Deconvoluting Graph Convolutional Networks

Answering the whats, whys and hows

Nagma Khan
M.Tech, 3rd Year
Vision and Image Processing Lab, Electrical Engineering

Outline

- Convolutional Neural Networks
- Why Graph Convolutional Networks (GCN)?
- Convolution in GCN
- Applications

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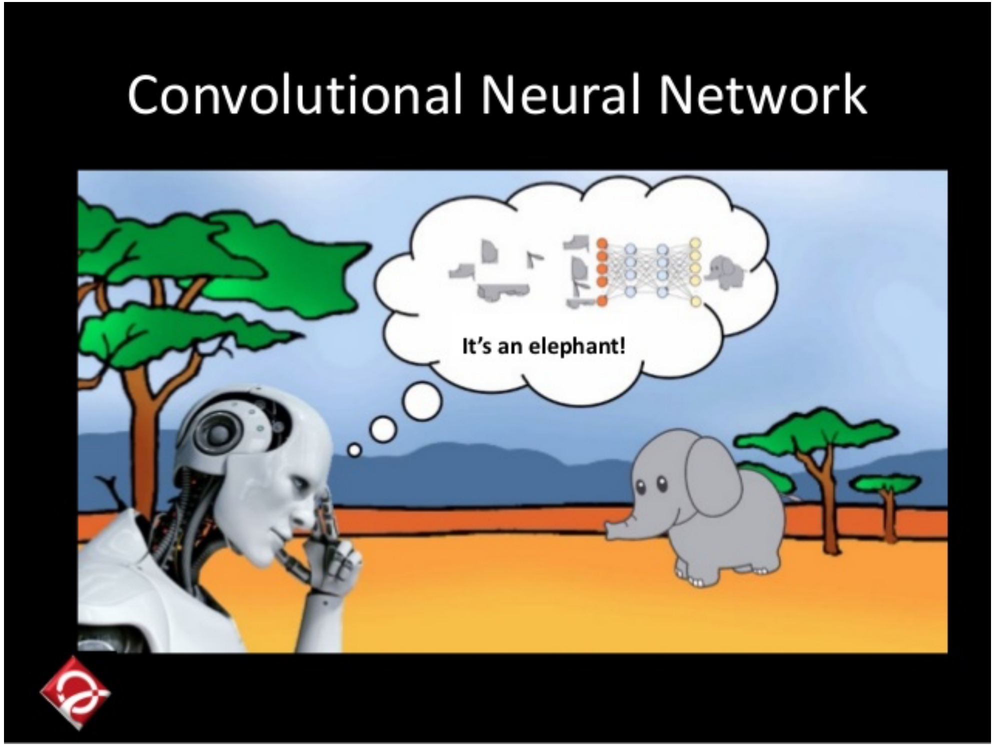
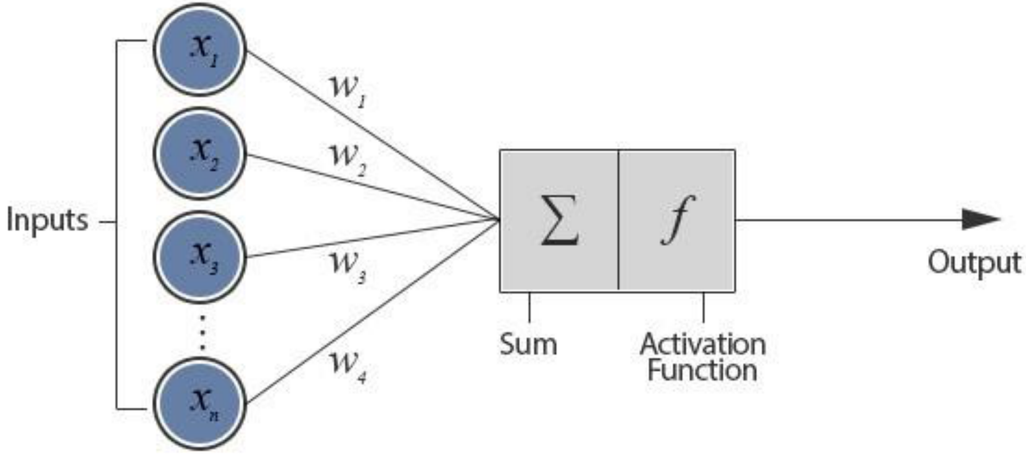
Convolutional Neural Networks - The revolution



- AlexNet brought about a revolution with its simple architecture and good performance
- This network achieved a top-5 error rate of 15.3% in ImageNet-2012 challenge
- Has just 8 layers, 5 convolutional followed by 3 fully-connected

Image courtesy: https://www.slideshare.net/Haxel/iisdv-2017-the-next-era-deep-learning-for-biomedical-research

Neural Networks - The starting point



A perceptron

- Perceptron consists of weights w, summing function and an activation function
- Output = f(Wx + b)

Image courtesy: https://medium.com/technologymadeeasy/for-dummies-the-introduction-to-neural-networks-we-all-need-c50f6012d5eb

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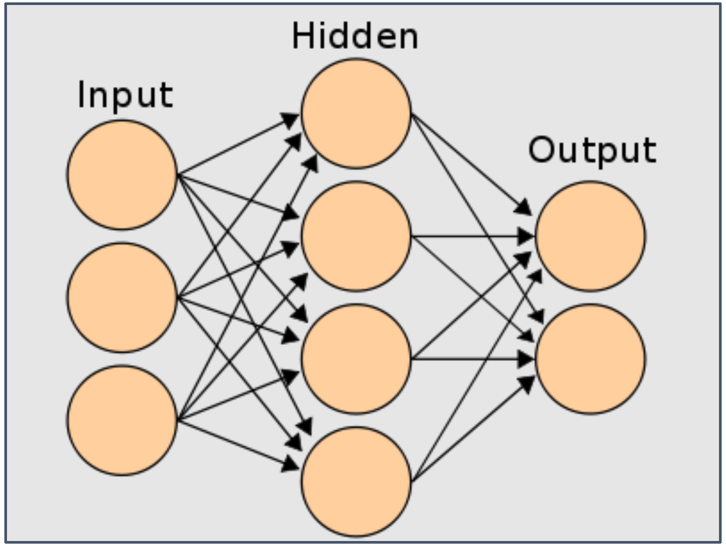


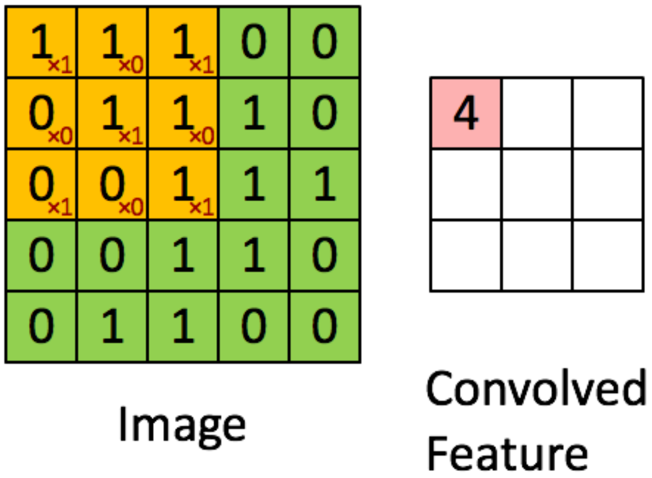
A multi-layer perceptron model

Multi-layer perceptron (MLP) models do not take spatial structure into account and suffer from curse of dimensionality!

Image courtesy: https://medium.com/technologymadeeasy/for-dummies-the-introduction-to-neural-networks-we-all-need-c50f6012d5eb

Convolutional Neural Networks (CNN)

- Operates on images - captures the spatial structure
- Consists of learnable set of filters which perform 2D convolution on the image to get activation map



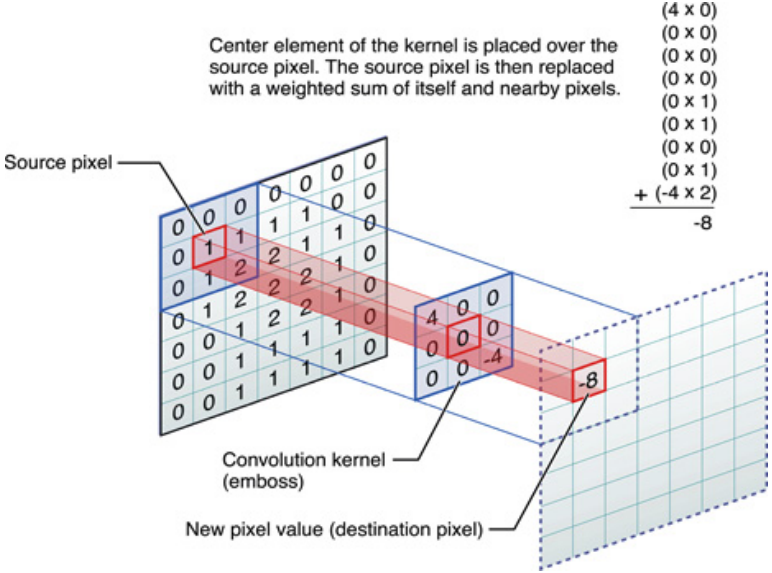
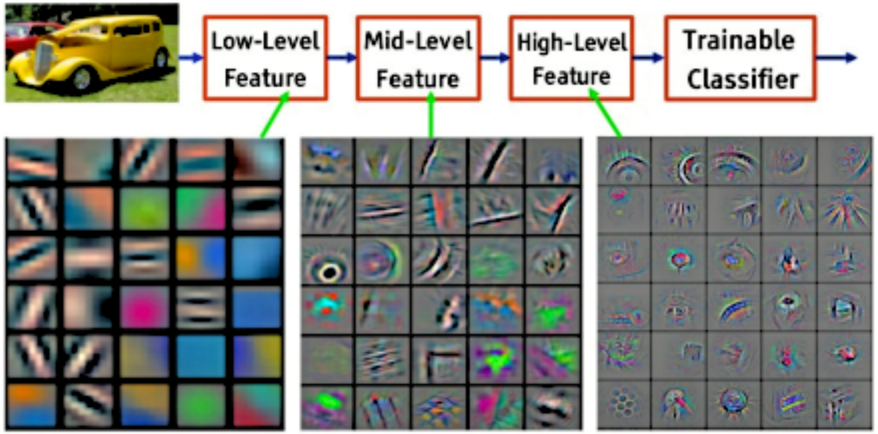


Image courtesy: https://media.giphy.com/media/6EjTPebp1oWxG/giphy.gif
https://stats.stackexchange.com/questions/114385/what-is-the-difference-between-convolutional-neural-networks-restricted-boltzma

Convolutional Neural Network - Activation Maps

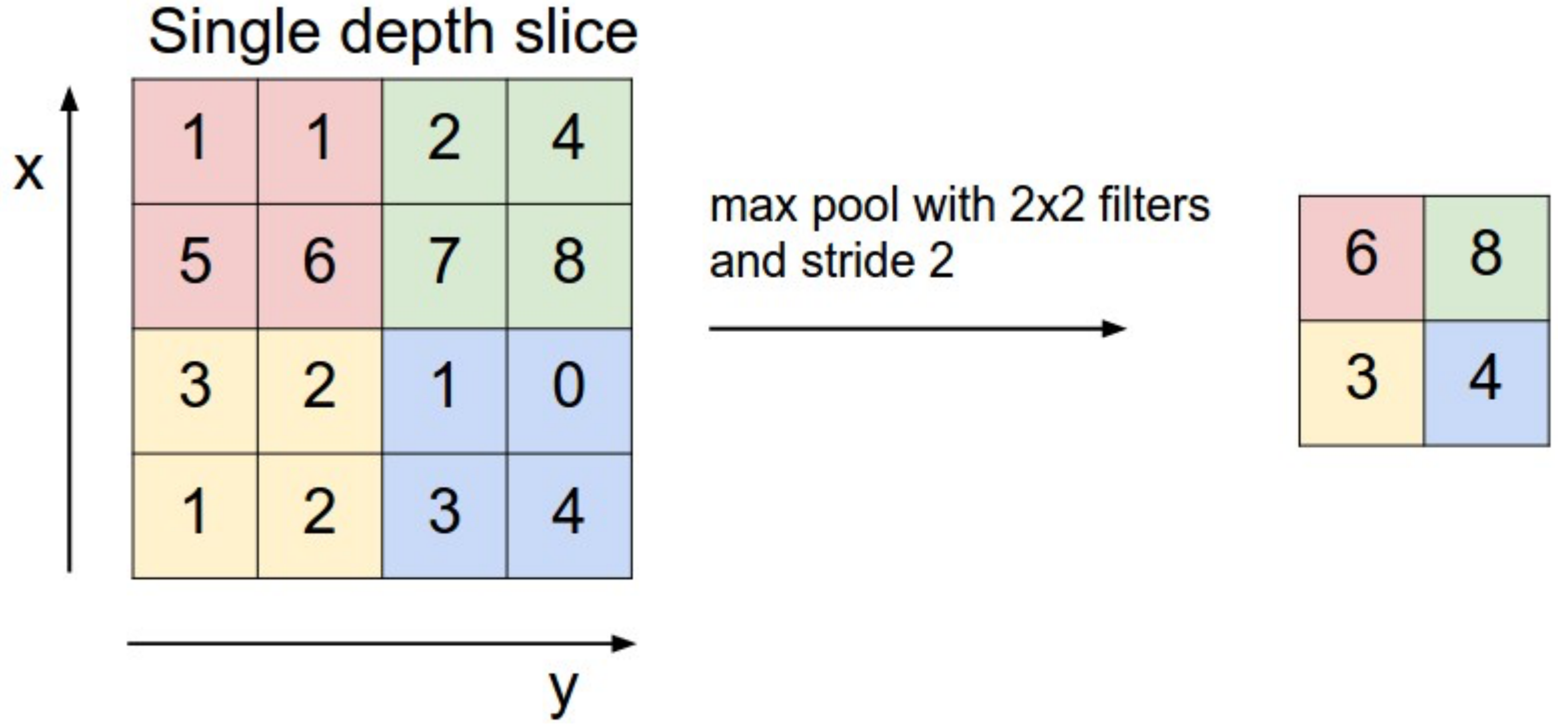


Example activation maps

- The 2D image obtained after convolution with filter is called activation map
- There can be multiple such maps in a given layer depending on number of filters
- Maps in the initial layers learn low level features like edges and deeper layers learn high-level features

Image courtesy: https://www.quora.com/What-is-a-convolutional-neural-network

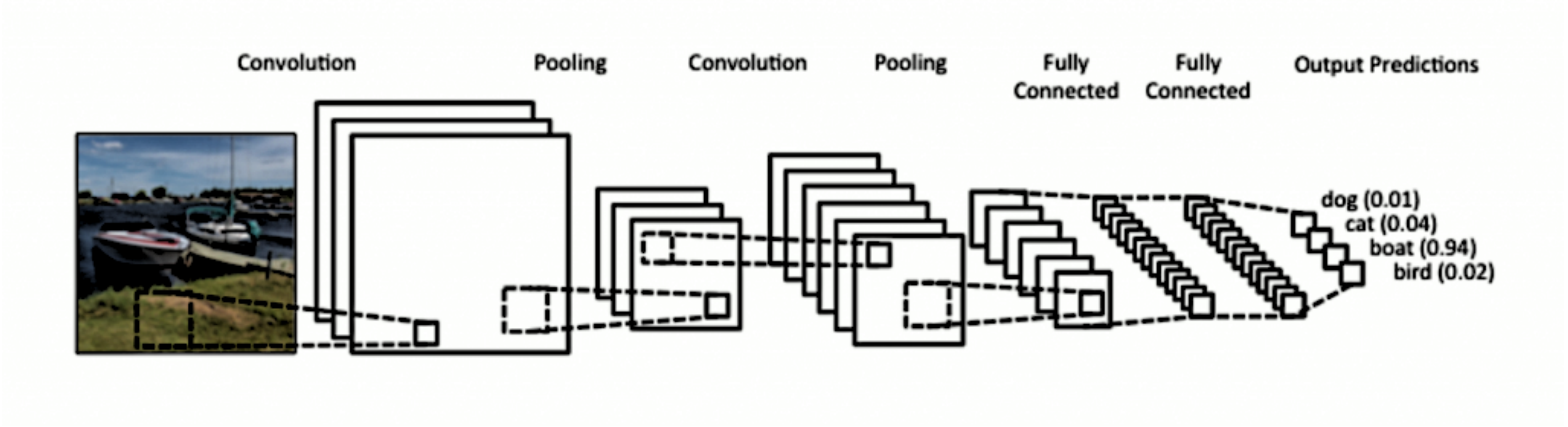
Convolutional Neural Network - Pooling



Max-pooling operation

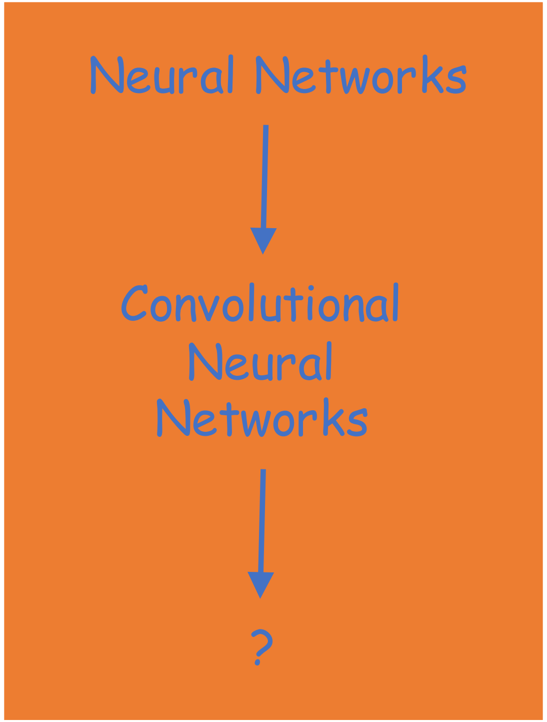
Image courtesy: http://cs231n.github.io/convolutional-networks/

Convolutional Neural Network



An example architecture of a CNN being used for classification

What next?



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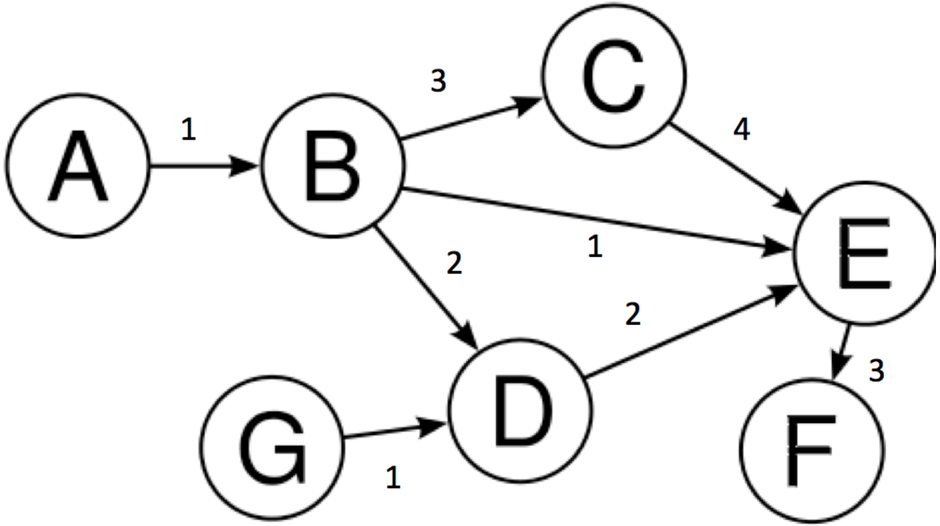
Graphs

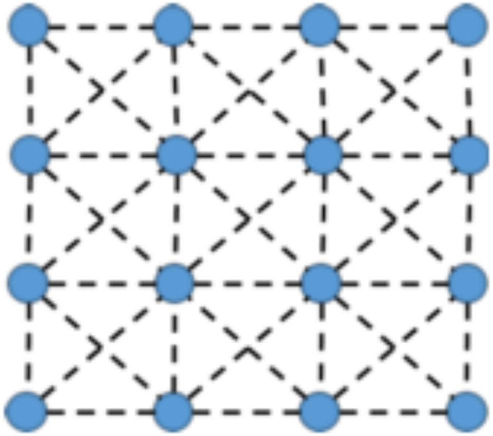
- A graph (directed or undirected) consists of a set of vertices V (or nodes) and a set of edges E
- Edges can be weighted (weights can be scalar or vector) or binary
- Nodes are represented by attribute values (can be scalar or vector)



A directed graph

Image courtesy: https://cs.stackexchange.com/questions/18138/dijkstra-algorithm-vs-breadth-first-search-for-shortest-path-in-graph

Image as a Graph



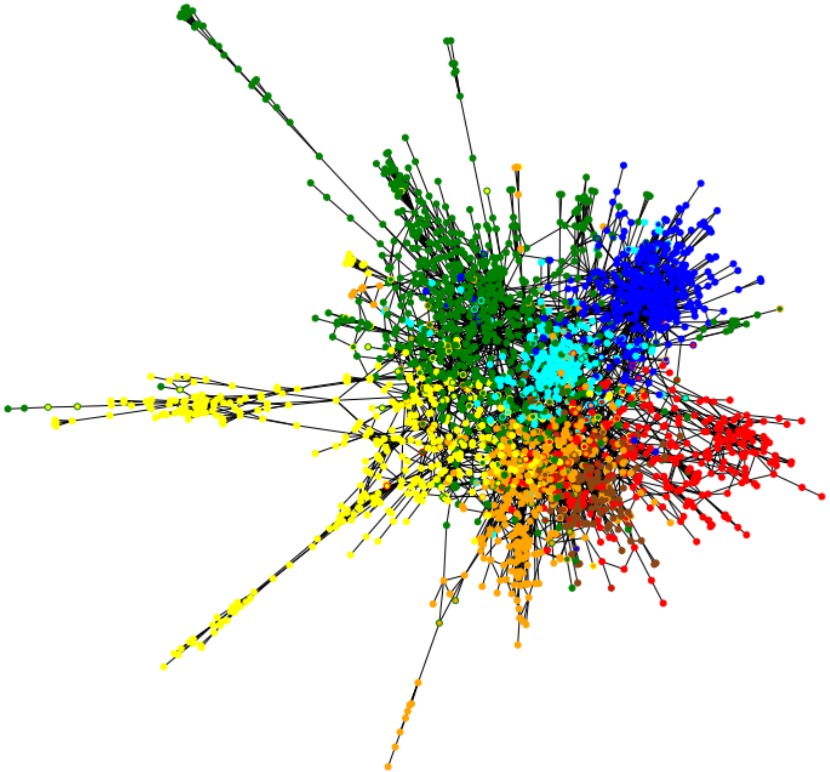
- Each pixel has 8 neighbors
- The node attributes are scalar values for grayscale image and 3-dimensional for RGB images
- The edge weights are binary (0 or 1), either present or absent

Graph Convolutional Networks (GCN)

Why?

Their arises many scenarios where the inherent structure of the data is that of a graph (for e.g. social networks) and one has to learn from it, one can employ GCN for classification/segmentation/clusterin g tasks!

Graph Convolutional Networks (GCN)



The Cora dataset

*Image courtesy: Monti et al.,Geometric deep learning on graphs and manifolds using mixture model CNNs, 2016

Graph Convolutional Networks (GCN)

What?

The architecture is similar to a traditional CNN but it takes graphs as input, also the convolution and pooling operations are different in principle

CNN vs GCN

Pooling

?

Convolution

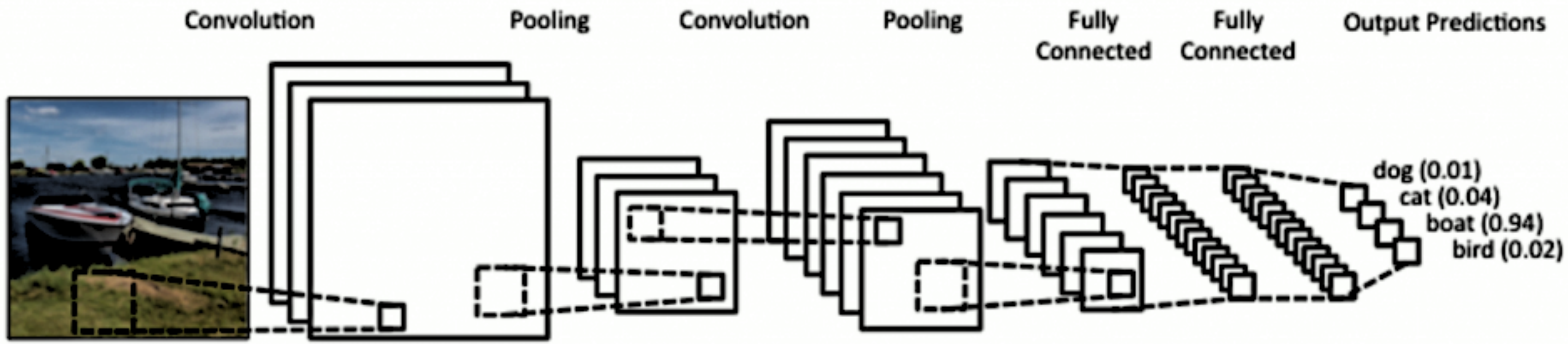
?

Fully-connected layer

Same as in CNN!

The three integral operations

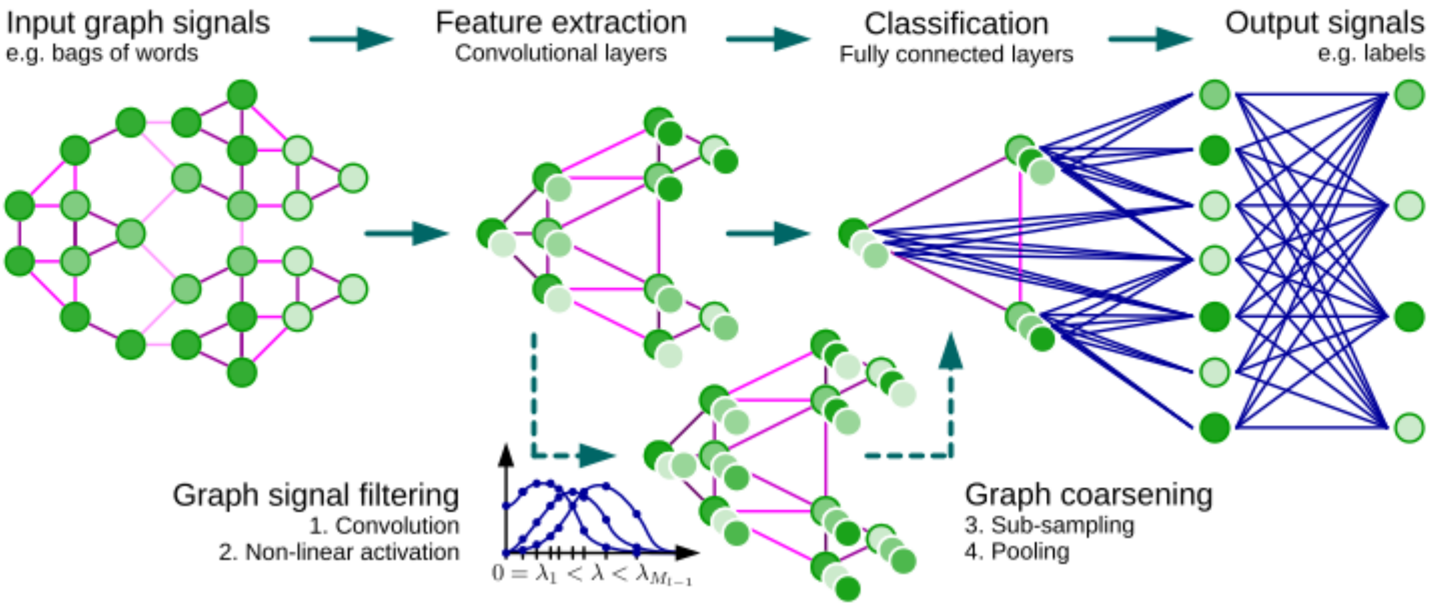
CNN vs GCN



An example architecture of a CNN being used
for classification

Image courtesy: https://ujjwalkarn.me/2016/08/11/intuitive-explanation-convnets/

CNN vs GCN



An example architecture of a GCN being used for classification

Image courtesy: Defferrard et al. Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering. 2016

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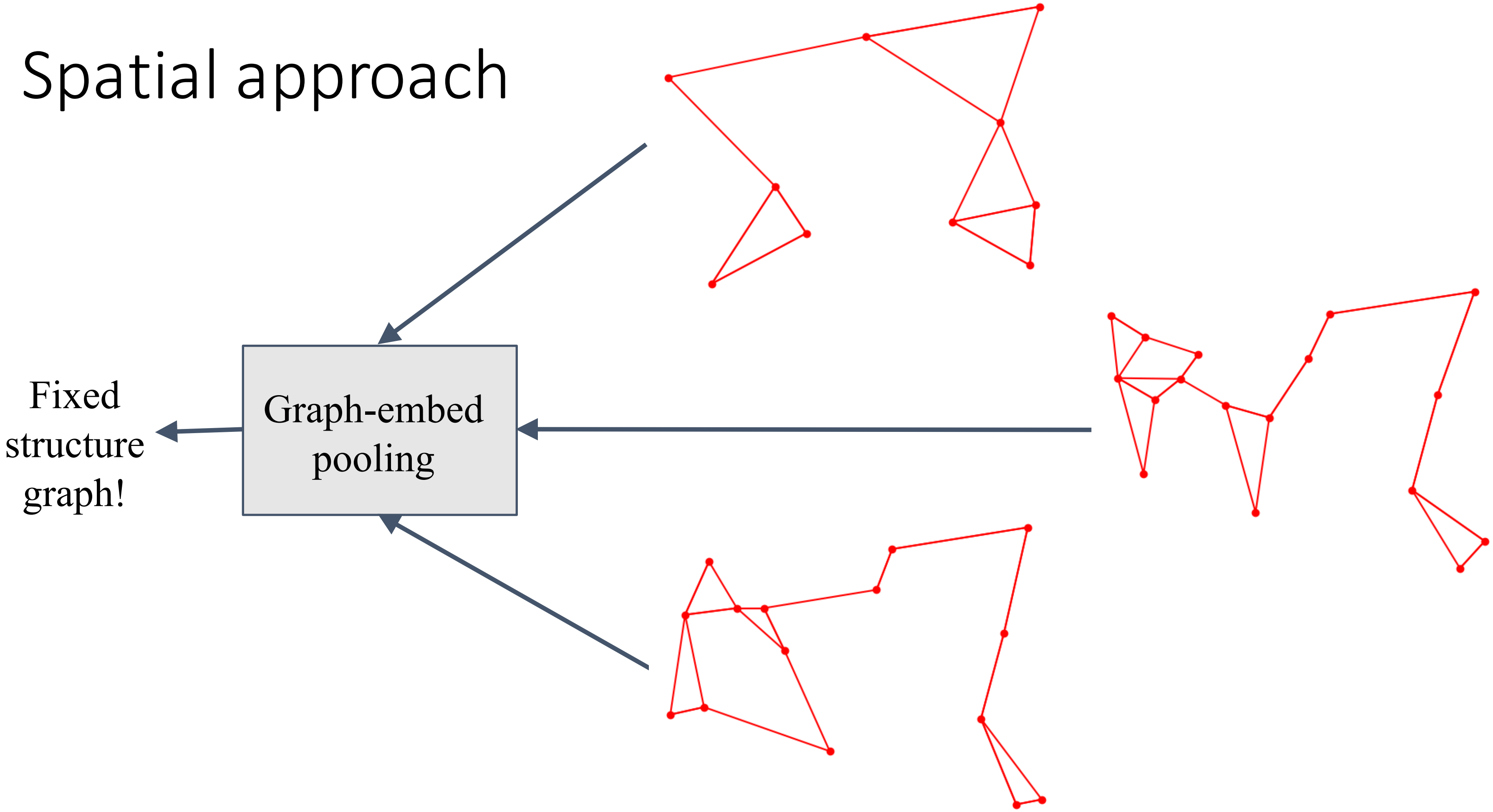
Convolution in GCN

- Spectral and Spatial approach exist for performing convolution in graphs
- Spectral approach has the limitation of the graph structure being same for all samples i.e. **homogeneous** structure
- It is a hard constraint, as most of the real-world graph data has different structures and size for different samples i.e. **heterogeneous structure**
- Spatial approach comes to the rescue!

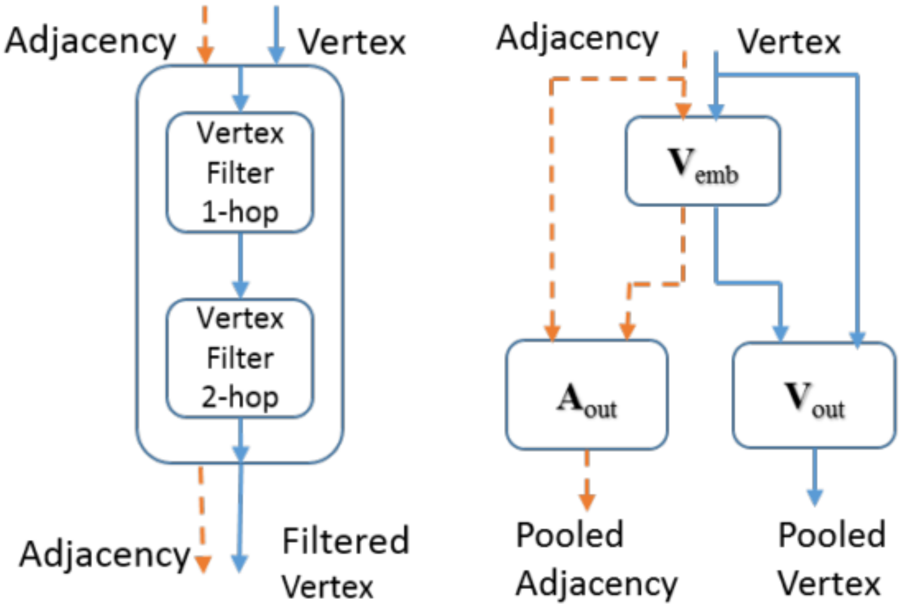
Spatial approach

- Does not require homogeneous graph structure
- In turn, requires preprocessing of graph to enable learning on it
- Recall in CNN, images had to be **same size** before being fed to the CNN
- So, in case of GCN also all the heterogeneous graph structures need to be **mapped to a fixed-size output** before learning is performed on it
- Luckily an approach exists - Graph Embed Pooling!

Spatial approach



Spatial approach



(a) Graph Convolution (b) Graph Pooling

Graph Convolution transforms only the Vertex values whereas and Graph Pooling transforms both the Vertex values as well as the Adjacency Matrix

Image courtesy: F.P. Such et al., Robust Spatial Filtering with Graph Convolutional Neural Networks, 2017

Spatial approach - Convolution

- Convolution of the vertices *V* with the filter *H* require matrix multiplication of the form,

$$\boldsymbol{V_{out}} = \boldsymbol{H}\boldsymbol{V_{in}} \text{ where } \boldsymbol{V_{in}}, \boldsymbol{V_{out}} \in \mathbb{R}^N$$

- The filter *H* is defined as the *k*-th degree polynomial of the graph adjacency matrix *A*,

$$\boldsymbol{H} = h_0\boldsymbol{I} + h_1\boldsymbol{A} + h_2\boldsymbol{A}^2 + ... + h_k\boldsymbol{A}^k, \boldsymbol{H} \in \mathbb{R}^{N\times N}$$

- Generally we have,

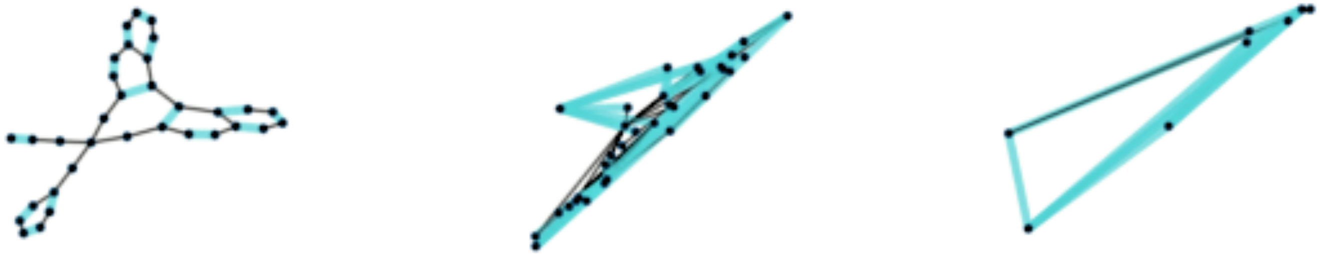
$$\boldsymbol{H} \approx h_0\boldsymbol{I} + h_1\boldsymbol{A}$$

- In case of node attributes being vector, the matrix *H* can be designed accordingly

Spatial approach - Pooling

- Just like in CNN, here too pooling has to be performed
- Graph embed pooling is the approach, it serves two purposes -
  - pooling of graphs to reduce size (and increase receptive field)
  - mapping of input to a fixed size output graph
- Unlike max-pooling in CNN, here a convolutional layer is learnt whose output gives the embedding matrix
- Using the embedding matrix, the vertex attributes and adjacency matrix are transformed

Spatial approach



(a) Input graph. (b) Pool to 32 vertex. (c) Pool to 8 vertex.

Graph Embed Pooling
demonstrated, geometry should not
be taken literally

Image courtesy: F.P. Such et al., Robust Spatial Filtering with Graph Convolutional Neural Networks, 2017

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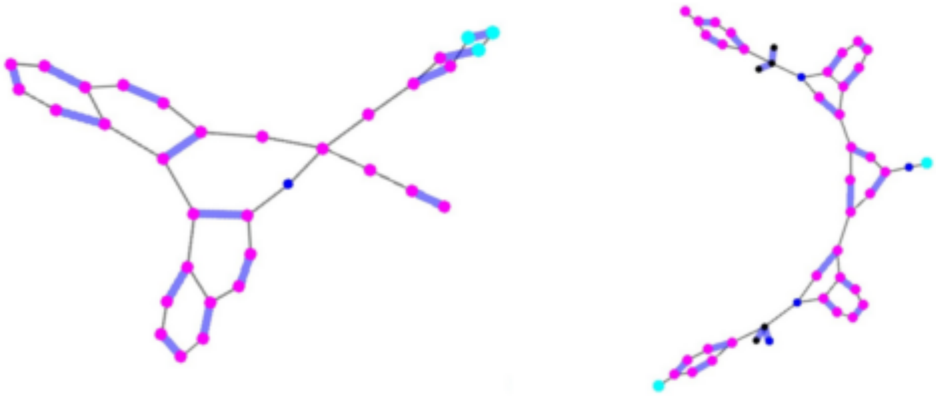
Applications

- Classification
  - Images/segments modelled as graph being labeled into classes
  - Chemical compound classification
- Clustering/Segmentation (subset of classification)
  - Image pixels, modelled as a graph, being labeled into semantic classes
  - Research paper classification depending on the citation and references relationship between different documents (Cora dataset)
  - To organize information in large datasets for faster access, say for social network analysis

Applications



Samples of chemical compounds which will be classified into positive or negative sample for detection of lung cancer

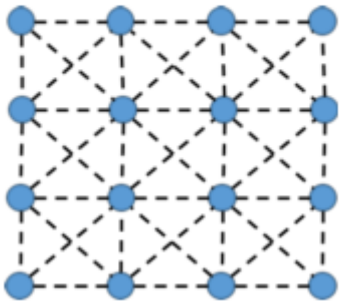
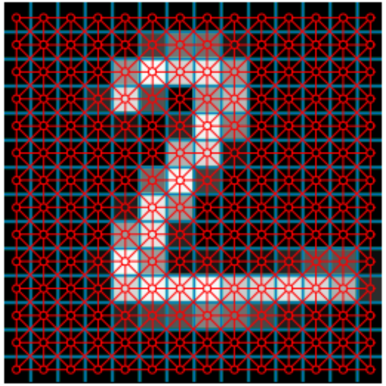


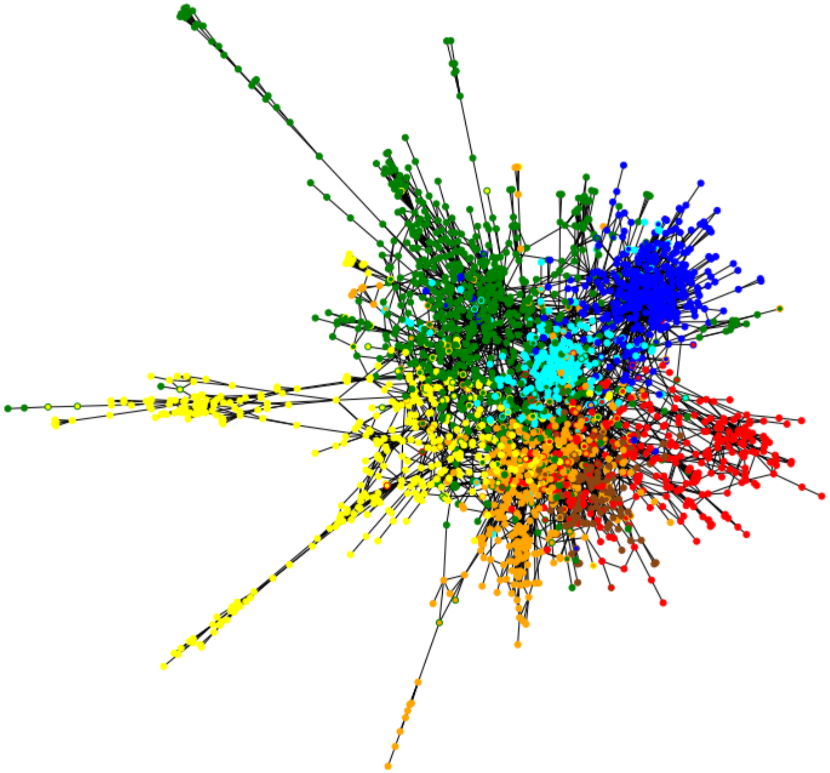
Image represented as a graph



MNIST digit image as a graph

*Image courtesy: F.P. Such et al., Robust Spatial Filtering with Graph Convolutional Neural Networks, 2017

Applications



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Important References

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Questions?

Thank You