

Graph Neural Networks on the Cora Dataset

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Objective: Implement and benchmark multiple neural network models (MLP, GCN, GraphSAGE, GAT) on a citation network (Cora dataset), explicitly formulating each model in terms of encoder (Enc), decoder (Dec), graph structure (Gt), and loss function (L). Compare performance across architectures and provide analysis.

1, Dataset

=>**Cora:** A citation network dataset consisting of 2,708 nodes (papers), 5,429 edges (citations), 1,433 features per node, and 7 classes.

=>**Train/Test Split:** Standard masks from PyTorch Geometric Planetoid dataset.

2, Models Implemented

Model	Enc	Gt	Dec	L
MLP	Linear layers	None	Linear layer + softmax	CrossEntropyLoss
GCN	GCNConv layers	Adjacency matrix	Linear layer + softmax	CrossEntropyLoss
GraphSAGE	SAGEConv layers	Edge list	Linear layer + softmax	CrossEntropyLoss
GAT	GATConv layers	Edge list + attention	Linear layer + softmax	CrossEntropyLoss

3, Training Configurations

-**Hidden Dimensions:** 16, 32, 64

-**Number of Layers:** 2, 3

-**Optimizer:** Adam (lr=0.01, weight_decay=5e-4)

-**Dropout:** 0.5 (MLP/GCN/SAGE), 0.6 (GAT)

-**Epochs:** 200

4, Results

Model	Hidden Layers	Accuracy	F1 Score
MLP	16	0.476	0.481
MLP	32	0.542	0.530
MLP	64	0.572	0.552
MLP	64	0.579	0.564
GCN	16	0.795	0.787
GCN	32	0.799	0.793
GCN	64	0.804	0.801
GCN	64	0.801	0.798
GraphSAGE	16	0.806	0.798
GraphSAGE	32	0.813	0.804
GraphSAGE	64	0.809	0.802
GraphSAGE	64	0.795	0.792
GAT	16	0.794	0.784
GAT	32	0.786	0.782
GAT	64	0.766	0.764
GAT	64	0.686	0.689

5, Analysis

1, Performance Comparison:

-Graph-based models (GCN, GraphSAGE, GAT) significantly outperform MLP due to utilization of graph structure.

-GraphSAGE achieves the highest Accuracy and F1 in most configurations, indicating effective neighborhood aggregation.

-GAT exhibits unstable performance with deeper layers and large hidden dimensions.

2,Effect of Hidden Dimension and Layers:

- Increasing hidden dimensions improves performance for all models initially.
- Adding more layers does not always improve performance, particularly for GAT, possibly due to overfitting or attention instability.

3,Encoder/Decoder Observation:

- MLP relies solely on node features (no graph information).
- GCN uses adjacency matrices to propagate node information.
- GraphSAGE aggregates neighbors via edges.
- GAT further incorporates attention mechanisms over neighbors.

6, Conclusion

- Graph Neural Networks outperform feature-only models (MLP) for node classification on citation networks.
- GraphSAGE demonstrates the most robust performance across configurations.
- Explicitly formulating Enc, Dec, Gt, and L helps in understanding model design and comparing architectures.