CS 768 Assignment Report

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MODEL DESCRIPTION

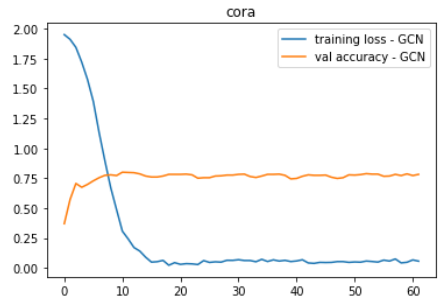
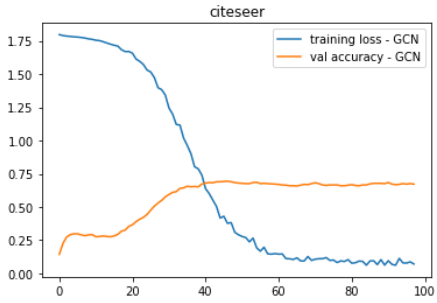
The GNNFactory class creates our GNN-based model to perform node classification on given datasets. Based on the arguments provided while creating a GNN instance, a user defined number of graph convolutional layers are defined using chosen convolutional model type (options include GCN, SAGE and GAT). If GAT is chosen, number of heads has been set to 1 in this assignment for the sake of simplicity. Each convolutional layer is followed by a ReLU activation and Dropout for regularization.

A post message passing module is also initialized, which in this case consists of a single linear layer which provides output that can be used for node classification. The model is trained using cross entropy loss (implemented by doing log-Softmax + NLL loss)

RESULTS

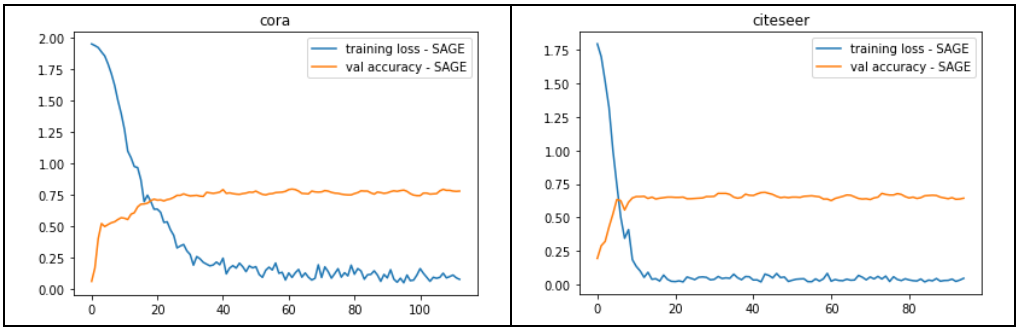
(1) Best Hyperparameters found using Grid Search and corresponding plots

a. GCN

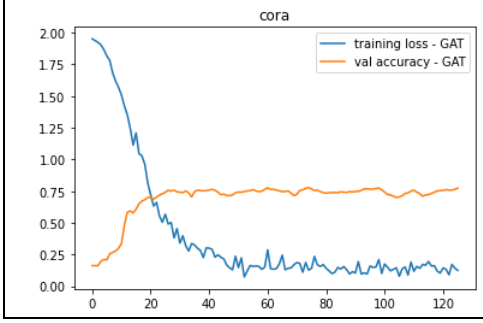
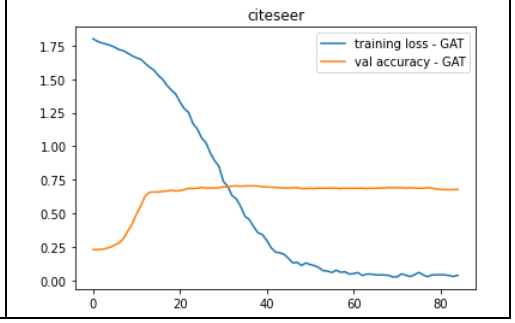
CORA	Citeseer
{'model_type': 'GCN', 'dataset': 'cora', 'num_layers': 2, 'batch_size': 32, 'hidden_dim': 64, 'dropout': 0.25, 'max_epochs': 1000, 'p': 50, 'opt': 'adam', 'weight_decay': 0.005, 'lr': 0.01, 'verbose': False}	{'model_type': 'GCN', 'dataset': 'citeseer', 'num_layers': 3, 'batch_size': 32, 'hidden_dim': 128, 'dropout': 0.5, 'max_epochs': 1000, 'p': 50, 'opt': 'adam', 'weight_decay': 0.005, 'lr': 0.001, 'verbose': False}
	

b. SAGE

CORA	Citeseer
{'model_type': 'SAGE', 'dataset': 'cora', 'num_layers': 3, 'batch_size': 32, 'hidden_dim': 32, 'dropout': 0.5, 'max_epochs': 1000, 'p': 50, 'opt': 'adam', 'weight_decay': 0.005, 'lr': 0.01, 'verbose': False}	{'model_type': 'SAGE', 'dataset': 'citeseer', 'num_layers': 2, 'batch_size': 32, 'hidden_dim': 64, 'dropout': 0.5, 'max_epochs': 1000, 'p': 50, 'opt': 'adam', 'weight_decay': 0.005, 'lr': 0.01, 'verbose': False}



c. GAT

CORA	Citeseer
{'model_type': 'GAT', 'dataset': 'cora', 'num_layers': 3, 'batch_size': 32, 'hidden_dim': 32, 'dropout': 0.5, 'max_epochs': 1000, 'p': 50, 'opt': 'adam', 'weight_decay': 0.005, 'lr': 0.01, 'verbose': False}	{'model_type': 'GCN', 'dataset': 'citeseer', 'num_layers': 3, 'batch_size': 32, 'hidden_dim': 128, 'dropout': 0.5, 'max_epochs': 1000, 'p': 50, 'opt': 'adam', 'weight_decay': 0.005, 'lr': 0.001, 'verbose': False}
	

(2) Test-set Accuracies

	GCN	SAGE	GAT
Cora	**0.8090**	0.7910	0.7710
Citeseer	0.6930	0.6790	**0.7090**

Note: GAT performance can be further improved by increasing number of heads