Graph Convolutional Network (GCN)

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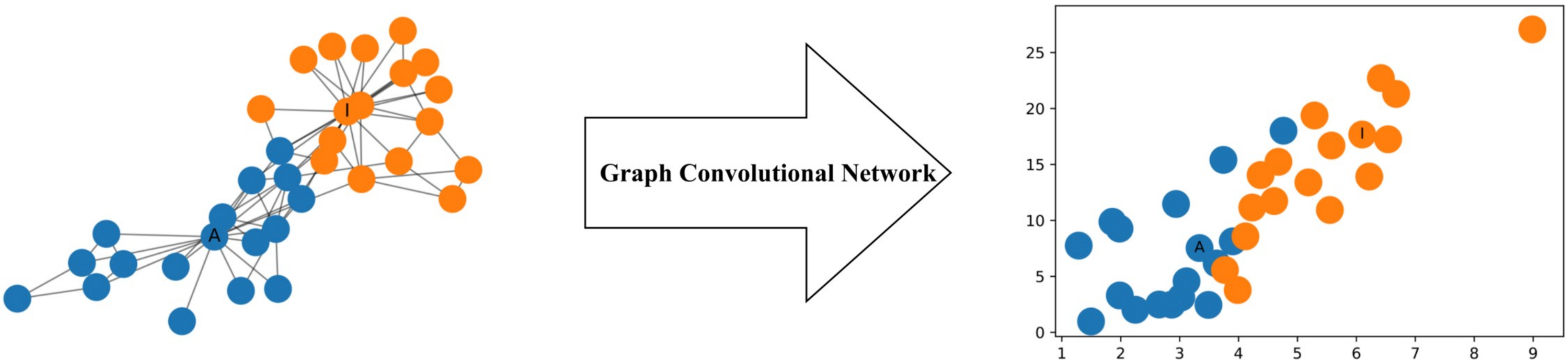


GCN is the most popular type of GNN. Similar to CNN, ‘convolution’ in GCN is similar to CNN.

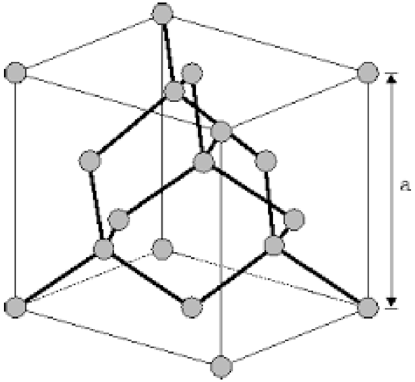
The main difference with CNN: GCNs are the generalized version of CNN that can work on data with underlying non-regular structures.

Other types of GNN -- Graph LSTM, Gated GNN.

Comparison between inputs of CNN and CGN

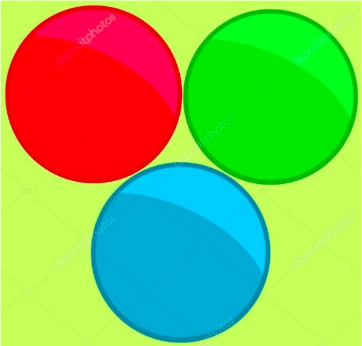
An image

A crystal

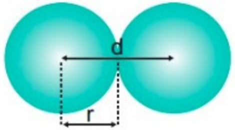


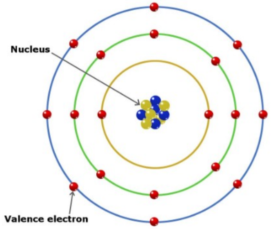
An atom in a lattice corresponds
To a pixel in the image

RGB values of pixel



Covalent radius,
Valence electrons





RGB values of a pixel corresponds to the
Covalent radius, valence electrons,
Electronegativity etc

Forward propagation in Neural Network

$$\underbrace{X^{[i+1]}}_{\text{feature representation at layer i+1}} = \underbrace{\sigma}_{\text{activation function}}(\underbrace{W^{[i]}}_{\text{weights at layer i}} \underbrace{X^{[i]}}_{\text{feature representation at layer i}} + \underbrace{b^{[i]}}_{\text{bias at layer i}})$$

Forward propagation in GCN

$$X^{[i+1]} = \sigma(W^{[i]} X^{[i]} A^{*})$$

A adjacency matrix = an N × N matrix representation of the graph structure

Normalization of adjacency matrix

$$X^{[i+1]} = \sigma(W^{[i]} X^{[i]} A^{*})$$

$$\text{normalized features} = D^{-1}AX$$

low-degree nodes would have bigger impacts on their neighbors, whereas high-degree nodes generate lower impacts as they scatter their influence at too many neighbors

Hyperparameter

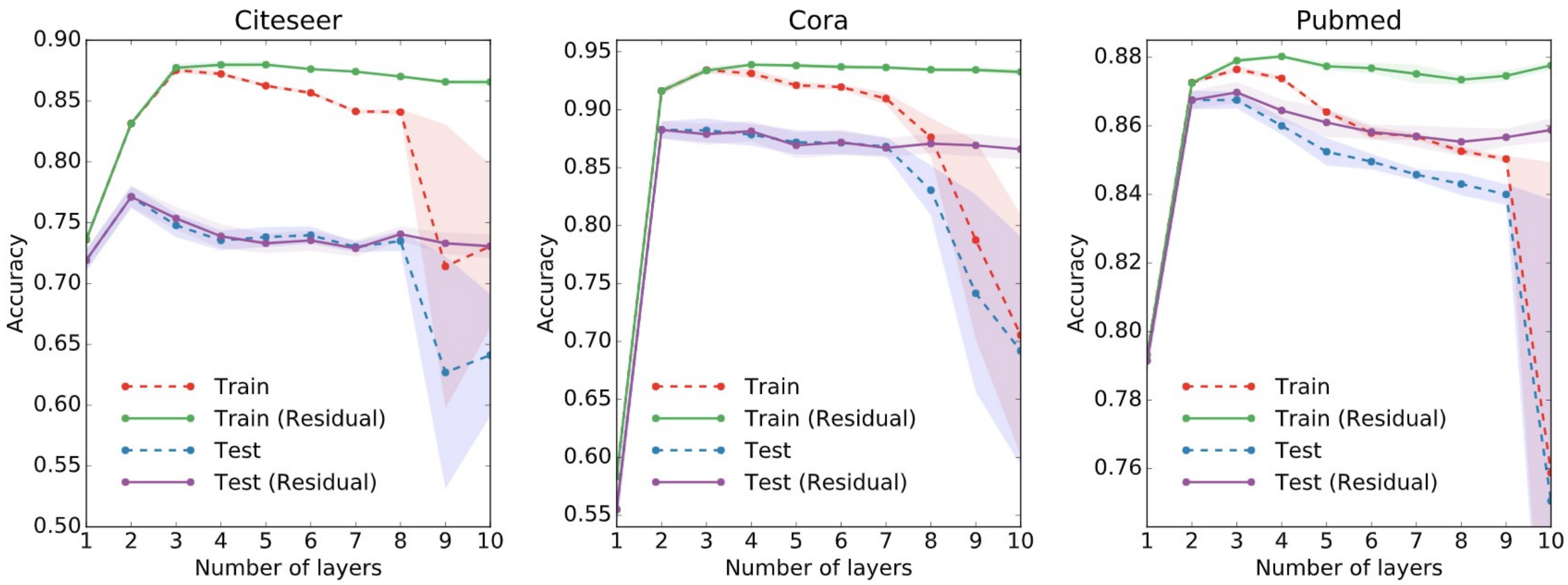
1. # of layers: The number of layers is the farthest distance that node features can travel. For example, with 1 layer GCN, each node can only get the information from its Neighbors.

2. So, depends on how far we think a node should get information from the networks, we can config a proper number for #layer.

3. With 6–7 hops, we almost get the entire graph, which makes the aggregation less meaningful

How many layers should we stack the GCN?

the best results are obtained with a 2- or 3-layer model



Applications

- Material Science: Predicting Crystal properties,
- Biology/Chemistry: Drug Discovery (Cancer drug prediction)
- Physics: Particle Collision.
- Computer Vision: Unstructured images, images contain multiple objects.
- Social Media: Fake News detection.

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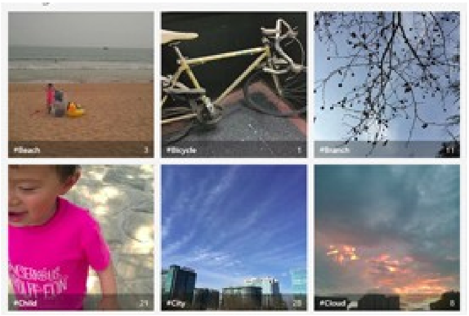
Comparison between CNN and CGN

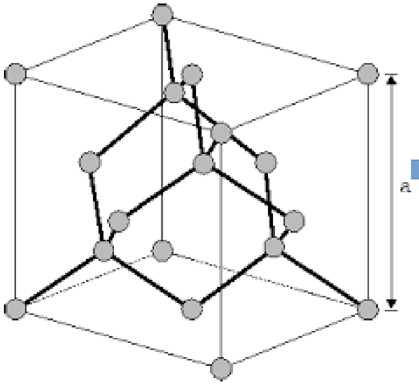
Imagenet

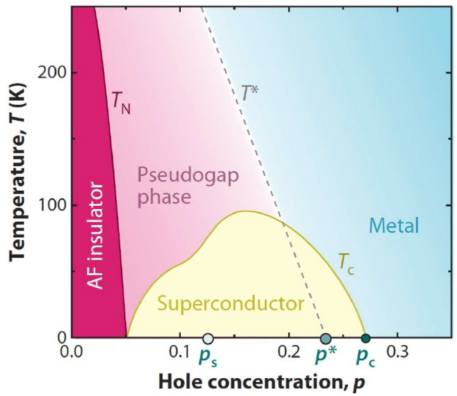


- Bike
- Child
- Beach
- City

For CNN:
1. Classification such as dog, cat, house etc, or fault detection.
2. Caption generation with RNN, Generate images with GAN.

Metal/ Insulator/ Superconductor





For CGCNN:
1. Classification: Metal, semiconductor, insulator etc.
2. Regression: Band gap, Fermi energy, Bulk modulus etc.

References

0. How to do Deep Learning on Graphs with Graph Convolutional Networks by Tobias Skovgaard Jepsen (Medium Article)

1. Graph neural network: Kipf and Welling (2016) – most cited paper on GCN

2. Multi-layer perceptron: Zaheer (2017) – send states through MLP

3. Graph attention networks: Velickovic (2017) – attention weights

4. Gated graph neural networks: Li (2015) – recurrent update

Thank You!