



KOREA ADVANCED INSTITUTE OF TECHNOLOGY

DEPARTMENT OF MATHEMATICAL SCIENCES

Semi-supervised graph node classification of CORA dataset using GCN

Author:
Junghyun Lee

Instructor:
Prof. Chang Dong Yoo

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Abstract

In this homework, I have implemented a simple version of GCN(Graph Convolutional Network) to do a semi-supervised graph node classification of CORA dataset. The algorithm is based upon the work by Kipf & Welling, 2016.

(Coding done in Google Colaboratory.)

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Chapter 1

Implementation

Implementation was done using the Google Colaboratory. All the modifications that I've done to the original template are accompanied by the comments that I've put.

Below, I've added additional explanations for some of the features that I've used or modified.

1.1 Initialization

I have initialized some boolean parameters to be used later on for the training/evaluation/testing.

```
# Dropout setting
#DROPOUT = 0
DROPOUT = 0.5

# Boolean value for Xavier initialization
# Used uniform xavier initialization from Glorot & Bengio, 2010[2]
XAVIER = True
#XAVIER = False
```

Figure 1.1: Initialization

1.2 TensorBoardColab

TensorBoard is a visualization toolkit that supports various experimentation. Especially, it is useful in tracking and visualizing metrics such as loss and accuracy.

It is supported in multiple platforms, including Tensorflow, Google Colaboratory...etc.

```
# Initialize tensorboard for visualization
# Note : click the Tensorboard link to see the visualization of training/testing results
tbc = TensorBoardColab()
```

Figure 1.2: TensorBoardColab

1.3 GraphConvolutionLayer

1.3.1 Parameter Initialization

Here I have given myself two choices for initializing weights:

1. Sampling from $U\left(-\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}\right)$ [2]
2. Xavier initialization[1]

For either case, bias was initialized by sampling from $U\left(-\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}\right)$.

```

def init_parameters(self):
    # ===== YOU CODE HERE =====
    # Initializing weight and bias
    stdv = 1. / math.sqrt(self.weight.size(1))

    # With Xavier Initialization
    if XAVIER:
        init.xavier_uniform_(self.weight)
    # Without Xavier Initialization
    else:
        self.weight.data.uniform_(-stdv, stdv)

    # Xavier Initialization is only applied to weights, not bias!
    self.bias.data.uniform_(-stdv, stdv)

    # =====

```

Figure 1.3: Parameter initialization

1.3.2 Forward Function

For forward propagation, I have used the heuristic of

$$forward(H) = AHW + b$$

where A is the adjacency matrix, H is the input matrix, W is the weight matrix, and b is the bias matrix.

```

def forward(self, input, adj):
    # ===== YOU CODE HERE =====
    # Convolve your input graph with your weight corresponding adjacent
    # matrix, don't forget to add bias
    s = torch.mm(input, self.weight)
    out = torch.mm(adj, s) + self.bias
    # =====
    return out

```

Figure 1.4: Forward propagation

1.4 GCN

1.4.1 Network Initialization

Following the work of Kipf & Welling[3], I have decided to implement the two-layered GCN. To do that, two *GraphConvolutionLayer*'s, along with *dropout*, were initialized.

```

def __init__(self, nfeat, nhid, nclass, dropout):
    super(GCN, self).__init__()

    # ===== YOU CODE HERE =====
    # Declaring your multiple graph convolution layers, remembering that
    # output of final layer has dimension equal to number of classes
    self.gc1 = GraphConvolutionLayer(nfeat, nhid)
    self.gc2 = GraphConvolutionLayer(nhid, nclass)
    self.dropout = dropout
    # =====

```

Figure 1.5: Network initialization

1.4.2 Forward Function

I have used the forward model of the form:

$$forward(X, A) = \text{softmax} \left(\hat{A} \text{ReLU} \left(\hat{A} X W^{(0)} \right) W^{(1)} \right)$$

```
def forward(self, x, adj):
    # ===== YOU CODE HERE =====
    # Feeding your input graph and adjacent matrix into multiple graph
    # convolution layers and activation function
    x = F.relu(self.gc1(x, adj))
    x = F.dropout(x, self.dropout, training = self.training)
    x = self.gc2(x, adj)
    # =====
    out = F.log_softmax(x, dim=1)
    return out
```

Figure 1.6: Forward propagation

1.5 Training/Validation/Testing

(Even though I only describe one of the three here, the rest are the same. Just change the index set to the appropriate one.)

I have utilized the negative log likelihood loss. Also, I have updated the tensorboard plot for every epoch.

```
# ===== YOU CODE HERE =====
# Feeding your input graph (nodes's feature and adjacent matrix) into your
# model and computing loss between prediction and ground truth

# input: feature matrix and the graph's adjacency matrix
# output: predicted labels
output = model(features, adj)
# Use negative log likelihood loss(nll_loss) for the datas assigned for training
# idx_train: range of indices for data to be used in the training process
loss_train = F.nll_loss(output[idx_train], labels[idx_train])

# Update the tensorboard plot
tbc.save_value('Loss', 'train_loss', epoch, loss_train.item())
# =====

acc_train = accuracy(output[idx_train], labels[idx_train])
# Update the tensorboard plot
tbc.save_value('Accuracy', 'train_accuracy', epoch, acc_train.item())
```

Figure 1.7: Training phase

1.6 Confusion Matrix

For the confusion matrix plot, I have utilized the external github open repository: <https://github.com/wcipriano/pretty-print-confusion-matrix>.

```
from sklearn.metrics import confusion_matrix

# Create numpy arrays for true/predicted labels
with torch.no_grad():
    true = labels[idx_test].cpu().numpy()
    predicted = model(features, adj)[idx_test].max(1)[1].type_as(labels).cpu().numpy()

# Plot confusion matrix
true_size = len(true) > 10

plot_confusion_matrix_from_data(true, predicted, columns,
    annot = True, cmap = 'Oranges', fmt = '.2f', fz = (lambda x: 12 if x else 9)(true_size),
    lw = 0.5, cbar = False, figsize = (lambda x: [9,9] if x else [12,12])(true_size),
    show_null_values = 2, pred_val_axis = 'y')
```

Figure 1.8: Confusion matrix

Chapter 2

Results

Here,

- Original model: One with uniform initialization with dropouts(rate=0.5).
- Ver. 1: Original model with Xavier (Uniform) Initialization
- Ver. 2: Original model without dropouts
- Ver. 3: Original model with Xavier Initialization and without dropouts

In all the plots, x-axis corresponds to the epoch. As for the graphs,

- Accuracy graph
 - Dark red: train accuracy
 - Bright red: validation accuracy
- Loss graph
 - Dark blue: train loss
 - Bright blue: validation loss

2.1 Original model

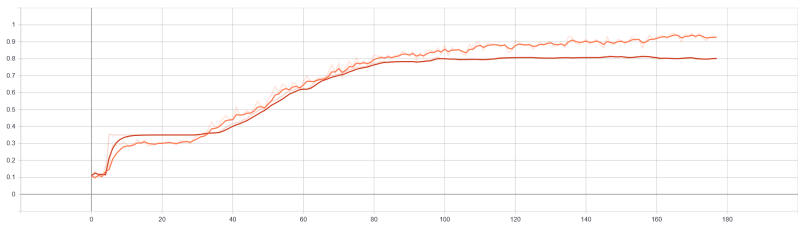


Figure 2.1: Accuracy graph

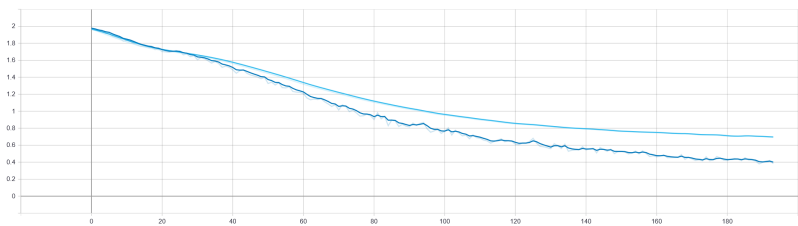


Figure 2.2: Loss graph

Confusion matrix

Predicted	class A	class B	class C	class D	class E	class F	class G	sum_col
	312 14.13%	1 0.05%	1 0.05%	3 0.14%	2 0.09%	0 0.0%	5 0.23%	324 96.30% 3.70%
	5 0.23%	206 9.33%	16 0.72%	22 1.00%	27 1.22%	15 0.68%	7 0.32%	298 69.13% 30.87%
	2 0.09%	10 0.45%	192 8.70%	12 0.54%	6 0.27%	4 0.18%	0 0.0%	226 94.96% 5.04%
	32 1.45%	31 1.40%	1 0.05%	538 24.37%	1 0.05%	40 1.81%	11 0.50%	654 82.26% 17.74%
	1 0.05%	8 0.36%	10 0.45%	2 0.09%	83 3.76%	3 0.14%	1 0.05%	108 76.85% 23.15%
	1 0.05%	23 1.04%	5 0.23%	44 1.99%	13 0.59%	275 12.45%	3 0.14%	364 75.55% 24.45%
	22 1.00%	12 0.54%	22 1.00%	32 1.45%	12 0.54%	9 0.41%	125 5.66%	234 53.42% 46.58%
sum_row	375 83.20% 16.80%	291 70.79% 29.21%	247 77.73% 22.27%	653 82.39% 17.61%	144 57.64% 42.36%	346 79.48% 20.52%	152 82.24% 17.76%	2208 95.49% 4.51%
Actual								sum_col

Figure 2.3: Confusion matrix

2.2 Modified Model (Ver. 1)

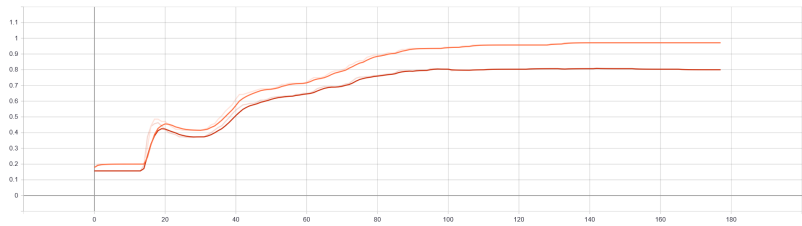


Figure 2.4: Accuracy graph

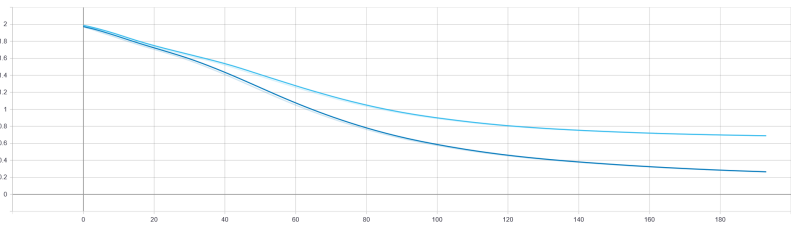


Figure 2.5: Loss graph

Confusion matrix								
Predicted	class A	class B	class C	class D	class E	class F	class G	sum_col
	549 24.86%	11 0.50%	51 2.31%	39 1.77%	2 0.09%	13 0.59%	28 1.27%	693 79.22% 20.78%
	27 1.22%	127 5.75%	4 0.18%	10 0.45%	17 0.77%	6 0.27%	24 1.09%	215 59.07% 40.93%
	36 1.63%	3 0.14%	260 11.78%	23 1.04%	4 0.18%	2 0.09%	1 0.05%	329 79.03% 20.97%
	22 1.00%	7 0.32%	17 0.77%	200 9.06%	19 0.86%	28 1.27%	6 0.27%	299 66.89% 33.11%
	12 0.54%	0 0.0%	10 0.45%	8 0.36%	193 8.74%	4 0.18%	4 0.18%	231 83.55% 16.45%
	3 0.14%	0 0.0%	4 0.18%	11 0.50%	11 0.50%	89 4.03%	3 0.14%	121 73.58% 26.42%
	4 0.18%	4 0.18%	0 0.0%	0 0.0%	1 0.05%	2 0.09%	309 13.99%	320 96.56% 3.44%
sum_col	653 84.07% 15.93%	152 83.55% 16.45%	346 75.14% 24.86%	291 68.73% 31.27%	247 78.14% 21.86%	144 61.81% 38.19%	375 82.40% 17.60%	2208 96.13% 3.87%
Actual								

Figure 2.6: Confusion matrix

2.3 Modified Model (Ver. 2)

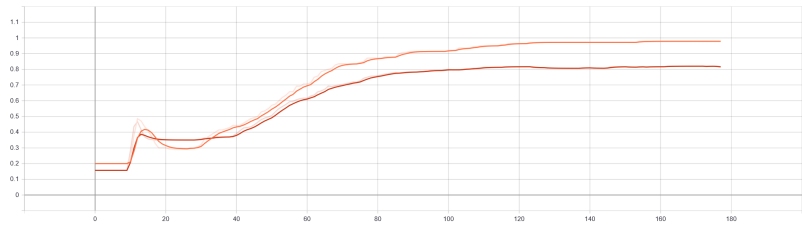


Figure 2.7: Accuracy graph

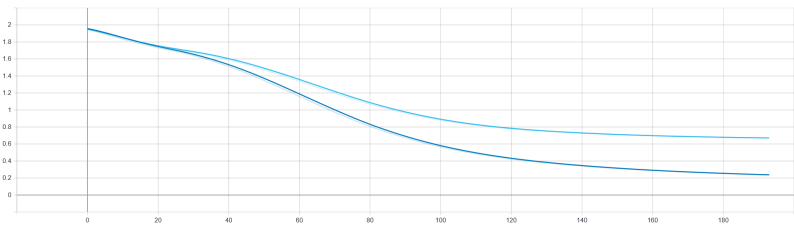


Figure 2.8: Loss graph

Confusion matrix								
Predicted	class A	class B	class C	class D	class E	class F	class G	sum_col
	124 5.62%	5 0.23%	17 0.77%	10 0.45%	7 0.32%	26 1.18%	26 1.18%	215 57.67% 40.33%
	3 0.14%	269 12.18%	4 0.18%	23 1.04%	5 0.23%	4 0.18%	43 1.95%	351 76.64% 23.36%
	0 0.0%	8 0.36%	194 8.79%	9 0.41%	6 0.27%	3 0.14%	12 0.54%	232 83.62% 16.38%
	8 0.36%	18 0.82%	16 0.72%	195 8.83%	15 0.68%	9 0.41%	24 1.09%	285 68.42% 31.58%
	0 0.0%	4 0.18%	13 0.59%	13 0.59%	102 4.62%	2 0.09%	4 0.18%	138 73.81% 26.19%
	6 0.27%	0 0.0%	1 0.05%	0 0.0%	2 0.09%	307 13.90%	4 0.18%	320 95.94% 4.06%
	11 0.50%	42 1.90%	2 0.09%	41 1.86%	7 0.32%	24 1.09%	540 24.46%	667 80.56% 19.44%
sum_row	152 81.58% 18.42%	346 77.75% 22.25%	247 78.54% 21.46%	291 67.01% 32.99%	144 70.83% 29.17%	375 81.87% 18.13%	653 82.70% 17.30%	2208 95.48% 21.60%
Actual								

Figure 2.9: Confusion matrix

2.4 Modified Model (Ver. 3)

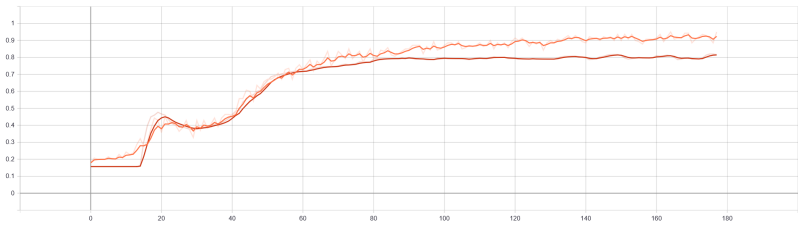


Figure 2.10: Accuracy graph

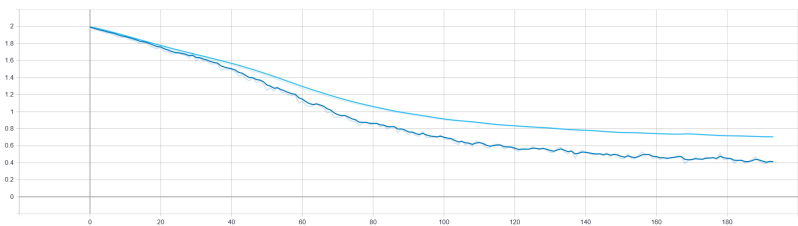


Figure 2.11: Loss graph

		Confusion matrix							
		class A	class B	class C	class D	class E	class F	class G	
Predicted	class A	547 24.77%	51 2.31%	36 1.63%	30 1.36%	11 0.50%	11 0.50%	3 0.14%	689 79.39% 20.61%
	class B	40 1.81%	256 11.59%	20 0.91%	1 0.05%	1 0.05%	2 0.09%	2 0.09%	322 79.50% 20.50%
	class C	19 0.86%	19 0.86%	211 9.56%	10 0.45%	56 2.54%	7 0.32%	17 0.77%	339 82.24% 17.76%
	class D	4 0.18%	0 0.0%	1 0.05%	311 14.09%	2 0.09%	5 0.23%	1 0.05%	324 99.99% 4.01%
	class E	2 0.09%	1 0.05%	4 0.18%	0 0.0%	58 2.63%	0 0.0%	10 0.45%	75 77.33% 22.67%
	class F	26 1.18%	5 0.23%	9 0.41%	18 0.82%	2 0.09%	126 5.71%	11 0.50%	197 83.96% 16.04%
	class G	15 0.68%	14 0.63%	10 0.45%	5 0.23%	14 0.63%	1 0.05%	203 9.19%	262 77.48% 22.52%
sum_col		653 83.77% 16.23%	346 73.99% 26.01%	291 72.51% 27.49%	375 82.93% 17.07%	144 40.28% 59.72%	152 82.89% 17.11%	247 82.19% 17.81%	2208 77.48% 22.46%
		class A	class B	class C	class D	class E	class F	class G	sum_row
		Actual							

Figure 2.12: Confusion matrix

Chapter 3

Conclusion

It seems that the slight modifications that I've tried did nothing to improve the model's accuracy. Indeed, the original model reports accuracy of 78.40%, which tied with Ver. 2 and is strictly greater than the other two versions.

This accuracy is actually lower than the reported accuracy from Kipf & Welling, which is actually 81.5%. I can't really explain why this is the case... But one guess is that maybe getting rid of the bias term might increase the accuracy? (<- just a wild guess)

One interesting observation is that Ver. 3, the model with the most complexity out of the 4 tested, performed the worst with accuracy 77.54%. It shows that adding in feature/model complexity doesn't always increase the accuracy; it might even decrease it!

Bibliography

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- [2] Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep Learning*. <http://www.deeplearningbook.org>. MIT Press, 2016.
- [3] Thomas N. Kipf and Max Welling. “Semi-Supervised Classification with Graph Convolutional Networks”. In: *5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings*. 2017. URL: <https://openreview.net/forum?id=SJU4ayYgl>.