Introduction to Deep Learning

Esther Puyol

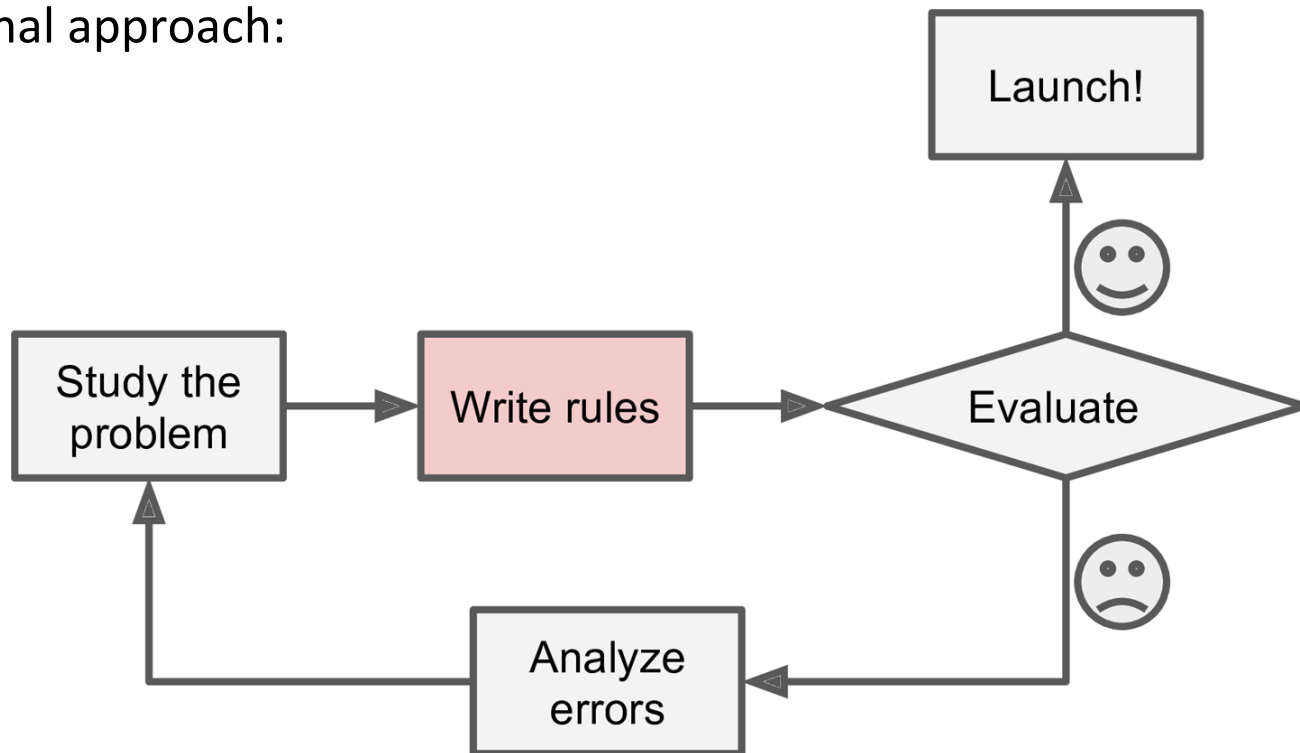Medical Imaging-Deep Learning (MIDL) satellite meeting

11 July 2019

What is AI?

The science (and art) of programming computers so they can *"learn from and make predictions on data"*
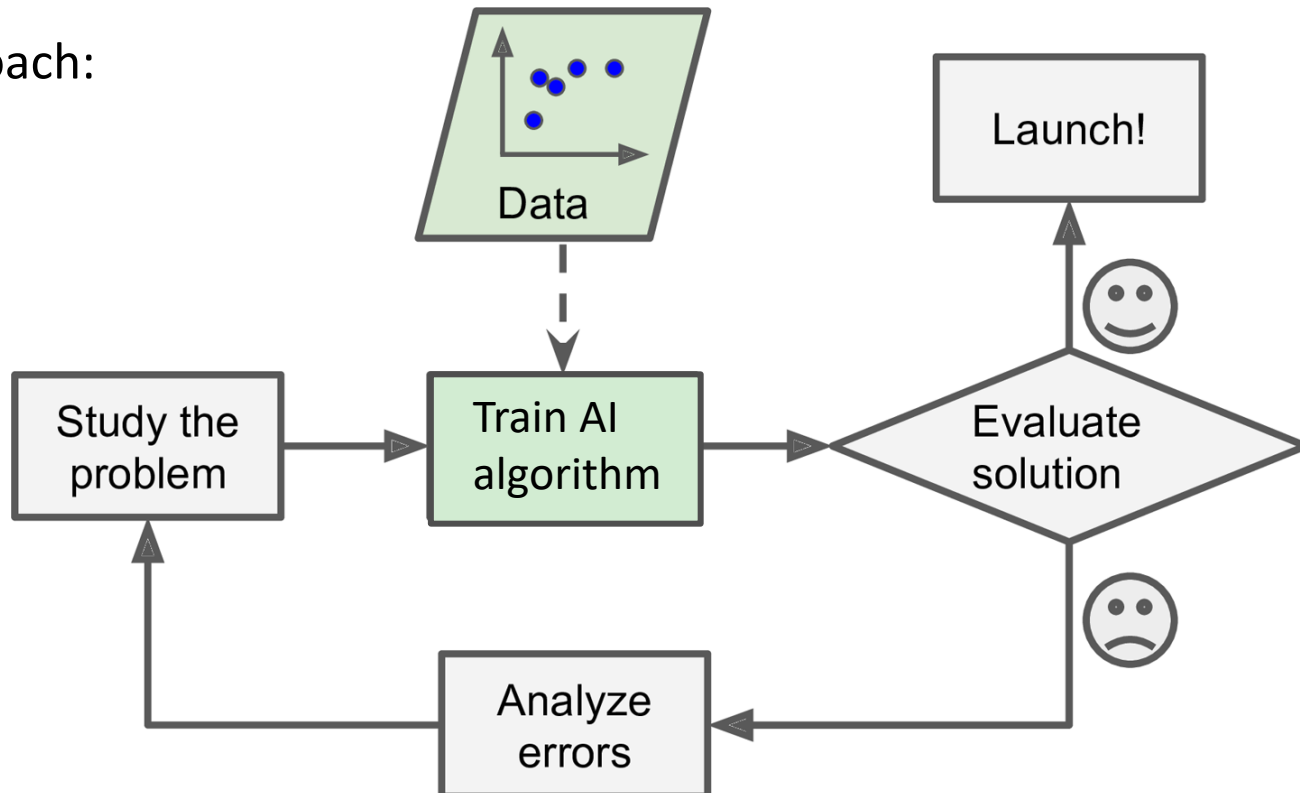
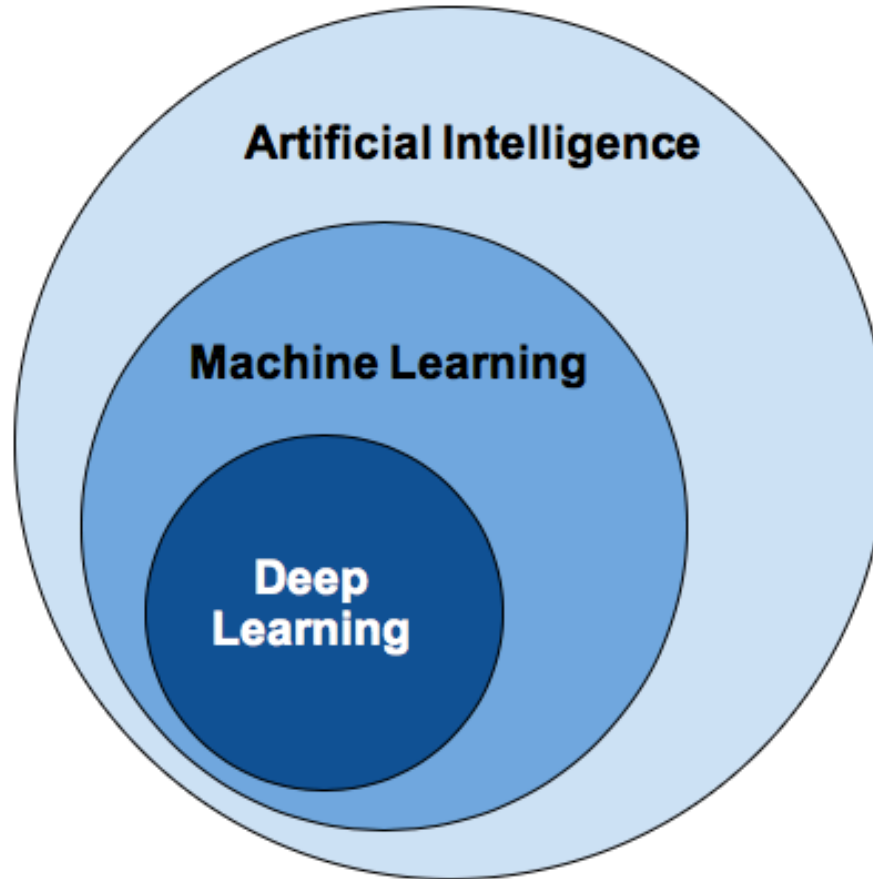Traditional approach:

What is AI?

The science (and art) of programming computers so they can *"learn from and make predictions on data"*
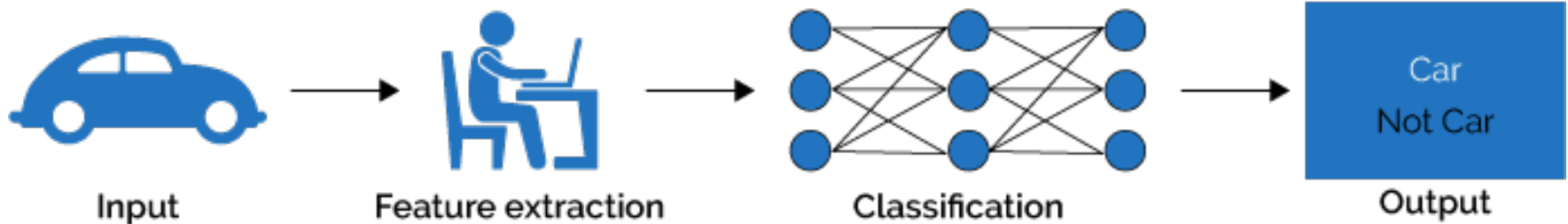
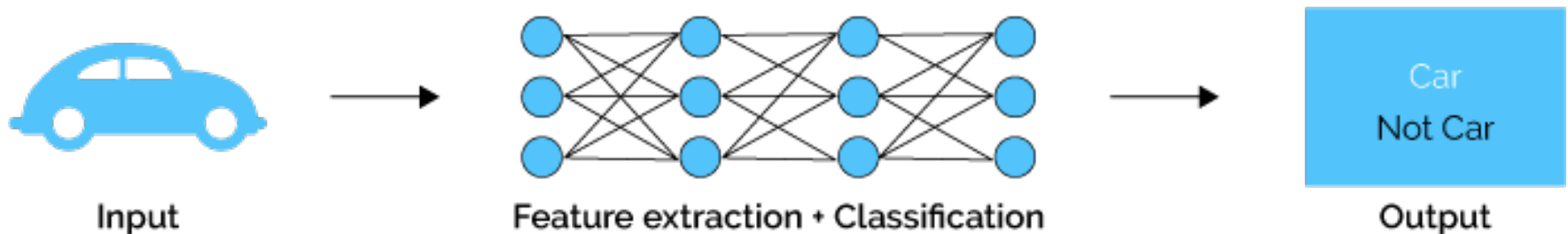AI approach:

AI, Machine Learning and Deep Learning:
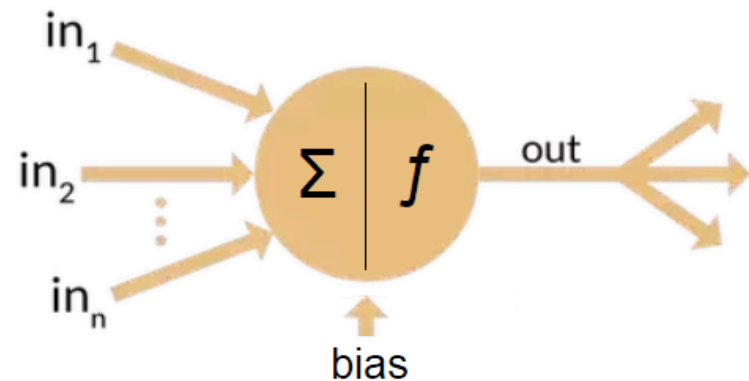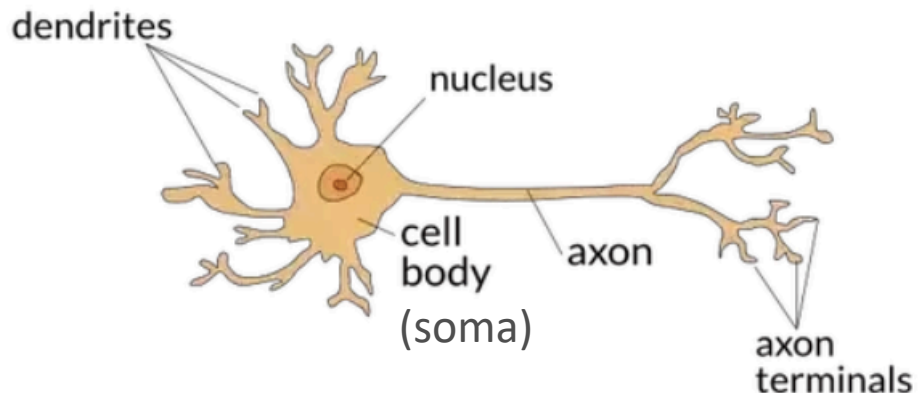
AI, Machine Learning and Deep Learning:

Artificial neural network (ANN)

- Machine learning has been around for decades
- First machine learning methods were inspired by how the brain works:

Perceptron

The first neural network (Frank Rosenblatt, 1957)
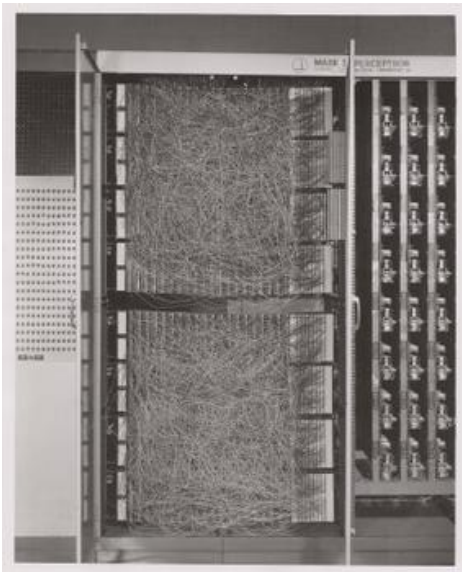
$$f(x) = \begin{cases} 1 & if \ \sum_i w_i . x_i > b \\ 0 & otherwise \end{cases}$$

"Mark 1 perceptron" - machine designed for image recognition: it had an array of 400 photocells, randomly connected to the "neurons". Weights were encoded in potentiometers, and weight updates during learning were performed by electric motors

A single-layer perceptron

A single-layer perceptron looks as follows:

Weights

Bias b_k

$$v_k = \sum_{j=1}^{m} w_{kj} x_j + b_k$$
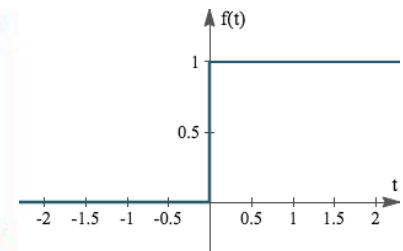
Activation function

$$y_k = \varphi(v_k)$$

Input signal

Summing junction

Output y_k

Discrete Perceptron:
$$\varphi(\cdot) = sign(\cdot)$$
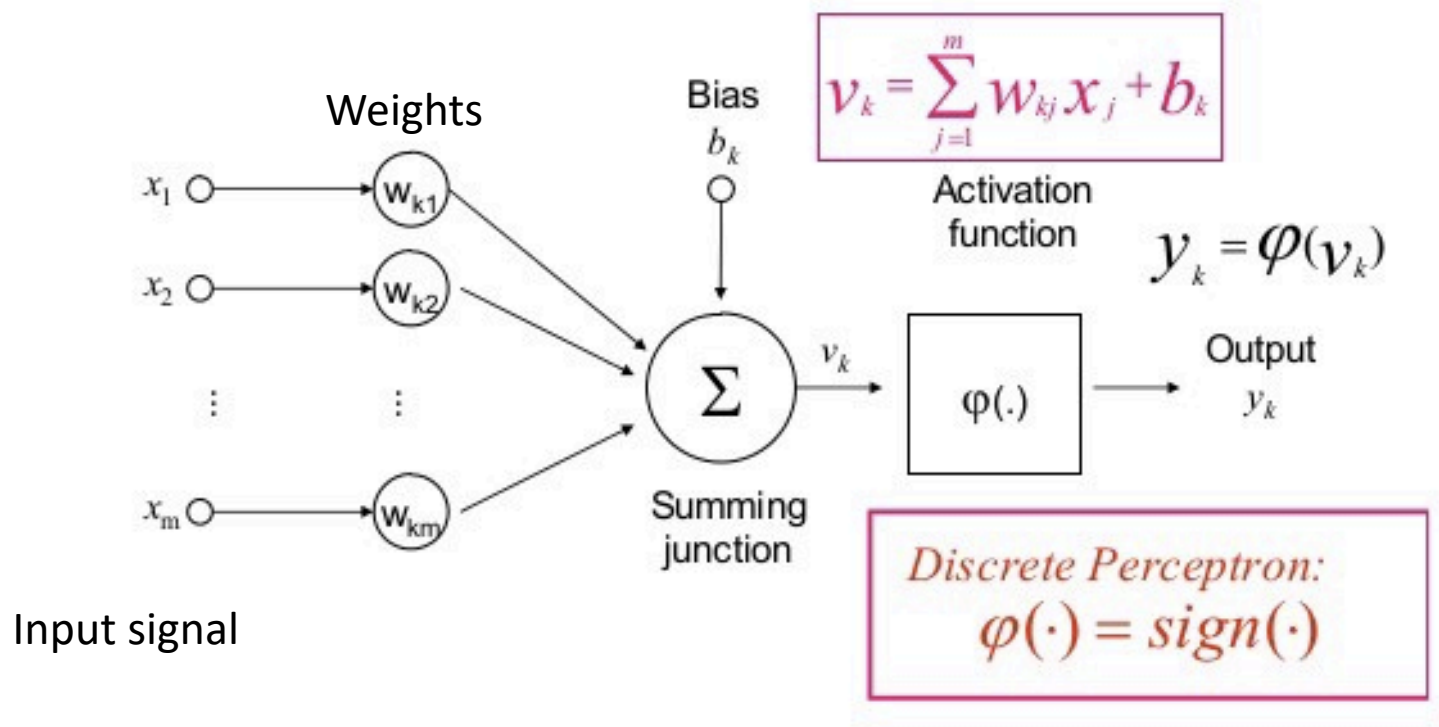
*This and the following slides follow the example on https://hackernoon.com/a-hands-on-introduction-to-neural-networks-6a03afb468b1

A single-layer perceptron

Input:

- Each input to the neuron (x_1, x_2, … x_n) is known as a **feature**

Weights:

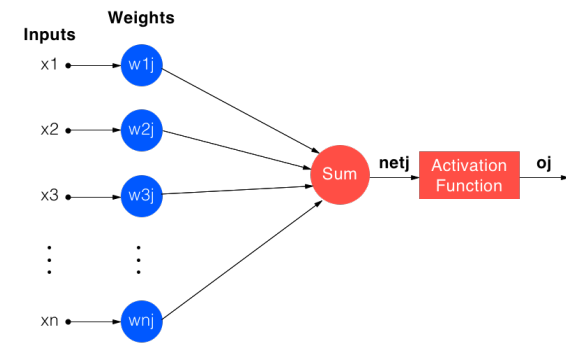- Each feature is weighted with a number to represent the strength of that input (w_{k1}, w_{k2}, … w_{km}).

Bias:

- Additional parameter (b_k) which is used to adjust the output along with the weighted sum of the inputs to the neuron.

Activation function:

- Calculate weighted sum of inputs (v_k) , pass through an **activation function** and threshold result y_k to 0 or 1

Activation function
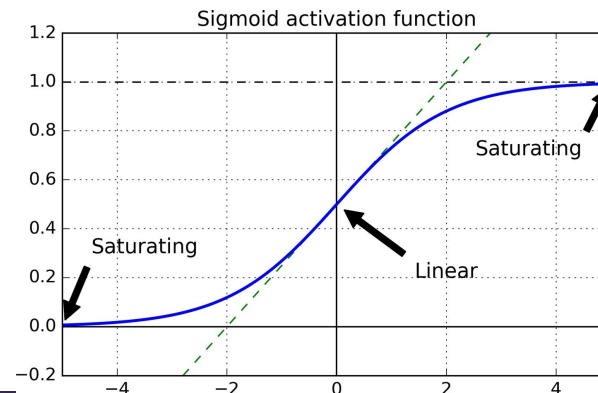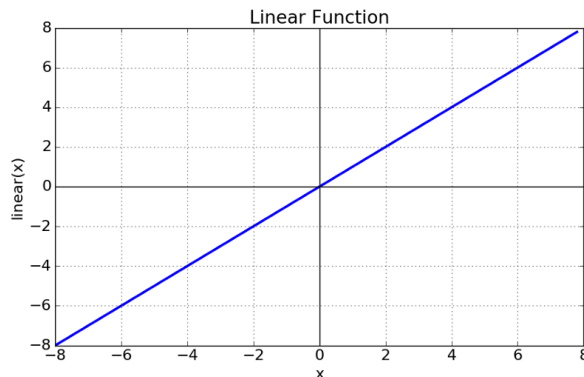

Added to the output end of any neural network

- Can be regarded as a **Transfer Function**

Used to determine whether the output of a neural network is 'yes' or 'no' (or something in between).

- Maps the resulting values in between 0 to 1 or -1 to 1 (depending upon the activation function)

We distinguish between (piecewise) linear and nonlinear activation functions
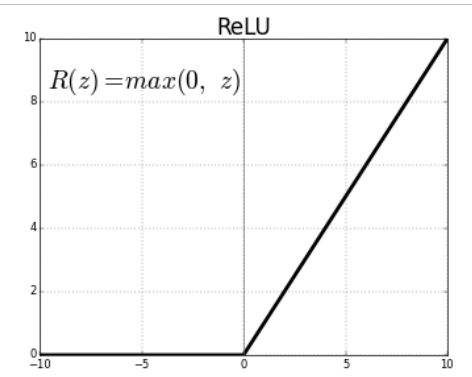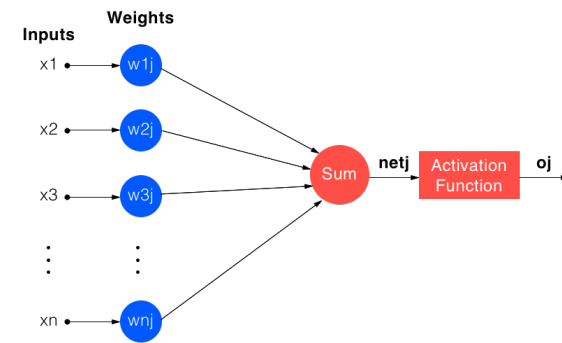
Training a perceptron
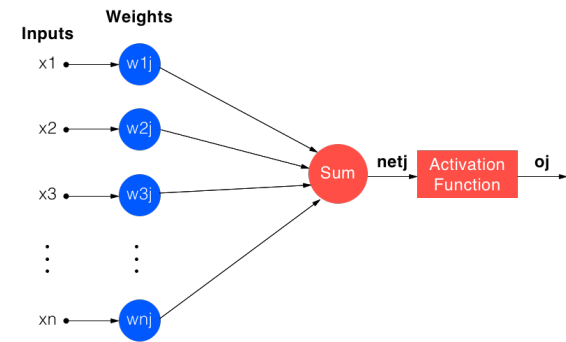
- Now that we see how a perceptron works, we need to train it

- **Training** a perceptron refers to iteratively updating the weights and bias associated with each of its inputs (Backpropagation)

- This allows to progressively approximate the underlying relationship in the given training dataset

- Once properly trained, it can be used to **classify** entirely new samples

Training a perceptron

What else do we need?

- We need **an error function (cost function** or **loss function):**
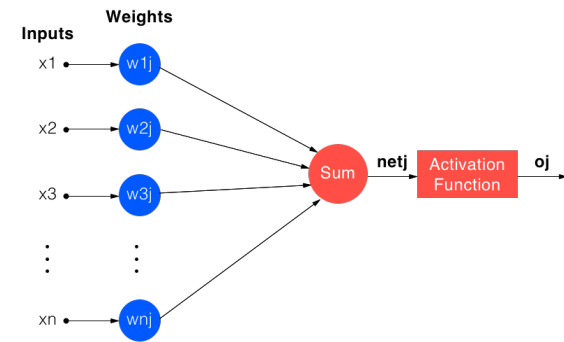 - Measure "how good" a neural network did with respect to it's given training sample and the expected output. The cost function must be able to be written as an average over cost functions Ei for individual training examples xi:

$$E = \frac{1}{N} \sum_{i=1}^{N} E_i$$

  - Examples of loss function: L1 norm $\rightarrow E = \sum_i |E_i|$
  - We want to minimize the cost function $\rightarrow$ need an **optimisation method** (e.g. gradient descent)
  - Our activation function should be **differentiable**

Training a perceptron - Overview

A single-layer perceptron can be trained as follows:

1. Ask the neuron* to classify a sample (**forward pass**)

2. Update the neuron's weights based on how wrong the prediction is.

3. Repeat for a set number of times (=**epochs**).

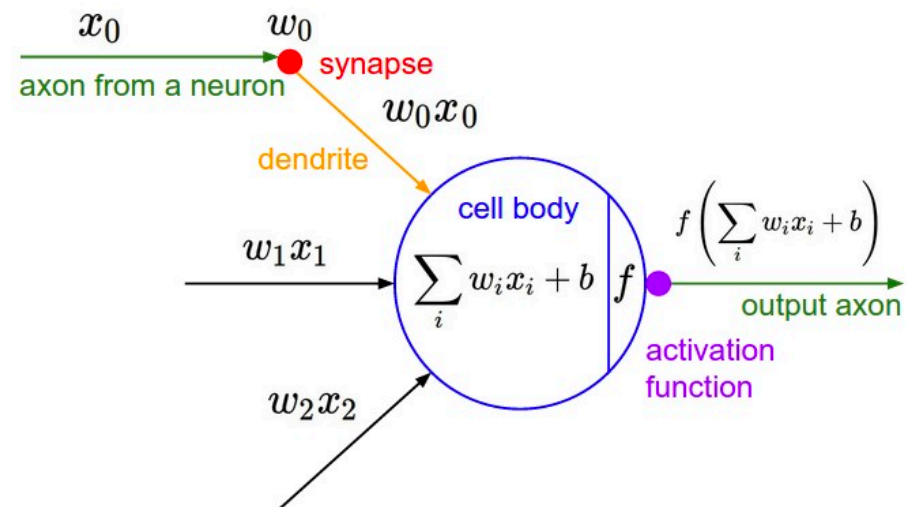*A perceptron is a neuron with a binary output

Training a perceptron – step 1

1. **Forward Pass**

- In the first step of training, we ask the neuron to make a prediction about the training samples.

- This is known as a **forward pass**, and it involves taking a weighted sum of the input features and passing that sum through the activation function.

- Mathematically:

  - $f(\sum_{i=1}^{N} w_{ij}x_i + b)$

Training a perceptron – step 2

2. **Reverse pass:**

- The second step to update the neuron's weights using the **Delta-rule** from the gradient descent algorithm:

$$\Delta w_{ij} = -n \frac{\partial E}{\partial w_{ij}}$$

- Ie each weight will be updated in the negative direction of the gradient, proportional to an additional term, ***n****.

- This scaling factor, n, determines how large a step we take when updating neuron weights, effectively controlling the rate at which the neuron learns. We call ***n*** the **learning rate**.

*Often called η

Training a perceptron – step 3

3. **Repeat for a set number of iterations (=epochs)**

    - We need to iterate through this several times:

    - **Either** until convergence (overall loss is smaller than ε)

    - **Or** until maximum number of **epochs**
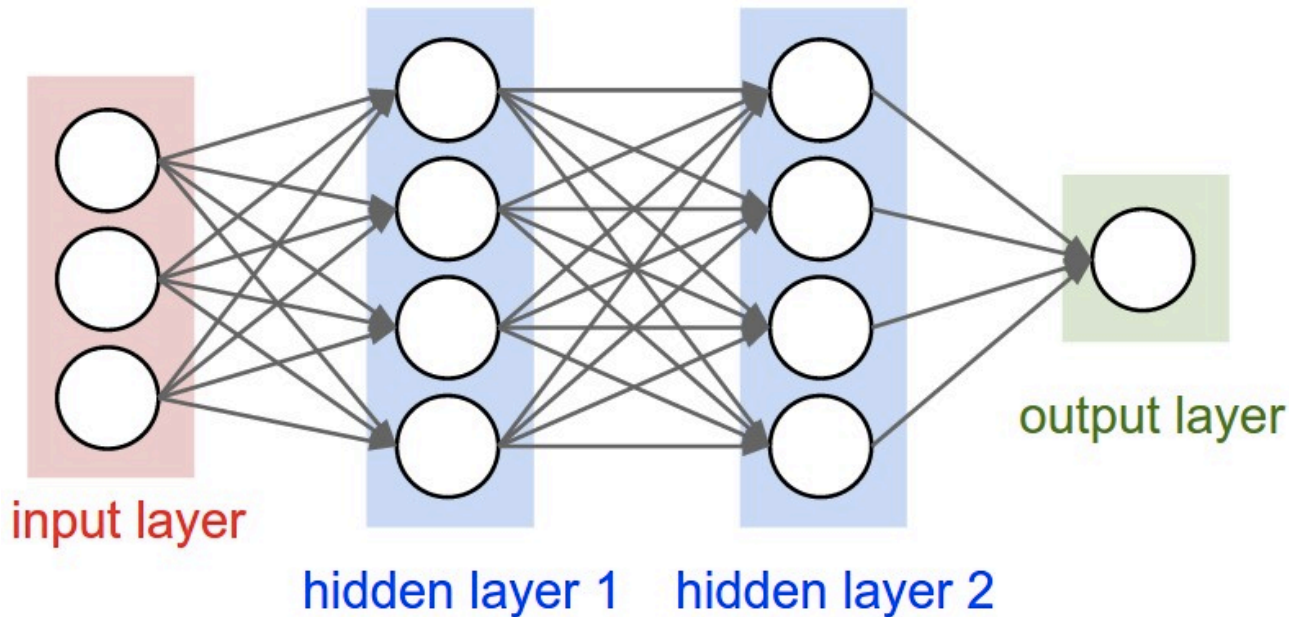
From single-layer to multi-layer perceptron

A more complex MLP is shown below (still only 1 hidden layer):

Input data:
***m* features**

Hidden Layer:
***n* hidden neurons**

Multi-Layer Neural Network
with 1 hidden layer
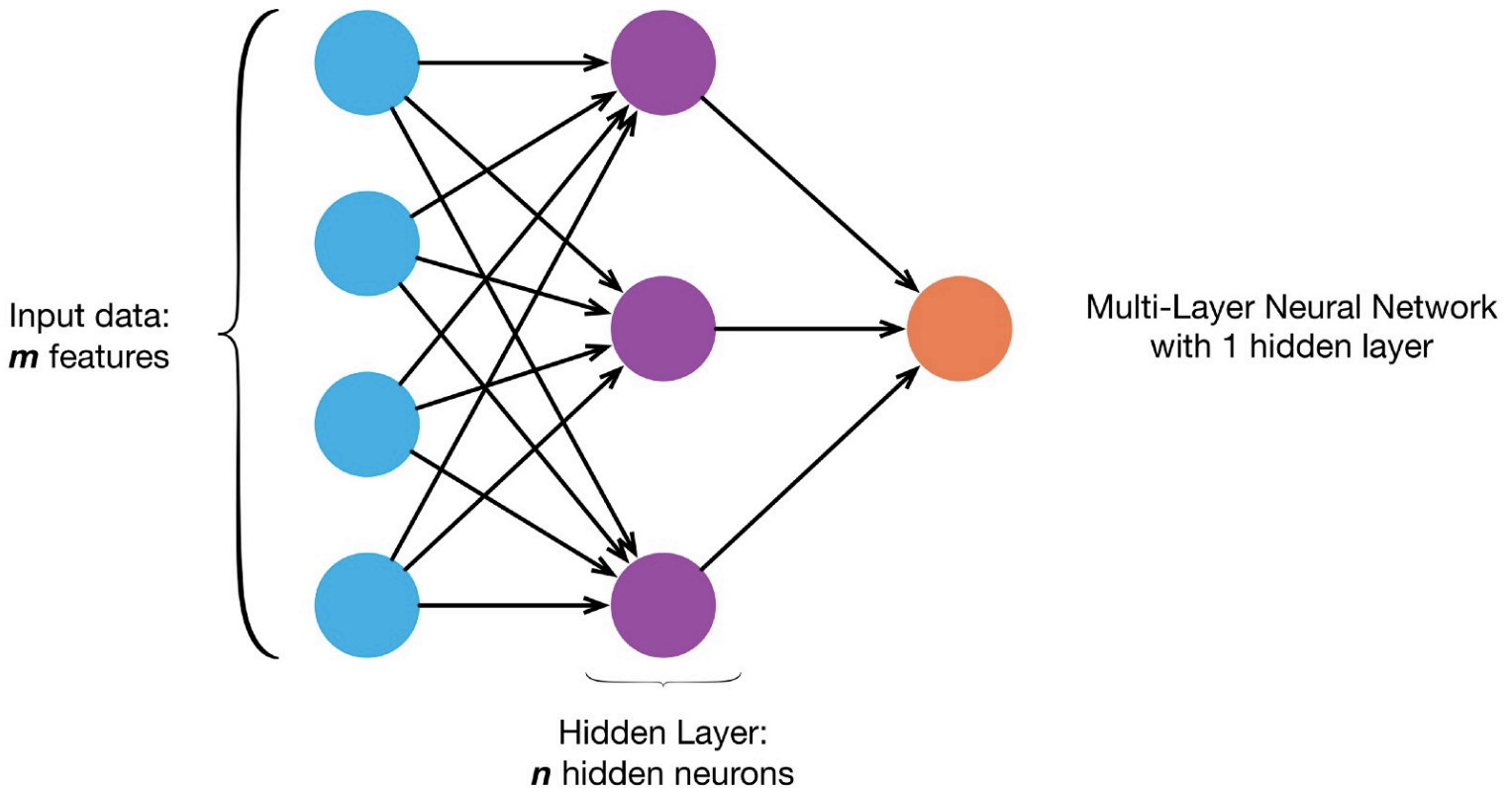
Multi-layer perceptron

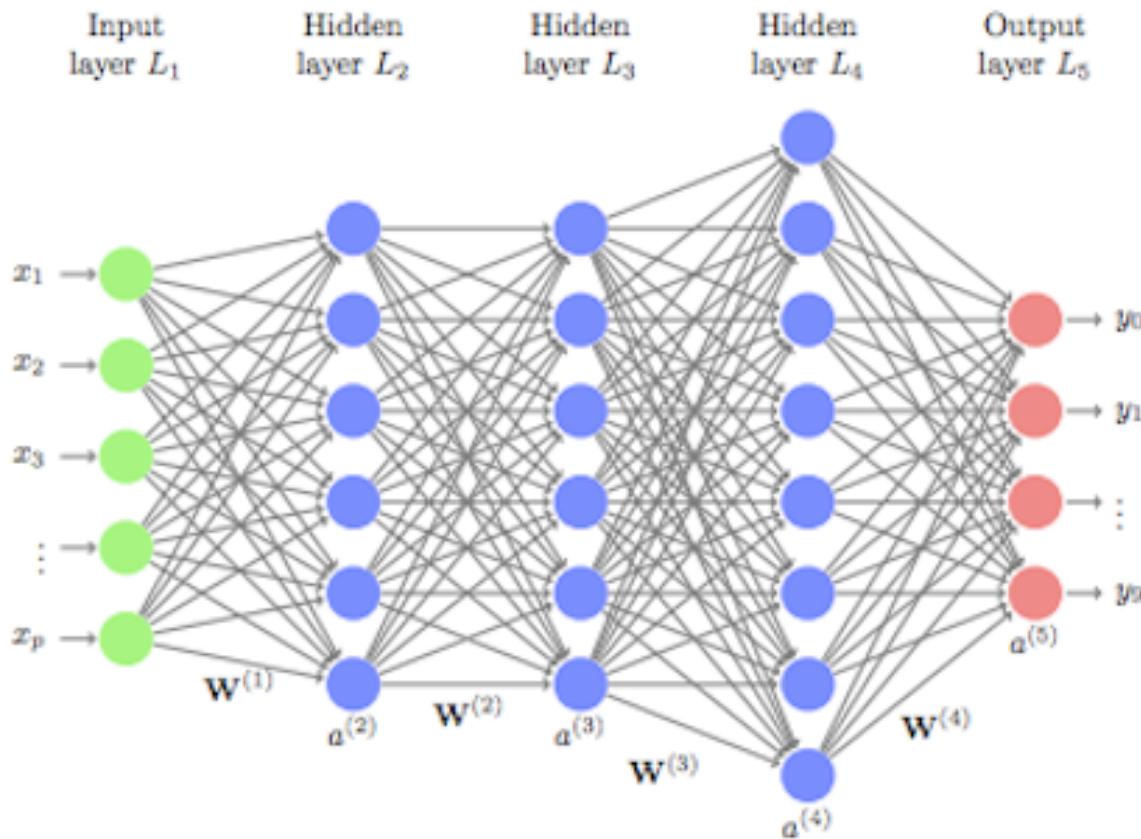We have stacked multiple perceptrons to generate hidden layers:

If we have more than one hidden layer, the neural network is considered to be "deep" and we move into **deep learning**

Deep fully connected networks (FCN)

Compare this to a deep fully-connected network with N hidden layers:

Training a FCN: **Backpropagation**

Backpropagation (BP) is a common method for training a neural network, and it is a generalization of the delta rule to multi-layered feedforward network, by **using the chain rule to iteratively compute gradients for each layer**.

For each training instance, the BP algorithm:

1. First make a prediction (**forward pass**) and measure the error

2. Then go through each layer in reverse to measure the error contribution from each connection (**reverse pass**)

3. And finally slightly tweak the connection weights to reduce the error (**Gradient Descent step**)

4. BP is a generalization of the delta rule to multi-layered feedforward network, by **using the chain rule to iteratively compute gradients for each layer**.

Training a FCN: **Backpropagation**

For BP the **step function is replaced by the (differentiable) sigmoid function**, so that the gradient is not flat

Other differentiable activation functions like tanh or ReLU also work
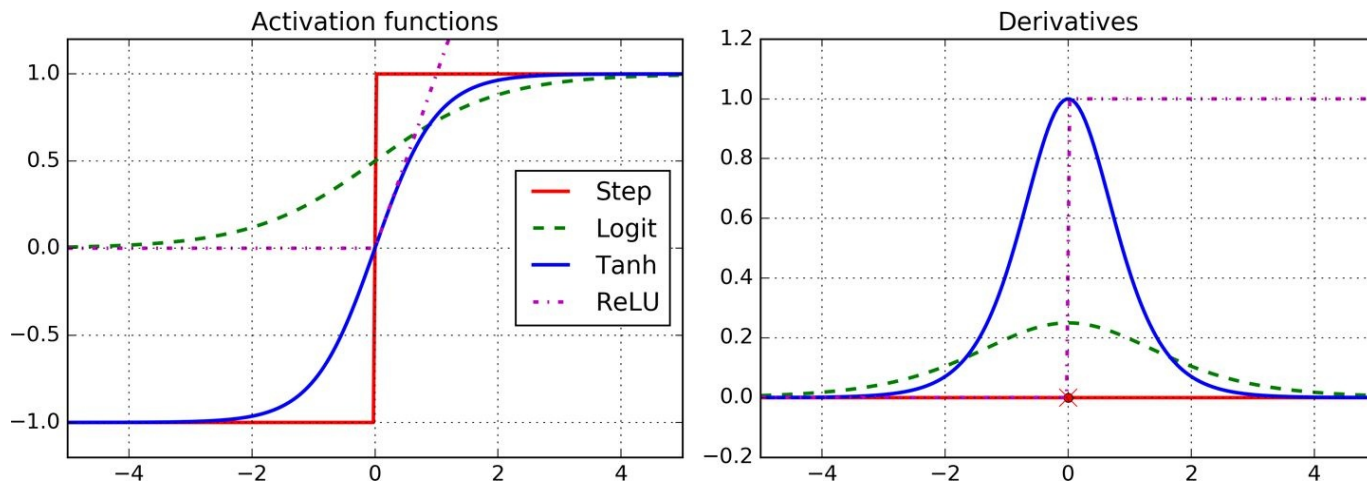
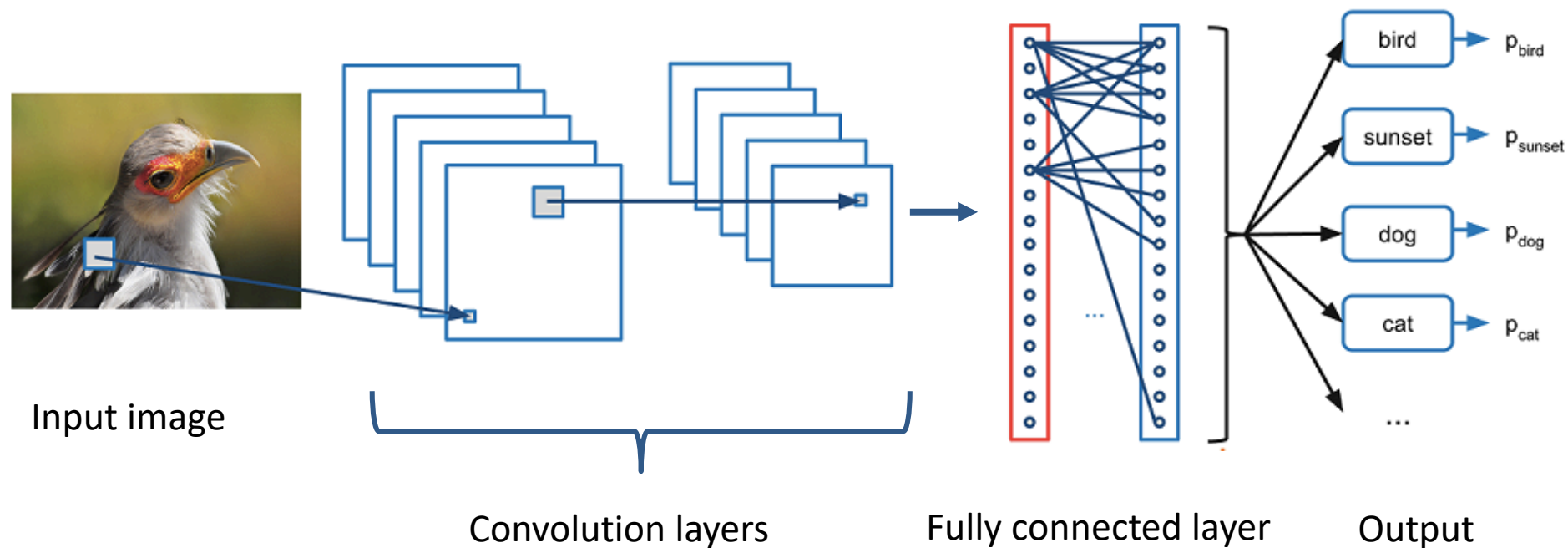# From FCN to Convolutional neural network

Disadvantages of FCN:

- Large number of parameters to be learn

- Incredibly computationally expensive.

- Slow

- Prone to overfitting data

Convolutional neural network (CNN):

- Regularized versions of multilayer perceptrons.

- Fully connected layers are replaced by one or more convolutional layers

Convolutional Neural Networks (CNNs)

Input image

Convolution layers

Fully connected layer

Output

Convolutional Neural Networks (CNNs)

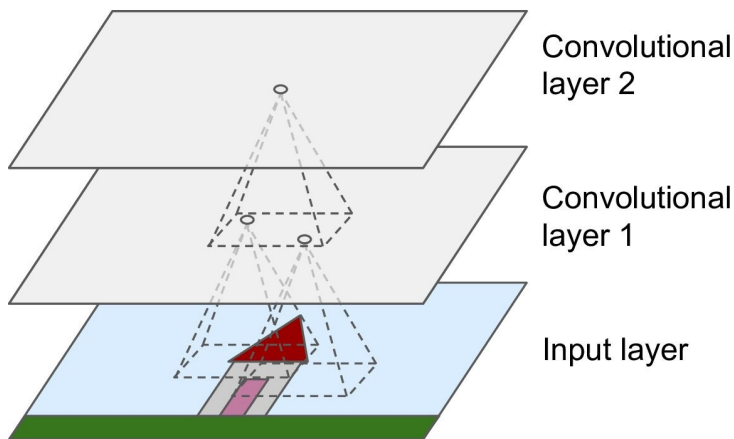CNNs have several important **building blocks**:

1. **2D (or 3D) input layer**
2. **Convolutional layer**
    - Neurons in the first convolutional layer are not connected to every single pixel, **but only to pixels in their receptive fields**
    - Neurons in the second convolutional layer are only connected to neurons within a small rectangular region in the first layer
3. **Pooling layer**
    - Goal is to **subsample** the input image to reduce computational load, memory usage, numbers of parameters (limits risk of overfitting)
4. **Fully-connected output layer**
    - This is a **regular feed-forward network** which produces final output prediction
    - E.g. **softmax layer** that outputs estimated class probabilities

Convolutional layer

Convolutional layers allow the network to:

- Concentrate on low-level features in the first hidden layer
- Assemble them to higher-level features in the next hidden layer

Convolutional layer 2

Convolutional layer 1

Input layer

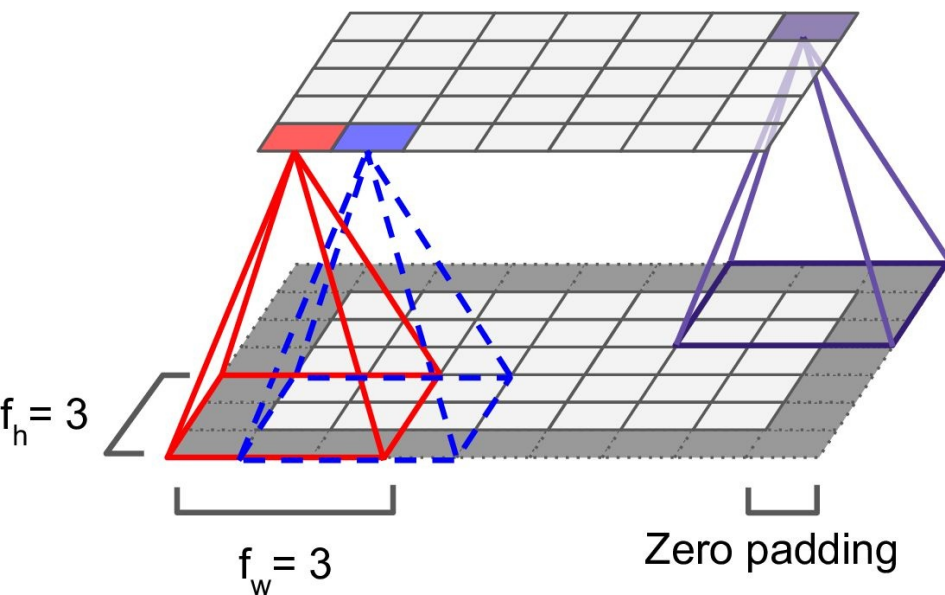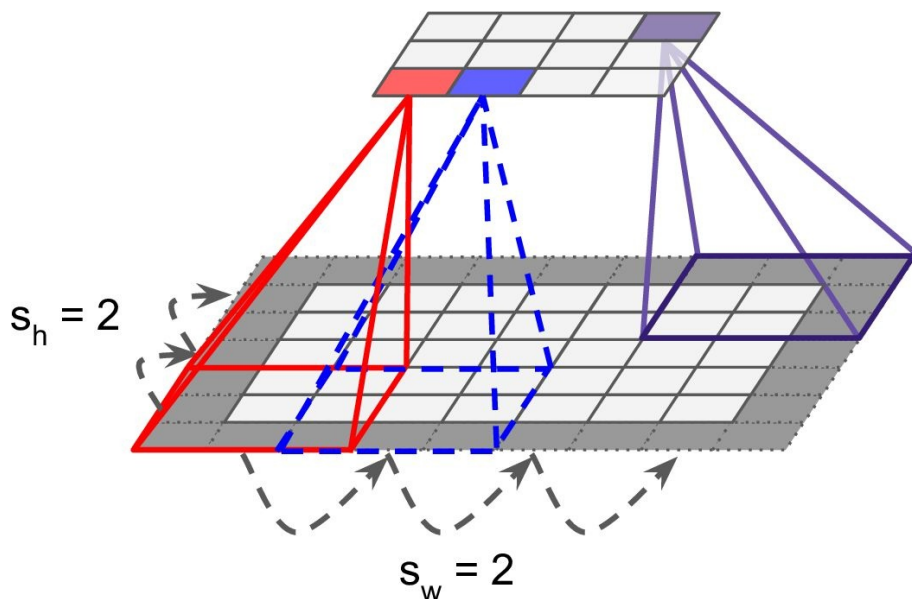Filter: $\begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$

Image

Convolved Feature

Convolutional layer

Need to apply **zero-padding** at each layer and also apply a stride for further **dimensionality reduction:**

$f_h = 3$

$f_w = 3$

Zero padding

$s_h = 2$

$s_w = 2$

Connections between layers and zero padding

Reducing dimensionality using a stride

Pooling layer

- Goal is to **subsample** the input image to reduce computational load, memory usage, numbers of parameters (limits risk of overfitting)

- Each neuron in pooling layer is connected to the outputs of limited number of neurons in previous layer, again located within a small rectangular receptive field

- Most common type is **max pooling**
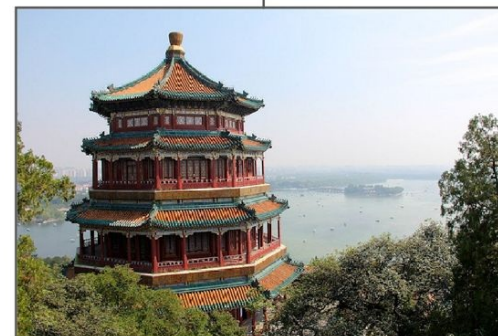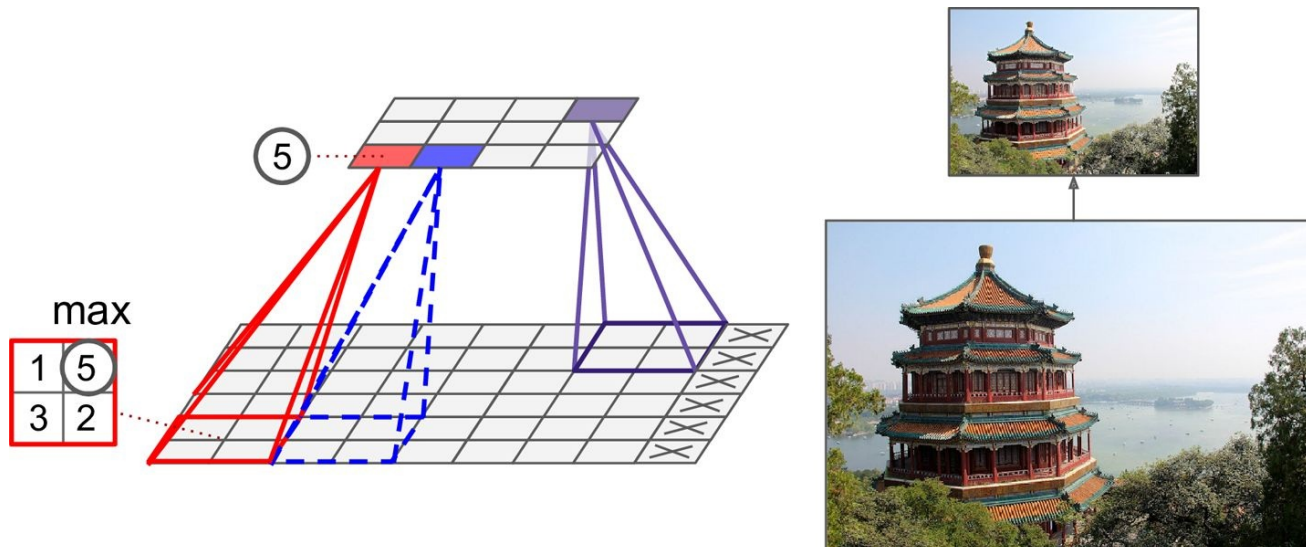
Convolutional Neural Networks (CNNs)
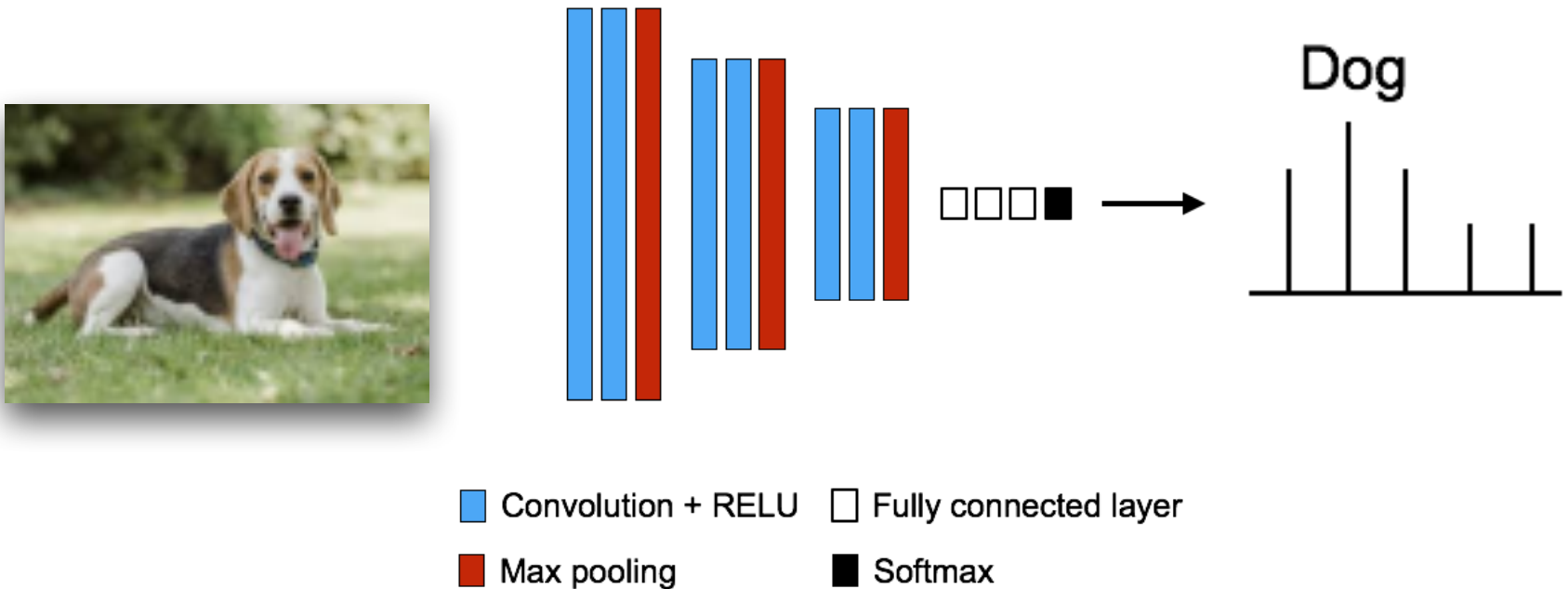
Putting it all together:
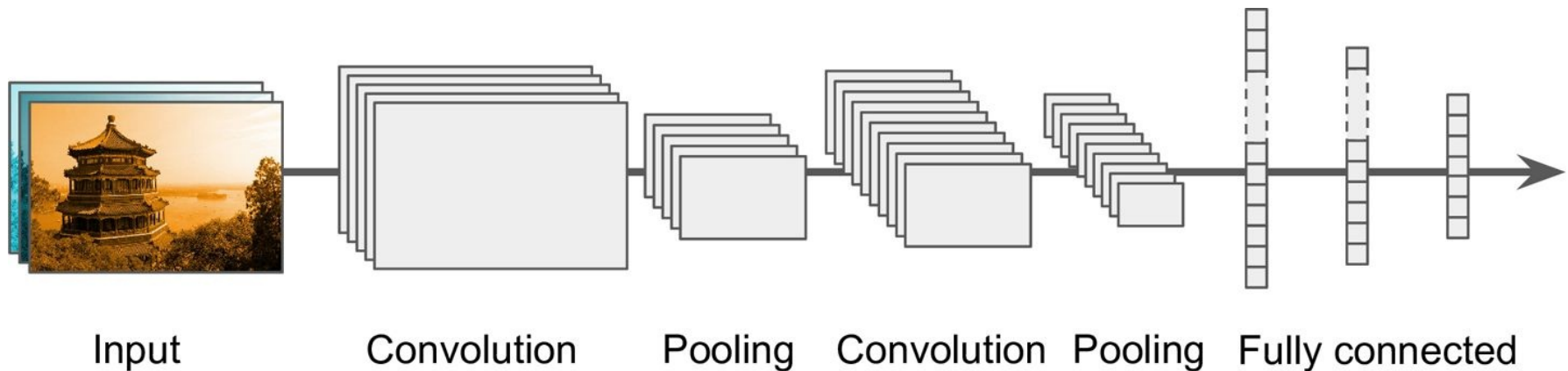
In this case, 3-channel RGB image)

Many variants of CNN exist and have been boosted by the advent of **ImageNet in 2010**
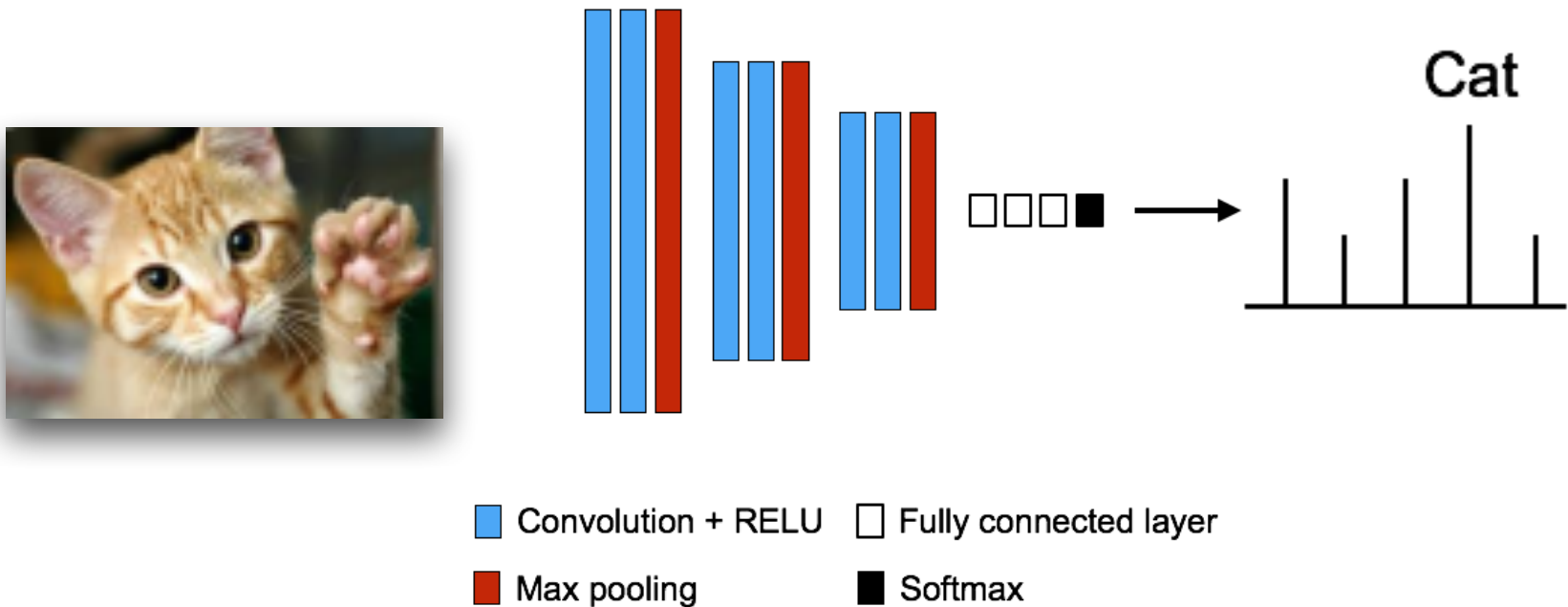
CNNs for image classification

First rewind and look at a simple CNN applied to real image classification

🟦 Convolution + RELU	⬜ Fully connected layer
🟥 Max pooling	⬛ Softmax

CNNs for image classification

First rewind and look at a simple CNN applied to real image classification

CNNs for image segmentation

One major focus in computer vision and medical imaging is on **image segmentation**

- Challenging in medical imaging due to variability in patient anatomy & pathology, patient pose and motion, image artefacts
- U-net is the most common used network , which was proposed by Ronneberger (Google DeepMind) in 2015:
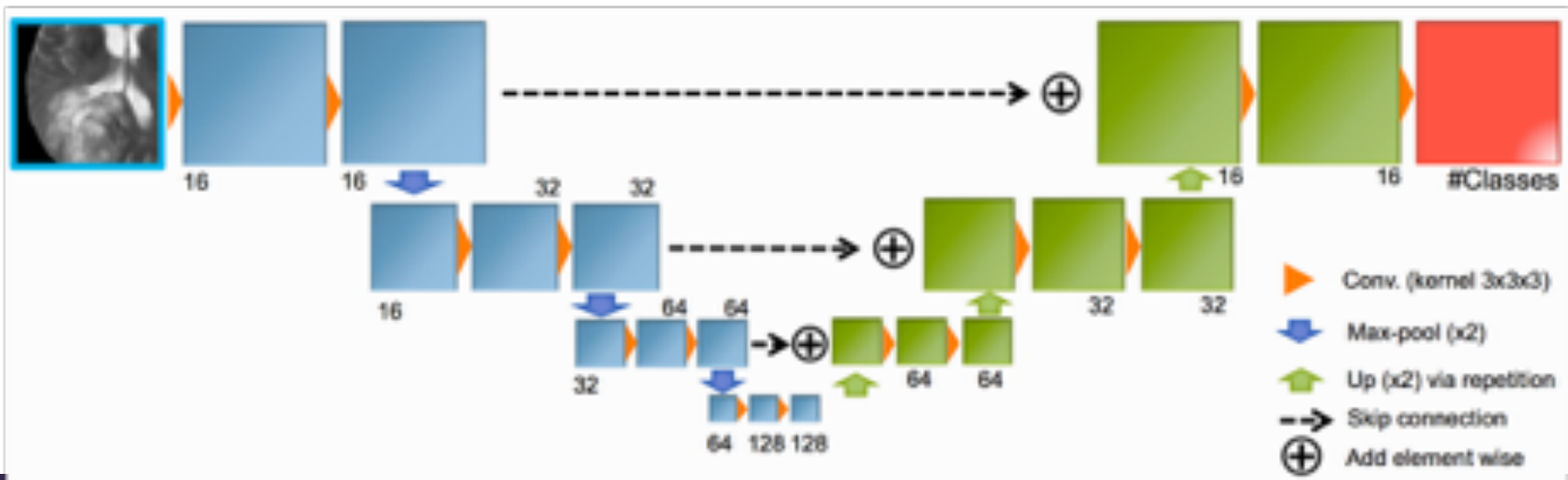
Bits & Bobs

All of the networks so far (deep neural networks, with our without convolutional layers), need to be carefully designed and trained:

Choice of:

- Number of hidden layers and neurons, stacking (AE)
- Loss function, activation function, learning rate, epochs
- **Optimisation methods**
- **Regularisation methods**

Optimisation

Choice of faster gradient-based optimisation methods for use with backpropagation:

1. **Gradient Descent**
2. **Momentum optimisation**
3. **Nesterov Accelerated Gradient**
4. **AdaGrad**
5. **RMSProp**
6. **Adam Optimiser**

Andrew Ng
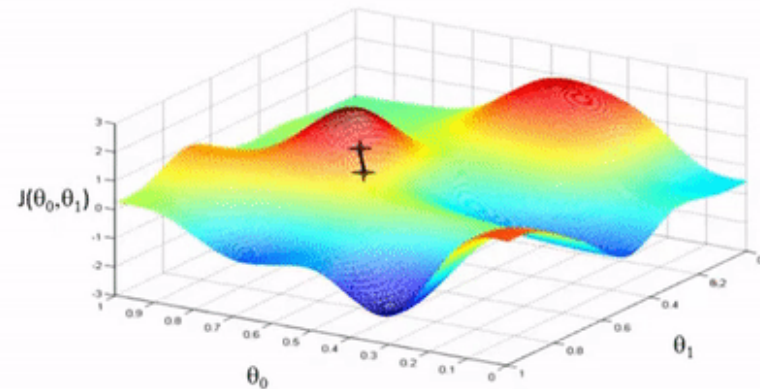
Regularisation

To avoid **overfitting**, we can do the following:

1. **Early stopping**: Interrupt training when its performance on the validation set starts dropping
2. *l_1 and l_2 regularization:* Add a regularization term in the cost function.
3. **Dropout**: At every training step, every neuron (input or hidden) has a probability p of being temporarily "dropped out"
4. **Data augmentation:** Generate new training instances from existing ones, artificially boosting the size of the training set.

    E.g. you can rotate, shift (translate), resize (scale), flip (reflect)

Summary

Input   Convolution   Pooling   Convolution   Pooling   Fully connected
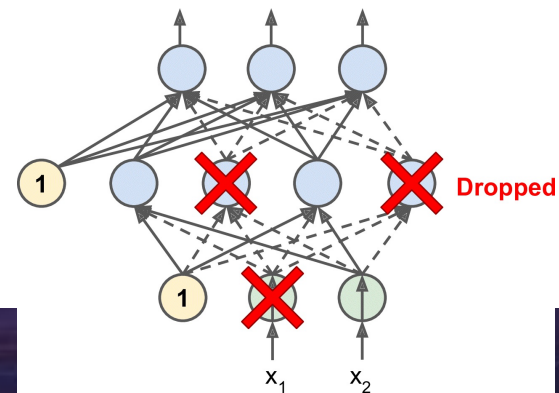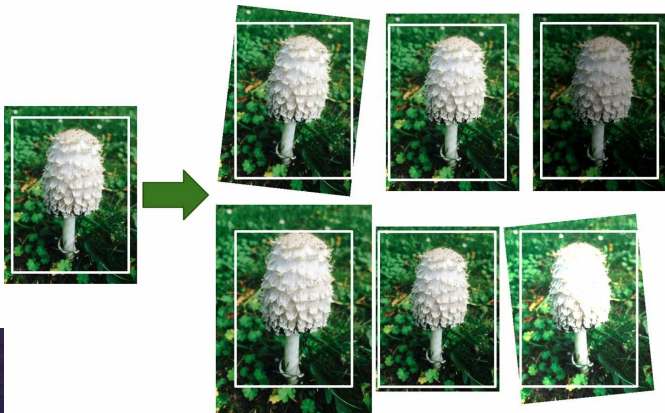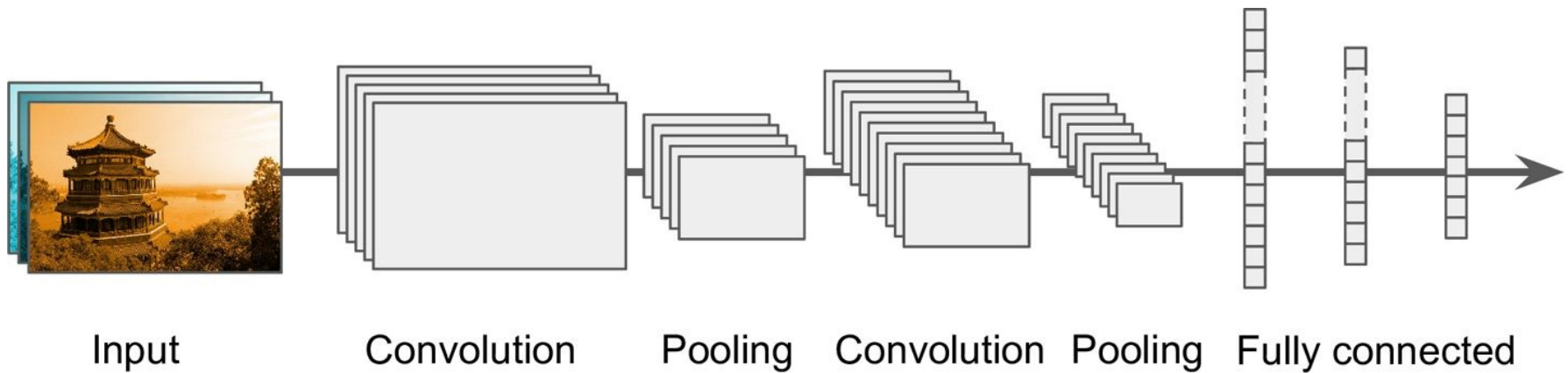
Hyperparameters:
- Number of layers
- Number of epochs
- Kernel size
- Stride
- Learning rate
- Dropout
- Optimisation method

Questions?

Slides adapted from the Machine Learning for Biomedical Application course from King's College of London