Introduction to Neural Networks – Part 2

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Convolutional Neural Networks

Convolutional Neural Networks - CNNs

- Specific type of Neural Networks (NNs)
- The popularity & success of Deep Learning owes much to CNNs
  - which have, in turn, benefitted from computational improvements allowing networks of ever-increasing depth
- CNNs can learn models which recognize objects in images and perform image classification
  - Learn directly from the images
- Input layer is large: one input for each pixel in the image
- Neurons in one layer not fully connected to all neurons in next layer
- Final output: Reduced to a single vector of probability scores
- Often illustrated and modelled in “3D”
  - Matrices of neurons in a layer rather than vectors
- CNNs have 2 key components:
  - Hidden layers – feature extraction part, where network performs convolution + pooling operations to detect features (e.g. stripes of a zebra, edges)
  - Classification: Fully connected layers serve as classifiers of these extracted features – assign probability

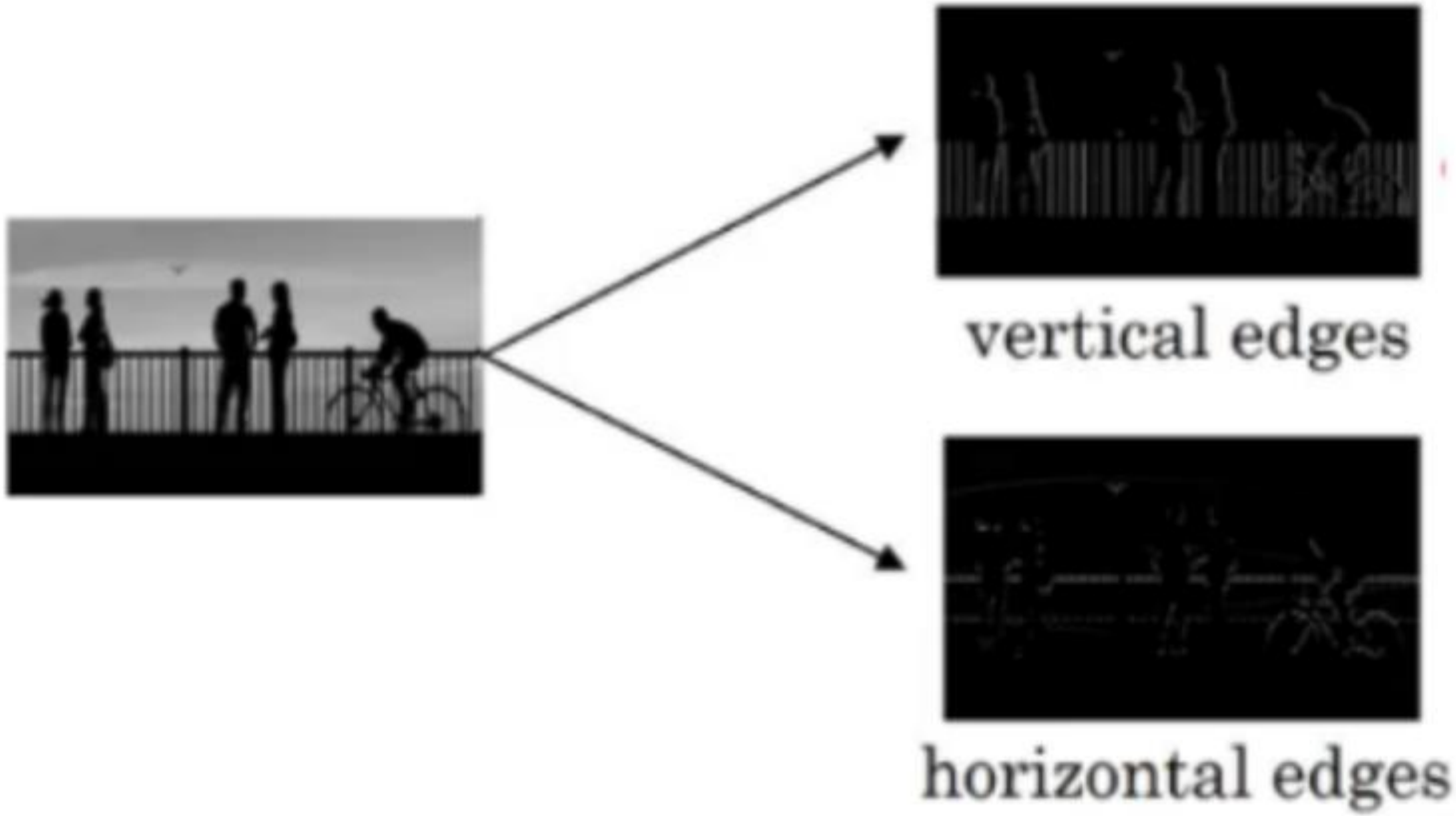
- CNNs are “just” deep neural networks with:
    - Particular kinds of layers which have
        - A particular kind of *connectivity* to previous layers, and
        - A particular kind of *activation function* which is designed to help identify features in images
- The two most important kinds of layers are
    - **convolution layers** which put the “C” in CNN, and
    - **pooling layers**

Convolution

- Using different **filters/kernels** on the input data to produce a **feature/activation map**
- Each filter corresponds to a receptive field
- After performing several convolutions (can be 100s of hidden layers), each with a different filter, we obtain a map of all features – the final output
- Training of CNNs:
  - Same as for regular NNs using backprop and gradient descent
  - Mathematically more complex due to convolutional operations

CNN example – Edge Detection

Start by taking a 6x6 grayscale image (one **channel**)



3	0	1	2	7	4
1	5	8	9	3	1
2	7	2	5	1	3
0	1	3	1	7	8
4	2	1	6	2	8
2	4	5	2	3	9

From https://www.analyticsvidhya.com/blog/2018/12/guide-convolutional-neural-network-cnn/
(which in turn may have been taken from Andrew Ng's videos…)

Edge Detection

"filter" or "kernel"

$$\begin{bmatrix}6&3&0&2&0&1\\3&1&6&6&7&2\\6&3&8&4&5&9\\0&1&3&1&6&5\\0&6&0&0&9&4\\7&8&2&4&5&7\end{bmatrix} * \begin{bmatrix}1&0&-1\\1&0&-1\\1&0&-1\end{bmatrix} = \begin{bmatrix}\ &\ &\ &\ \\\ &\ &\ &\ \\\ &\ &\ &\ \\\ &\ &\ &\ \end{bmatrix}$$

convolution

Edge Detection

$$\begin{bmatrix} 6^{1} & 3^{0} & 0^{-1} & 2 & 0 & 1 \\ 3^{1} & 1^{0} & 6^{-1} & 6 & 7 & 2 \\ 6^{1} & 3^{0} & 8^{-1} & 4 & 5 & 9 \\ 0 & 1 & 3 & 1 & 6 & 5 \\ 0 & 6 & 0 & 0 & 9 & 4 \\ 7 & 8 & 2 & 4 & 5 & 7 \end{bmatrix} * \begin{bmatrix} 1 & 0 & -1 \\ 1 & 0 & -1 \\ 1 & 0 & -1 \end{bmatrix} = \begin{bmatrix} \boxed{1} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix}$$

$$6 \times 1 + 3 \times 0 + 0 \times -1 + 3 \times 1 + 1 \times 0 + 6 \times -1 + 6 \times 1 + 3 \times 0 + 8 \times -1$$
$$= 6 + 0 + 0 + 3 + 0 + -6 + 6 + 0 + -8 = 1$$

Edge Detection

$$\overset{6\times6}{\begin{bmatrix} 6 & 3 & 0 & 2 & 0 & 1 \\ 3 & 1 & 6 & 6 & 7 & 2 \\ 6 & 3 & 8 & 4 & 5 & 9 \\ 0 & 1 & 3 & 1 & 6 & 5 \\ 0 & 6 & 0 & 0 & 9 & 4 \\ 7 & 8 & 2 & 4 & 5 & 7 \end{bmatrix}} * \overset{3\times3}{\begin{bmatrix} 1 & 0 & -1 \\ 1 & 0 & -1 \\ 1 & 0 & -1 \end{bmatrix}} = \overset{4\times4}{\begin{bmatrix} 1 & \boxed{-5} & & \\ & & & \\ & & & \\ & & & \end{bmatrix}}$$

$$3\times1 + 0\times0 + 2\times-1 + 1\times1 + 6\times0 + 6\times-1 + 3\times1 + 8\times0 + 4\times-1$$

$$= 3 + 0 - 2 + 1 + 0 - 6 + 3 + 0 - 4 = -5$$

Convolving a 6x6 image with a 3x3 filter

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3	0	1	2	7	4
1	5	8	9	3	1
2	7	2	5	1	3
0	1	3	1	7	8
4	2	1	6	2	8
2	4	5	2	3	9

6 X 6 image

*

1	0	-1
1	0	-1
1	0	-1

3 X 3 filter

for vertical edges

=

-5	-4	0	8
-10	-2	2	3
0	-2	-4	-7
-3	-2	-3	-16

- Dot product for first output element:
  - $3*1 + 0*0 + 1*(-1) + 1*1 + 5*0 + 8*(-1) + 2*1 + 7*0 + 2*(-1) = -5$
- Type of filter helps to detect horizontal or vertical edges
- Higher-magnitude values in output matrix will represent areas where edges have been located

$$\underbrace{\begin{bmatrix} 1 & 0 & -1 \\ 1 & 0 & -1 \\ 1 & 0 & -1 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & -1 \\ 2 & 0 & -2 \\ 1 & 0 & -1 \end{bmatrix}}_{\text{vertical edge detection}} \qquad \underbrace{\begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \end{bmatrix} \quad \begin{bmatrix} 1 & 2 & 1 \\ 0 & 0 & 0 \\ -1 & -2 & -1 \end{bmatrix}}_{\text{horizontal edge detection}}$$

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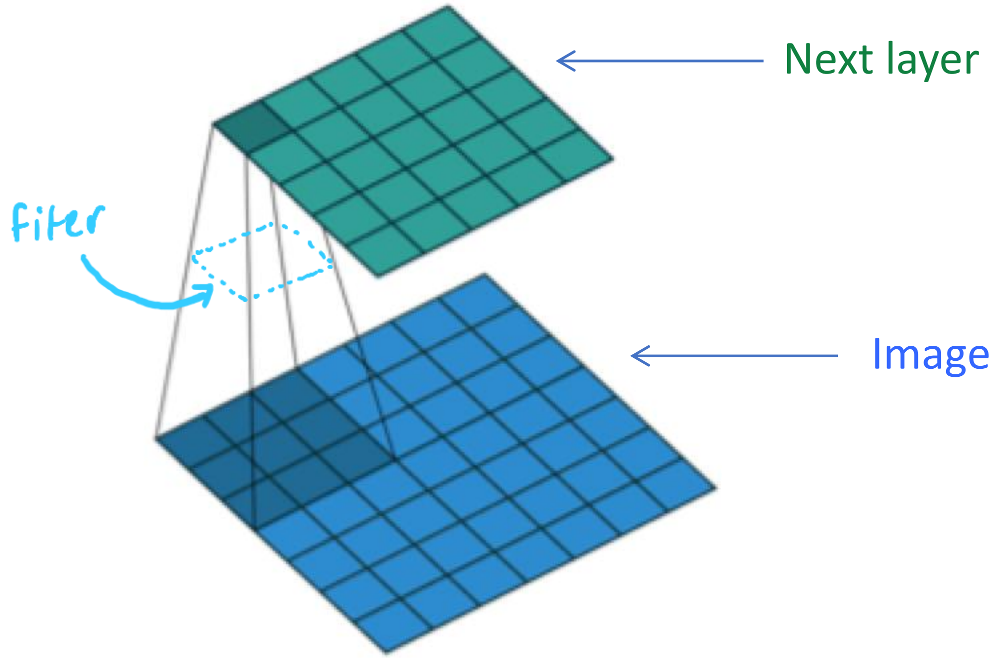
$$\begin{bmatrix} 1 & 0 & -1 \\ 1 & 0 & -1 \\ 1 & 0 & -1 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & -1 \\ 2 & 0 & -2 \\ 1 & 0 & -1 \end{bmatrix} \quad \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \end{bmatrix} \quad \begin{bmatrix} 1 & 2 & 1 \\ 0 & 0 & 0 \\ -1 & -2 & -1 \end{bmatrix}$$

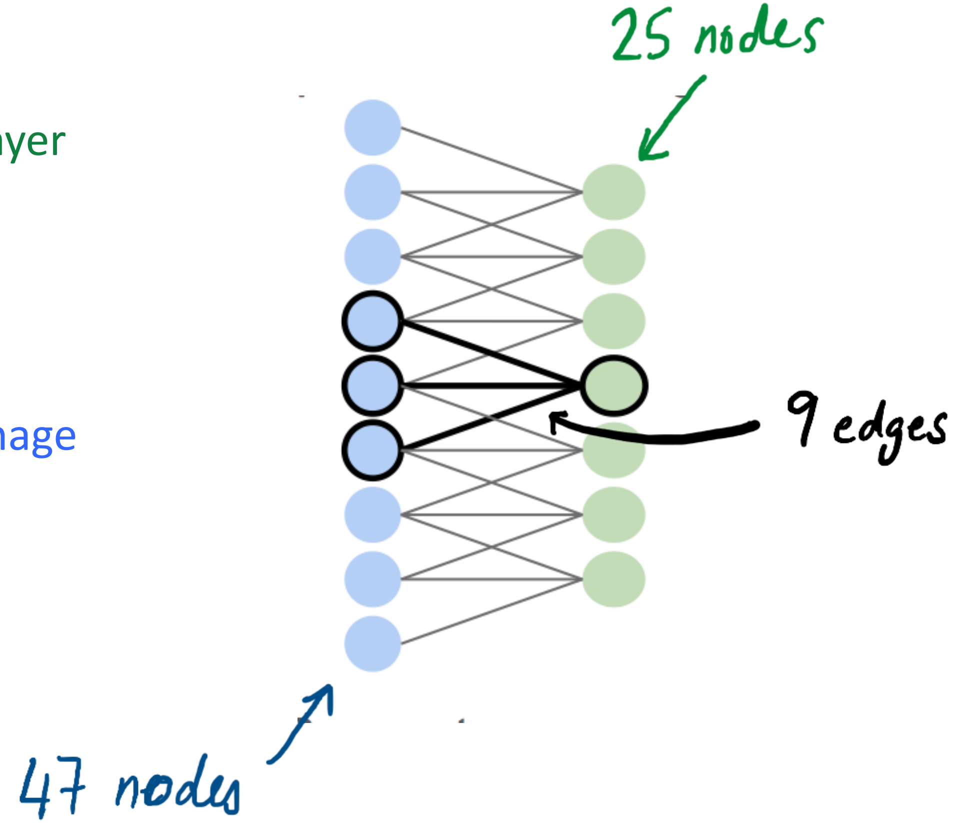
but in a CNN we let the NN find useful filters itself

$$\begin{bmatrix} w_1 & w_2 & w_3 \\ w_4 & w_5 & w_6 \\ w_7 & w_8 & w_9 \end{bmatrix}$$

Convolution

- CNNs slide the same kernel of weights across their input (**compute dot product**), thus have local sparse connectivity + tied weights

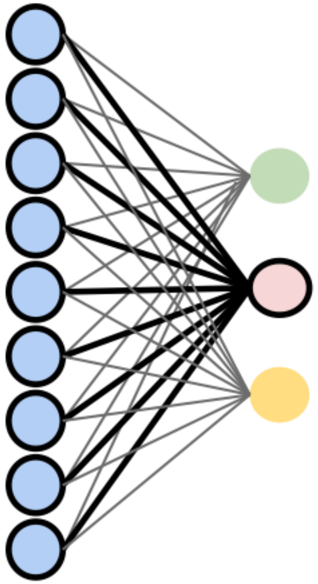




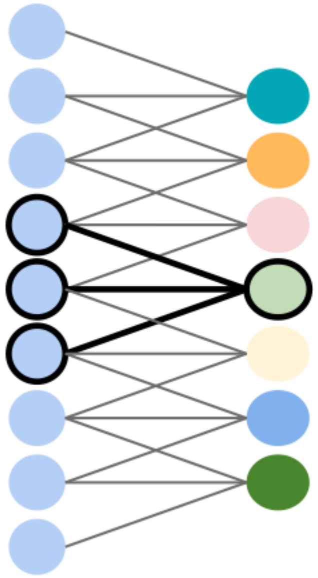
Connectivity

Fully connected (dense):

Every neuron is connected to all components of the input vector

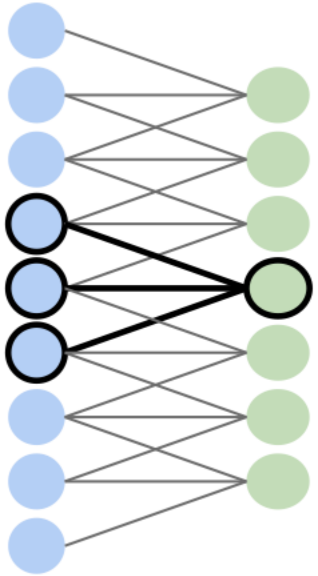


Sparse connectivity



Every neuron is only affected by a limited input “receptive field”; 3 in this example.

Sparse connectivity + parameter sharing



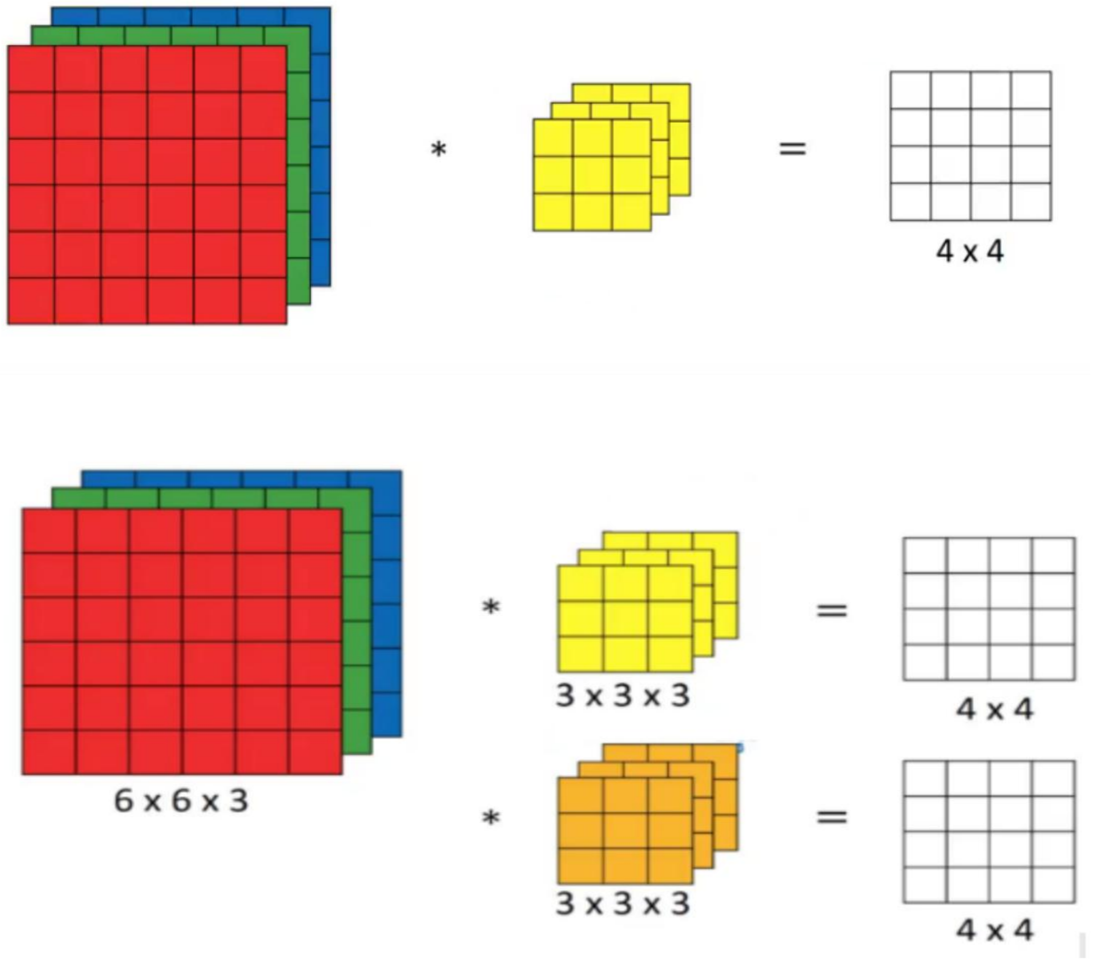
Parameters are shared (tied weights) across all neurons

From: M, Mustafa, Introduction to Deep Learning, NERSC

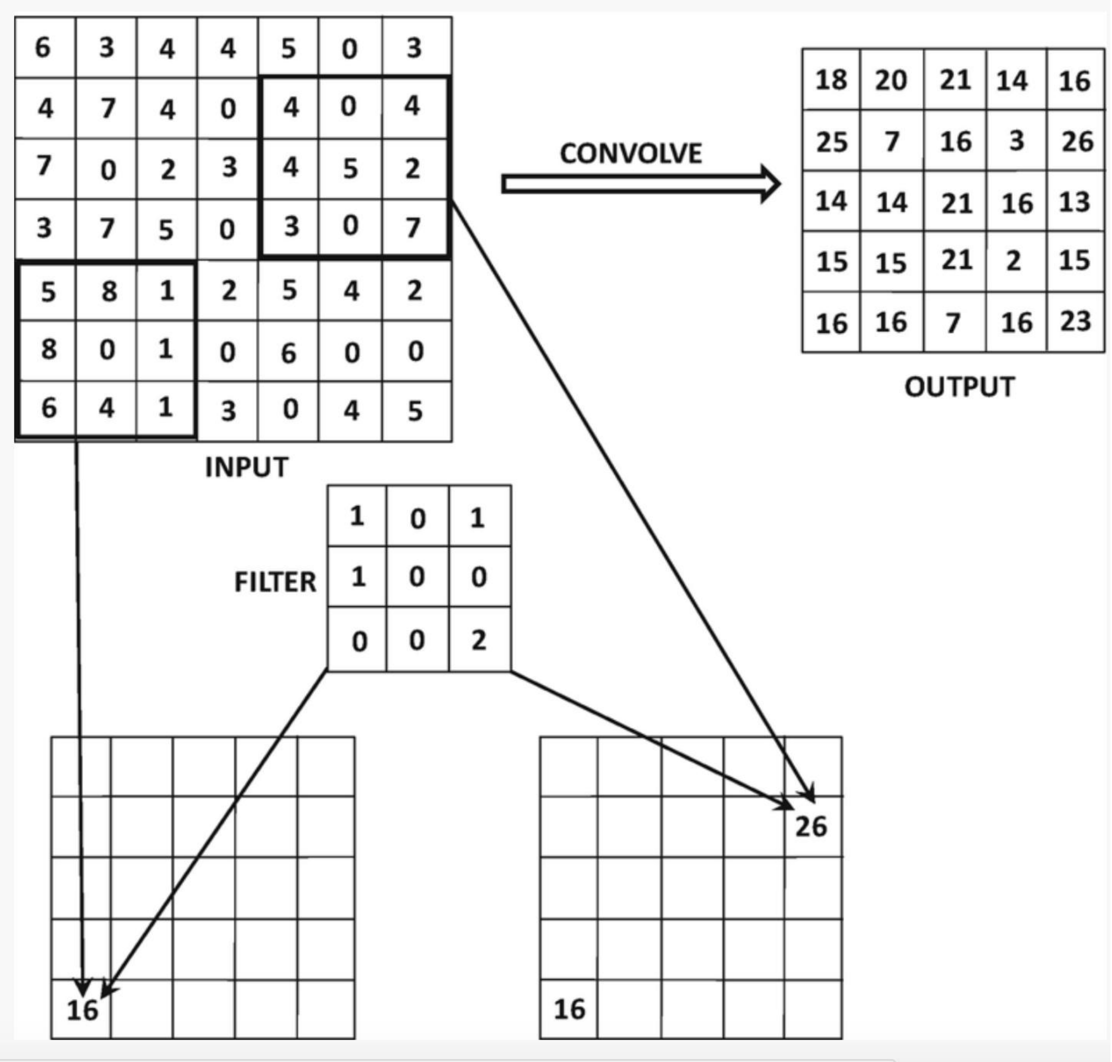
Shared weights + Biases

- Weights + biases are usually all the same for all neurons in a given layer
- So all hidden neurons **detect the same hidden feature** (e.g. edge) in different regions of the image
- This makes the network tolerant re translations of objects in an image – it doesn’t matter where the object is in the image

CNNs with multiple channels



From https://www.analyticsvidhya.com/blog/2018/12/guide-convolutional-neural-network-cnn/



From https://link.springer.com/chapter/10.1007/978-3-319-94463-0_8

Padding

- From https://link.springer.com/chapter/10.1007/978-3-319-94463-0_8

6	3	4	4	5	0	3
4	7	4	0	4	0	4
7	0	2	3	4	5	2
3	7	5	0	3	0	7
5	8	1	2	5	4	2
8	0	1	0	6	0	0
6	4	1	3	0	4	5

PAD $\Longrightarrow$

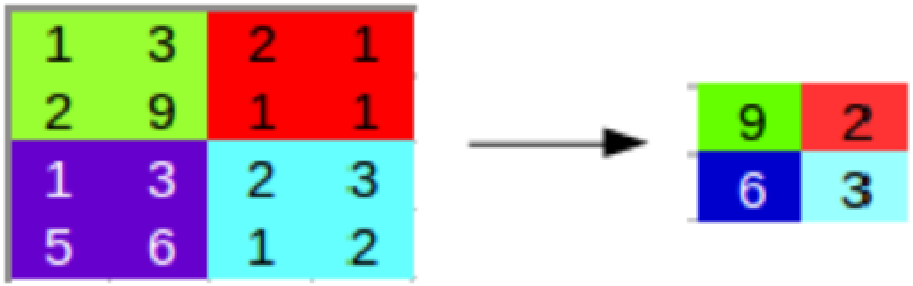
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	6	3	4	4	5	0	3	0	0
0	0	4	7	4	0	4	0	4	0	0
0	0	7	0	2	3	4	5	2	0	0
0	0	3	7	5	0	3	0	7	0	0
0	0	5	8	1	2	5	4	2	0	0
0	0	8	0	1	0	6	0	0	0	0
0	0	6	4	1	3	0	4	5	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0

Pooling

1	3	2	1
2	9	1	1
1	3	2	3
5	6	1	2

Input

Applying **‘max’ pooling** with a filter of stride = 2, size = 2
(Pooling layer hyperparameters)

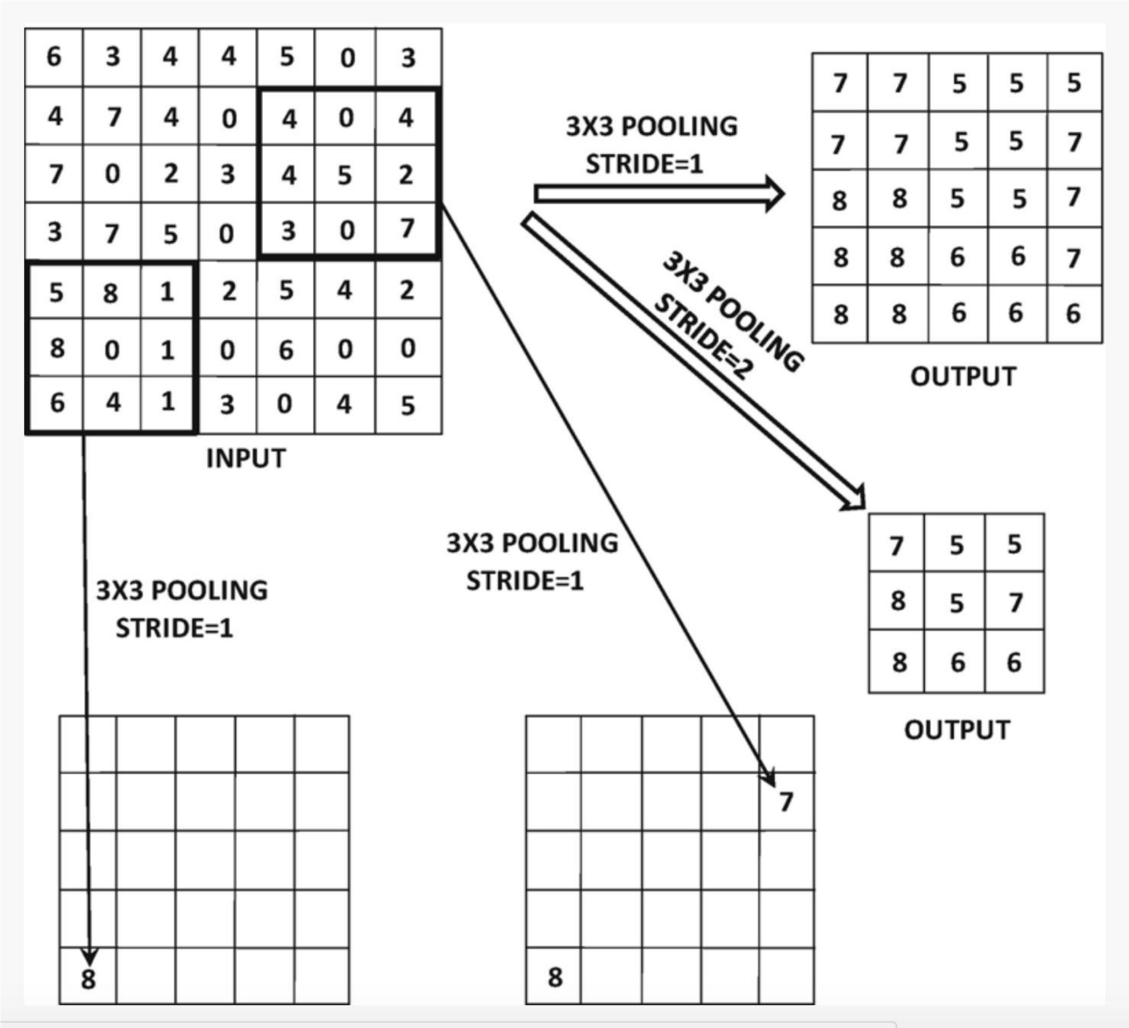


Strides in Padding & Pooling

- Stride: Size of the step the convolution filter moves each time. Usually (and in example on previous slides) slides pixel by pixel. Stride > 2 is uncommon, bad on accuracy if too large.
- Padding: Size of feature map is always smaller than input. Corner pixels are covered less often than centre pixels. To prevent it from shrinking: add layer of zero-valued pixels.
- Pooling:
  - Makes the model invariant to small local translations of input
  - ‘Max’ (introduces non-linearity + greater translational invariance) or ‘Average’ pooling are most common pooling layers
  - Used to reduce dimension of input feature map (condenses output of small regions) , reduces #parameters that the model needs to learn => speeds up training time; stride > 1
  - Controls overfitting
  - Interleafed with convolution/ReLu layers, but less frequently applied

Max Pooling example

- From https://link.springer.com/chapter/10.1007/978-3-319-94463-0_8

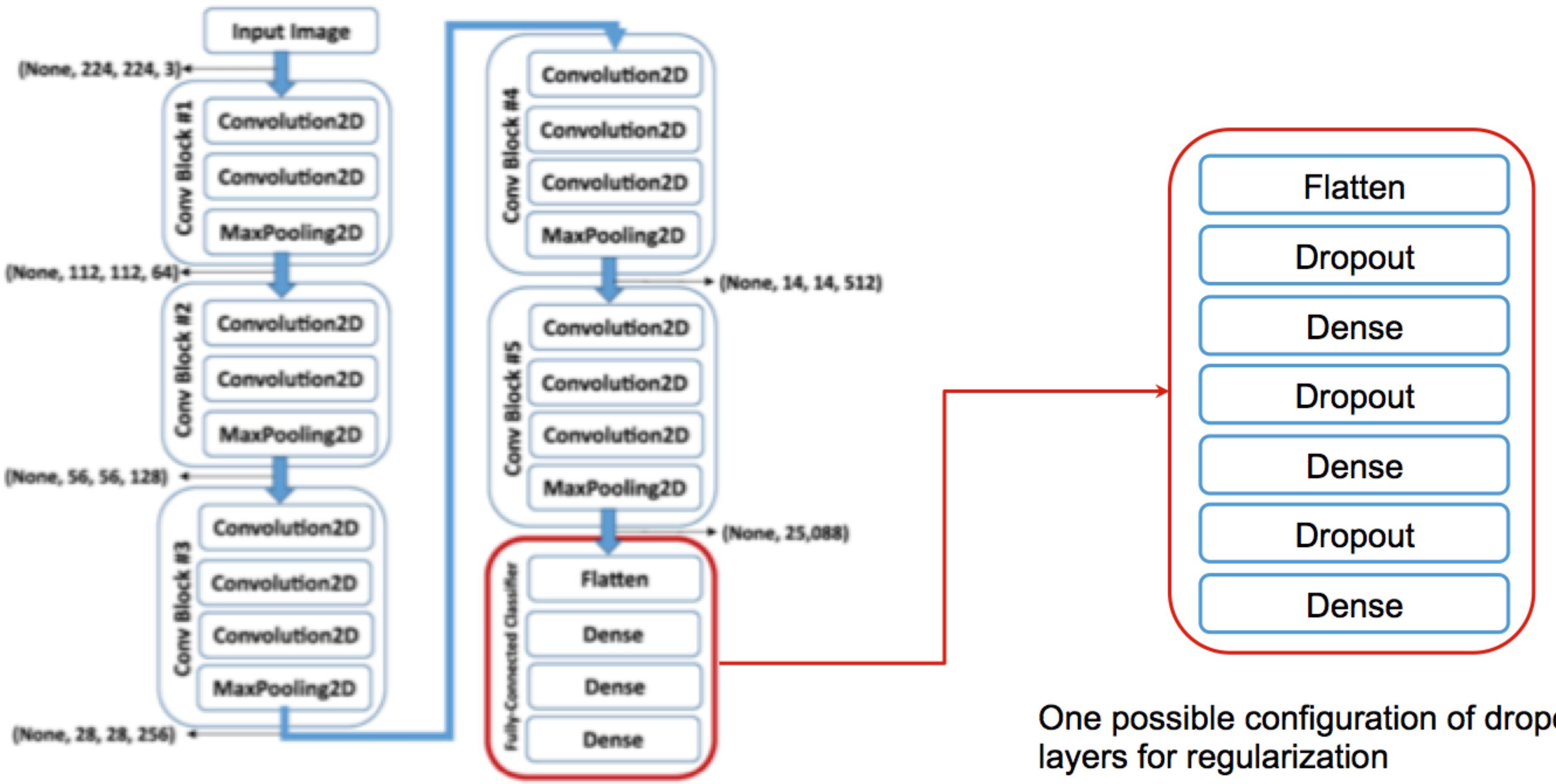


Classification – fully connected layer

- After convolution + pooling layers
- A few fully connected layers (like regular NN)
- Can only accept 1D data
  - Conversion from 3D -> 1D (e.g. 'flatten' in Python)
- Where most parameters are
  - E.g. Two fully connected layers with 4096 hidden units have $4096^2 \sim 16$ million weights

(Convolutional layers have more activations)

Example for a full CNN architecture
…pulling all the bits together from the previous slides



One possible configuration of dropout layers for regularization

A schematic of VGG-16 Deep Convolutional Neural Network (DCNN) architecture

trained on ImageNet (2014 ILSVRC winner)

Dropout

- Dropping out units/neurons during the training phase =>
  - These neurons are not considered during a particular forward or backward propagation
- Chosen at random
- To avoid overfitting
- Used between fully connected layers of the classification part to improve the generalization error

Residual Networks and Depth

- Increasing network depth: (see Goodfellow et al. arXiv:1312.6082)
  - Accuracy increases
  - Outperform wider models with same number of parameters
  - Harder to train due to the vanishing gradient problem
  - (exploding gradients are also possible!)

- As gradient is back-propagated to earlier layers:
  - Repeated multiplication can make gradient very small
  - Solution: Skip Connections

Skip Connections

- Partial architecture of **ResNet**
  - Connections between layers i and (i+r), r>1
- Copy features from earlier layers i into later ones (i+r)
- Inputs classified with a small amount of non-linearity (simple ones) will skip many connections
- Inputs with more complex structures will travel across more connections so all relevant features can be covered
- Side-steps the vanishing gradient problem
  - Effective gradient flow because the backprop algorithm can now use a fast lane using the skip connections

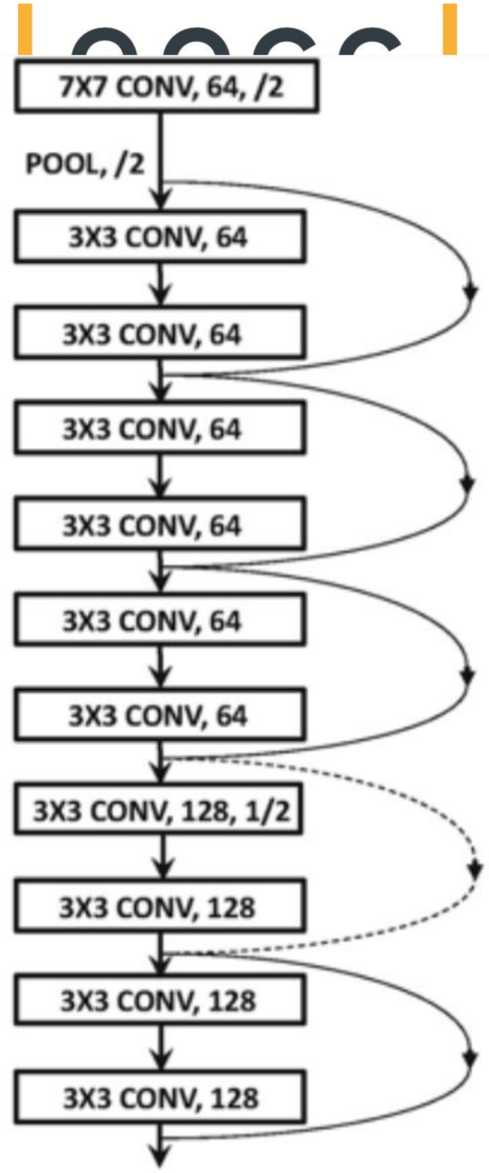
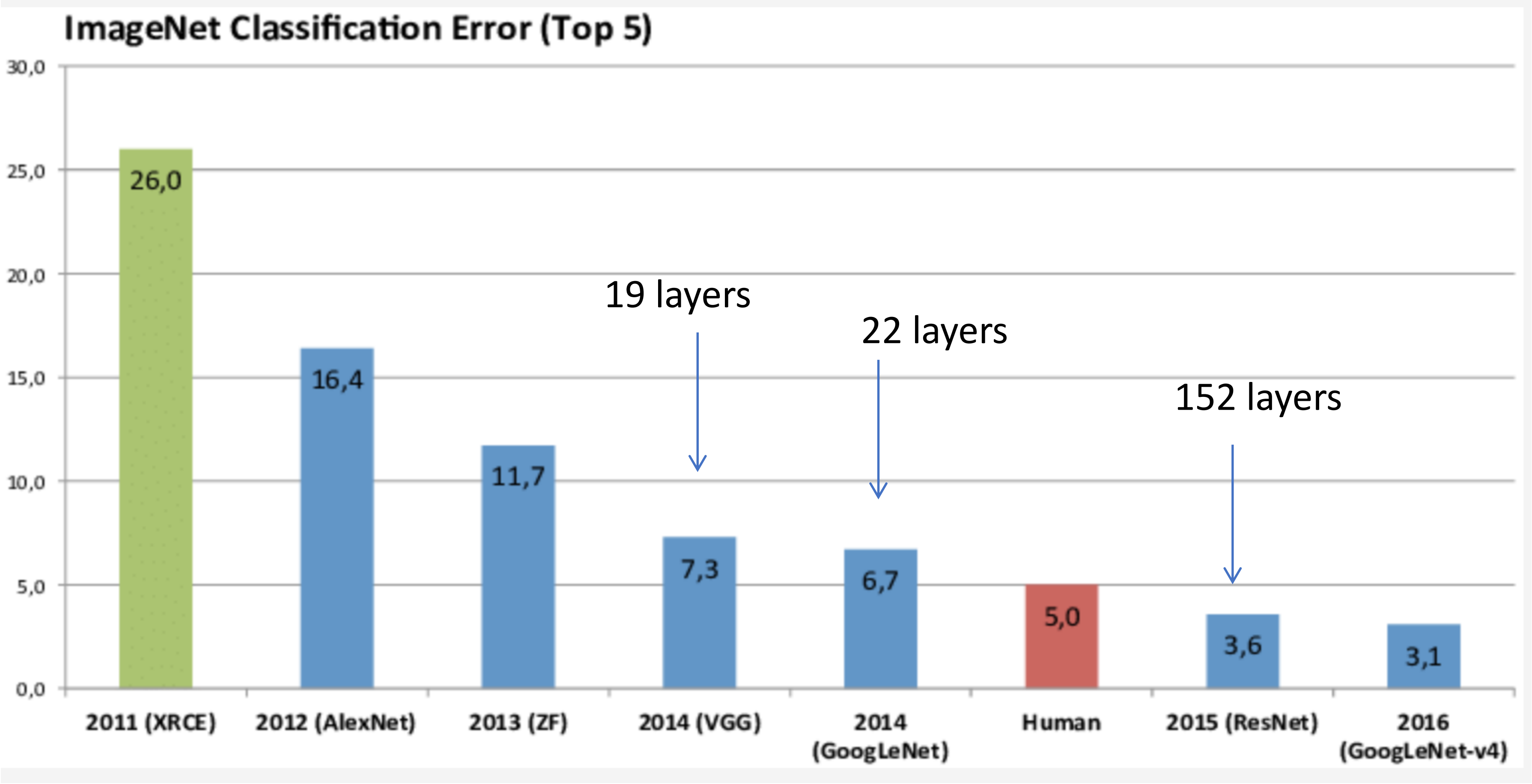


Image Source: https://link.springer.com/chapter/10.1007/978-3-319-94463-0_8

CNN architectures - depth



Zitzewitz, Gustav. "Survey of neural networks in autonomous driving." (2017)

Some Popular Architectures

- ResNet
  - A ”residual network” : Links to skip layers
- Inception Network
  - Multiple filters combined so that the network can learn the best filter to use
- MobileNet
  - An attempt to lower computation cost using a lower-dimensional filter (“depthwise-seperable convolution”)
- EfficientNet
  - Includes features to trade-off resolution, depth and width to get the best results with the computational resources available

- Earlier networks
  - LeNet, 1989: 7 layers, including convolution, pooling and dense, using sigmoid
  - AlexNet, ~2012: 11 layers, using ReLU
  - GoogLeNet, ~2014: 22 layers
  - VGG-16, ~2018: 21 layers (of which 16 parameterised) aiming to lower number of parameters. More, smaller kernels.

Other Neural Network Architectures

Natural Language Processing
as a key driver in NN architecture design

Bag of Words

- Vector of length *n* to represent occurrence of words from a dictionary of *n* words
- Can be suitable for basic document classification
- Issue: Does not take order into account

RNN

- Has some memory
- Issue: Vanishing & Exploding Gradients

LSTM

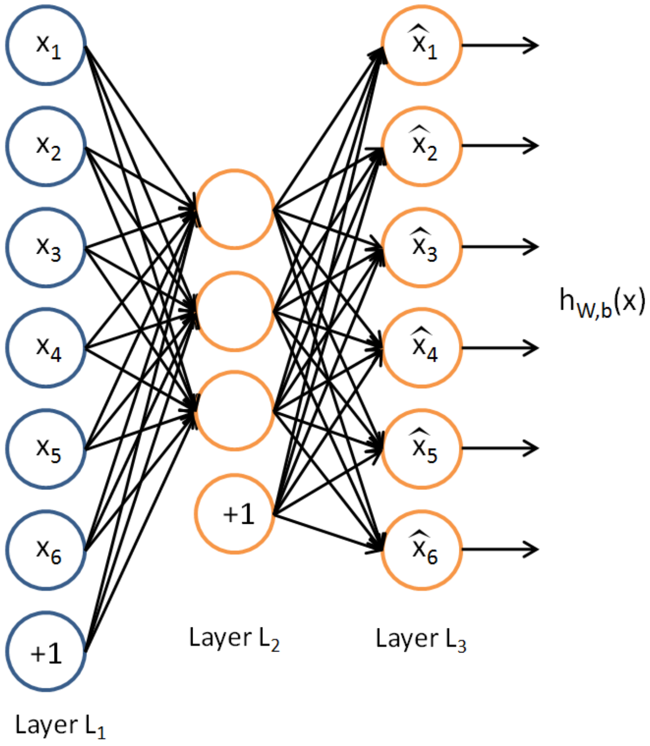
- Proposed 1997
- Introduce a mechanism for long-term memory
- Issue: Difficult to train
- Issue: Transfer Learning doesn't work well
- Issue: Sequential calculation

Transformers

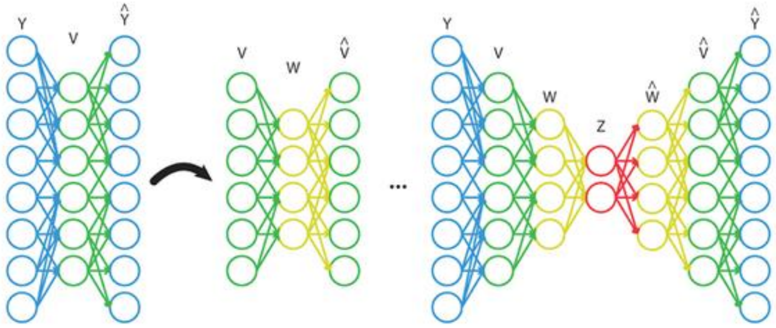
- Use self attention
- Can process data in parallel
  - Although still computationally expensive
- Appear to give better results than LSTM
- Better at keeping track of context

Types of DNN

- Autoencoder
  - Neural network used for dimensionality reduction and feature learning
  - Comprises an encoder to map data to a lower-dimensional representation and a decoder for reconstruction
  - Layers trained separately with input == output
  - Data compression, image denoising, anomaly detection.
  - Feature learning for subsequent tasks
- Can also use multiple DNN together, i.e. Generative Adversarial Network (GAN)
  - Generator network to create data
  - Discriminator network to try and identify genuine data
  - Generator aims to produce data like the real data
  - Discriminator distinguishes between real and fake data
  - Loss functions to optimise real data production and identification

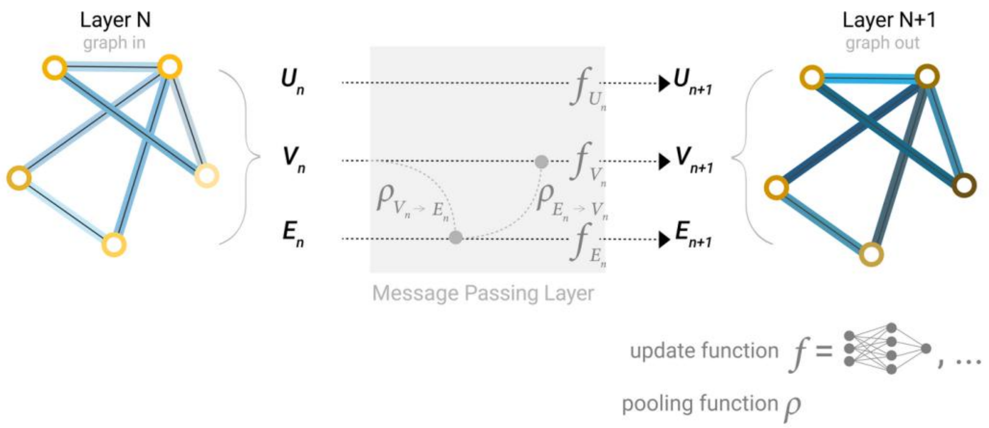


http://ufldl.stanford.edu/tutorial/unsupervised/Autoencoders/



Berniker M, Kording KP. Deep networks for motor control functions. *Frontiers in Computational Neuroscience*. 2015;9(32). doi:10.3389/fncom.2015.00032.

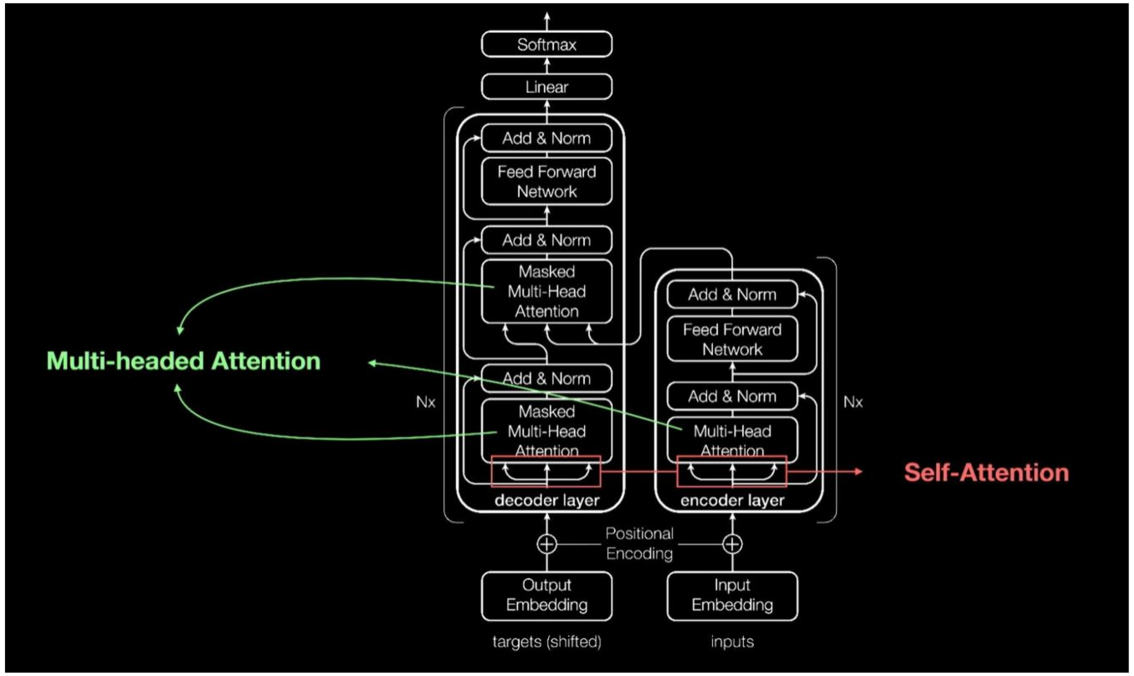
Graph Neural Networks (GNN)



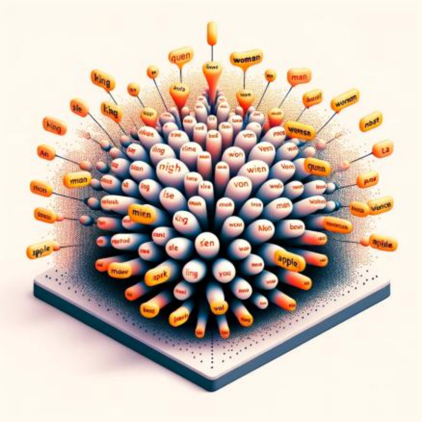
https://distill.pub/2021/gnn-intro/

- Different approaches to GNN
  - Graph: Whole structure categorisation
  - Node: Classification of elements
  - Edge: Relationship between elements
  - Collapsing graphs to matrices for computation so care about adjacency
- Typically have a multi-level perceptron (MLP) for each aspect of the graph (nodes, edges, etc…)
  - Plus pooling layers to couple these together (nodes influence edges, etc…)
- Nearest neighbour message passing to maintain locality
  - Variable form of convolution (no fixed kernels)

Transformers

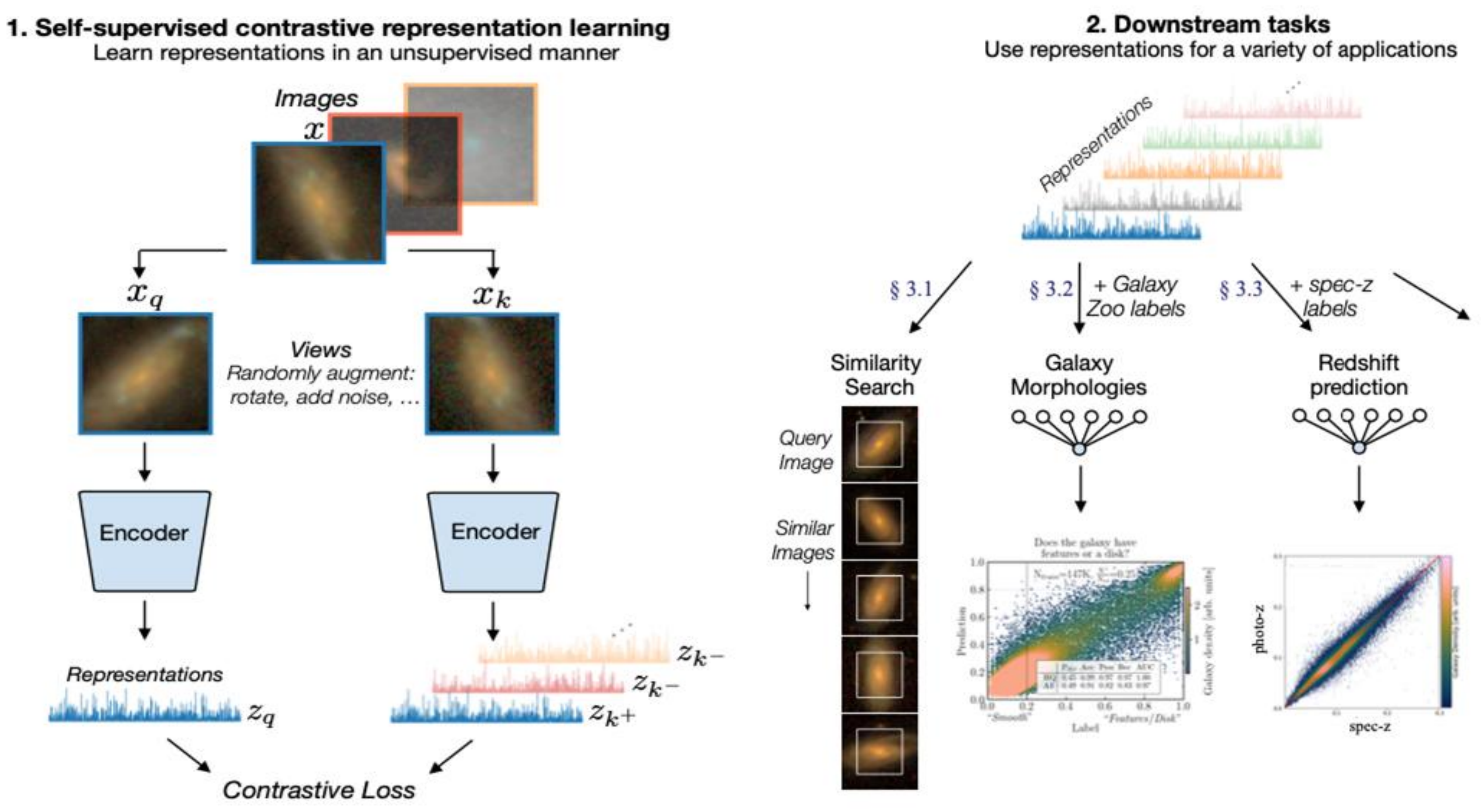


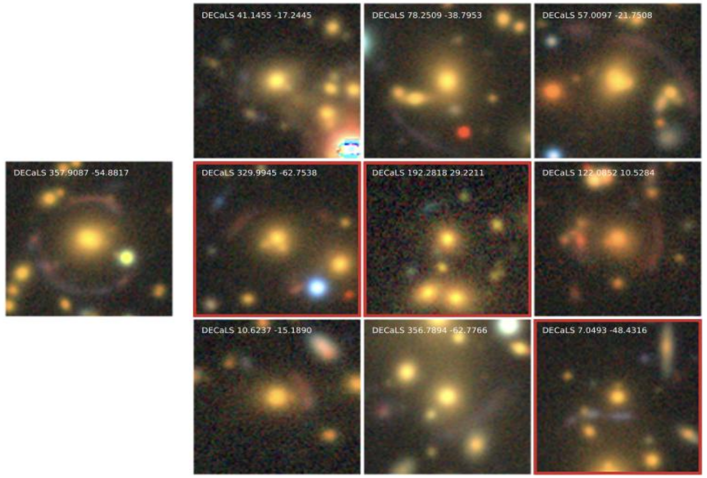
https://blogs.nvidia.com/blog/what-is-a-transformer-model/



- LLM built on transformer models
  - The feed forward network in the encoder and decoder is still a standard DNN (if often very large)
  - GPT-3 has something like 95 layers, 175 billion parameters (proportional to neurons)
  - Attention calculations are small matrix operations on word placement
    - Attention scores
- Word embeddings key part of transformers
  - Mapping words into high dimensional space
  - Embedding is learned as the model is trained

Example use: Identifying galaxy features





Initial approach: Hayat et. al. (2020) arXiv:2012.13083
Strong-lens analysis: Stein et. al. (2021) arXiv:2110.00023

DNNs

- Neural Networks are **highly-parameterised**, **non-linear** models where the parameters (the **weights** and **biases**) are calculated using **back propagation** to calculate **gradients** which are, in-turn, used to **minimise** a loss function.
- Increasing depth gives more parameters:
  - Tends to allow for a more accurate model
  - Run the risk of overfitting
  - Computationally costly
- NN architectures are often selected for the problem at hand but often this boils down to finding different ways to try to optimally trade off
  - Accuracy
  - Training time & convergence
  - Prediction time

DNNs

- Key to DNNs usefulness are
  - Growth in computing to enable large linear algebra operations to be undertaken quickly
  - Depth and breadth of the network has improved performance
- Still many challenges to functionality
  - Over fitting
  - Exploding or vanishing gradients
  - Reliability/Generalisability
  - Network design
  - Data availability
- HPC challenges are common
  - Parallelisation
  - Memory capacity
  - Communication
  - Load balance
- Try out some network features for yourselves
  - https://playground.tensorflow.org