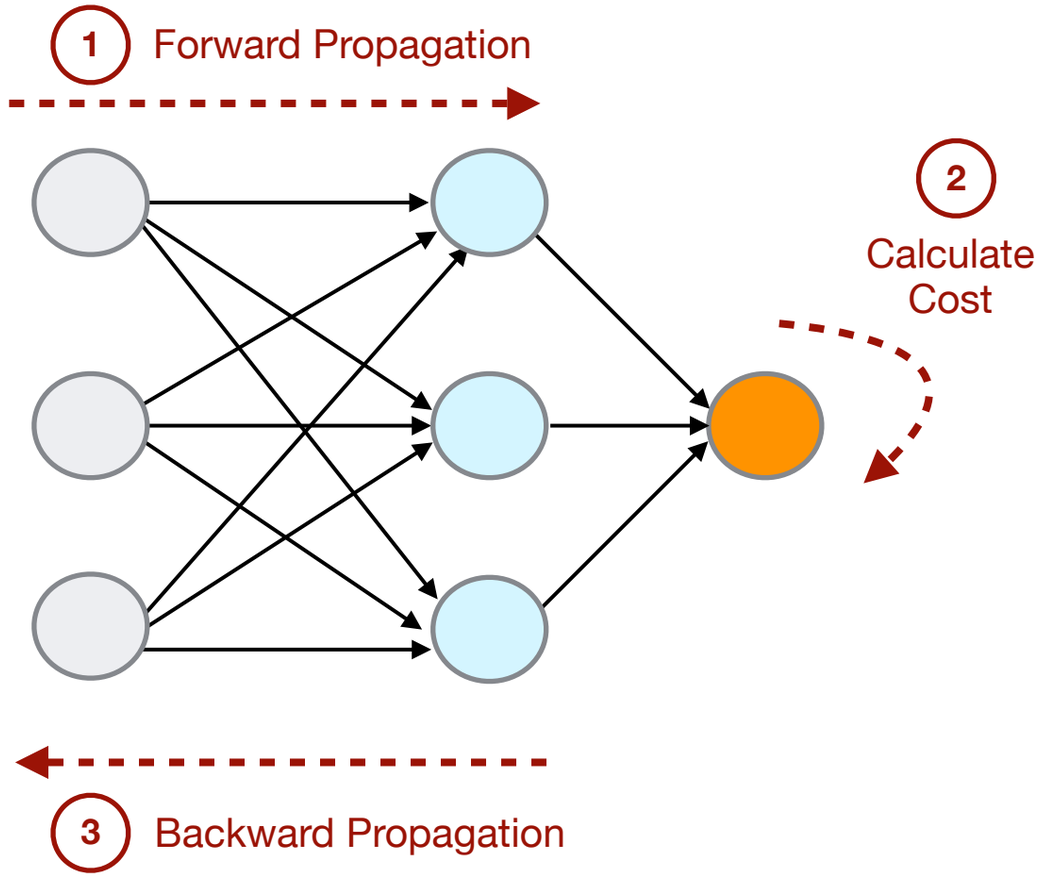
Update rule for weights

Update rule for biases

- When learning on large training sets, repeatedly computing the gradients can be very slow with batch gradient descent.
- In practice, stochastic gradient descent is often applied to speed up learning, which involves estimating the gradient ∇C for only a small batch of randomly selected training examples.
- This can provide a good estimate, while significantly reducing the time required to train a network.

Backpropagation

- To train the network, we start with random initial guesses for the weights and biases in the model. The optimisation algorithm then repeats a cycle of propagations and weight updates.
- Forward propagation: Feed training examples through the network layers, and calculate the resulting outputs. Use the cost function to measure the difference between the outputs and the correct answers.
- Backpropagation: Starting at the output layer, propagate errors back through the network, which allows us to calculate the gradient of the cost function.
- Weight update: The gradient is fed to the optimisation method, which in turn uses it to update the weights, in an attempt to minimise the cost function.



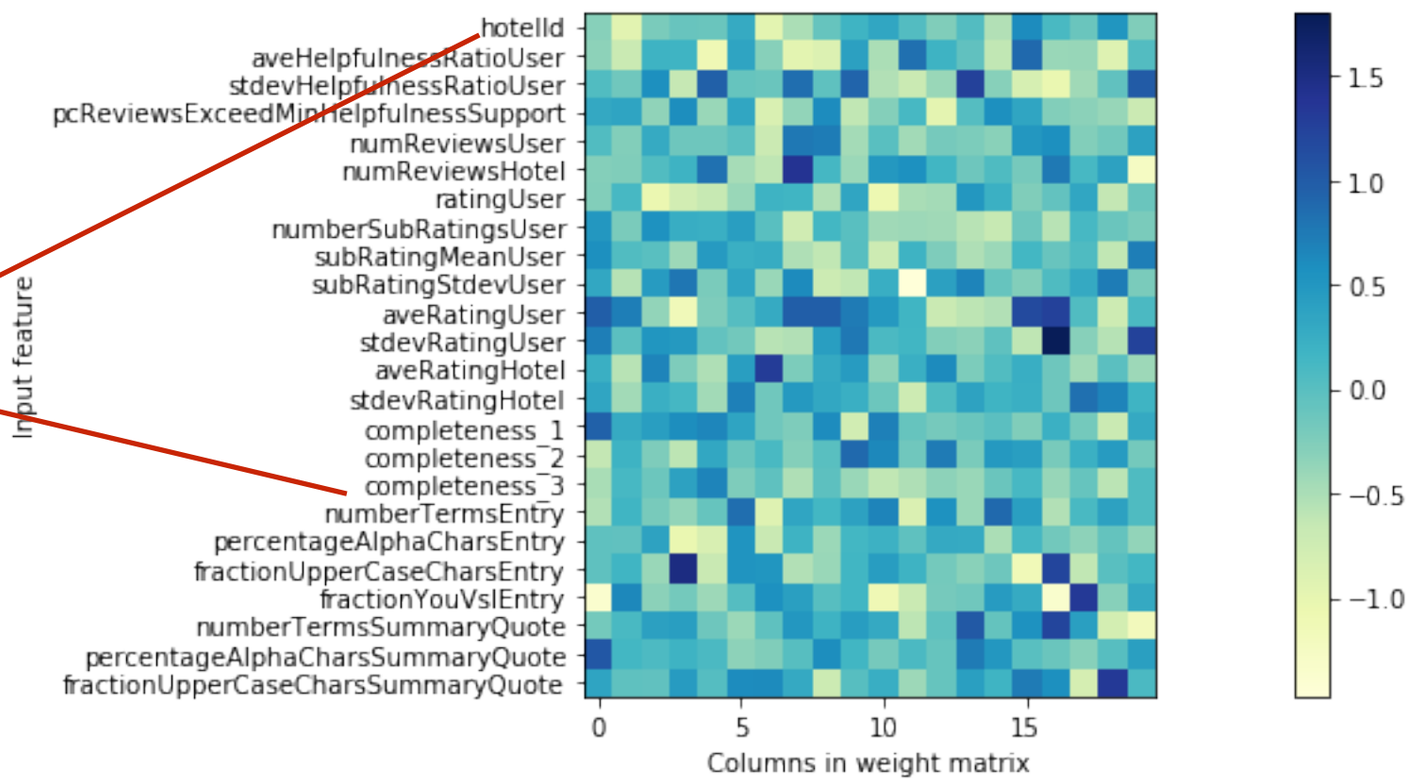
Training Neural Networks

- Applying gradient descent in the context of training neural networks involves the following steps:
  - Choose initial weights (typically small random values)
  - Until convergence repeat:
    1. Set all gradients to 0
    2. For each training example
       a. Predict the output from the model
       b. Calculate the resulting cost
       c. Update the gradients for each weight and bias term
    3. Update the weights and biases using weight update rule

Neural Networks in sklearn

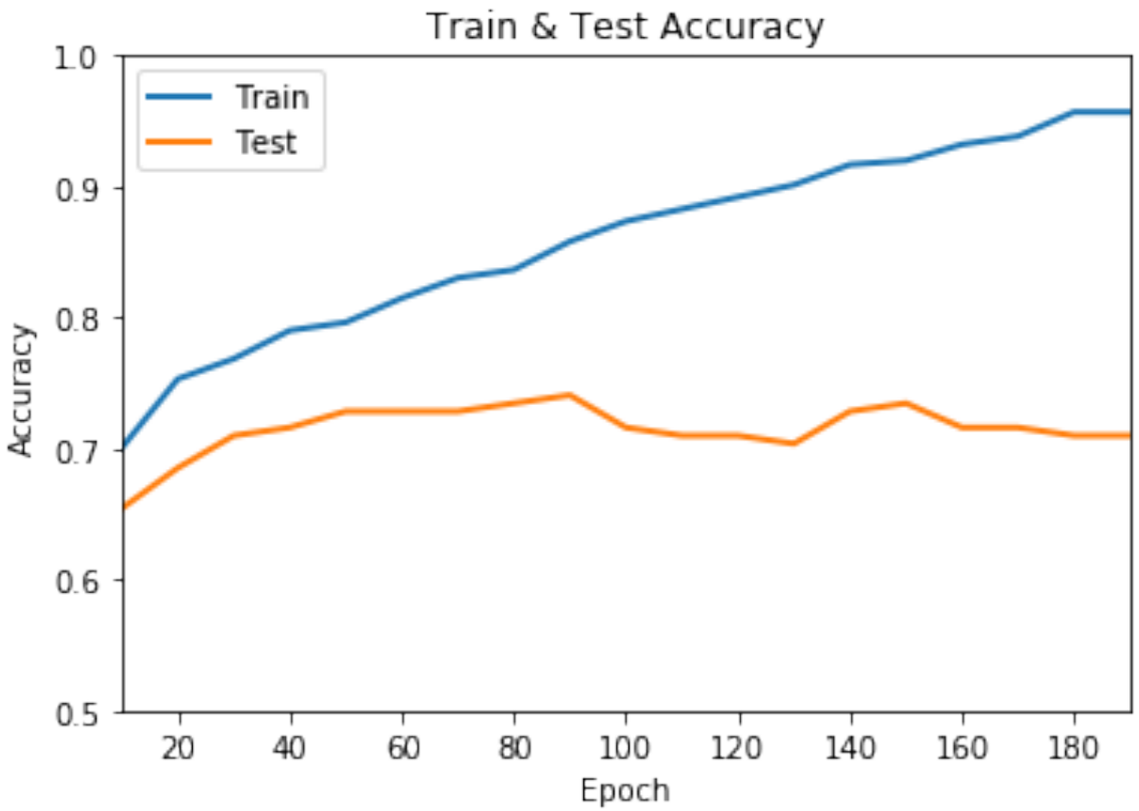
```
y = HR.pop('reviewHelpfulness').values
scaler = preprocessing.StandardScaler().fit(HR)
X_scaled = scaler.transform(HR)
In [55]:
mlp = MLPClassifier(max_iter=2000, random_state=2,
                    hidden_layer_sizes=[20])
mlp.fit(X_scaled, y)
acc = mlp.score(X_scaled, y)
print("Accuracy on training set: {:.2f}".format(acc))

Accuracy on training set: 1.00
```

Weights
Some features not Influential

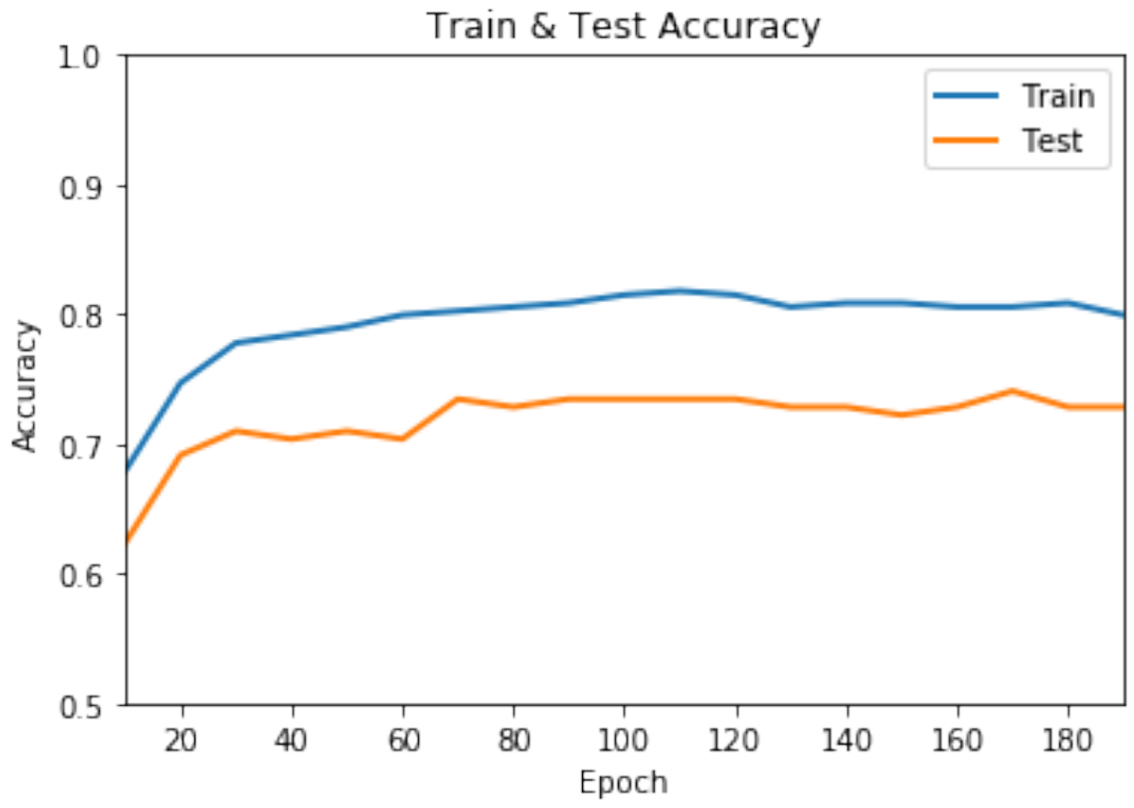


Holdout Testing

Overfitting



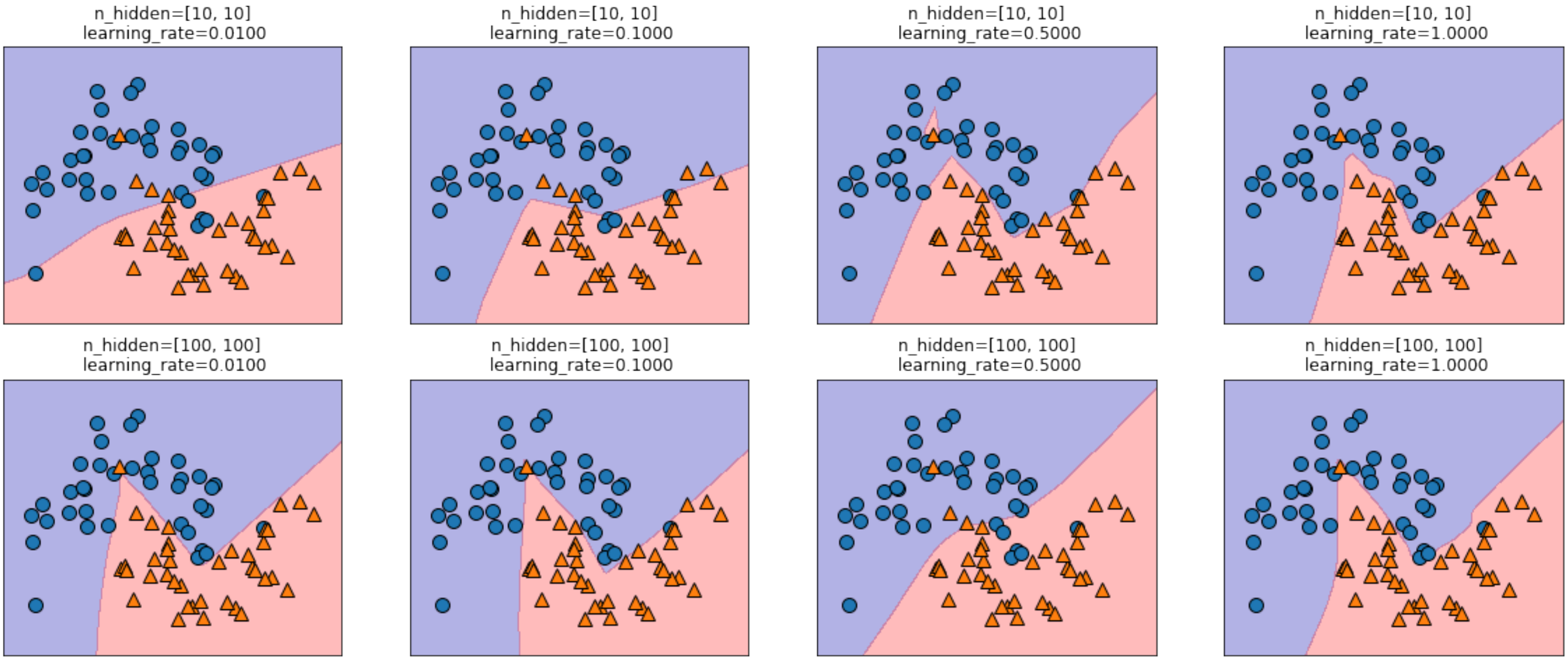
Use regularisation to control overfitting (alpha = 5)



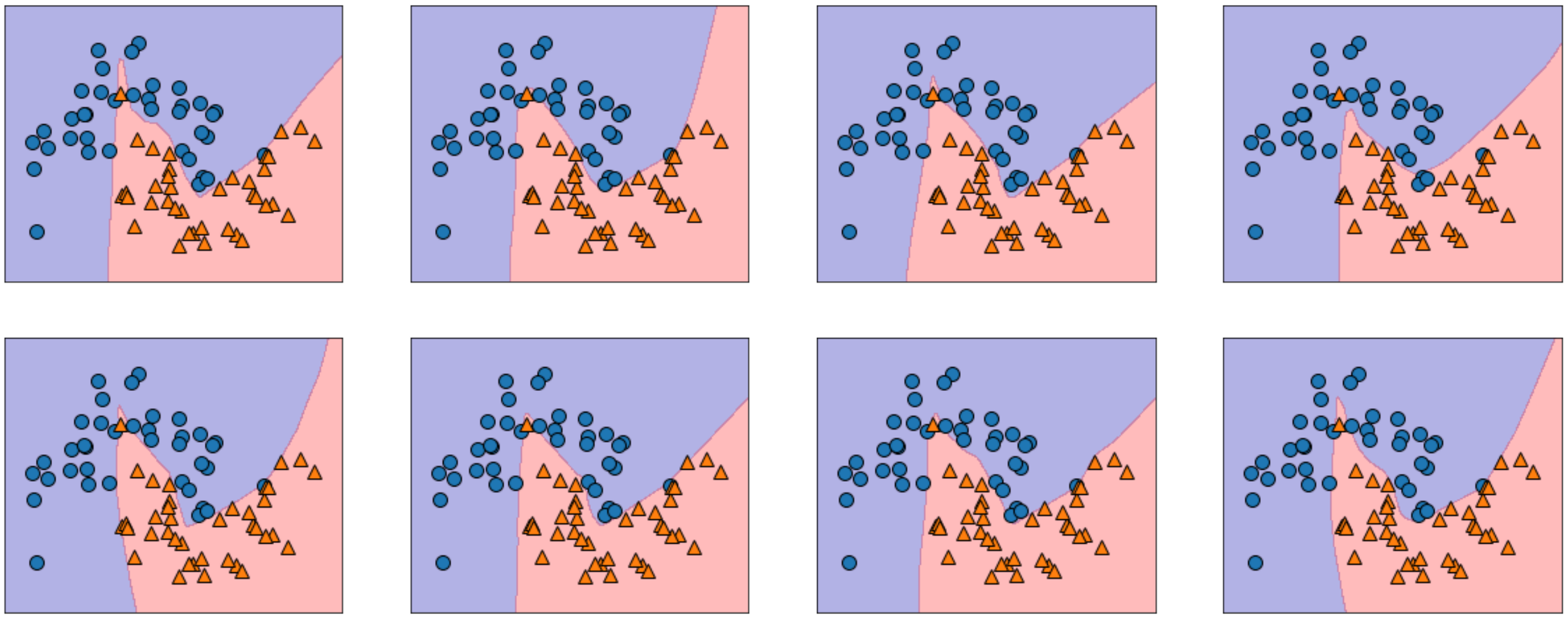
- alpha restricts the weights
- Overfitting can also be controlled by restricting network complexity,
  - e.g. reduce units in hidden layer

NNs very sensitive to model parameters

- 2 hidden layers [10,10] or [100,100]
- Learning rate 0.01, 0.1, 0.5, 1



Also sensitive to weight initialisation



Aside: Grid Search

- Neural Networks particularly sensitive to parameter selection.
  - e.g. learning rate, momentum, alpha, hidden layers, activation function
- Grid Search
  - Search through a grid of parameter values (2 params, 2D grid)
  - Scikit Learn has:
    - GridSearchCV: cross validation search over grid of parameters
      - Grid defined by a dictionary
    - RandomizedSearchCV: random search over parameters
    - e.g

```
mlp = MLPClassifier(random_state=2, max_iter=1000)

grid = [{'alpha': [0.01, 0.1, 1, 10, 100],
         'hidden_layer_sizes': [[5], [10], [50], [100]]}]
clf = GridSearchCV(mlp, grid, n_jobs = -1, cv=8, scoring = 'accuracy')
clf.fit(X_train, y_train)
```

See Neural Network Tutorial notebook

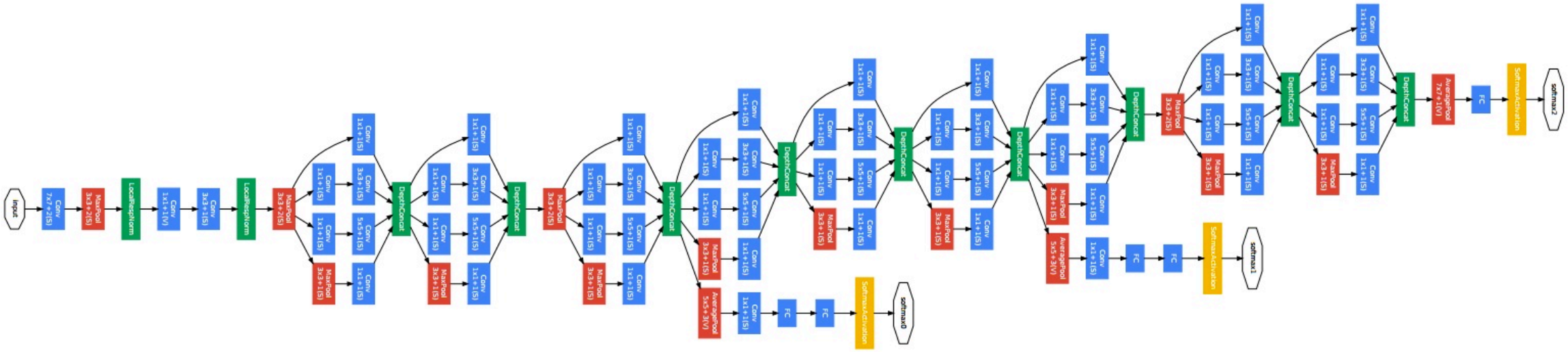
What are Neural Networks Good For?

- **Advantages**
  - Can learn and model non-linear and complex relationships.
  - Work well when training data is noisy or inaccurate.
  - Fast performance once a network is trained.
- **Disadvantages**
  - Often require a large number of training examples.
  - Training time can be very long.
  - Network is like a “black box”. A human cannot look inside and easily understand the model or interpret the outputs.

➡ Recent work has sought to address these issues...

Deep Learning

- Recent developments in neural networks have led to a step change in the performance of machine learning models.
- Difference: Deeper networks, more complex architectures, huge performance improvements, many past issues have been solved.
- Gradient descent is still the core algorithm behind deep learning.



(Szegedy et al, 2015)

That's a lot of hyper parameters!

Learn More:

COMP47650 Deep Learning
COMP47590 Advanced Machine Learning
COMP47980 Generative AI: Language Models

References

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