torch

February 10, 2022

1 Links

https://chrsmrrs.github.io/datasets/docs/datasets/

```
[34]: ## Standard libraries
      import os
      import json
      import math
      import numpy as np
      import time
      import pandas as pd
      import sklearn
      from sklearn.linear_model import LogisticRegression
      ## Imports for plotting
      import matplotlib
      import matplotlib.pyplot as plt
      %matplotlib inline
      from IPython.display import set_matplotlib_formats
      set_matplotlib_formats('svg', 'pdf') # For export
      from matplotlib.colors import to_rgb
      from mpl_toolkits.mplot3d import Axes3D
      matplotlib.rcParams['lines.linewidth'] = 2.0
      import seaborn as sns
      sns.reset_orig()
      sns.set()
      # Plotly
      import plotly.graph_objects as go
      # NetworkX
      import networkx as nx
      # Gensim
      import gensim
      import gensim.downloader as api
      from gensim.models.word2vec import Word2Vec
```

```
## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.nn import Linear
import torch.utils.data as data
import torch.optim as optim
# Geometric
import torch_geometric
import torch geometric.nn as geom nn
from torch_geometric.nn import GCNConv, GraphConv, global_mean_pool
import torch_geometric.data as geom_data
from torch_geometric.datasets import TUDataset
from torch_geometric.loader import DataLoader, ClusterData, ClusterLoader
from torch_geometric.utils import to_networkx
# PyTorch Lightning
import pytorch_lightning as pl
```

```
[245]: def visualize_graph(ax, G, color=None, labels=False, title=None, layout=lambda_
       →G : nx.spring_layout(G, seed=42)):
          ax.set_xticks([])
          ax.set_yticks([])
          node_color = 'white'
          if color is not None: node_color = color
          nx.draw_networkx(G, pos=layout(G), with_labels=labels,
                            node_color=node_color, cmap="Set2", node_size=100, ax=ax)
          if title: ax.set_title(title)
      def visualize_embedding(ax, h, color, epoch=None, loss=None, title=None):
          ax.set xticks([])
          ax.set_yticks([])
          h = h.detach().cpu().numpy()
          ax.scatter(h[:, 0], h[:, 1], s=140, c=color, cmap="Set2")
          if epoch is not None and loss is not None:
               ax.set_xlabel(f'Epoch: {epoch}, Loss: {loss.item():.4f}', fontsize=10)
          if title: ax.set_title(title)
      def visualize_model_embedding_spaces(models, modelnames):
          fig, ax = plt.subplots(1, len(models), figsize=(len(models)*4,4))
          x_min, x_max = -1, 1
          y_min, y_max = -1, 1
          xx, yy = np.meshgrid(np.arange(x_min, x_max, 0.02), np.arange(y_min, y_max,_u
       →0.02))
          for i, model in enumerate(models):
               assert model.classifier.in_features == 2
```

```
name = modelnames[i]
        pred = model.classifier(torch.from_numpy(np.c_[xx.ravel(), yy.ravel()]).
 →float()).detach().numpy()
        zz = np.argmax(pred, axis=1).reshape(xx.shape)
        ax[i].pcolormesh(xx, yy, zz)
        ax[i].set title(name)
    plt.tight_layout()
def plot_results(losses, acc, modelnames):
    assert list(losses.keys()) == modelnames and list(acc.keys()) == modelnames
    n_models = len(modelnames)
    fig, ax = plt.subplots(2, n_models, figsize=(3*n_models,6))
    for i in range(n_models):
        model_acc = acc[modelnames[i]]
        ax[0,i].set_title(f'{modelnames[i]}: accuracy')
        ax[0,i].plot(np.arange(len(model_acc)), [x[0] for x in model_acc],_u
 →label='train acc')
        ax[0,i].plot(np.arange(len(model_acc)), [x[1] for x in model_acc],__
 →label='test acc')
        ax[0,i].set_xlabel('# epochs')
        ax[0,i].legend(loc='lower right')
        ax[0,i].set_ylim(([0,1]))
        model_losses = losses[modelnames[i]]
        ax[1,i].set title(f'{modelnames[i]}: loss')
        ax[1,i].plot(np.arange(len(model_losses)), model_losses)
        ax[1,i].set_xlabel('# epochs')
        ax[1,i].set_ylim(([0,1]))
    plt.tight_layout()
def plot_subgraph_3d(graph, data, N=100):
    subgraph_idx = np.random.choice(np.arange(len(graph.nodes)), N,__
→replace=False)
    subgraph labels = data.y[subgraph idx]
    subgraph = graph.subgraph(subgraph_idx)
    spring_3D = nx.spring_layout(subgraph, dim = 3, k = 0.7) # k regulates the_
\rightarrow distance between nodes
    nodes3d = [[spring_3D[key][i] for key in spring_3D.keys()] for i in_
\rightarrowrange(3)]
    edges3d = [[], [], []]
    for edge in subgraph.edges():
        for i in range(3):
            edges3d[i] += [spring_3D[edge[0]][i],spring_3D[edge[1]][i],None]
```

```
trace_edges = go.Scatter3d(x=edges3d[0], y=edges3d[1], z=edges3d[2],
    mode='lines',
    line=dict(
        color='black',
        width=.1),
    hoverinfo='none')

trace_nodes = go.Scatter3d(x=nodes3d[0], y=nodes3d[1], z=nodes3d[2],
    mode='markers',
    marker=dict(
        symbol='circle',
        size=6,
        color=subgraph_labels),
    hovertemplate=[f'<b>{1}</b><extra></extra>' for 1 in subgraph_labels])

fig = go.Figure(data=[trace_edges, trace_nodes])
fig.show()
```

2 Twitter

- 2.0.1 Each graph in this dataset represents a tweet, and each node in a graph is represented by a 1323-dimensional vector, corresponding to one of 1323 different words listed in the readme.txt file.
- 2.0.2 Each graph is labeled with 0 or 1, corresponding to sentiment. The source doesn't indicate what the sentiment is. So far, no clear sentiment seems apparent from observation.

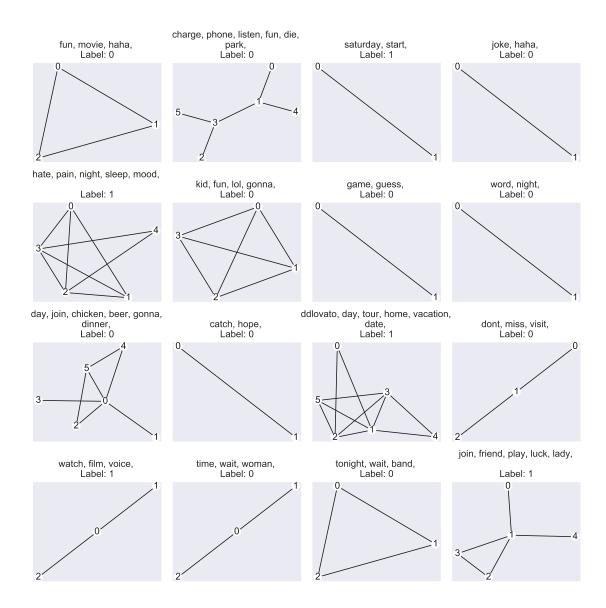
2.0.3 Because nodes correspond to words, we will consider using word embeddings as feature representations of the nodes in a tweet.

2.0.4 If tweets include words not in the embedding corpus, we embed the word as a zero vector

```
[127]: # convert integers to their corresponding words
       id2word = {}
       word2id = \{\}
       with open('data/TWITTER-Real-Graph-Partial/raw/readme.txt') as f:
           lines = f.readlines()
           for n in range(51, 51+1323):
               1 = lines[n].split()
               id2word[int(1[0])] = 1[1]
               word2id[1[1]] = int(1[0])
       # get word embeddings from GenSim word2vec.
       word2vec_model = Word2Vec.load("word2vec.model")
       # get word embeddings from Gensim glove-twitter-25
       glove vectors = api.load('glove-twitter-25')
       embeddings = {
           'word2vec' : {'size' : 100, 'model' : word2vec_model.wv},
           'glove' : {'size' : 25, 'model' : glove_vectors}
       # add unused words as a zero embedding
       for w in word2id.keys():
          for emb in embeddings:
               if w not in embeddings[emb]['model'].index_to_key:
                   embeddings[emb][w] = np.zeros(embeddings[emb]['size'])
       keywords = ['nervous', 'palms']
       for emb in embeddings:
           print(f'{emb} similar to {keywords}: ', [x[0] for x in_
       →embeddings[emb]['model'].most similar(positive=keywords, topn=3)])
      word2vec similar to ['nervous', 'palms']: ['digestive', 'vascular',
      'endocrine']
      glove similar to ['nervous', 'palms']: ['rough', 'resting', 'dragging']
      /Users/maxcembalest/opt/anaconda3/lib/python3.8/site-
      packages/gensim/models/keyedvectors.py:772: RuntimeWarning:
      invalid value encountered in true_divide
```

2.1 According to the dataset source on github, words are connected if they "co-occur". What does that mean in a tweet?

```
[44]: def format_ax_title(tweets, words):
          title = ''
          for i in range(len(words)):
              title += words[i] + ', '
              if i\%4==0 and i > 0:
                   title += '\n'
          title += '\n' + 'Label: ' + str(tweets.y[0].numpy())
          return title
      fig, ax = plt.subplots(4, 4, figsize=(10,10))
      sample_idx = np.random.choice(np.arange(len(twitter)), 16, replace=False)
      feature_vector_to_word = lambda v : id2word[np.where(v)[0][0]]
      for i, idx in enumerate(sample_idx):
          tweets = twitter[idx]
          words = [feature_vector_to_word(tweets.x[j]) for j in range(tweets.x.
       \hookrightarrowshape[0])]
          tweetG = to_networkx(tweets, to_undirected=True)
          title = format_ax_title(tweets, words)
          \label{limits} visualize\_graph(ax[i//4,i\%4], \ tweetG, \ labels=True, \ title=title)
      plt.tight_layout()
```



2.2 Load data

```
[184]: N_train = 50000
N_test = 1000
batch_size_train=128
batch_size_test=32

twitter_train_idx = np.random.choice(np.arange(len(twitter)), N_train, uperplace=False)

twitter_test_idx = np.random.choice(np.arange(len(twitter)), N_test, uperplace=False)
```

2.3 Build models

```
[185]: class TwitterGNN(torch.nn.Module):
           def __init__(self, hidden_channels, embedding=None):
               super(TwitterGNN, self).__init__()
               if embedding:
                   in D = embeddings[embedding]['size']
                   self.embedding_map = lambda x : torch.
        →tensor(embeddings[embedding]['model'][torch.where(x)[1].numpy()])
                   in_D = twitter.num_features
                   self.embedding_map = None
               self.conv1 = GraphConv(in_D, hidden_channels)
               self.conv2 = GraphConv(hidden channels, hidden channels//2)
               self.lin = Linear(hidden_channels//2, twitter.num_classes)
           def forward(self, x, edge_index, batch):
               # O. apply optional word embeddings
               if self.embedding_map:
                   x = self.embedding map(x)
               # 1. GCN embeddings
               x = self.conv1(x, edge_index)
               x = x.relu()
               x = self.conv2(x, edge_index)
               # 2. Readout layer, to obtain a graph-level representation
               x = global_mean_pool(x, batch)
               # 3. Apply a final classifier
               x = F.dropout(x, p=0.5, training=self.training)
               x = self.lin(x)
               return x
       # todo: compare these models against nlp-only baselines to see the impact of
       \rightarrow the GCN
       twitter_gnn_model = TwitterGNN(64)
       twitter_gnnword2vec_model = TwitterGNN(64, embedding='word2vec')
```

```
twitter_gnnglove_model = TwitterGNN(64, embedding='glove')
       twitter_models = [twitter_gnn_model, twitter_gnnword2vec_model,_
       →twitter_gnnglove_model]
       twitter modelnames = ['GNN', 'Word2Vec GNN', 'Glove GNN']
       for i in range(len(twitter_models)):
           print(twitter modelnames[i], ':', twitter models[i])
      GNN : TwitterGNN(
        (conv1): GraphConv(1323, 64)
        (conv2): GraphConv(64, 32)
        (lin): Linear(in_features=32, out_features=2, bias=True)
      Word2Vec GNN : TwitterGNN(
        (conv1): GraphConv(100, 64)
        (conv2): GraphConv(64, 32)
        (lin): Linear(in_features=32, out_features=2, bias=True)
      Glove GNN : TwitterGNN(
        (conv1): GraphConv(25, 64)
        (conv2): GraphConv(64, 32)
        (lin): Linear(in_features=32, out_features=2, bias=True)
      )
      2.4 Train models
[186]: learning_rate = .001
       optimizers = [torch.optim.Adam(m.parameters(), lr=learning_rate) for m in_
       →twitter models]
       criterion = torch.nn.CrossEntropyLoss()
       assert len(twitter_models) == len(twitter_modelnames) == len(optimizers)
       def train_step(model, loader, optimizer):
           model.train()
           losses = 0
           for data in loader: # Iterate in batches over the training dataset.
               out = model(data.x, data.edge_index, data.batch) # Perform a single_i
        \hookrightarrow forward pass.
               loss = criterion(out, data.y) # Compute the loss.
               losses += loss
               loss.backward() # Derive gradients.
               optimizer.step() # Update parameters based on gradients.
               optimizer.zero_grad() # Clear gradients.
           return losses.detach().numpy()/len(loader) # average batch loss
       def test(model, loader):
           model.eval()
```

correct = 0

```
for data in loader: # Iterate in batches over the training/test dataset.
        out = model(data.x, data.edge_index, data.batch)
        pred = out.argmax(dim=1) # Use the class with highest probability.
        correct += int((pred == data.y).sum()) # Check against ground-truth_
 \rightarrow labels.
    return correct / len(loader.dataset) # percent correct label
evaluate = lambda model : (test(model, twitter_train_loader), test(model, __
→twitter_test_loader))
twitterlosses = {m : [] for m in twitter_modelnames}
twitteracc = {m : [] for m in twitter modelnames}
for i, model in enumerate(twitter_models):
    print(twitter_modelnames[i])
    for epoch in range(100):
        loss = train_step(model, twitter_train_loader, optimizers[i])
        train_acc, test_acc = evaluate(model)
        twitterlosses[twitter_modelnames[i]].append(loss)
        twitteracc[twitter_modelnames[i]].append((train_acc, test_acc))
        if epoch%10==9: print(f'Epoch: {epoch}, loss: {np.around(loss, 2)}, acc:
 → {np.around(test_acc, 2)}')
```

GNN

```
Epoch: 0, loss: 0.63, acc: 0.68
Epoch: 9, loss: 0.37, acc: 0.72
Epoch: 18, loss: 0.21, acc: 0.7
Epoch: 27, loss: 0.16, acc: 0.71
Epoch: 36, loss: 0.14, acc: 0.72
Epoch: 45, loss: 0.13, acc: 0.71
Epoch: 54, loss: 0.12, acc: 0.72
Epoch: 63, loss: 0.12, acc: 0.72
Epoch: 72, loss: 0.11, acc: 0.72
Epoch: 81, loss: 0.11, acc: 0.71
Epoch: 90, loss: 0.11, acc: 0.72
Epoch: 99, loss: 0.1, acc: 0.71
Word2Vec GNN
Epoch: 0, loss: 0.67, acc: 0.62
Epoch: 9, loss: 0.58, acc: 0.67
Epoch: 18, loss: 0.54, acc: 0.68
Epoch: 27, loss: 0.51, acc: 0.68
Epoch: 36, loss: 0.49, acc: 0.67
Epoch: 45, loss: 0.48, acc: 0.69
Epoch: 54, loss: 0.47, acc: 0.68
Epoch: 63, loss: 0.46, acc: 0.68
Epoch: 72, loss: 0.45, acc: 0.68
Epoch: 81, loss: 0.45, acc: 0.67
Epoch: 90, loss: 0.44, acc: 0.68
```

```
Epoch: 99, loss: 0.44, acc: 0.68 Glove GNN

Epoch: 0, loss: 0.69, acc: 0.55

Epoch: 9, loss: 0.63, acc: 0.64

Epoch: 18, loss: 0.62, acc: 0.65

Epoch: 27, loss: 0.61, acc: 0.66

Epoch: 36, loss: 0.6, acc: 0.68

Epoch: 45, loss: 0.6, acc: 0.65

Epoch: 54, loss: 0.59, acc: 0.66

Epoch: 63, loss: 0.59, acc: 0.66

Epoch: 72, loss: 0.59, acc: 0.66

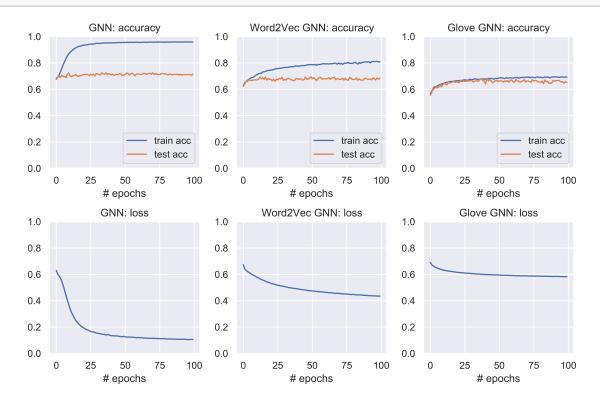
Epoch: 81, loss: 0.59, acc: 0.66

Epoch: 90, loss: 0.58, acc: 0.66

Epoch: 99, loss: 0.58, acc: 0.66
```

2.5 Plot evaluation

[243]: plot_results(twitterlosses, twitteracc, twitter_modelnames)



3 Airports

- 3.1 Withouth knowing which airport is which, we will plot them as points in 3d, and draw lines between nodes if their airports are connected in the UsaAirports dataset
- 3.2 Without knowing what the labels mean, it seems the labels have something to do with the connectedness of the nodes. The labels are equally balanced (1190=297+297+297+299)
- 3.3 Here we are viewing approximately 40% of the nodes of the graph, since it is too dense to view the whole thing

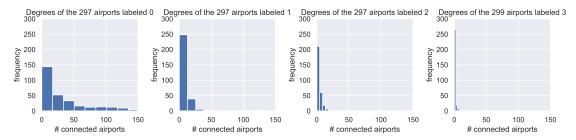
```
[246]: plot_subgraph_3d(airport_graph, airport_data, N=500)
```

3.3.1 A correlation between node degree (# of neighbors) and the label

```
[35]: fig, ax = plt.subplots(1, 4, figsize=(12,3))

for i in range(4):
    subdf= airports_df[airports_df['label']==i]
    ax[i].hist(subdf.num_neighbors)
    ax[i].set_xlabel('# connected airports')
    ax[i].set_ylabel('frequency')
    ax[i].set_xlim((0,150))
```

```
ax[i].set_ylim((0,300))
ax[i].set_title(f'Degrees of the {len(subdf)} airports labeled {i}')
plt.tight_layout()
```

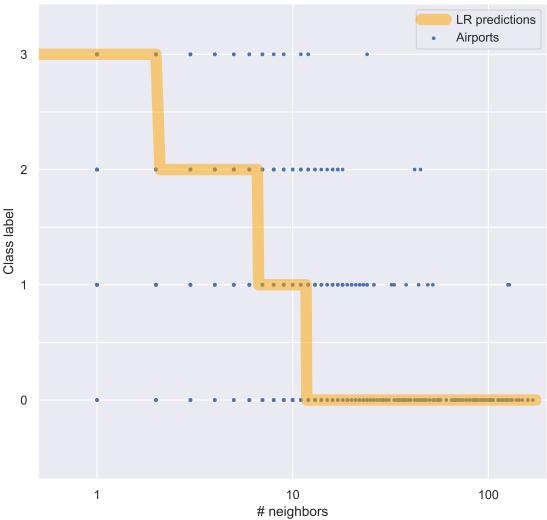


3.4 As a baseline against a GNN, here is a logistic regression model using the # of neighbors as its only feature

```
[194]: fig, ax = plt.subplots(figsize=(7,7))
       # plot airports by their # of neighbors and class label
       ax.scatter(airports df.num neighbors, airports_df.label, sizes=5*np.
       →ones(len(airports_df)), label='Airports')
       # fit logistic regression model just using the # neighbors to predict the label
       train idx = np.random.choice(np.arange(len(airports df)), 700, replace=False)
       test_idx = np.random.choice(np.arange(len(airports_df)), 300, replace=False)
       dftrain, dftest = airports_df.loc[train_idx], airports_df.loc[test_idx]
       xtrain, ytrain, xtest, ytest = dftrain.num_neighbors.values, dftrain.label.
       →values, dftest.num_neighbors.values, dftest.label.values
       lr = LogisticRegression()
       lr.fit(xtrain.reshape(-1,1), ytrain)
       ypred = lr.predict(xtest.reshape(-1,1))
       probs = lr.predict_proba(xplot.reshape(-1,1))
       accuracy = sklearn.metrics.accuracy_score(ytest, ypred)
       # plot logistic regression model predictions
       xplot = np.arange(0,175,.1)
       plotpreds = lr.predict(xplot.reshape(-1,1))
       ax.plot(xplot, plotpreds, linewidth=10, color='orange', alpha=0.5, label = 'LR_U
       →predictions')
       # fill a region of space whose width changes proportional to the predicted \Box
       →probabiltiy of the LR model for each class
       for i in range(4):
           ax.fill_between(xplot, i - 0.5*probs[:,i], i + 0.5*probs[:,i], linewidth=5,__
        ⇔color='blue', alpha=0.3)
```

```
# format
title = f'Baseline Logistic Regression model using # neighbors as predictor: u
title += '\nThe widths of the blue regions are the model\'s predicted_{\sqcup}
→probability of each class'
ax.set_title(title)
ax.set_xscale('log')
ax.set_xlim([.5,200])
ax.set_xticks([1, 10, 100])
ax.set_xticklabels(['1', '10', '100'])
ax.set_yticks(np.arange(0,3.5,0.5))
ax.set_yticklabels(['0','','1','','2','','3'])
ax.set_xlabel('# neighbors')
ax.set_ylabel('Class label')
ax.legend(loc='best')
plt.tight_layout()
```

Baseline Logistic Regression model using # neighbors as predictor: 49.33% accurate The widths of the blue regions are the model's predicted probability of each class



3.5 Load data

3.6 Build models

```
[225]: class AirportGNN(torch.nn.Module):
           def __init__(self, layer):
               super().__init__()
               self.conv1 = layer(airports.num_features, 100)
               self.conv2 = layer(100, 10)
               self.conv3 = layer(10, 2)
               self.classifier = Linear(2, airports.num_classes)
           def forward(self, x, edge_index):
               h = self.conv1(x, edge_index)
               h = h.tanh()
               h = self.conv2(h, edge_index)
               h = h.tanh()
               h = self.conv3(h, edge_index)
               h = h.tanh() # Final GNN embedding space.
               # Apply a final (linear) classifier.
               out = self.classifier(h)
               return out, h
       airport_gcnconv_model = AirportGNN(GCNConv)
       airport_graphconv_model = AirportGNN(GraphConv)
       airport_models = [airport_gcnconv_model, airport_graphconv_model]
       airport_modelnames = ['GCNConv', 'GraphConv']
       for i in range(len(airport_models)):
           print(airport_modelnames[i], ':', airport_models[i])
      GCNConv : AirportGNN(
        (conv1): GCNConv(1190, 100)
        (conv2): GCNConv(100, 10)
        (conv3): GCNConv(10, 2)
        (classifier): Linear(in_features=2, out_features=4, bias=True)
      GraphConv : AirportGNN(
        (conv1): GraphConv(1190, 100)
        (conv2): GraphConv(100, 10)
        (conv3): GraphConv(10, 2)
        (classifier): Linear(in_features=2, out_features=4, bias=True)
      )
```

3.7 Train models

```
[231]: learning_rate = .003
       optimizers = [torch.optim.Adam(m.parameters(), lr=learning_rate) for m in_
       →airport_models]
       criterion = torch.nn.CrossEntropyLoss()
       assert len(airport models) == len(airport modelnames) == len(optimizers)
       def train step(model, optimizer):
           model.train()
           optimizer.zero_grad() # Clear gradients
           out, h = model(airports_data.x, airports_data.edge_index) # Forward pass_u
       \hookrightarrow on whole graph
           loss = criterion(out[airport_train_mask], airports_data.
       →y[airport_train_mask]) # Loss on training nodes
           loss.backward() # Calculate gradients
           optimizer.step() # Update parameters based on gradients
           return loss.detach().numpy(), out, h
       def test(out, mask):
           pred = out[mask].argmax(dim=1) # Use the class with highest probability
           acc = int((pred == airports_data.y[mask]).sum()) / mask.sum() # Percent_
        \hookrightarrow correct
           return acc
       evaluate = lambda out : (test(out, airport_train_mask), test(out,__
       →airport_test_mask))
       airportlosses = {m : [] for m in airport_modelnames}
       airportacc = {m : [] for m in airport_modelnames}
       airportemb = {m : [] for m in airport_modelnames}
       # sample_idx = np.random.choice(np.arange(airports.num_features), 100)
       n_epochs=30
       for i, model in enumerate(airport_models):
           name = airport_modelnames[i]
           print(name)
           for epoch in range(n_epochs):
               loss, out, h = train_step(model, optimizers[i])
               train_acc, test_acc = evaluate(out)
               airportlosses[name].append(loss)
               airportacc[name].append((train_acc, test_acc))
               airportemb[name].append(h)
               if epoch%10==9:
                   print(f'Epoch: {epoch}, loss: {np.around(loss, 2)}, acc: {np.
        →around(test acc, 2)}')
```

GCNConv

Epoch: 9, loss: 0.8700000047683716, acc: 0.43 Epoch: 19, loss: 0.8299999833106995, acc: 0.5 Epoch: 29, loss: 0.7900000214576721, acc: 0.43

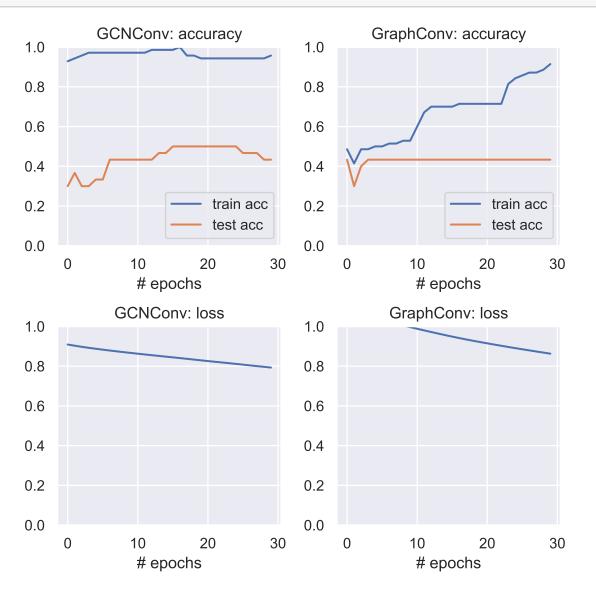
 ${\tt GraphConv}$

Epoch: 9, loss: 1.0, acc: 0.43

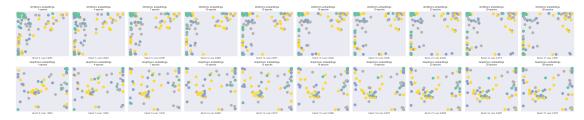
Epoch: 19, loss: 0.9200000166893005, acc: 0.43 Epoch: 29, loss: 0.8600000143051147, acc: 0.43

3.8 Plot evaluation

[248]: plot_results(airportlosses, airportacc, airport_modelnames)



3.9 Visualize the change in the last layer embeddings during training

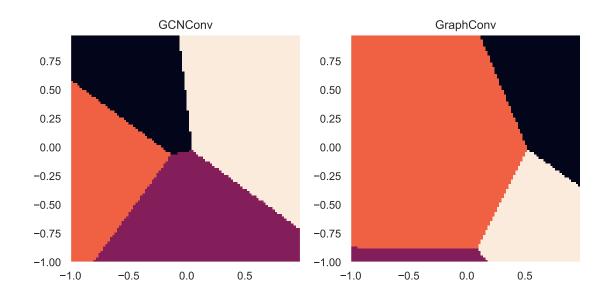


3.10 Visualize the the last layer embedding space after training

```
[316]: visualize_model_embedding_spaces(airport_models, airport_modelnames)
```

<ipython-input-297-e4104e03d506>:13: MatplotlibDeprecationWarning:

shading='flat' when X and Y have the same dimensions as C is deprecated since 3.3. Either specify the corners of the quadrilaterals with X and Y, or pass shading='auto', 'nearest' or 'gouraud', or set rcParams['pcolor.shading']. This will become an error two minor releases later.



[]:[