

## Task IV: Classical Graph Neural Network (GNN) Part

For Task IV, you will use ParticleNet's data for Quark/Gluon jet classification available [here](#) with its corresponding description.

- Choose 2 Graph-based architectures of your choice to classify jets as being quarks or gluons. Provide a description on what considerations you have taken to project this point-cloud dataset to a set of interconnected nodes and edges.
- Discuss the resulting performance of the 2 chosen architectures.

### Downloading the Dataset

```
In [1]: !wget https://zenodo.org/record/3164691/files/QG_jets.npz?download=1 -O QG_jets.npz

--2021-03-19 13:56:00-- https://zenodo.org/record/3164691/files/QG_jets.npz?download=1
Resolving zenodo.org (zenodo.org)... 137.138.76.77
Connecting to zenodo.org (zenodo.org)|137.138.76.77|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 106689379 (102M) [application/octet-stream]
Saving to: 'QG_jets.npz'

QG_jets.npz      100%[=====] 101.75M  22.1MB/s   in 5.0s

2021-03-19 13:56:06 (20.3 MB/s) - 'QG_jets.npz' saved [106689379/106689379]
```

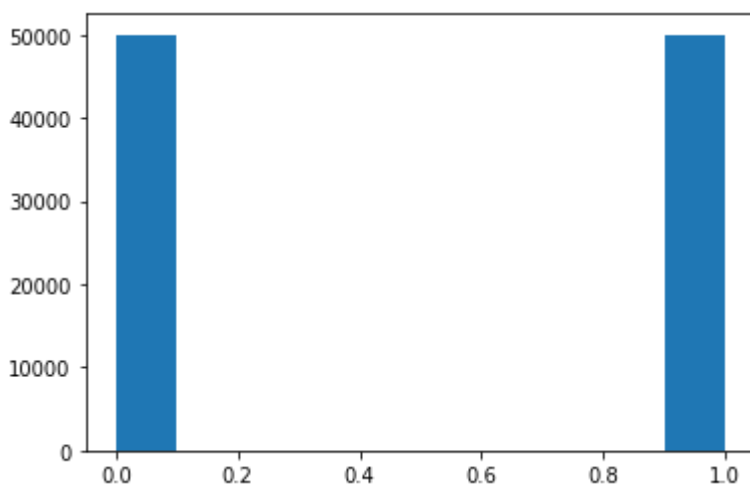
```
In [2]: import numpy as np

%matplotlib inline
import matplotlib.pyplot as plt
```

```
In [3]: with np.load('./QG_jets.npz') as data:
        X = data['X']
        y_train = data['y']
        print(X.shape)
        print(y_train.shape)

(100000, 139, 4)
(100000,)
```

```
In [4]: plt.hist(y_train)
plt.show()
```



```
In [5]: x_train = []
        for i in X:
            x_train.append(i[0])
        x_train = np.array(x_train)
        print(x_train.shape)

(100000, 4)
```

```
In [6]: !pip install dgl-cu101
import dgl
import torch
import networkx as nx
```

```
Requirement already satisfied: dgl-cu101 in /usr/local/lib/python3.7/dist-packages (0.6.0.post1)
Requirement already satisfied: requests>=2.19.0 in /usr/local/lib/python3.7/dist-packages (from dgl-cu101) (2.23.0)
Requirement already satisfied: scipy>=1.1.0 in /usr/local/lib/python3.7/dist-packages (from dgl-cu101) (1.4.1)
Requirement already satisfied: numpy>=1.14.0 in /usr/local/lib/python3.7/dist-packages (from dgl-cu101) (1.19.5)
Requirement already satisfied: networkx>=2.1 in /usr/local/lib/python3.7/dist-packages (from dgl-cu101) (2.5)
Requirement already satisfied: idna<3,>=2.5 in /usr/local/lib/python3.7/dist-packages (from requests>=2.19.0->dgl-cu101) (2.10)
Requirement already satisfied: urllib3!=1.25.0,!1.25.1,<1.26,>=1.21.1 in /usr/local/lib/python3.7/dist-packages (from requests>=2.19.0->dgl-cu101) (1.24.3)
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.7/dist-packages (from requests>=2.19.0->dgl-cu101) (2020.12.5)
Requirement already satisfied: chardet<4,>=3.0.2 in /usr/local/lib/python3.7/dist-packages (from requests>=2.19.0->dgl-cu101) (3.0.4)
Requirement already satisfied: decorator>=4.3.0 in /usr/local/lib/python3.7/dist-packages (from networkx>=2.1->dgl-cu101) (4.4.2)
Using backend: pytorch
```

### Approach

I am choosing the following two graph-based architectures:

1. Node Classification

## Node Classification

In this approach, I will encode the data as nodes of a graph and then train a GNN to learn to classify these nodes. In this way we can build a classifier which classifies quarks from gluons.

## Graph Classification

In this approach, I will encode each training sample as a graph, resulting in a training data of different graphs. I will then train a GNN to learn to classify different graphs. In this way too we can build a classifier which classifies quarks from gluons.

## Node Classification

Let us begin by preparing the dataset. We will use a small subset of the training data for demonstration.

```
In [47]: x_train_small = x_train[:2000].astype(np.float32)
y_train_small = y_train[:2000]
class NodeClassificationDataset(dgl.data.DGLDataset):
    """A Class to process and convert the numpy training data into Graphs so that it can be used in GNNs"""
    def __init__(self):
        super().__init__(name='node_classification')
        self.num_classes = 2

    def process(self):
        node_features = torch.from_numpy(x_train_small)
        node_labels = torch.from_numpy(y_train_small).long()

        self.graph = dgl.from_networkx(nx.generators.fast_gnp_random_graph(x_train_small.shape[0], 0.008, seed=1337))
        self.graph.ndata['feat'] = node_features
        self.graph.ndata['label'] = node_labels
        # self.graph.ndata['weight'] = None

        n_nodes = x_train_small.shape[0]
        n_train = int(n_nodes * 0.8)
        n_val = int(n_nodes * 0.1)
        train_mask = torch.zeros(n_nodes, dtype=torch.bool)
        val_mask = torch.zeros(n_nodes, dtype=torch.bool)
        test_mask = torch.zeros(n_nodes, dtype=torch.bool)
        train_mask[:n_train] = True
        val_mask[n_train:n_train+n_val] = True
        test_mask[n_train+n_val:] = True
        self.graph.ndata['train_mask'] = train_mask
        self.graph.ndata['val_mask'] = val_mask
        self.graph.ndata['test_mask'] = test_mask

    def __getitem__(self, idx):
        return self.graph

    def __len__(self):
        return 1

node_classif_dataset = NodeClassificationDataset()
node_classif_graph = node_classif_dataset[0]

print(node_classif_graph)
```

```
Graph(num_nodes=2000, num_edges=31988,
      ndata_schemes={'feat': Scheme(shape=(4,), dtype=torch.float32), 'label': Scheme(shape=(), dtype=torch.int64), 'train_mask': Scheme(shape=(), dtype=torch.bool), 'val_mask': Scheme(shape=(), dtype=torch.bool), 'test_mask': Scheme(shape=(), dtype=torch.bool)}
      edata_schemes={})
```

## Defining the Model

```
In [48]: from dgl.nn import GraphConv

class NodeClassificationModel(torch.nn.Module):
    """A Model Class having the methods to implement and forward pass a GNN."""
    def __init__(self, in_feats, num_classes):
        super(NodeClassificationModel, self).__init__()
        self.conv1 = GraphConv(in_feats, 16)
        self.conv2 = GraphConv(16, 32)
        self.conv3 = GraphConv(32, 64)
        self.conv4 = GraphConv(64, num_classes)

    def forward(self, g, in_feat):
        h = self.conv1(g, in_feat)
        h = torch.nn.functional.elu(h)
        h = self.conv2(g, h)
        h = torch.nn.functional.relu(h)
        h = self.conv3(g, h)
        h = torch.nn.functional.relu(h)
        h = self.conv4(g, h)
        return h

node_classif_model = NodeClassificationModel(node_classif_graph.ndata['feat'].shape[1], node_classif_dataset.num_classes)
```

## Defining the Training Loop

```
In [49]: def train(g, model, num_epochs):
    """The function implementing the main train loop."""
```

```

losses = []
accs = {'train': [], 'val': [], 'test': []}
optimizer = torch.optim.Adam(model.parameters(), lr=1*1e-5, betas=(0.6, 0.7))
best_val_acc = 0.0
best_test_acc = 0.0

features = g.ndata['feat']
labels = g.ndata['label']
train_mask = g.ndata['train_mask']
val_mask = g.ndata['val_mask']
test_mask = g.ndata['test_mask']

for e in range(num_epochs):
    model.train()
    logits = model(g, features)
    preds = logits.argmax(1)

    loss = torch.nn.functional.cross_entropy(logits[train_mask], labels[train_mask])

    train_acc = (preds[train_mask] == labels[train_mask]).float().mean()
    val_acc = (preds[val_mask] == labels[val_mask]).float().mean()
    test_acc = (preds[test_mask] == labels[test_mask]).float().mean()
    losses.append(loss)
    accs['train'].append(train_acc)
    accs['val'].append(val_acc)
    accs['test'].append(test_acc)

    if best_val_acc < val_acc:
        best_val_acc = val_acc
        best_test_acc = test_acc

    with torch.no_grad():
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

    if e % 5 == 0:
        print('In epoch {}, loss: {:.8f}, val acc: {:.8f} (best {:.8f}), test acc: {:.8f} (best {:.8f})'.format(
            e, loss, val_acc, best_val_acc, test_acc, best_test_acc))

return losses, accs

```

In [50]:

```

node_classif_graph = node_classif_graph.to('cuda')
node_classif_model = node_classif_model.to('cuda')
node_classif_losses, node_classif_accs = train(node_classif_graph, node_classif_model, 5000)

```

```

In epoch 0, loss: 7.58675766, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 5, loss: 7.52613258, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 10, loss: 7.46548605, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 15, loss: 7.40483522, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 20, loss: 7.34418201, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 25, loss: 7.28349257, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 30, loss: 7.22277641, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 35, loss: 7.16203165, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 40, loss: 7.10127878, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 45, loss: 7.04049969, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 50, loss: 6.97972059, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 55, loss: 6.91894579, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 60, loss: 6.85817337, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 65, loss: 6.79738712, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 70, loss: 6.73660135, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 75, loss: 6.67581320, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 80, loss: 6.61501265, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 85, loss: 6.55420113, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 90, loss: 6.49337482, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 95, loss: 6.43254089, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 100, loss: 6.37171125, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 105, loss: 6.31088257, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 110, loss: 6.25004530, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 115, loss: 6.18919373, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 120, loss: 6.12830448, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 125, loss: 6.06740475, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 130, loss: 6.00650215, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 135, loss: 5.94559526, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 140, loss: 5.88468790, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 145, loss: 5.82376814, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 150, loss: 5.76285076, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 155, loss: 5.70193863, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 160, loss: 5.64101458, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 165, loss: 5.58008289, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 170, loss: 5.51917171, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 175, loss: 5.45826530, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 180, loss: 5.39735985, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 185, loss: 5.33644342, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 190, loss: 5.27552843, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 195, loss: 5.21461868, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 200, loss: 5.15370750, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 205, loss: 5.09279680, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 210, loss: 5.03188276, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 215, loss: 4.97097397, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 220, loss: 4.91007376, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 225, loss: 4.84918690, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 230, loss: 4.78831148, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 235, loss: 4.72745705, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 240, loss: 4.66661358, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 245, loss: 4.60578108, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 250, loss: 4.54496861, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 255, loss: 4.48415995, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 260, loss: 4.42335796, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)
In epoch 265, loss: 4.36256027, val acc: 0.47999999 (best 0.47999999), test acc: 0.52499998 (best 0.52499998)

```

In epoch 270,	loss:	4.30177927,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 275,	loss:	4.24101162,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 280,	loss:	4.18026304,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 285,	loss:	4.11953497,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 290,	loss:	4.05883217,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 295,	loss:	3.99813819,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 300,	loss:	3.93746114,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 305,	loss:	3.87680888,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 310,	loss:	3.81618595,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 315,	loss:	3.75558925,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 320,	loss:	3.69501686,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 325,	loss:	3.63446736,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 330,	loss:	3.57394814,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 335,	loss:	3.51345515,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 340,	loss:	3.45300221,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 345,	loss:	3.39258385,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 350,	loss:	3.33219910,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 355,	loss:	3.27186465,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 360,	loss:	3.21156645,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 365,	loss:	3.15131855,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 370,	loss:	3.09112120,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 375,	loss:	3.03098631,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 380,	loss:	2.97090626,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 385,	loss:	2.91088462,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 390,	loss:	2.85092783,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 395,	loss:	2.79104614,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 400,	loss:	2.73125172,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 405,	loss:	2.67154765,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 410,	loss:	2.61193562,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 415,	loss:	2.55242968,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 420,	loss:	2.49305105,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 425,	loss:	2.43380952,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 430,	loss:	2.37470722,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 435,	loss:	2.31575871,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 440,	loss:	2.25698709,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.52499998)
In epoch 445,	loss:	2.19841099,	val acc:	0.47999999	(best 0.47999999),	test acc:	0.52499998	(best 0.524



In epoch 785,	loss: 0.69364572,	val acc: 0.51999998	(best 0.52999997),	test acc: 0.44999999	(best 0.42999998)
In epoch 790,	loss: 0.69357771,	val acc: 0.51499999	(best 0.52999997),	test acc: 0.44999999	(best 0.42999998)
In epoch 795,	loss: 0.69350785,	val acc: 0.51999998	(best 0.52999997),	test acc: 0.45499998	(best 0.42999998)
In epoch 800,	loss: 0.69344223,	val acc: 0.52999997	(best 0.53499997),	test acc: 0.45999998	(best 0.45999998)
In epoch 805,	loss: 0.69337636,	val acc: 0.52999997	(best 0.53999996),	test acc: 0.45499998	(best 0.45999998)
In epoch 810,	loss: 0.69331336,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.44999999	(best 0.45999998)
In epoch 815,	loss: 0.69325083,	val acc: 0.52999997	(best 0.53999996),	test acc: 0.44999999	(best 0.45999998)
In epoch 820,	loss: 0.69319117,	val acc: 0.52999997	(best 0.53999996),	test acc: 0.44999999	(best 0.45999998)
In epoch 825,	loss: 0.69313407,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.45499998	(best 0.45999998)
In epoch 830,	loss: 0.69308221,	val acc: 0.52999997	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 835,	loss: 0.69303054,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 840,	loss: 0.69297707,	val acc: 0.52999997	(best 0.53999996),	test acc: 0.45999998	(best 0.45999998)
In epoch 845,	loss: 0.69291991,	val acc: 0.52999997	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 850,	loss: 0.69286638,	val acc: 0.52999997	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 855,	loss: 0.69281232,	val acc: 0.52999997	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 860,	loss: 0.69275606,	val acc: 0.52499998	(best 0.53999996),	test acc: 0.47000000	(best 0.45999998)
In epoch 865,	loss: 0.69270307,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.47000000	(best 0.45999998)
In epoch 870,	loss: 0.69265276,	val acc: 0.51499999	(best 0.53999996),	test acc: 0.47000000	(best 0.45999998)
In epoch 875,	loss: 0.69260162,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 880,	loss: 0.69255155,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 885,	loss: 0.69250512,	val acc: 0.51499999	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 890,	loss: 0.69246137,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 895,	loss: 0.69241792,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 900,	loss: 0.69237709,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 905,	loss: 0.69233721,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.45999998	(best 0.45999998)
In epoch 910,	loss: 0.69229662,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.45999998	(best 0.45999998)
In epoch 915,	loss: 0.69225693,	val acc: 0.52499998	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 920,	loss: 0.69221914,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 925,	loss: 0.69218206,	val acc: 0.51999998	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 930,	loss: 0.69214731,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.45999998	(best 0.45999998)
In epoch 935,	loss: 0.69211280,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.45999998	(best 0.45999998)
In epoch 940,	loss: 0.69207799,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.45999998	(best 0.45999998)
In epoch 945,	loss: 0.69204628,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 950,	loss: 0.69201708,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.45999998	(best 0.45999998)
In epoch 955,	loss: 0.69198942,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.45499998	(best 0.45999998)
In epoch 960,	loss: 0.69196296,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.45999998	(best 0.45999998)
In epoch 965,	loss: 0.69193602,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.45999998	(best 0.45999998)
In epoch 970,	loss: 0.69190824,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)
In epoch 975,	loss: 0.69188291,	val acc: 0.53499997	(best 0.53999996),	test acc: 0.46500000	(best 0.45999998)

In epoch 1300,	loss: 0.69095492,	val acc: 0.53499997	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1305,	loss: 0.69094604,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1310,	loss: 0.69094050,	val acc: 0.53499997	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1315,	loss: 0.69093019,	val acc: 0.52999997	(best 0.56999999),	test acc: 0.49499997	(best 0.48999998)
In epoch 1320,	loss: 0.69092447,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1325,	loss: 0.69091660,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1330,	loss: 0.69091278,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.49499997	(best 0.48999998)
In epoch 1335,	loss: 0.69090104,	val acc: 0.52999997	(best 0.56999999),	test acc: 0.47999999	(best 0.48999998)
In epoch 1340,	loss: 0.69089389,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.48499998	(best 0.48999998)
In epoch 1345,	loss: 0.69088727,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.48499998	(best 0.48999998)
In epoch 1350,	loss: 0.69088119,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.47999999	(best 0.48999998)
In epoch 1355,	loss: 0.69087541,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.47999999	(best 0.48999998)
In epoch 1360,	loss: 0.69086897,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.47999999	(best 0.48999998)
In epoch 1365,	loss: 0.69086105,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.47999999	(best 0.48999998)
In epoch 1370,	loss: 0.69085431,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.47999999	(best 0.48999998)
In epoch 1375,	loss: 0.69084775,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.47999999	(best 0.48999998)
In epoch 1380,	loss: 0.69084001,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1385,	loss: 0.69083667,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.47999999	(best 0.48999998)
In epoch 1390,	loss: 0.69082999,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1395,	loss: 0.69082785,	val acc: 0.55000001	(best 0.56999999),	test acc: 0.50000000	(best 0.48999998)
In epoch 1400,	loss: 0.69081897,	val acc: 0.52999997	(best 0.56999999),	test acc: 0.49499997	(best 0.48999998)
In epoch 1405,	loss: 0.69081491,	val acc: 0.53499997	(best 0.56999999),	test acc: 0.50000000	(best 0.48999998)
In epoch 1410,	loss: 0.69080931,	val acc: 0.52999997	(best 0.56999999),	test acc: 0.50000000	(best 0.48999998)
In epoch 1415,	loss: 0.69080973,	val acc: 0.54500002	(best 0.56999999),	test acc: 0.49499997	(best 0.48999998)
In epoch 1420,	loss: 0.69080061,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.49499997	(best 0.48999998)
In epoch 1425,	loss: 0.69079691,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.50000000	(best 0.48999998)
In epoch 1430,	loss: 0.69079900,	val acc: 0.51499999	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1435,	loss: 0.69079053,	val acc: 0.53499997	(best 0.56999999),	test acc: 0.50000000	(best 0.48999998)
In epoch 1440,	loss: 0.69078583,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.49499997	(best 0.48999998)
In epoch 1445,	loss: 0.69078273,	val acc: 0.53499997	(best 0.56999999),	test acc: 0.50000000	(best 0.48999998)
In epoch 1450,	loss: 0.69077981,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.50500000	(best 0.48999998)
In epoch 1455,	loss: 0.69077712,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.50000000	(best 0.48999998)
In epoch 1460,	loss: 0.69077611,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1465,	loss: 0.69076991,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.50500000	(best 0.48999998)
In epoch 1470,	loss: 0.69077039,	val acc: 0.51999998	(best 0.56999999),	test acc: 0.48999998	(best 0.48999998)
In epoch 1475,	loss: 0.69076246,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.49499997	(best 0.48999998)
In epoch 1480,	loss: 0.69075942,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.50000000	(best 0.48999998)
In epoch 1485,	loss: 0.69076180,	val acc: 0.52499998	(best 0.56999999),	test acc: 0.49499997	(best 0.48999998)
In epoch 1490,	loss: 0.69075340,	val acc: 0.53499997	(best 0.56999999),</		

[illegible]

[illegible]



[illegible]

[illegible]

In epoch 3875,	loss:	0.69012070,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.51499999	(best 0.48999998)
In epoch 3880,	loss:	0.69012070,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3885,	loss:	0.69011819,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3890,	loss:	0.69011998,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.50500000	(best 0.48999998)
In epoch 3895,	loss:	0.69011736,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3900,	loss:	0.69011748,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.52499998	(best 0.48999998)
In epoch 3905,	loss:	0.69011438,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3910,	loss:	0.69011360,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3915,	loss:	0.69011301,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3920,	loss:	0.69011098,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0.51499999	(best 0.48999998)
In epoch 3925,	loss:	0.69011086,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3930,	loss:	0.69011062,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.52499998	(best 0.48999998)
In epoch 3935,	loss:	0.69010848,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3940,	loss:	0.69010901,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.52499998	(best 0.48999998)
In epoch 3945,	loss:	0.69010943,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.52499998	(best 0.48999998)
In epoch 3950,	loss:	0.69010681,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.52499998	(best 0.48999998)
In epoch 3955,	loss:	0.69010663,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.52499998	(best 0.48999998)
In epoch 3960,	loss:	0.69010329,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3965,	loss:	0.69010293,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3970,	loss:	0.69010347,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.52499998	(best 0.48999998)
In epoch 3975,	loss:	0.69010043,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 3980,	loss:	0.69010466,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.52999997	(best 0.48999998)
In epoch 3985,	loss:	0.69009781,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.51499999	(best 0.48999998)
In epoch 3990,	loss:	0.69009680,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0.51499999	(best 0.48999998)
In epoch 3995,	loss:	0.69009590,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 4000,	loss:	0.69009477,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0.51499999	(best 0.48999998)
In epoch 4005,	loss:	0.69009471,	val	acc:	0.52999997	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 4010,	loss:	0.69009417,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 4015,	loss:	0.69009173,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0.50999999	(best 0.48999998)
In epoch 4020,	loss:	0.69009078,	val	acc:	0.52499998	(best 0.56999999),	test	acc:	0.50999999	(best 0.48999998)
In epoch 4025,	loss:	0.69009066,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0.51999998	(best 0.48999998)
In epoch 4030,	loss:	0.69009292,	val	acc:	0.51499999	(best 0.56999999),	test	acc:	0.50500000	(best 0.48999998)
In epoch 4035,	loss:	0.69008768,	val	acc:	0.51999998	(best 0.56999999),	test	acc:	0	

[illegible]



```

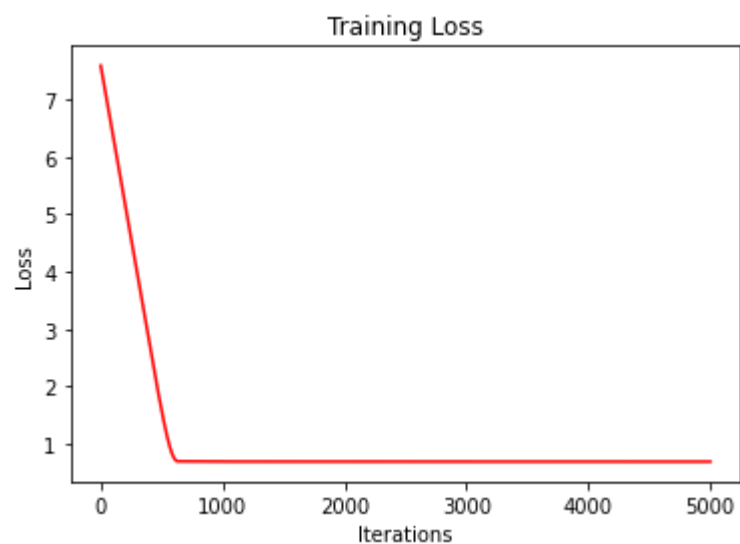
In epoch 4905, loss: 0.68991303, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4910, loss: 0.68991208, val acc: 0.50999999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4915, loss: 0.68991226, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4920, loss: 0.68991113, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4925, loss: 0.68991119, val acc: 0.50999999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4930, loss: 0.68990934, val acc: 0.50999999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4935, loss: 0.68990844, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4940, loss: 0.68990809, val acc: 0.50999999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4945, loss: 0.68990862, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4950, loss: 0.68990576, val acc: 0.50999999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4955, loss: 0.68990868, val acc: 0.51999998 (best 0.56999999), test acc: 0.51499999 (best 0.48999998)
In epoch 4960, loss: 0.68990219, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4965, loss: 0.68990189, val acc: 0.51999998 (best 0.56999999), test acc: 0.52499998 (best 0.48999998)
In epoch 4970, loss: 0.68990052, val acc: 0.52499998 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4975, loss: 0.68990219, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4980, loss: 0.68989825, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4985, loss: 0.68989730, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4990, loss: 0.68989635, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)
In epoch 4995, loss: 0.68989527, val acc: 0.51499999 (best 0.56999999), test acc: 0.51999998 (best 0.48999998)

```

```

In [51]: plt.plot(node_classif_losses, 'r-')
plt.title('Training Loss')
plt.xlabel('Iterations')
plt.ylabel('Loss')
plt.show()

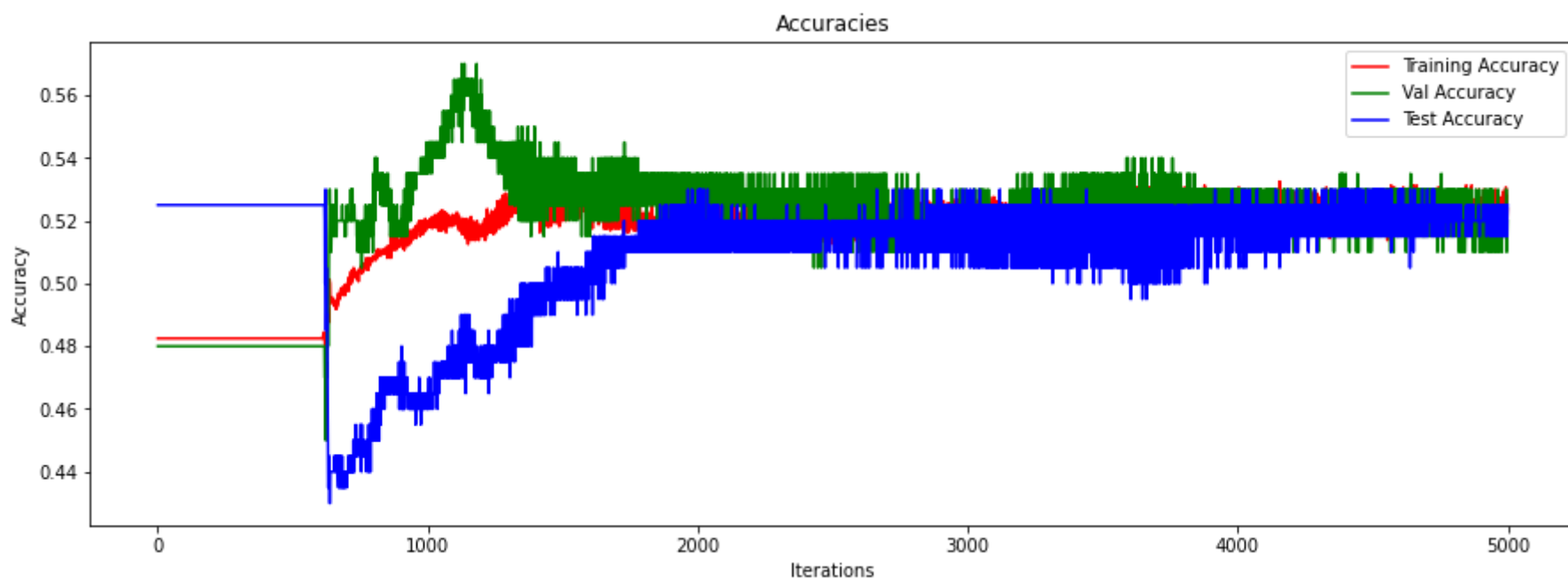
```



```

In [52]: plt.figure(figsize=(15, 5))
plt.plot(node_classif_accs['train'], 'r-', label='Training Accuracy')
plt.plot(node_classif_accs['val'], 'g-', label='Val Accuracy')
plt.plot(node_classif_accs['test'], 'b-', label='Test Accuracy')
plt.title('Accuracies')
plt.xlabel('Iterations')
plt.ylabel('Accuracy')
plt.legend()
plt.show()

```



```

In [53]: logits = node_classif_model(node_classif_graph, node_classif_graph.ndata['feat'])
pred = logits.argmax(1)
pred

```

```

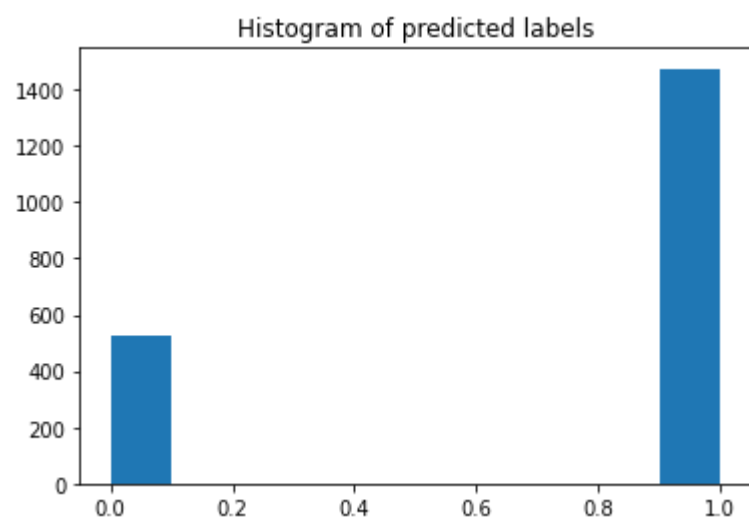
Out[53]: tensor([1, 0, 0, ..., 1, 1, 1], device='cuda:0')

```

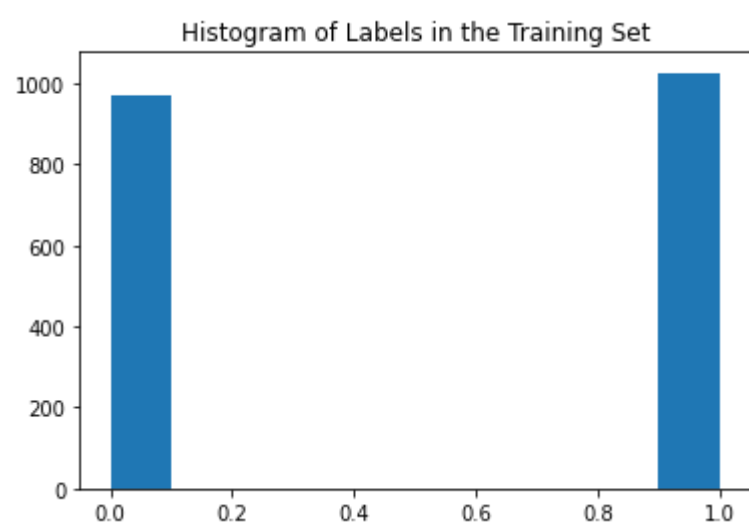
```

In [54]: plt.hist(pred.cpu().numpy())
plt.title("Histogram of predicted labels")
plt.show()

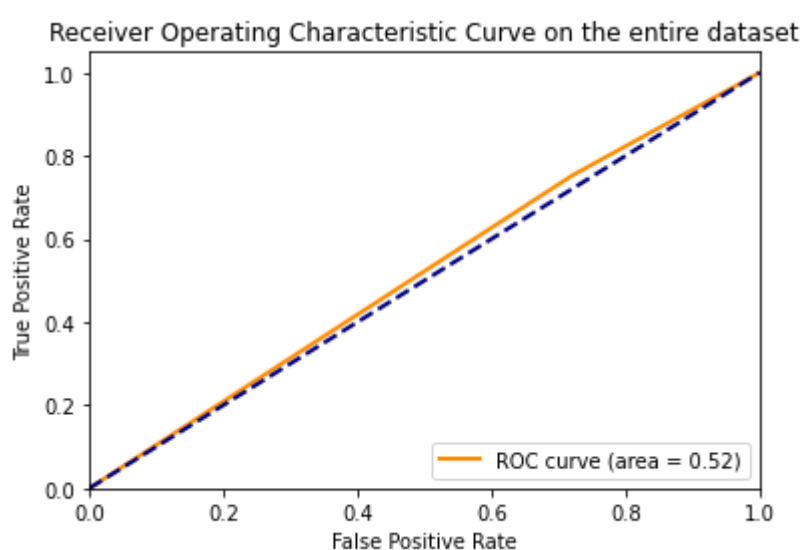
```



```
In [55]: label = node_classif_graph.ndata['label']
plt.hist(label.cpu().numpy())
plt.title("Histogram of Labels in the Training Set")
plt.show()
```



```
In [56]: from sklearn.metrics import auc, roc_curve
fpr, tpr, _ = roc_curve(label.cpu().numpy(), pred.cpu().numpy())
roc_auc = auc(fpr, tpr)
plt.figure()
lw = 2
plt.plot(fpr, tpr, color='darkorange',
lw=lw, label='ROC curve (area = %0.2f)' % roc_auc)
plt.plot([0, 1], [0, 1], color='navy', lw=lw, linestyle='--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Receiver Operating Characteristic Curve on the entire dataset')
plt.legend(loc="lower right")
plt.show()
```



## Graph Classification

We now begin with this approach. Like before, we begin with creating a dataloader. We will fix the number of nodes in each graph (a tunable parameter) and then generate random graphs for each point in the dataset. We will give a label for each such graph.

In this approach, we can take the entire dataset provided as we can load the graphs in batches while training. But for the sake of fair comparison, we will take the same smaller dataset that we used for the Node Classification Approach.

```
In [17]: x_train_small[0].shape
```

```
Out[17]: (4,)
```

```
In [18]: class GraphClassificationDataset(dgl.data.DGLDataset):
        """A Class to process and convert the numpy training data into Graphs so that it can be used in GNNs."""
        def __init__(self):
            super().__init__(name='graph_classification')
            self.num_classes = 2
            self.dim_nfeats = 4

        def process(self):
```

```

self.graphs = []
self.labels = []
num_examples = len(x_train_small)
num_train = int(num_examples * 0.8)
num_val = int(num_examples * 0.1)
train_mask = torch.zeros(num_examples, dtype=torch.bool)
val_mask = torch.zeros(num_examples, dtype=torch.bool)
test_mask = torch.zeros(num_examples, dtype=torch.bool)
train_mask[:num_train] = True
val_mask[num_train:num_train+num_val] = True
test_mask[num_train+num_val:] = True
self.train_mask = train_mask
self.test_mask = test_mask
self.val_mask = val_mask

for id in range(len(x_train_small)):
    g = dgl.from_networkx(nx.generators.fast_gnp_random_graph(20, p=0.6))
    g.ndata['feat'] = torch.from_numpy(np.repeat(x_train_small[id].reshape(1,4),20,0))
    g.ndata['label'] = torch.LongTensor([y_train_small[id]]*20)
    self.graphs.append(g)
    self.labels.append(y_train_small[id])

self.labels = torch.LongTensor(self.labels)

def __getitem__(self, idx):
    return self.graphs[idx], self.labels[idx]

def __len__(self):
    return len(self.graphs)

```

```

In [19]: graph_classif_dataset = GraphClassificationDataset()
g_sample, label_sample = graph_classif_dataset[0]
print(g_sample, label_sample)

```

```

Graph(num_nodes=20, num_edges=234,
      ndata_schemes={'feat': Scheme(shape=(4,), dtype=torch.float32), 'label': Scheme(shape=(), dtype=torch.int64)}
      edata_schemes={}) tensor(1)

```

We will now create a dataloader

```

In [20]: from dgl.data.loading import GraphDataLoader
from torch.utils.data.sampler import SubsetRandomSampler

num_examples = len(graph_classif_dataset)
num_train = int(num_examples * 0.8)
num_val = int(num_examples * 0.1)

train_sampler = SubsetRandomSampler(torch.arange(num_train))
val_sampler = SubsetRandomSampler(torch.arange(num_train, num_train+num_val))
test_sampler = SubsetRandomSampler(torch.arange(num_train+num_val, num_examples))

train_dataloader = GraphDataLoader(graph_classif_dataset, sampler=train_sampler, batch_size=5, drop_last=False)
val_dataloader = GraphDataLoader(graph_classif_dataset, sampler=val_sampler, batch_size=5, drop_last=False)
test_dataloader = GraphDataLoader(graph_classif_dataset, sampler=test_sampler, batch_size=5, drop_last=False)

```

```

In [21]: it = iter(train_dataloader)
batch = next(it)
print(batch)

```

```

[Graph(num_nodes=100, num_edges=1132,
      ndata_schemes={'feat': Scheme(shape=(4,), dtype=torch.float32), 'label': Scheme(shape=(), dtype=torch.int64)}
      edata_schemes={}), tensor([1, 1, 1, 0, 1])]

```

```

In [22]: batched_graph, labels = batch
print('Number of nodes for each graph element in the batch:', batched_graph.batch_num_nodes())
print('Number of edges for each graph element in the batch:', batched_graph.batch_num_edges())

# Recover the original graph elements from the minibatch
graphs = dgl.unbatch(batched_graph)
print('The original graphs in the minibatch:')
print(graphs)

```

```

Number of nodes for each graph element in the batch: tensor([20, 20, 20, 20, 20])
Number of edges for each graph element in the batch: tensor([228, 234, 218, 220, 232])
The original graphs in the minibatch:
[Graph(num_nodes=20, num_edges=228,
      ndata_schemes={'feat': Scheme(shape=(4,), dtype=torch.float32), 'label': Scheme(shape=(), dtype=torch.int64)}
      edata_schemes={}), Graph(num_nodes=20, num_edges=234,
      ndata_schemes={'feat': Scheme(shape=(4,), dtype=torch.float32), 'label': Scheme(shape=(), dtype=torch.int64)}
      edata_schemes={}), Graph(num_nodes=20, num_edges=218,
      ndata_schemes={'feat': Scheme(shape=(4,), dtype=torch.float32), 'label': Scheme(shape=(), dtype=torch.int64)}
      edata_schemes={}), Graph(num_nodes=20, num_edges=220,
      ndata_schemes={'feat': Scheme(shape=(4,), dtype=torch.float32), 'label': Scheme(shape=(), dtype=torch.int64)}
      edata_schemes={}), Graph(num_nodes=20, num_edges=232,
      ndata_schemes={'feat': Scheme(shape=(4,), dtype=torch.float32), 'label': Scheme(shape=(), dtype=torch.int64)}
      edata_schemes={})]

```

## Defining the Model

```

In [23]: from dgl.nn import GraphConv

class GraphClassificationModel(torch.nn.Module):
    """A Model Class having the methods to implement and forward pass a GNN."""
    def __init__(self, in_feats, num_classes):
        super(GraphClassificationModel, self).__init__()
        self.conv1 = GraphConv(in_feats, 16)
        self.conv2 = GraphConv(16, 32)

```

```

self.conv3 = GraphConv(32, num_classes)
# self.conv3 = GraphConv(32, 64)
# self.conv4 = GraphConv(64, num_classes)

```

```

def forward(self, g, in_feat):
    h = self.conv1(g, in_feat)
    h = torch.nn.functional.relu(h)
    h = self.conv2(g, h)
    h = torch.nn.functional.relu(h)
    h = self.conv3(g, h)
    # h = torch.nn.functional.relu(h)
    # h = self.conv4(g, h)
    g.ndata['h'] = h
    return dgl.mean_nodes(g, 'h')

```

```
In [24]: graph_classif_model = GraphClassificationModel(graph_classif_dataset.dim_nfeats, graph_classif_dataset.num_classes)
```

## Defining the Training Loop

```
In [25]: def train(train_loader, val_loader, test_loader, model, num_epochs):
    """The function implementing the main train loop."""
    losses = []
    accs = {'train': [], 'val': [], 'test': []}
    optimizer = torch.optim.Adam(model.parameters(), lr=0.01, betas=(0.9, 0.9999))
    best_val_acc = 0.0
    best_test_acc = 0.0

    for e in range(num_epochs):
        train_acc_batch = []
        val_acc_batch = []
        test_acc_batch = []
        train_loss_batch = []
        for batched_graph, labels in train_loader:
            model.train()
            batched_graph, labels = batched_graph.to('cuda'), labels.to('cuda')
            logits = model(batched_graph, batched_graph.ndata['feat'].float())
            pred = logits.argmax(1)
            loss = torch.nn.functional.cross_entropy(logits, labels)
            train_loss_batch.append(loss)
            train_acc = (pred == labels).float().mean()
            train_acc_batch.append(train_acc)
            with torch.no_grad():
                optimizer.zero_grad()
                loss.backward()
                optimizer.step()
        accs['train'].append(sum(train_acc_batch) / len(train_acc_batch))
        losses.append(sum(train_loss_batch) / len(train_loss_batch))

        model.eval()
        for batched_graph_val, labels_val in val_loader:
            batched_graph_val, labels_val = batched_graph_val.to('cuda'), labels_val.to('cuda')
            logits_val = model(batched_graph_val, batched_graph_val.ndata['feat'].float())
            pred_val = logits_val.argmax(1)
            val_acc = (pred_val == labels_val).float().mean()
            val_acc_batch.append(val_acc)
        accs['val'].append(sum(val_acc_batch) / len(val_acc_batch))

        for batched_graph_test, labels_test in test_loader:
            batched_graph_test, labels_test = batched_graph_test.to('cuda'), labels_test.to('cuda')
            logits_test = model(batched_graph_test, batched_graph_test.ndata['feat'].float())
            pred_test = logits_test.argmax(1)
            test_acc = (pred_test == labels_test).float().mean()
            test_acc_batch.append(test_acc)
        accs['test'].append(sum(test_acc_batch) / len(test_acc_batch))

        if best_val_acc < val_acc:
            best_val_acc = val_acc
            best_test_acc = test_acc

        if e % 5 == 0:
            print('In epoch {}, loss: {:.8f}, val acc: {:.8f} (best {:.8f}), test acc: {:.8f} (best {:.8f})'.format(
                e, loss, val_acc, best_val_acc, test_acc, best_test_acc))

    return losses, accs

```

```
In [26]: graph_classif_model = graph_classif_model.to('cuda')
graph_classif_losses, graph_classif_accs = train(train_dataloader, val_dataloader, test_dataloader, graph_classif_model, 700)
```

```

In epoch 0, loss: 1.32255912, val acc: 0.80000001 (best 0.80000001), test acc: 0.80000001 (best 0.80000001)
In epoch 5, loss: 0.71140397, val acc: 0.80000001 (best 0.80000001), test acc: 0.20000000 (best 0.80000001)
In epoch 10, loss: 0.69860405, val acc: 0.40000001 (best 0.80000001), test acc: 0.60000002 (best 0.80000001)
In epoch 15, loss: 0.65682209, val acc: 0.60000002 (best 0.80000001), test acc: 0.80000001 (best 0.80000001)
In epoch 20, loss: 0.69134969, val acc: 0.60000002 (best 0.80000001), test acc: 0.20000000 (best 0.80000001)
In epoch 25, loss: 0.68840706, val acc: 0.40000001 (best 1.00000000), test acc: 0.40000001 (best 0.60000002)
In epoch 30, loss: 0.64081395, val acc: 0.80000001 (best 1.00000000), test acc: 0.60000002 (best 0.60000002)
In epoch 35, loss: 0.68934125, val acc: 0.40000001 (best 1.00000000), test acc: 0.40000001 (best 0.60000002)
In epoch 40, loss: 0.65559149, val acc: 0.60000002 (best 1.00000000), test acc: 0.40000001 (best 0.60000002)
In epoch 45, loss: 0.80932617, val acc: 0.40000001 (best 1.00000000), test acc: 0.40000001 (best 0.60000002)
In epoch 50, loss: 0.70110434, val acc: 0.60000002 (best 1.00000000), test acc: 0.00000000 (best 0.60000002)
In epoch 55, loss: 0.60884756, val acc: 0.20000000 (best 1.00000000), test acc: 0.40000001 (best 0.60000002)
In epoch 60, loss: 0.78330880, val acc: 0.40000001 (best 1.00000000), test acc: 0.60000002 (best 0.60000002)
In epoch 65, loss: 0.61864960, val acc: 0.20000000 (best 1.00000000), test acc: 1.00000000 (best 0.60000002)
In epoch 70, loss: 0.65097696, val acc: 0.40000001 (best 1.00000000), test acc: 0.40000001 (best 0.60000002)
In epoch 75, loss: 0.68667787, val acc: 0.80000001 (best 1.00000000), test acc: 0.40000001 (best 0.60000002)
In epoch 80, loss: 0.71602374, val acc: 0.60000002 (best 1.00000000), test acc: 1.00000000 (best 0.60000002)
In epoch 85, loss: 0.71640110, val acc: 0.40000001 (best 1.00000000), test acc: 0.60000002 (best 0.60000002)

```





```

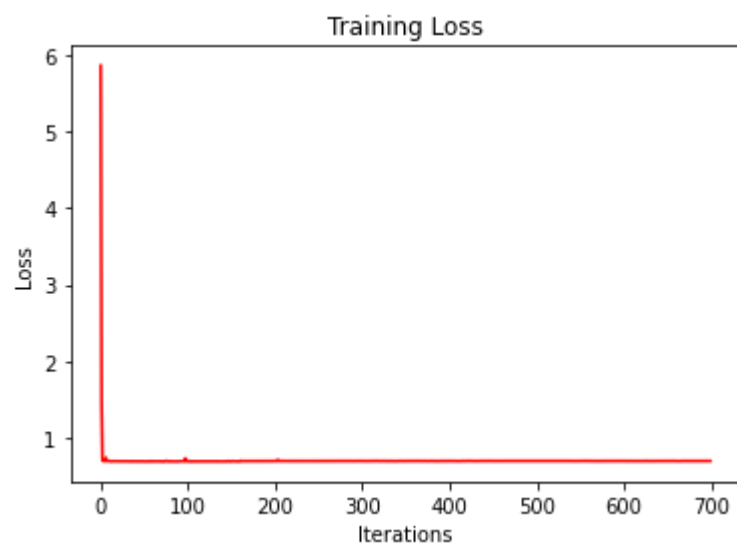
In epoch 605, loss: 0.71804667, val acc: 0.40000001 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)
In epoch 610, loss: 0.65557688, val acc: 0.80000001 (best 1.0000000), test acc: 0.20000000 (best 0.60000002)
In epoch 615, loss: 0.65636319, val acc: 0.60000002 (best 1.0000000), test acc: 0.80000001 (best 0.60000002)
In epoch 620, loss: 0.64237678, val acc: 0.20000000 (best 1.0000000), test acc: 0.20000000 (best 0.60000002)
In epoch 625, loss: 0.69880027, val acc: 0.40000001 (best 1.0000000), test acc: 1.00000000 (best 0.60000002)
In epoch 630, loss: 0.66862571, val acc: 0.40000001 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)
In epoch 635, loss: 0.71697938, val acc: 0.20000000 (best 1.0000000), test acc: 0.20000000 (best 0.60000002)
In epoch 640, loss: 0.69136047, val acc: 0.40000001 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)
In epoch 645, loss: 0.70799369, val acc: 0.60000002 (best 1.0000000), test acc: 0.00000000 (best 0.60000002)
In epoch 650, loss: 0.66819632, val acc: 0.80000001 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)
In epoch 655, loss: 0.62669951, val acc: 0.80000001 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)
In epoch 660, loss: 0.71225512, val acc: 0.60000002 (best 1.0000000), test acc: 0.20000000 (best 0.60000002)
In epoch 665, loss: 0.71507406, val acc: 0.80000001 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)
In epoch 670, loss: 0.68541181, val acc: 0.80000001 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)
In epoch 675, loss: 0.69149733, val acc: 0.60000002 (best 1.0000000), test acc: 0.20000000 (best 0.60000002)
In epoch 680, loss: 0.73088843, val acc: 0.20000000 (best 1.0000000), test acc: 0.40000001 (best 0.60000002)
In epoch 685, loss: 0.70393020, val acc: 0.40000001 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)
In epoch 690, loss: 0.69476098, val acc: 0.20000000 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)
In epoch 695, loss: 0.68425953, val acc: 0.80000001 (best 1.0000000), test acc: 0.60000002 (best 0.60000002)

```

```

In [33]: plt.plot(graph_classif_losses, 'r-')
plt.title('Training Loss')
plt.xlabel('Iterations')
plt.ylabel('Loss')
plt.show()

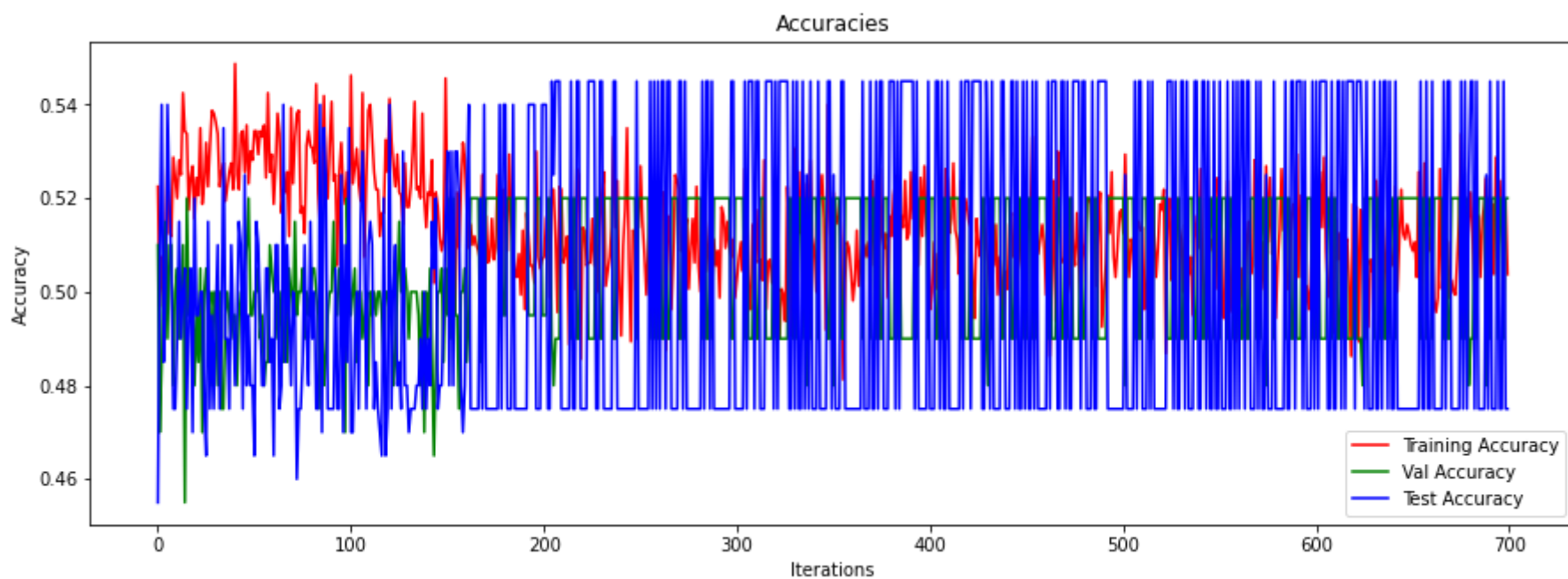
```



```

In [36]: plt.figure(figsize=(15, 5))
plt.plot(graph_classif_accs['train'], 'r-', label='Training Accuracy')
plt.plot(graph_classif_accs['val'], 'g-', label='Val Accuracy')
plt.plot(graph_classif_accs['test'], 'b-', label='Test Accuracy')
plt.title('Accuracies')
plt.xlabel('Iterations')
plt.ylabel('Accuracy')
plt.legend()
plt.show()

```



```

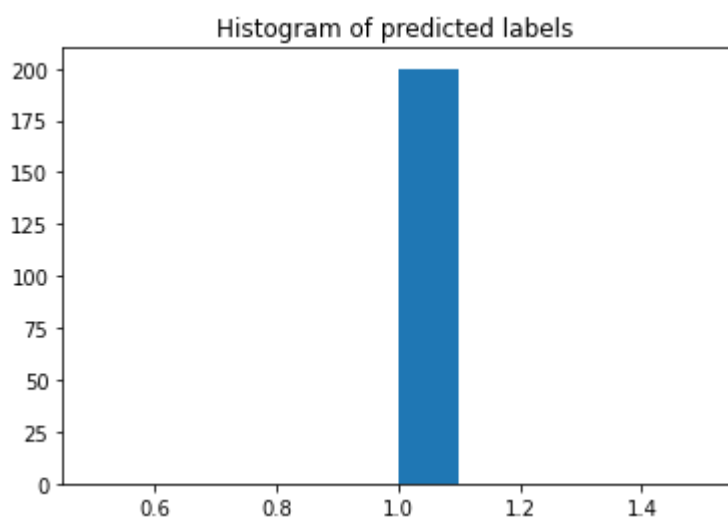
In [29]: all_preds_graph_classif = []
for batched_graph_test, labels_test in test_dataloader:
    batched_graph_test = batched_graph_test.to('cuda')
    labels_test = labels_test.to('cuda')
    logits_test = graph_classif_model(batched_graph_test, batched_graph_test.ndata['feat'].float())
    pred_test = logits_test.argmax(1)
    all_preds_graph_classif = all_preds_graph_classif + [*pred_test.cpu().numpy()]

```

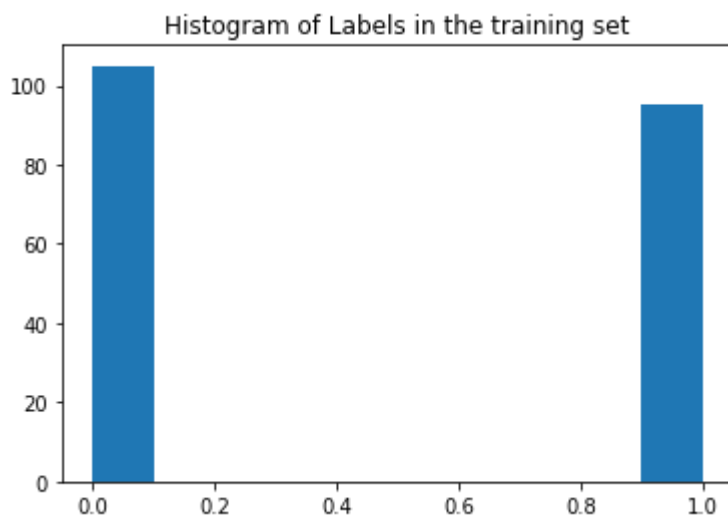
```

In [35]: plt.hist(all_preds_graph_classif)
plt.title("Histogram of predicted labels ")
plt.show()

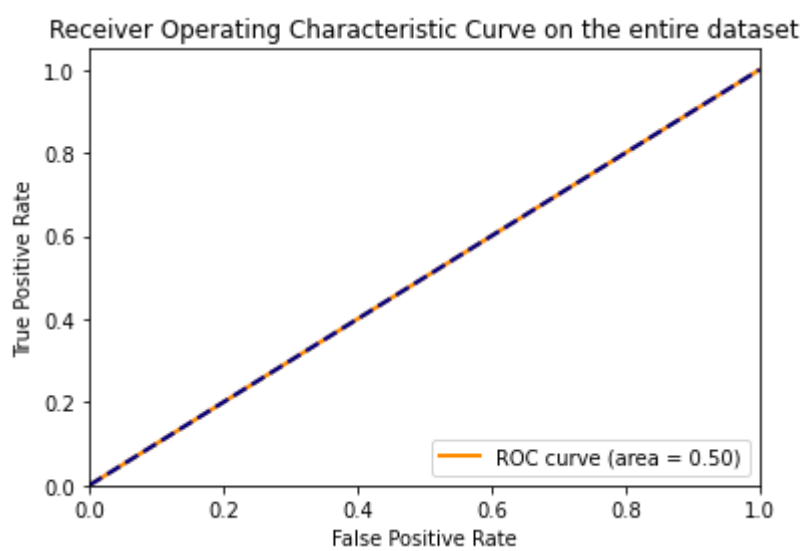
```



```
In [34]: label = graph_classif_dataset.labels[graph_classif_dataset.test_mask]
plt.hist(label.cpu().numpy())
plt.title("Histogram of Labels in the training set")
plt.show()
```



```
In [32]: from sklearn.metrics import auc, roc_curve
fpr, tpr, _ = roc_curve(label.cpu().numpy(), all_preds_graph_classif)
roc_auc = auc(fpr, tpr)
plt.figure()
lw = 2
plt.plot(fpr, tpr, color='darkorange',
lw=lw, label='ROC curve (area = %0.2f)' % roc_auc)
plt.plot([0, 1], [0, 1], color='navy', lw=lw, linestyle='--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Receiver Operating Characteristic Curve on the entire dataset')
plt.legend(loc="lower right")
plt.show()
```



## Comparison

As we can see above, theoretically both the architectures will work. The loss vs iteration curve and the ROC suggest that the graph classification approach has failed to learn and it is predicting the same output for all inputs. The main reason for this result is that:

1. I used very less training data
2. The training data has very less number of features.
3. The limited computational resource. The colab notebook's RAM was getting used up even before training for 1000 epochs. As we can see in the Node Classification approach, the GNN required atleast a 1000 epochs to stabilize.

Because of the above reasons, I think the Graph Classification approach gave inferior performance.

## Possible Improvements

- Neural Message Passing Models have shown good results on other particle jet classification tasks like [here](#).
- Studying and applying better ways of encoding the train data in the form of graphs