Graph Neural Networks for Spatial Clustering and Classification

By: Aidan Gao
Mentored by: Junhong Lin
Special Thanks to: Julian Shun

Background

01

Graph Neural Networks

02

Spatial Clustering

03

K Nearest Neighbors

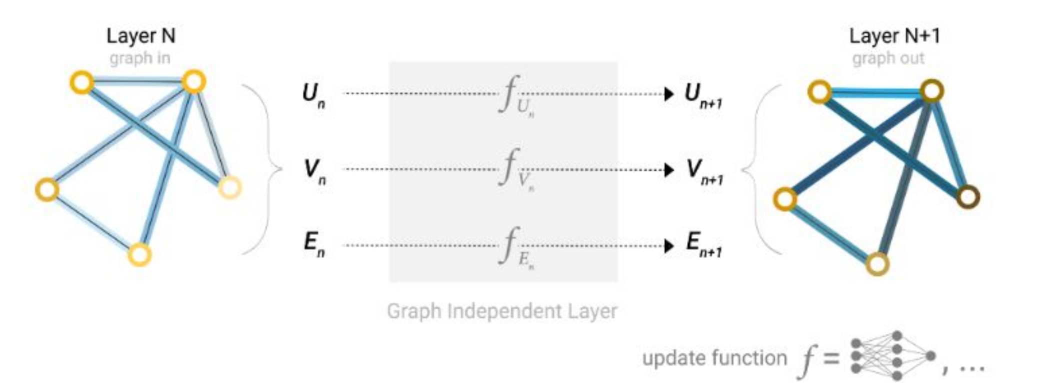
04

Previous Work

Graph Neural Networks

What's a Graph Neural Network?

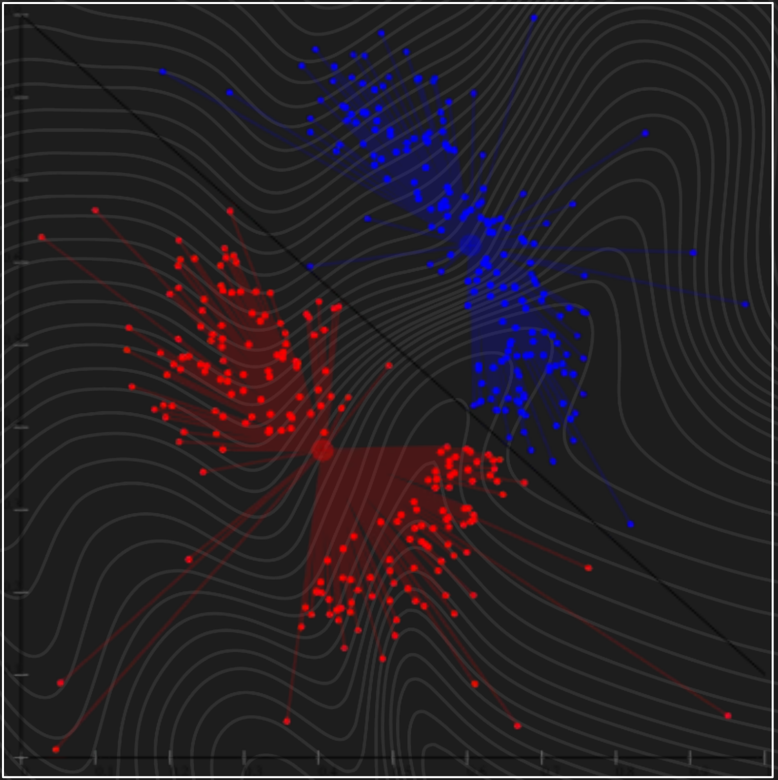
A trainable transform on a all aspects of a graph that is permutation invariant



Left - An example of a basic graph neural network. Nodes, and edges are updated through a basic MLP

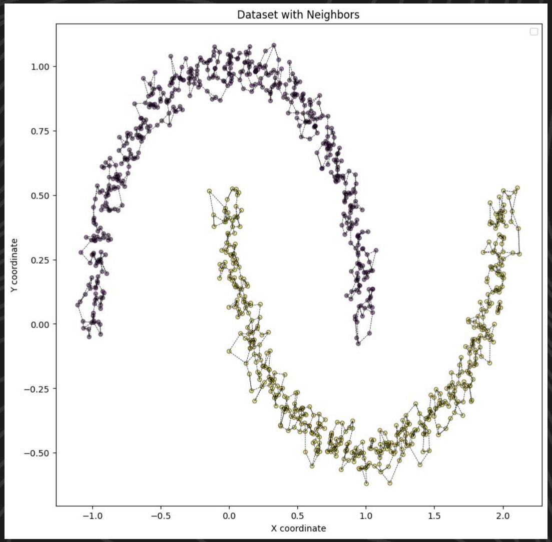
Spatial Clustering

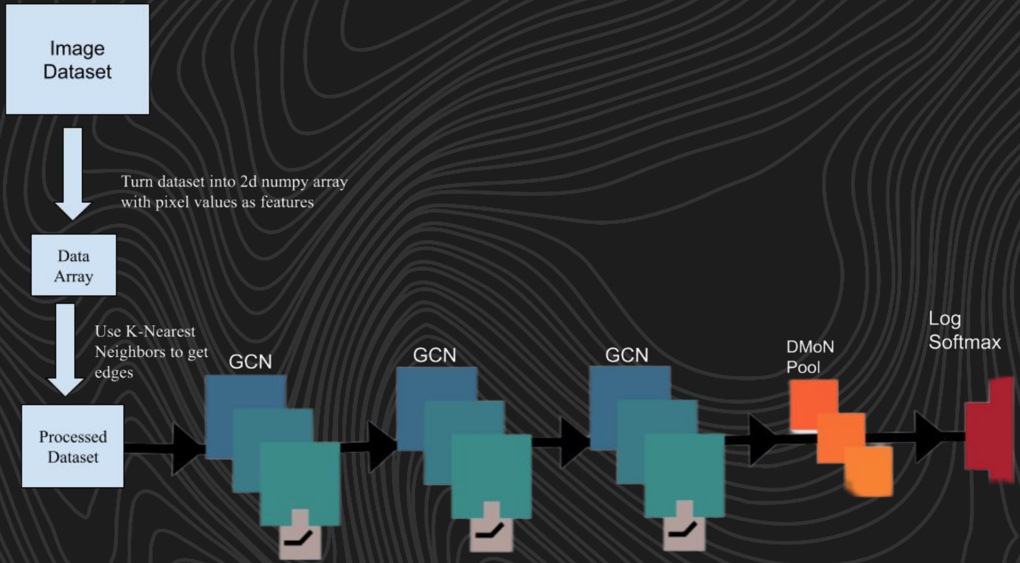
- Instead of dealing with graphs, spatial clustering deals with points in space,
- This is the main form of clustering in literature
- Examples: K-means, DBScan, etc.



K - Nearest Neighbors

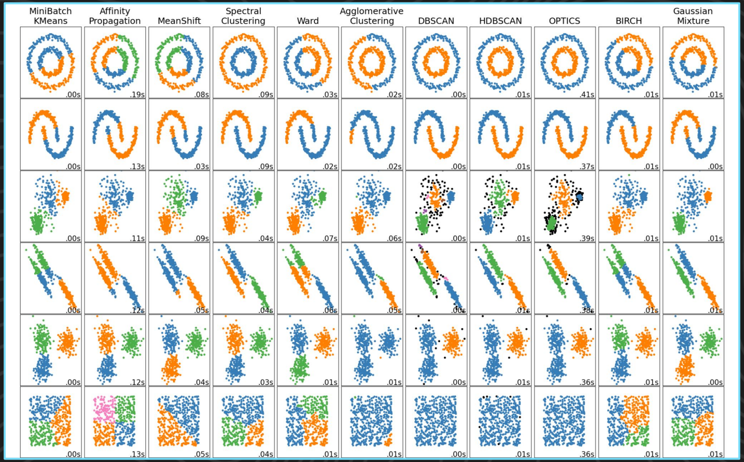
- Information is typically retrieved from neighbors in graphs, but such information isn't available.
- By using a spatial clustering algorithm to create edges between nodes (usually k-nearest neighbors), we can utilize a graph neural network for classification and clustering on spatial datasets.



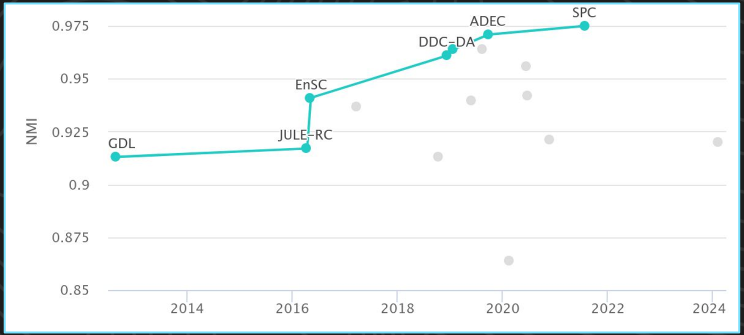


Previous Work

- There exists many works on spatial clustering, on the same datasets.
- There also exists some work on clustering with graph neural networks
- Recently, there has been work done in spatial clustering with graph neural networks, mainly a paper on cell spatial clustering



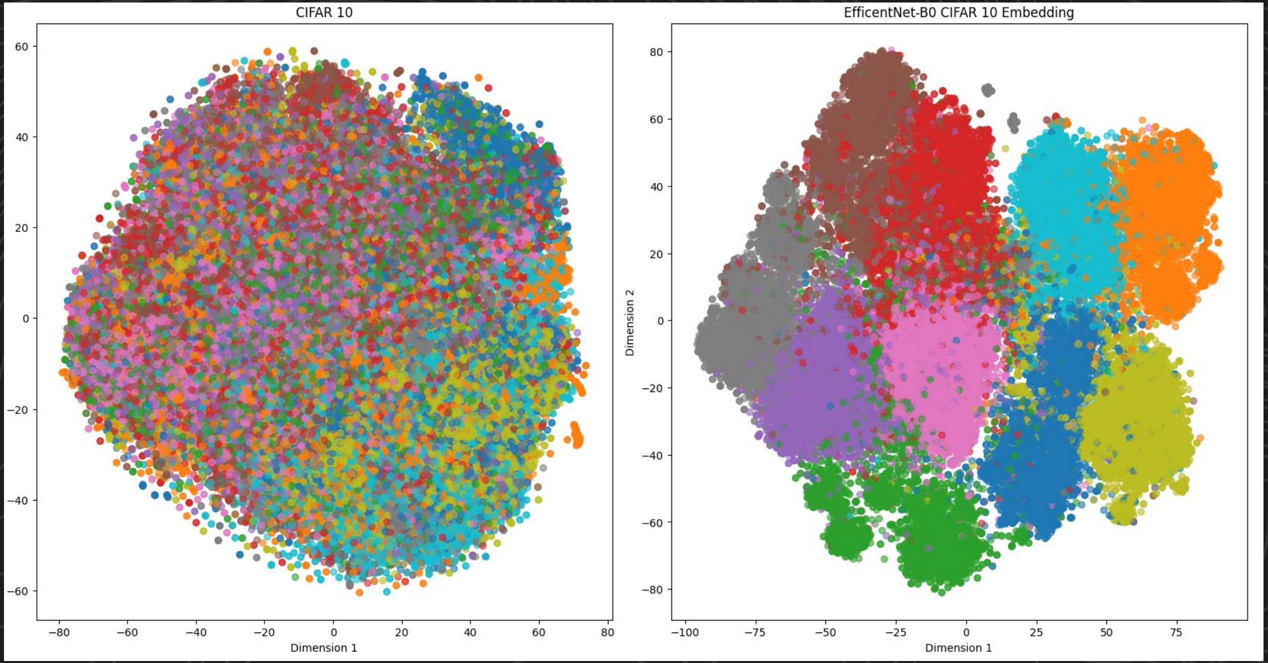
Cell clustering for spatial transcriptomics data with graph neural networks



Li, J., Chen, S., Pan, X. *et al.* Cell clustering for spatial transcriptomics data with graph neural networks. *Nat Comput Sci* 2, 399–408 (2022). https://doi.org/10.1038/s43588-022-00266-5

Methods

CNN Embedding



- CNN embedding reduces dimensionality and enhances features

DMoN Operator

Purpose:

- The DMoN operator is combination of loss and clustering assignment functions that aims to optimize soft cluster assignments for graphs

- Given cluster assignments C from a model, a GCN in the paper's case, the DMoN operator is defined as the following:

$$\mathcal{L}_{\text{DMoN}}(\mathbf{C};\mathbf{A}) = \underbrace{-\frac{1}{2m}\operatorname{Tr}(\mathbf{C}^\top\mathbf{B}\mathbf{C})}_{\text{modularity}} + \underbrace{\frac{\sqrt{k}}{n}\left\|\sum_i \mathbf{C}_i^\top\right\|_F - 1}_{\text{collapse regularization}},$$

Where A is the normalized adjacency matrix.

In addition to optimizing clustering assignments, it also returns the spectral and collapse regularization loss.

Spatial Clustering with GNNs

Supervised Learning

Analogous to image classification

Contributions

CNN-GNN classification that beats state of the art and introduces graph augmented predictions

Unsupervised Learning

In line with spatial clustering literature

Contributions

GNN based clustering that beats baselines and embeddings/transforms that make models competitive with state of the art

GNNs Used

GCN

Aggregates information from neighbors like CNN

GIN

handles Isomorphism and improves power

GAT

GNN with attention mechanism

NAGPhormer

Node adaptive attention transformer

HGT

Node/edge attention on heterogeneous graphs

SuperGAT

Self-supervised attention

CNN-GNN Framework

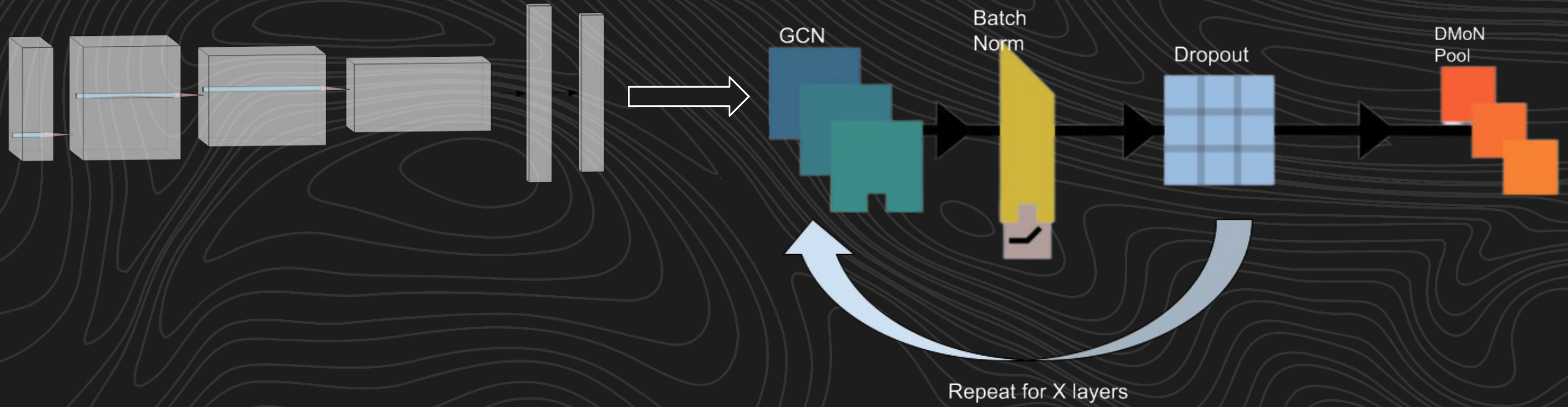
Pipeline

	Data Normalized	Data is normalized and an edge index is built via KNN
	CNN Transforms	A pretrained or untrained CNN reduces dimensionality
	Models Trained	The CNN/GNN are trained on training set
	GNN Classifies	The final GNN performs clustering/node classification

01

Supervised

CNN-GNN Architecture



99.96% MNIST

#1 on State of the Art

99.67% CIFAR

#1 on State of the Art

91.1% Imagenet*

#2 on State of the Art

*only 100k samples used

02

Unsupervised

Unsupervised Losses

01 Orthogonal Loss

Unsupervised loss that encourages orthogonality between rows and columns in weight matrices to encourage more diversity

02 Clustering Loss

Encourages balanced clusters via Frobenius norm of gram matrix of cluster assignments

03 Spectral Loss

Sums modularity diagonally to provide clustering quality based on intra vs extra node connections

04 Collapse Regularization Loss

Sums modularity diagonally to provide clustering quality based on intra vs extra node connections

Unsupervised Data Processing

No Outside Information

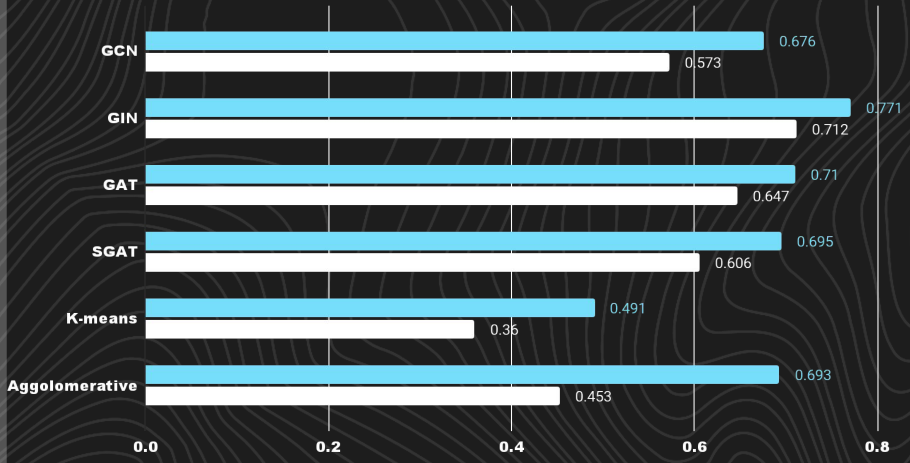
- Once again, the graph is built with KNN, and planar graphs are also tested
- Once the graph is built, the main dimensionality reduction method used is Umap
- Various GNNs can also be used as trainable data transforms

Outside Information

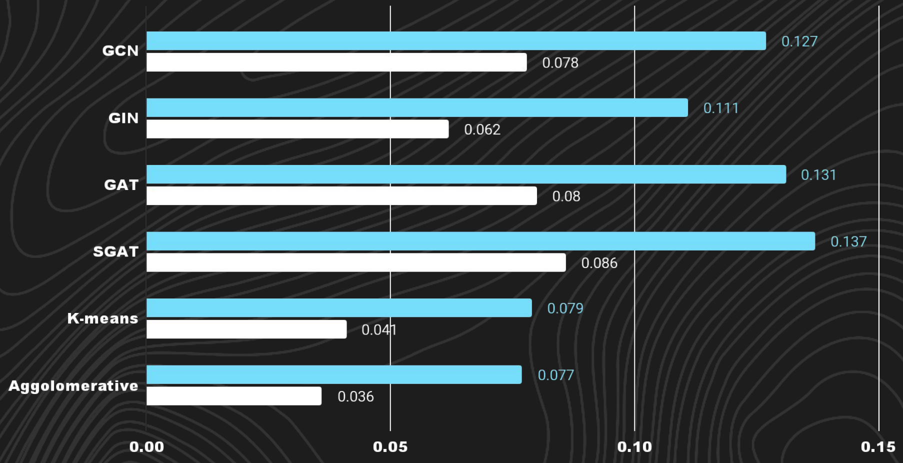
- The graph construction is still built with a KNN, before or after the transform
- A CNN pretrained on general information embeds data
- Umap/GNNs can be used as further dimensionality reductions

GNN Baselines (No Outside Information)

MNIST



CIFAR 10



ARI

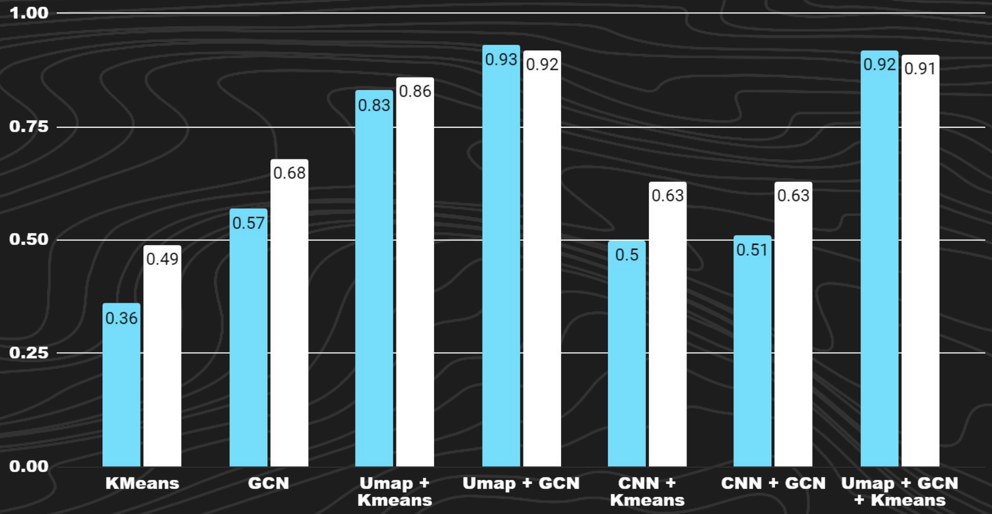
Over 2x top baseline for CIFAR 10 and 1.5 x on MNIST

NMI

1.5x top baseline for CIFAR 10 and 1.1 x on MNIST

No Prior Information

- Testing on MNIST with K-means/GCN
- Umap significantly improves model accuracy to be competitive with state of the art
- CNNs and GCNs can both be used as transforms, but function better when data is more distinct
- Due to its learnability a GNN functions better as an end classifier than static baselines



ARI

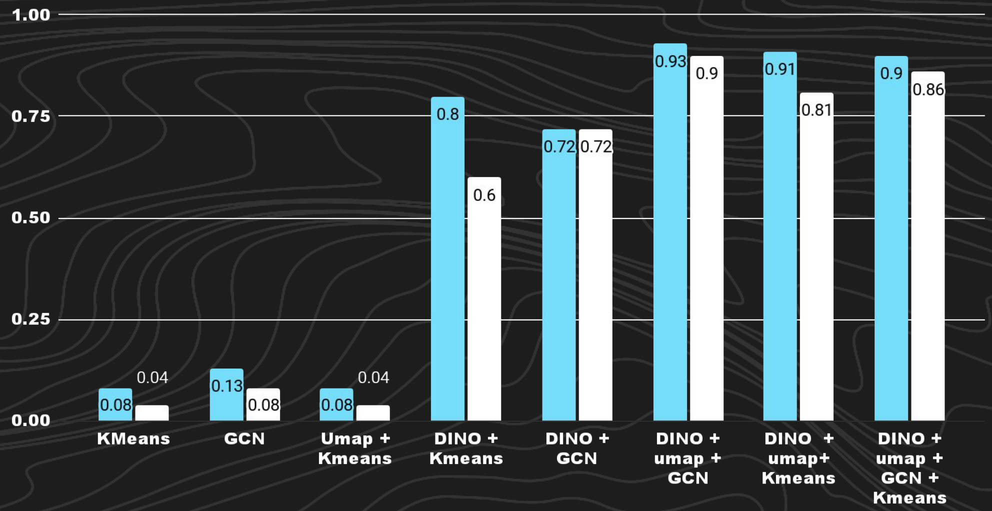
Not Measured in most papers

NMI

Top 10 amongst leaderboards

Prior Information

- Testing on CIFAR with Dino V2 L, K-means/GCN
- Umap functions as a feature enhancer and is only useful when features are already distinguished
- Pre Learned CNN Architecture very powerful for separating features as an embedding



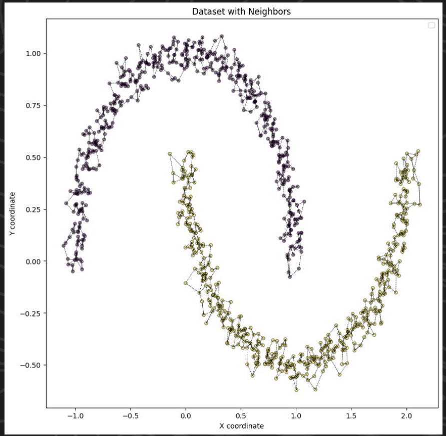
ARI

#3 in CIFAR 10 leaderboards

NMI

#2 in CIFAR 10 leaderboards

Conclusion



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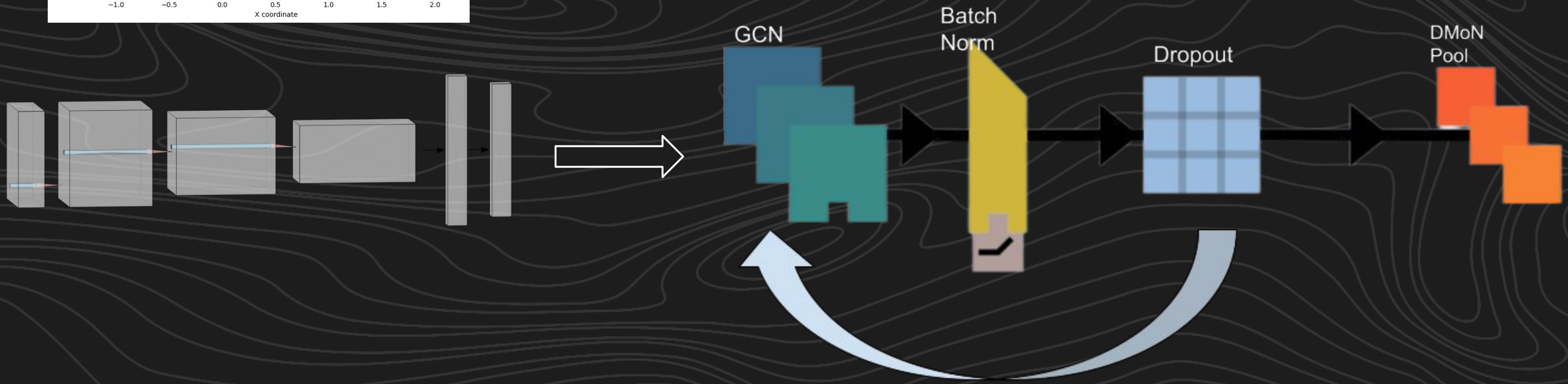

Acknowledgements

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- Thanks to PRIMES, for giving me this continued opportunity
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Any Questions?