IMPORTS

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import KFold
from sklearn.inspection import DecisionBoundaryDisplay
import torch
import torch.nn as nn
import torch.optim as optim
from torch_geometric.datasets import TUDataset
from torch_geometric.utils import to_networkx
import networkx as nx
from torch_geometric.loader import DataLoader
from torch_geometric.nn import GINConv, global_mean_pool
from torch.utils.data import Subset
from scipy.stats import binom_test # library for p-value
```

```
c:\Users\matsa\AppData\Local\Programs\Python\Python310\lib\site-packages\tqdm\auto.p
y:21: TqdmWarning: IProgress not found. Please update jupyter and ipywidgets. See ht
tps://ipywidgets.readthedocs.io/en/stable/user_install.html
  from .autonotebook import tqdm as notebook_tqdm
```

LOAD THE DATA

In [2]:
```
# https://www.edureka.co/community/72971/how-to-load-numpy-array-in-jupyter-noteboo

features = np.load("data/data/features.npy")
labels = np.load("data/data/labels.npy")

print(features.shape)
print(labels.shape)

print(set(labels))
```

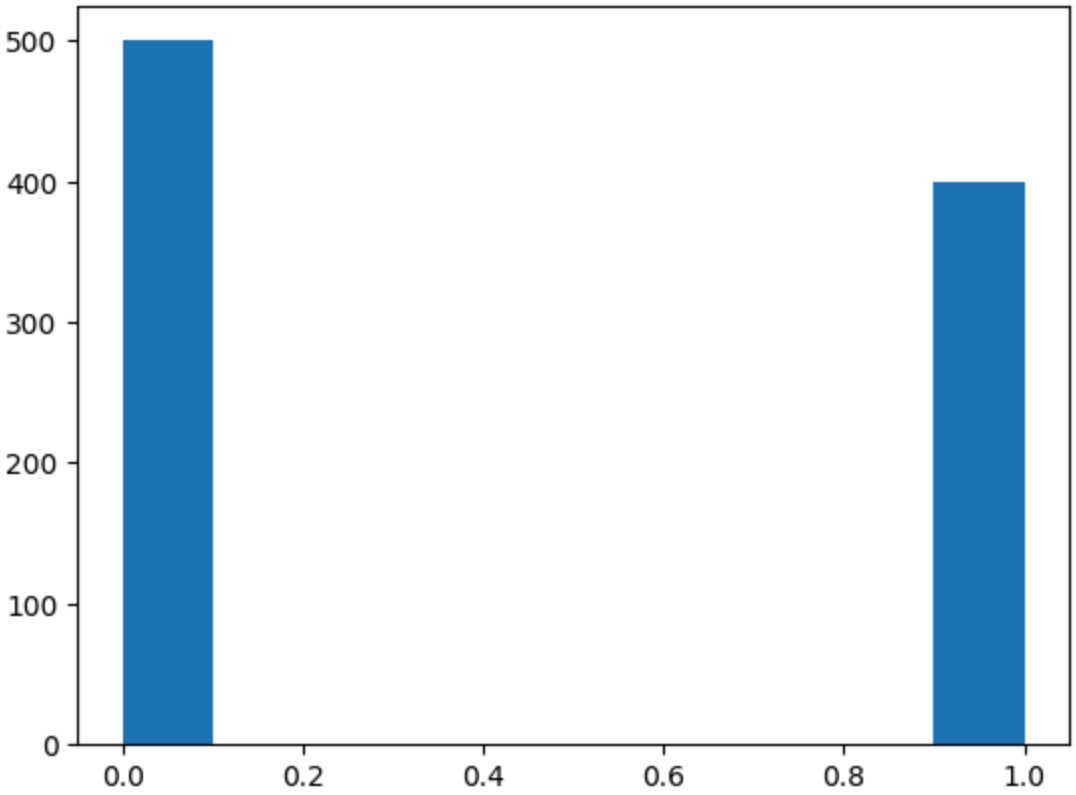
```
(900, 2)
(900,)
{0.0, 1.0}
```

PART 1

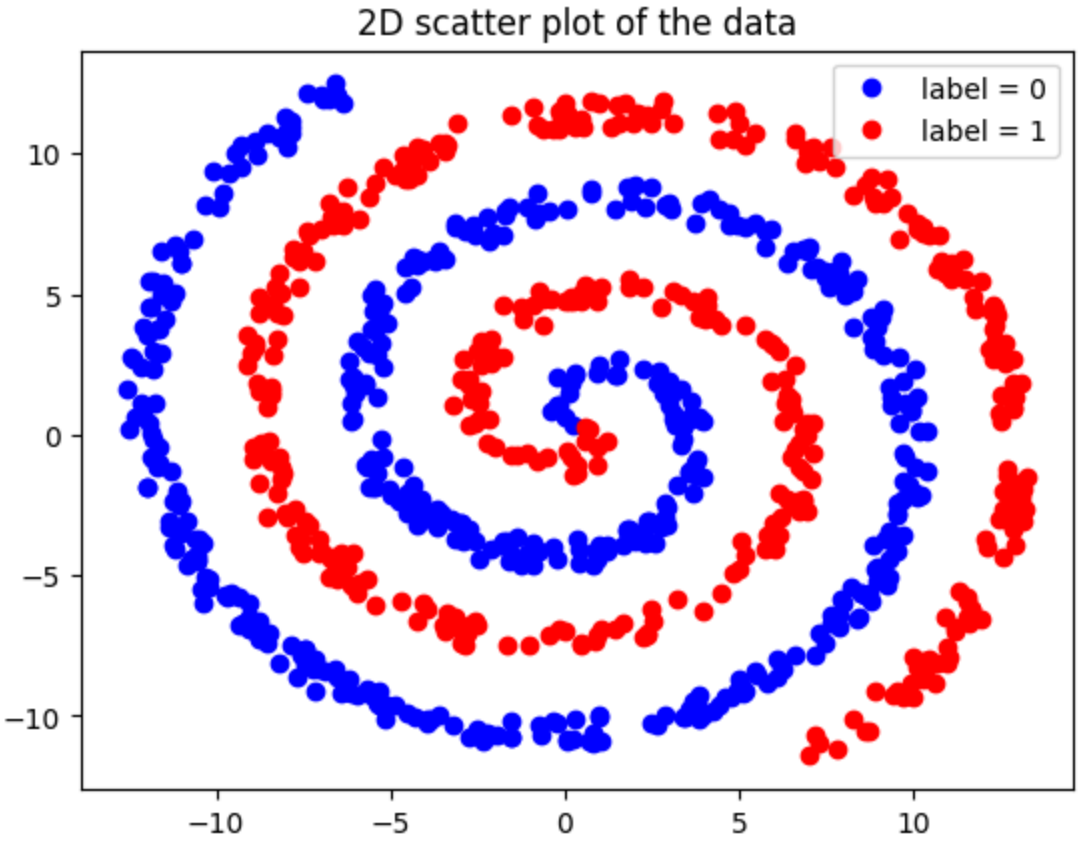
In [3]:
```
"""
1.
a) 2 features, 900 samples
b) binary classification since we only have 2 label values, 0 and 1
c) we can infer that we have 500 0 samples and 400 1 samples
"""
```

```
# c:
plt.hist(labels)
```

Out[3]:
```
(array([500.,   0.,   0.,   0.,   0.,   0.,   0.,   0.,   0., 400.]),
 array([0. , 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1. ]),
 <BarContainer object of 10 artists>)
```



In [4]:
```
# Go through all the points, check ther label and plot them with the appropriate co
label_1 = "label = 1"
label_0 = "label = 0"
for i in range(features.shape[0]):

    if labels[i] == 0:
        if label_0:
            plt.plot(features[i][0], features[i][1], "bo", label=f"{label_0}")
            label_0 = None
        else:
            plt.plot(features[i][0], features[i][1], "bo")
    else:
        if label_1:
            plt.plot(features[i][0], features[i][1], "ro", label=f"{label_1}")
            label_1 = None
        else:
            plt.plot(features[i][0], features[i][1], "ro")

plt.title("2D scatter plot of the data")
plt.legend()
plt.show()
```



In [5]:
```
"""
2.
a)...
b) the data does not look linearly speperable at first glance, since it has a spira
c) no since the data is not linearly seperable
d) the bayes optimal lassifier would follow the spiral pattern that we can observe
   It would be able to achieve an empirical risk of 0, since the data can
   be perfectly seperated due to the lack of noise (the only somewhat problematic p
   but since I am not completely sure I am making a bit of an assumption that we ha
"""
```

Out[5]:
```
'\n2.\na)...\nb) the data does not look linearly speperable at first glance, since
it has a spiral-like shape\nc) no since the data is not linearly seperable\nd) the
bayes optimal lassifier would follow the spiral pattern that we can observe in the
image.\n   It would be able to achieve an empirical risk of 0, since the data can
\n   be perfectly seperated due to the lack of noise (the only somewhat problemati
c part might be at the very middle\n   but since I am not completely sure I am mak
ing a bit of an assumption that we have 0 noise overall)\n'
```

In [5]:
```
# Split data into train and test sets (80-20 split)
X_train, X_test, y_train, y_test = train_test_split(features, labels, test_size=0.2
print(X_train.shape)
print(X_test.shape)
```

```
(720, 2)
(180, 2)
```

In [ ]:
```
"""
3.
a) The split is neccesary, because you want to be abel to train on a part of the da
```

```
   a good model, you can verify it by using your test data, since if the model is r
   otherwise it might have overfitted.
b) TODO Well LDA is out of the question since it makes the assumption that we have
   as for the other 2, I would choose Logistic Regression, mainly because it is sim
   it works with probabilities, which might be usefull in this case since a poor re
   3 classifiers are linear classifiers. But I can't find any other reason to not u
c) 0.6333333333333333, well the classifier is learning but still isn't performing w
d) ...
"""
```

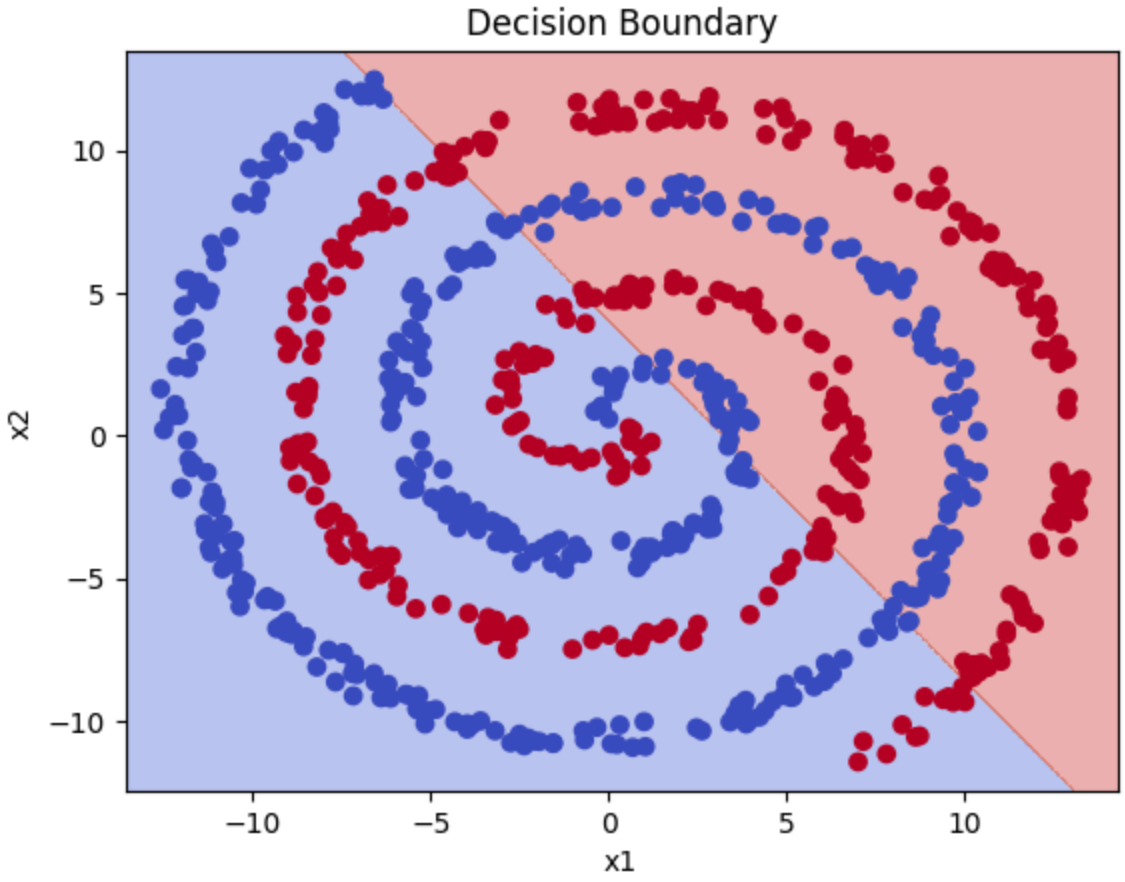
Out[ ]:
```
'\n3.\na)...\nb) Well LDA is out of the question since it makes the assumption tha
t we have Gaussian distributions\n   as for the other 2, I would choose Logistic R
egression, mainly because it is simplier and because\n   it works with probabiliti
es, which might be usefull in this case since a poor result is a given, considerin
g all\n   3 classifiers are linear classifiers.\n'
```

In [7]:
```python
def calculate_accuracy(predictions, y_test):
    correct = 0
    for i in range(len(predictions)):
        if predictions[i] == y_test[i]:
            correct += 1
    return correct/len(predictions)
```

In [8]:
```python
# Create a logistic classifier, train it and check the accuracy
#log_reg_classifier = LinearDiscriminantAnalysis()
#log_reg_classifier = SVC(kernel='linear', C=1.0)
log_reg_classifier = LogisticRegression()
log_reg_classifier.fit(X_train, y_train)
predictions = log_reg_classifier.predict(X_test)
print(calculate_accuracy(predictions, y_test))
```

```
0.6333333333333333
```

In [9]:
```python
# https://scikit-learn.org/stable/modules/generated/sklearn.inspection.DecisionBoun
# Decision boundary display
decision_boundary = DecisionBoundaryDisplay.from_estimator(
    log_reg_classifier,
    X_train,
    response_method="predict",
    grid_resolution=1000,
    alpha=0.4,
    cmap="coolwarm",
    xlabel="x1",
    ylabel="x2",
)

decision_boundary.ax_.scatter(X_train[:, 0], X_train[:, 1], c=y_train, cmap="coolwa
plt.title("Decision Boundary")
plt.show()
```



In [ ]:
```
"""
4.
a) 0.6, almsost the same as the classifier
b) ...
c) the plot suggests that we are pretty much guessing. We are doing slightly better
   this accuracy could be reached.
d) well I repeated it 1000 times (as suggested in the pdf). I believe a 1000 is eno
   distributed. If we used less then there exists the possibility that outlier valu
   (when I say less, I mean considerably less, like 100 or 50. Obviously 900 would
e) 0.65, so they are not the same which is to be expected. Afterall the chance accu
   of that cell, whereas this accuracy will always statys the same, since the numbe
f) So from what we can observe guessing, picking the label that belongs to the majo
   because the classifier simply cant do that good of a job, because the data is no
   depends on the task and as I stated there is some accuracy benefit but it's mini
"""
```

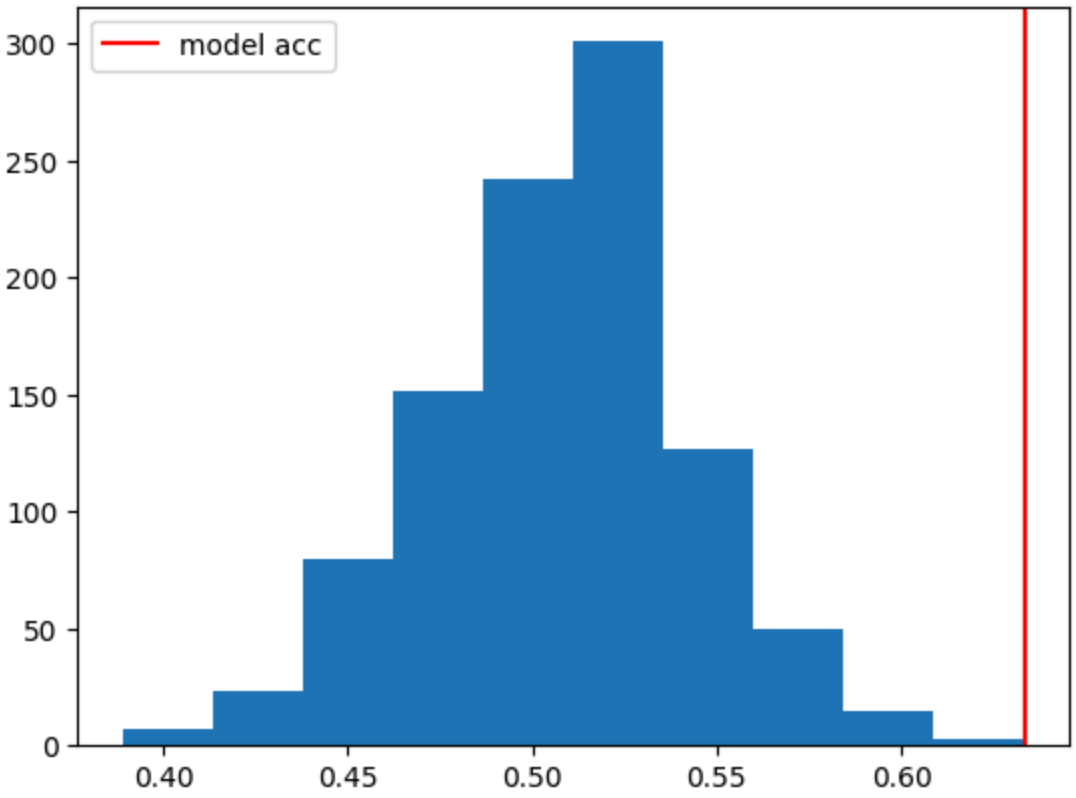
In [38]:
```
# https://www.w3schools.com/python/numpy/numpy_random_permutation.asp
y_test_random = np.random.permutation(y_test)
print(calculate_accuracy(y_test_random, y_test))
```

```
0.6
```

In [17]:
```
# Get 1000 accuracy scores and plot them into a histogram
accuracies = []
for i in range(1000):
    y_test_random = np.random.permutation(y_test)
    accuracies.append(calculate_accuracy(y_test_random, y_test))
```

```
model_accuracy = 0.6333333333333333

plt.hist(accuracies)
plt.axvline(model_accuracy, color="red", label="model acc") # https://www.geeksforg
plt.legend()
```

Out[17]: <matplotlib.legend.Legend at 0x23bce1b9c90>



In [41]:
```
# Count 0's, if it's greater than the half of the total in the test then 0, else 1
count = 0
choise = np.zeros_like(y_test)
for value in y_test:
    if value == 0:
        count += 1
if count <= len(y_test)/2:
    choise = np.ones_like(y_test)
print(calculate_accuracy(choise, y_test))
```

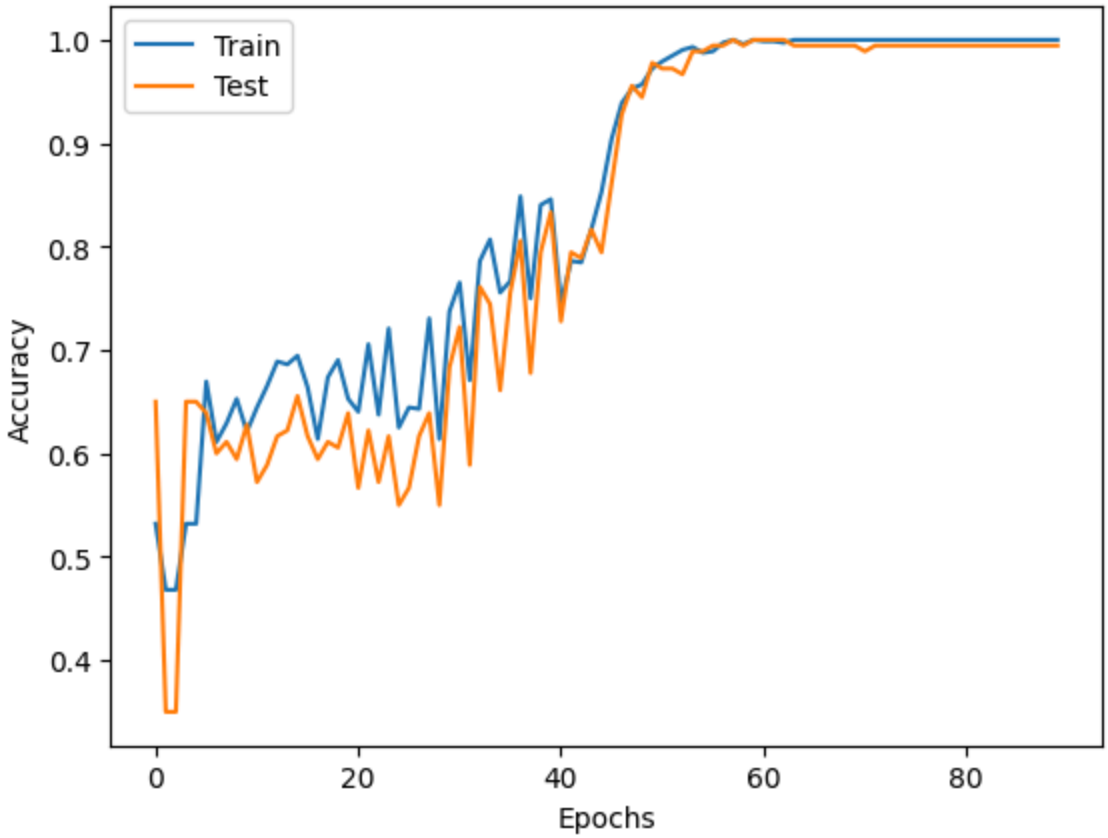
```
0.65
```

In [ ]:
```
"""
5.
a) ...
b) The learning curves suggest robustness and good generalization, due to both curv
c) Well my idea was to first find a good architecture, where with enough epochs we
   I did this by adding one layer at the time, while also increasing the number of
   you won't be able to get a better accuracy without adding another layer). After
   I used 10Fold cross validation to fine tune the learning rate (There are countle
   which show that just by tuning the learning rate, you should achieve the best re
d) ...
"""
```

In [ ]:
```
# We need to convert to pytorch tensors
X_train_nn = torch.FloatTensor(X_train)
X_test_nn = torch.FloatTensor(X_test)
y_train_nn = torch.LongTensor(y_train)
y_test_nn = torch.LongTensor(y_test)

# NN architecture
class Model(nn.Module):
    def __init__(self):
        super(Model, self).__init__()
        self.l1 = nn.Linear(2, 64)
        self.l2 = nn.Linear(64, 128)
        self.l3 = nn.Linear(128, 256)
        self.l4 = nn.Linear(256, 512)
        self.l5 = nn.Linear(512, 1024)
        self.l6 = nn.Linear(1024, 2)
        self.relu = nn.ReLU()

    def forward(self, x):
        x = self.relu(self.l1(x))
        x = self.relu(self.l2(x))
        x = self.relu(self.l3(x))
        x = self.relu(self.l4(x))
        x = self.relu(self.l5(x))
        x = self.l6(x)
        return x

# Initialize some stuff
model = Model()
criterion = nn.CrossEntropyLoss()
optimizer = optim.Adam(model.parameters(), lr=0.01)

# Training loop
train_acc, test_acc = [], []
for epoch in range(90):
    model.train()
    optimizer.zero_grad()
    outputs = model(X_train_nn)
    loss = criterion(outputs, y_train_nn)
    loss.backward()
    optimizer.step()

    with torch.no_grad():
        model.eval()
        # Train
        train_pred = model(X_train_nn).argmax(1)
        train_acc.append((train_pred == y_train_nn).float().mean())
        # Test
        test_pred = model(X_test_nn).argmax(1)
        test_acc.append((test_pred == y_test_nn).float().mean())
```

```
c:\Users\matsa\AppData\Local\Programs\Python\Python310\lib\site-packages\tqdm\auto.p
y:21: TqdmWarning: IProgress not found. Please update jupyter and ipywidgets. See ht
tps://ipywidgets.readthedocs.io/en/stable/user_install.html
  from .autonotebook import tqdm as notebook_tqdm
```

In [ ]:
```
plt.plot(train_acc, label="Train")
plt.plot(test_acc, label="Test")
plt.xlabel("Epochs")
plt.ylabel("Accuracy")
plt.legend()
plt.show()
```

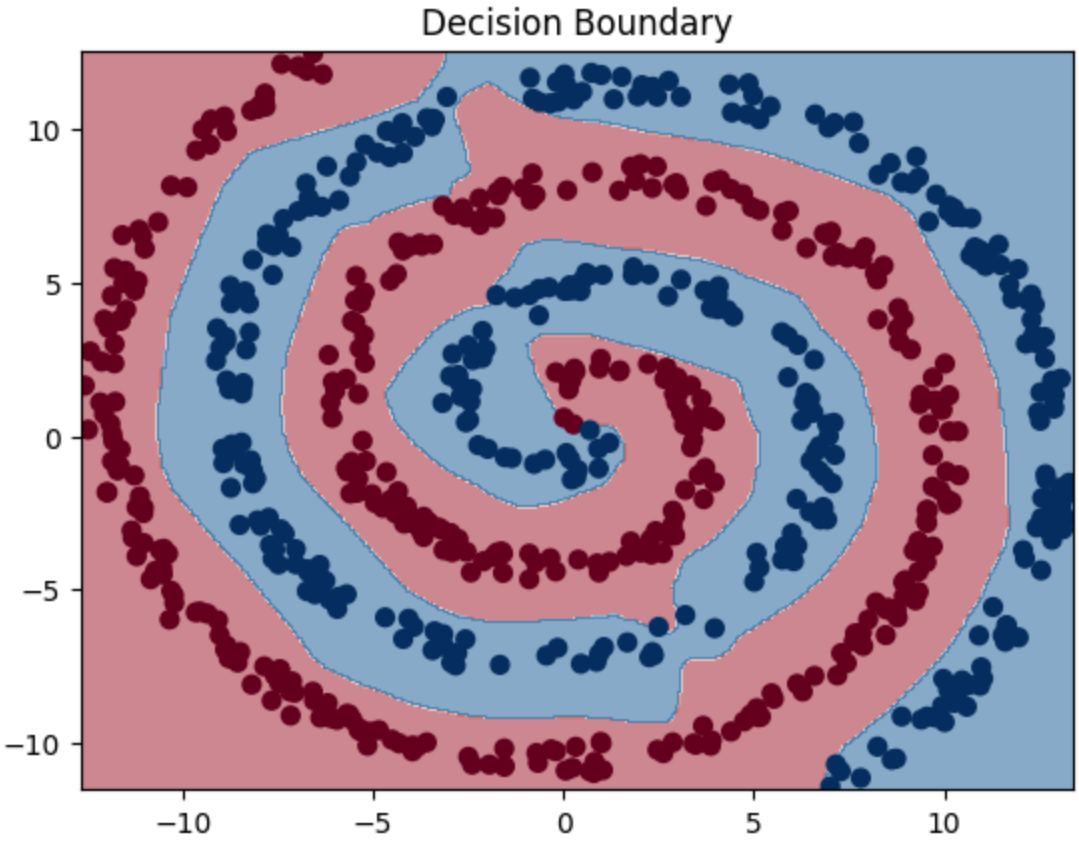


In [ ]:
```
# Learning rates
learning_rates = [0.0001, 0.001, 0.005, 0.01, 0.05]
k = 10
kf = KFold(n_splits=k, shuffle=True)

results = {}

for lr in learning_rates:
    print(f"Testing learning rate: {lr}")
    fold_accuracies = []

    for train_index, val_index in kf.split(X_train_nn):
        # Split data
        X_train_cv, X_val_cv = X_train_nn[train_index], X_train_nn[val_index]
        y_train_cv, y_val_cv = y_train_nn[train_index], y_train_nn[val_index]

        model1 = Model()
        optimizer = optim.Adam(model1.parameters(), lr=lr)

        for epoch in range(90):
            model1.train()
            optimizer.zero_grad()
```

```
            outputs = model1(X_train_nn)
            loss = criterion(outputs, y_train_nn)
            loss.backward()
            optimizer.step()

            with torch.no_grad():
                model1.eval()
                # Validation accuracy
                val_pred = model1(X_val_cv).argmax(1)
                fold_accuracies.append((val_pred == y_val_cv).float().mean())

    avg_acc = np.mean(fold_accuracies)
    results[lr] = avg_acc
    print(f"Average validation accuracy: {avg_acc}")

# Best learning rate
best_lr = max(results, key=results.get)
print("\nBest learning rate:", best_lr)
```

In [ ]:

```
# https://psrivasin.medium.com/plotting-decision-boundaries-using-numpy-and-matplot

# Create mesh grid
# Range for visualization
x_min, x_max = X_train[:, 0].min() - 0.1, X_train[:, 0].max() + 0.1
y_min, y_max = X_train[:, 1].min() - 0.1, X_train[:, 1].max() + 0.1

# Create "points" (not yet points) that will use to draw the decision boundary
xx, yy = np.meshgrid(np.linspace(x_min, x_max, 400), np.linspace(y_min, y_max, 400)

# Create the actuall points
x_in = np.c_[xx.ravel(), yy.ravel()]
x_in_tensor = torch.FloatTensor(x_in)

# Predict
model.eval()
with torch.no_grad():
    y_pred = model(x_in_tensor).argmax(1).reshape(xx.shape)

# Plot
plt.contourf(xx, yy, y_pred, cmap=plt.cm.RdBu, alpha=0.5)
plt.scatter(X_train[:, 0], X_train[:, 1], c=y_train, s=40, cmap=plt.cm.RdBu)
plt.title("Decision Boundary")
plt.show()
```



PART 2

In [ ]:
```
"""
1.
a) 188, 7, 2
b) Per the ai model (prompt: Can you explain what the MUTAG dataset represents? Spe
   and google (https://paperswithcode.com/dataset/mutag)
   Sample: Chemical compound modeled as a graph
   Nodes: Atoms
   Edges: Bonds between the atoms
   Features: Features are one-hot encodings, so in essense the feature vector tells
   Labels: 1 if chemical compound is mutagenic, 0 if not

c) The first sample has 17 nodes and 38 edges (prompt: how to get the nodes and edg
d) ...

"""
```

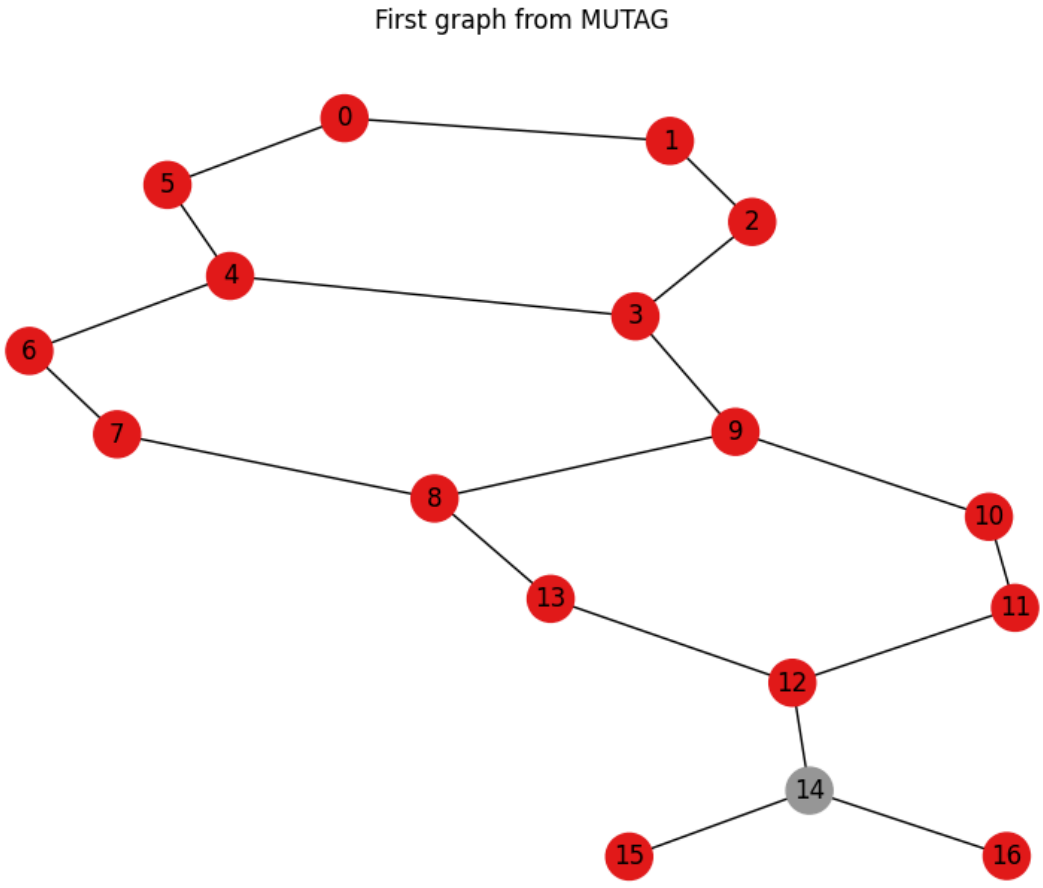
In [19]:
```
# (https://medium.com/@james-coffey/gcn-with-neo4j-and-pytorch-using-mutag-dataset-
dataset = TUDataset(root="data", name="MUTAG")
samples = len(dataset)
features = dataset.num_node_features
classes = dataset.num_classes
print(f"Samples: {samples}, Features: {features}, Classes: {classes}")
```

```
Samples: 188, Features: 7, Classes: 2
```

In [93]:
```
# Nodes and edges in first graph
sample = dataset[0]
nodes = sample.x
edges = sample.edge_index
print(f"First sample has {nodes.shape[0]} nodes and {edges.shape[1]} edges")
```

```
First sample has 17 nodes and 38 edges
```

In [ ]:
```
# Plot graph of the first sample with nodes colored by second feature (index 1)
graph = to_networkx(sample, to_undirected=True)
node_colors = sample.x[:, 1].tolist()

plt.figure(figsize=(8, 6))
nx.draw(graph, with_labels=True, node_color=node_colors, cmap=plt.cm.Set1, node_siz
plt.title("First graph from MUTAG")
plt.show()
```



In [ ]:
```
"""
We shall use the same linear modle as before, so Linear Regression.
2.
a) After asking the AI "How can I prep the data so that I can train without using g
   add them together and then devide the whole vector by the number of nodes in tha
b) ..., fairly poor results, we are learning just not all that much, peaking at aro
c) Choosing most frequent label = 0.6648936170212766, Guessing = 0.4210526315789473
   that even with the NN the accuracy remains low (plateauing at around 60%)
```

```
"""
```

In [7]:
```
# Prep the data
features = []
labels = []

# Loop through each graph in the dataset
for data in dataset:
    # data.x is a tensor that for each node in the graph, will have it's feature ve
    graph_features = data.x.mean(dim=0).numpy()

    features.append(graph_features)

    labels.append(data.y.item())  # Convert to a single number rather than a tensor


# Split data into train and test sets (80-20 split)
train_idx, test_idx = train_test_split(range(len(dataset)), test_size=0.2)

# Split the training set further so that we can later use this for the validation p
train_idx_val, val_idx = train_test_split(range(len(train_idx)), test_size=0.2)

# Get the actual training splits
X_train = np.array([features[i] for i in train_idx])
X_test = np.array([features[i] for i in test_idx])
y_train = np.array([labels[i] for i in train_idx])
y_test = np.array([labels[i] for i in test_idx])

#X_train, X_test, y_train, y_test =
#X_train, X_test, y_train, y_test = train_test_split(features, labels, test_size=0.
#print(len(X_train))
#print(len(X_test))
```

In [8]:
```
# GREAT DATA IMBALANCE NEEDS TO BE TAKEN INTO ACCOUNT!
# What if we choose the most frequent class?
count = 0
for label in labels:
    if label == 1:
        count += 1
print(count/samples)
```

```
0.6648936170212766
```

In [15]:
```
# Guessing
y_test_shuffled = np.random.permutation(y_test)
print(calculate_accuracy(y_test_shuffled, y_test))
```

```
0.42105263157894735
```

In [14]:
```
# Linear model
log_reg_classifier = LogisticRegression()
log_reg_classifier.fit(X_train, y_train)
predictions = log_reg_classifier.predict(X_test)
print(calculate_accuracy(predictions, y_test))
```

```
# The results are better than before. Still not great but better!
```

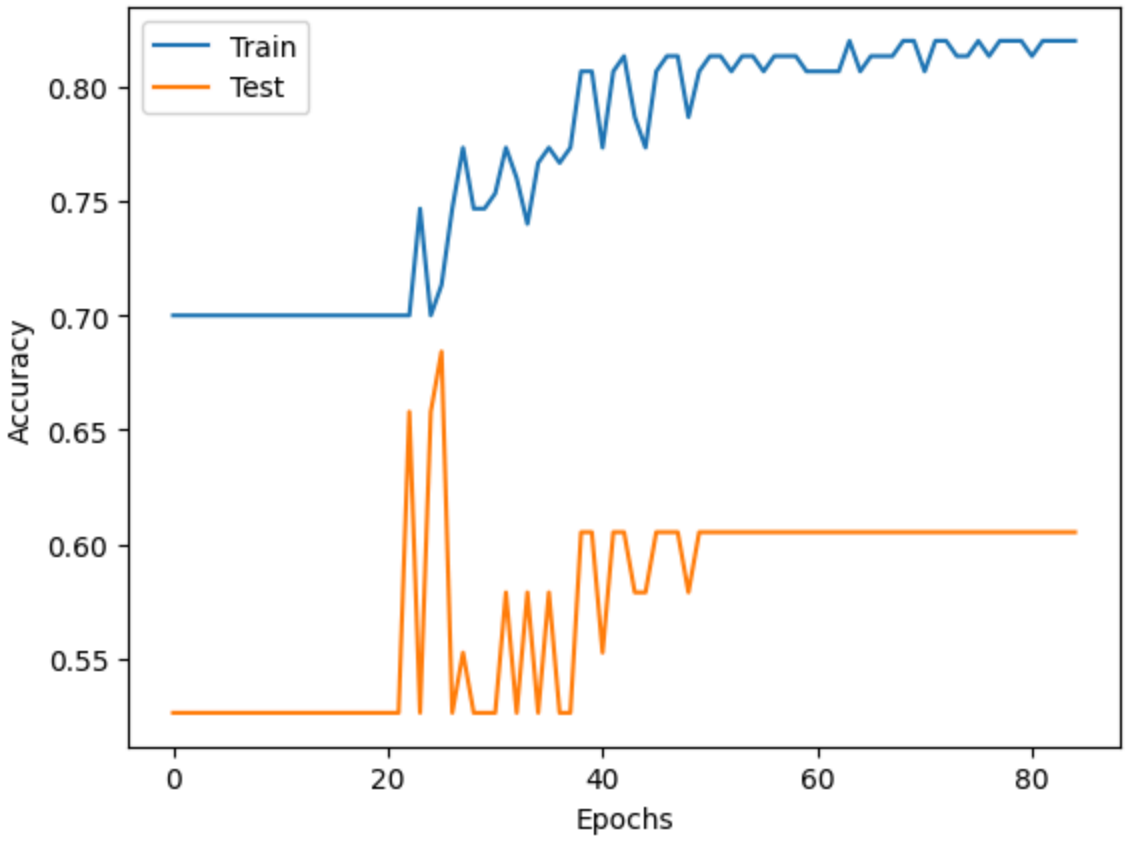
```
0.5263157894736842
```

In [ ]:

```
# NN
import torch
import torch.nn as nn
import torch.optim as optim
import matplotlib.pyplot as plt

# We need to convert to pytorch tensors
X_train_nn = torch.FloatTensor(X_train)
X_test_nn = torch.FloatTensor(X_test)
y_train_nn = torch.LongTensor(y_train)
y_test_nn = torch.LongTensor(y_test)

# NN architecture
class Model(nn.Module):
    def __init__(self):
        super(Model, self).__init__()
        self.l1 = nn.Linear(7, 64)
        self.l2 = nn.Linear(64, 128)
        self.l3 = nn.Linear(128, 256)
        self.l4 = nn.Linear(256, 512)
        self.l5 = nn.Linear(512, 512)
        self.l6 = nn.Linear(512, 2)
        self.relu = nn.ReLU()

    def forward(self, x):
        x = self.relu(self.l1(x))
        x = self.relu(self.l2(x))
        x = self.relu(self.l3(x))
        x = self.relu(self.l4(x))
        x = self.relu(self.l5(x))
        x = self.l6(x)
        return x

# Initialize some stuff
model = Model()
criterion = nn.CrossEntropyLoss()
optimizer = optim.Adam(model.parameters(), lr=0.01)

# Training loop
train_acc, test_acc = [], []
for epoch in range(85):
    model.train()
    optimizer.zero_grad()
    outputs = model(X_train_nn)
    loss = criterion(outputs, y_train_nn)
    loss.backward()
    optimizer.step()

    with torch.no_grad():
        model.eval()
        # Train
```

```
        train_pred = model(X_train_nn).argmax(1)
        train_acc.append((train_pred == y_train_nn).float().mean())
        # Test
        test_pred = model(X_test_nn).argmax(1)
        test_acc.append((test_pred == y_test_nn).float().mean())
```

In [ ]:
```
plt.plot(train_acc, label="Train")
plt.plot(test_acc, label="Test")
plt.xlabel("Epochs")
plt.ylabel("Accuracy")
plt.legend()
plt.show()
```



In [27]:
```
print(test_acc[-1])
```

```
tensor(0.6053)
```

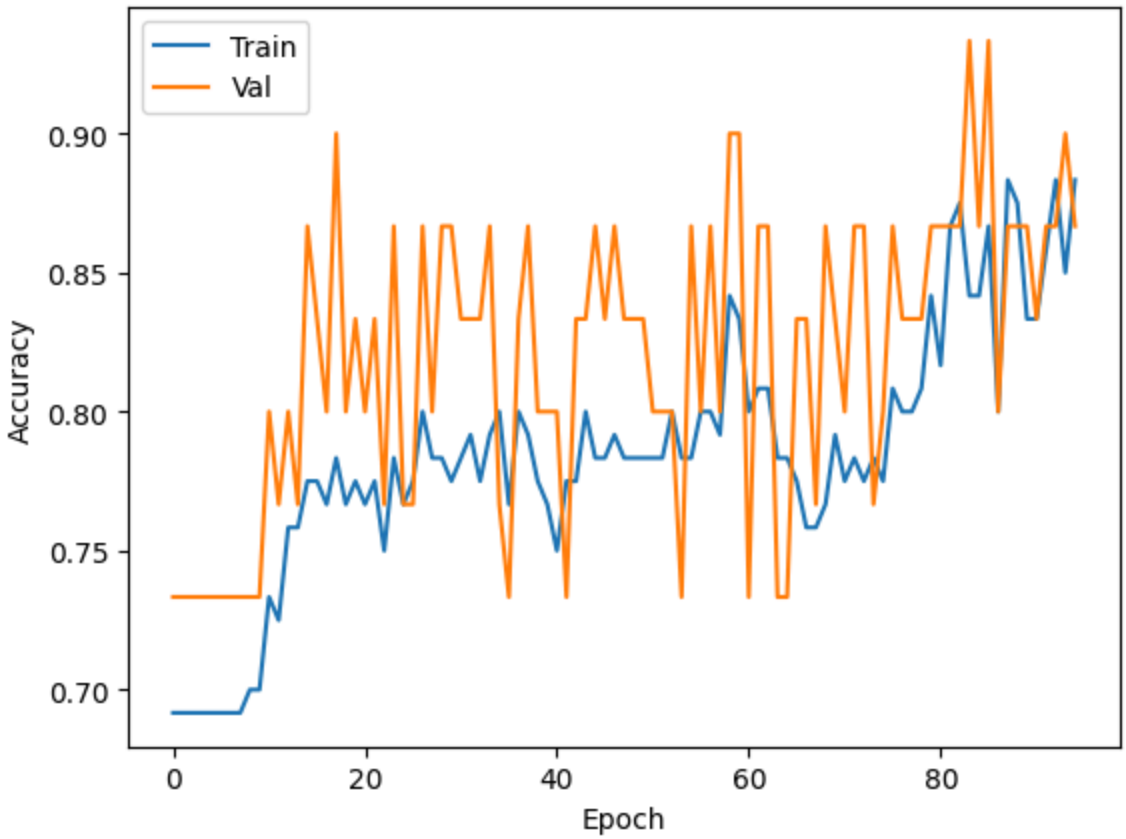
In [ ]:
```
"""
3.
a) ...
b) AI prompt : "How does a GNN take into account graph info and what does the layer
   Per the ai and a bit of crossreferencing on google I understood that the high le
   is that each node doesn't just use it's own information but through message pass
   into account information of its surrounding/ neighboring nodes before updating i
   how far the neighbor you receive onfo from can be. Layer 1 -> immediate neighbor
   neighbor of neighor, etc.
c) ..., in essense I just created a validation dataset from the training dataset an
   looked a bit on batch sizes but didn't get much of a change (even though I belie
d) Accuracy = 0.79, P-value = 4.051328899727381e-06 (not exactly 0 probably but pre
```

```
   as mine should reach around 85-90% accuracy and considering the fact that that's
"""
```

In [ ]:

```
# THIS PART IS USED FOR FINDING THE BEST HYPERPARAMETERS

train_dataset = Subset(dataset, train_idx)

# Create subsets for train and validation
train_subdataset = Subset(train_dataset, train_idx_val)
val_subdataset = Subset(train_dataset, val_idx)

# DataLoaders for these subsets
train_loader = DataLoader(train_subdataset, batch_size=32, shuffle=True)
val_loader = DataLoader(val_subdataset, batch_size=32, shuffle=False)

# Model with GINConv layers
class Model2(nn.Module):
    def __init__(self):
        super(Model2, self).__init__()

        part1 = nn.Sequential(
            nn.Linear(7, 64),
            nn.ReLU(),
            nn.Linear(64, 128)
        )
        self.l1 = GINConv(part1)

        part2 = nn.Sequential(
            nn.Linear(128, 256),
            nn.ReLU(),
            nn.Linear(256, 256)
        )
        self.l2 = GINConv(part2)

        part3 = nn.Sequential(
            nn.Linear(256, 512),
            nn.ReLU(),
            nn.Linear(512, 512)
        )
        self.l3 = GINConv(part3)

        self.l4 = nn.Linear(512, 2)
        self.relu = nn.ReLU()

    def forward(self, x, edge_index, batch):
        x = self.relu(self.l1(x, edge_index))
        x = self.relu(self.l2(x, edge_index))
        x = self.relu(self.l3(x, edge_index))
        x = global_mean_pool(x, batch)
        x = self.l4(x)
        return x

model = Model2()
criterion = nn.CrossEntropyLoss()
optimizer = optim.Adam(model.parameters(), lr=0.01)
```

```python
train_acc, val_acc = [], []
for epoch in range(95):
    model.train()
    for batch in train_loader:
        optimizer.zero_grad()
        outputs = model(batch.x, batch.edge_index, batch.batch)
        loss = criterion(outputs, batch.y)
        loss.backward()
        optimizer.step()

    with torch.no_grad():
        model.eval()
        # Train
        correct = 0
        total = 0
        for batch in train_loader:
            out = model(batch.x, batch.edge_index, batch.batch)
            pred = out.argmax(dim=1)
            correct += (pred == batch.y).sum().item()
            total += batch.y.size(0)
        train_acc.append(correct / total)

        # Val
        correct = 0
        total = 0
        for batch in val_loader:
            out = model(batch.x, batch.edge_index, batch.batch)
            pred = out.argmax(dim=1)
            correct += (pred == batch.y).sum().item()
            total += batch.y.size(0)
        val_acc.append(correct / total)

# Plot results
plt.plot(train_acc, label="Train")
plt.plot(val_acc, label="Val")
plt.xlabel("Epoch")
plt.ylabel("Accuracy")
plt.legend()
plt.show()
```



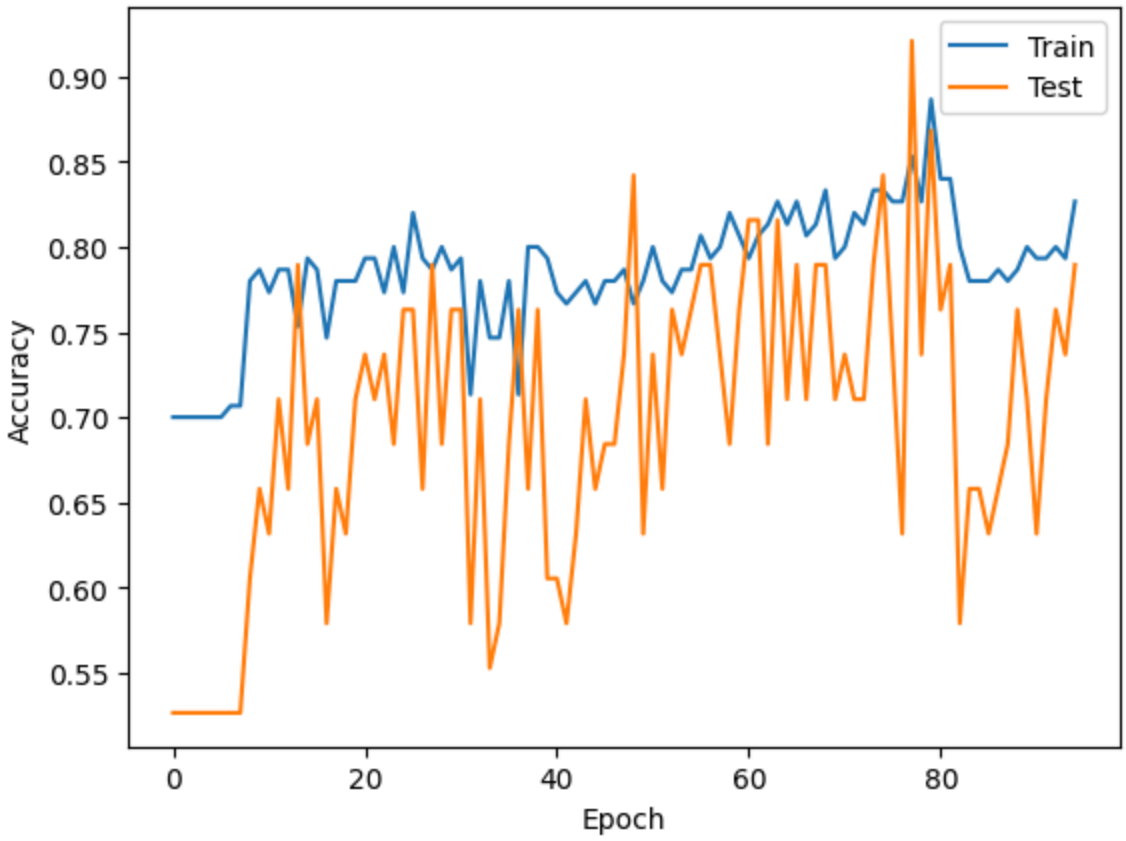
In [48]:
```
print(train_acc[-1])
print(val_acc[-1])
```

```
0.8833333333333333
0.8666666666666667
```

In [ ]:
```
train_dataset = Subset(dataset, train_idx)
test_dataset = Subset(dataset, test_idx)

train_loader = DataLoader(train_dataset, batch_size=32, shuffle=True)
test_loader = DataLoader(test_dataset, batch_size=32, shuffle=False)

# Model with GINConv layers
class Model2(nn.Module):
    def __init__(self):
        super(Model2, self).__init__()

        part1 = nn.Sequential(
            nn.Linear(7, 64),
            nn.ReLU(),
            nn.Linear(64, 128)
        )
        self.l1 = GINConv(part1)

        part2 = nn.Sequential(
            nn.Linear(128, 256),
            nn.ReLU(),
            nn.Linear(256, 256)
        )
        self.l2 = GINConv(part2)
```

```
        part3 = nn.Sequential(
            nn.Linear(256, 512),
            nn.ReLU(),
            nn.Linear(512, 512)
        )
        self.l3 = GINConv(part3)


        self.l4 = nn.Linear(512, 2)
        self.relu = nn.ReLU()

    def forward(self, x, edge_index, batch):
        x = self.relu(self.l1(x, edge_index))
        x = self.relu(self.l2(x, edge_index))
        x = self.relu(self.l3(x, edge_index))
        x = global_mean_pool(x, batch)
        x = self.l4(x)
        return x

model = Model2()
criterion = nn.CrossEntropyLoss()
optimizer = optim.Adam(model.parameters(), lr=0.01)

train_acc, test_acc = [], []
for epoch in range(95):
    model.train()
    for batch in train_loader:
        optimizer.zero_grad()
        outputs = model(batch.x, batch.edge_index, batch.batch)
        loss = criterion(outputs, batch.y)
        loss.backward()
        optimizer.step()

    with torch.no_grad():
        model.eval()
        # Train
        correct = 0
        total = 0
        for batch in train_loader:
            out = model(batch.x, batch.edge_index, batch.batch)
            pred = out.argmax(dim=1)
            correct += (pred == batch.y).sum().item()
            total += batch.y.size(0)
        train_acc.append(correct / total)

        # Test
        correct = 0
        total = 0
        for batch in test_loader:
            out = model(batch.x, batch.edge_index, batch.batch)
            pred = out.argmax(dim=1)
            correct += (pred == batch.y).sum().item()
            total += batch.y.size(0)
        test_acc.append(correct / total)
```

```
# Plot results
plt.plot(train_acc, label="Train")
plt.plot(test_acc, label="Test")
plt.xlabel("Epoch")
plt.ylabel("Accuracy")
plt.legend()
plt.show()
```



In [50]:
```
print(train_acc[-1])
print(test_acc[-1])
```

```
0.8266666666666667
0.7894736842105263
```

In [ ]:
```
# P-value calculation
correct = int(len(test_idx)*test_acc[-1])
total = len(test_idx)
p_value = binom_test(correct, total, p=0.42105263157894735, alternative="greater")

print(f"P-value: {p_value}")
```

```
P-value: 4.051328899727381e-06
C:\Users\matsa\AppData\Local\Temp\ipykernel_20960\1323653989.py:8: DeprecationWarnin
g: 'binom_test' is deprecated in favour of 'binomtest' from version 1.7.0 and will b
e removed in Scipy 1.12.0.
  p_value = binom_test(correct, total, p=0.42105263157894735, alternative='greater')
```

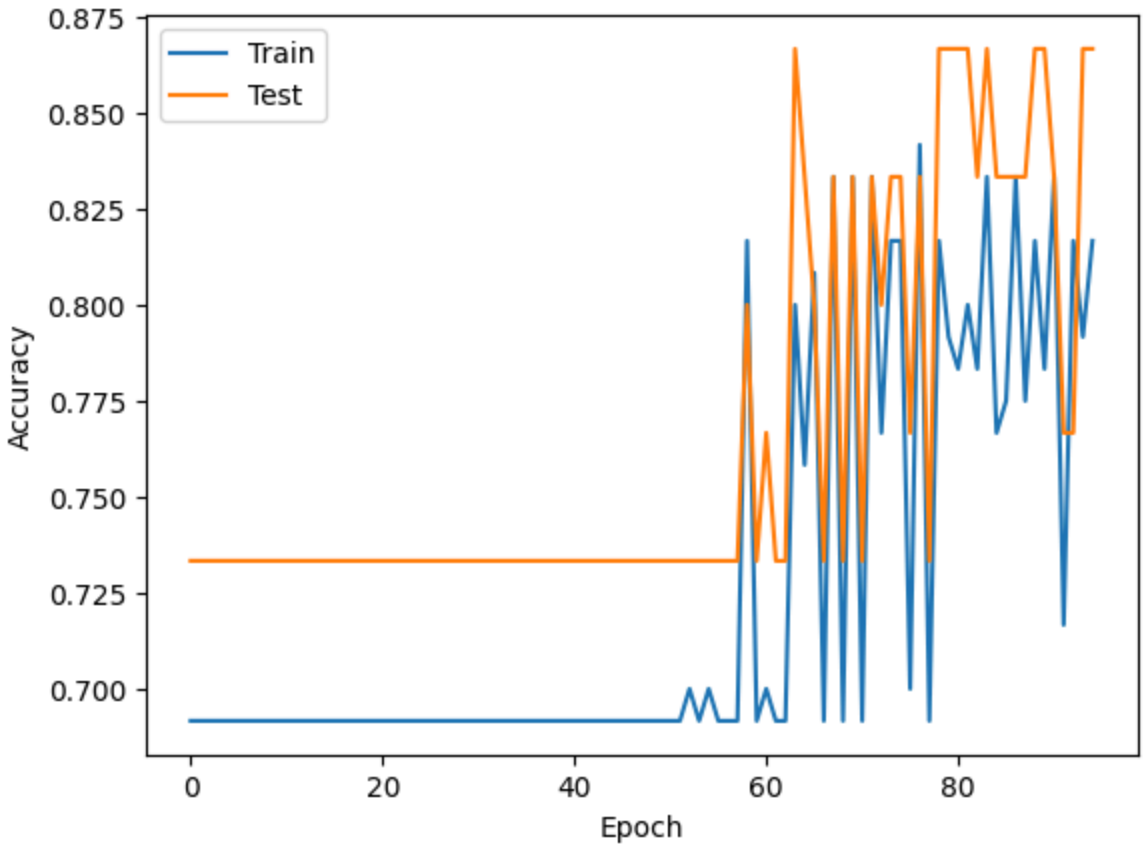
In [ ]:
```
"""
4.
a) ...
```

```
b) After some tests I found that using 2 + 16*2 (16 GIN layers with 2 linear layers
   and 2in 2out respectively) gave me pretty good results (around 80% accuracy) on
c)
"""
```

In [ ]:

```
# THIS PART IS USED FOR FINDING THE BEST HYPERPARAMETERS

train_dataset = Subset(dataset, train_idx)

# Subsets for train and validation
train_subdataset = Subset(train_dataset, train_idx_val)
val_subdataset = Subset(train_dataset, val_idx)

# DataLoaders for these subsets
train_loader = DataLoader(train_subdataset, batch_size=32, shuffle=True)
val_loader = DataLoader(val_subdataset, batch_size=32, shuffle=False)

# Model with GINConv layers
class Model2(nn.Module):
    def __init__(self):
        super(Model2, self).__init__()

        self.convs = nn.ModuleList()

        part1 = nn.Sequential(
            nn.Linear(7, 6),
            nn.ReLU(),
            nn.Linear(6, 6)
        )
        self.convs.append(GINConv(part1))

        for _ in range(15):
            part = nn.Sequential(
                nn.Linear(6, 6),
                nn.ReLU(),
                nn.Linear(6, 6)
            )
            self.convs.append(GINConv(part))

        self.em = nn.Linear(6, 2) # Embedding layer
        self.fin = nn.Linear(2, 2)
        self.relu = nn.ReLU()

    def forward(self, x, edge_index, batch):
        for conv in self.convs:
            x = self.relu(conv(x, edge_index))
        x = global_mean_pool(x, batch)
        embedding = self.em(x) # Embedding
        out = self.fin(embedding)
        return out, embedding


model = Model2()
criterion = nn.CrossEntropyLoss()
optimizer = optim.Adam(model.parameters(), lr=0.01)
```

```
train_acc, val_acc = [], []
embeddings = []
predictions = []
true_labels = []
for epoch in range(95):
    model.train()
    for batch in train_loader:
        optimizer.zero_grad()
        outputs, embedding = model(batch.x, batch.edge_index, batch.batch)
        loss = criterion(outputs, batch.y)
        loss.backward()
        optimizer.step()

    with torch.no_grad():
        model.eval()
        # Train
        correct = 0
        total = 0
        for batch in train_loader:
            out, embedding = model(batch.x, batch.edge_index, batch.batch)
            pred = out.argmax(dim=1)
            correct += (pred == batch.y).sum().item()
            total += batch.y.size(0)
        train_acc.append(correct / total)

        # Val
        correct = 0
        total = 0
        for batch in val_loader:
            out, embedding = model(batch.x, batch.edge_index, batch.batch)
            pred = out.argmax(dim=1)

            embeddings.append(embedding)
            true_labels.append(batch.y)
            predictions.append(pred)

            correct += (pred == batch.y).sum().item()
            total += batch.y.size(0)
        val_acc.append(correct / total)

# Plot results
plt.plot(train_acc, label="Train")
plt.plot(val_acc, label="Test")
plt.xlabel("Epoch")
plt.ylabel("Accuracy")
plt.legend()
plt.show()
```

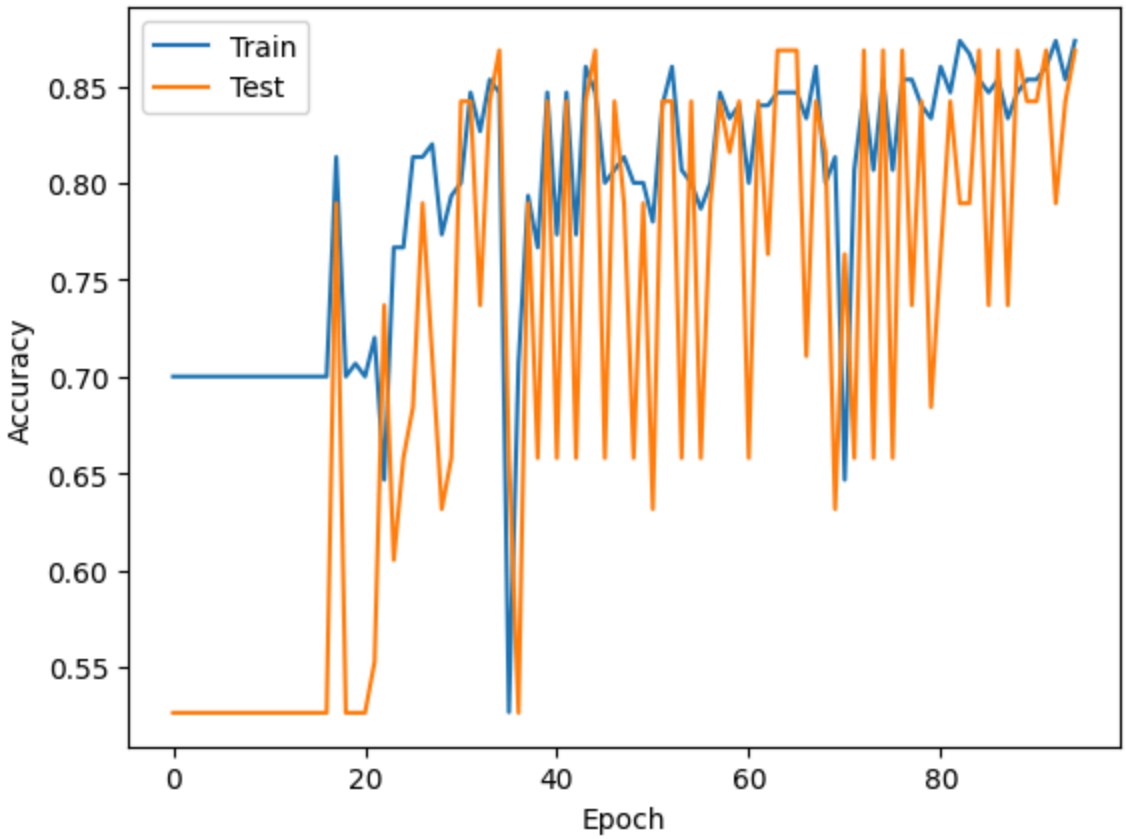


In [ ]:

```
train_dataset = Subset(dataset, train_idx)
test_dataset = Subset(dataset, test_idx)

train_loader = DataLoader(train_dataset, batch_size=32, shuffle=True)
test_loader = DataLoader(test_dataset, batch_size=32, shuffle=False)

# Model with GINConv layers
class Model2(nn.Module):
    def __init__(self):
        super(Model2, self).__init__()

        self.convs = nn.ModuleList()

        part1 = nn.Sequential(
            nn.Linear(7, 6),
            nn.ReLU(),
            nn.Linear(6, 6)
        )
        self.convs.append(GINConv(part1))

        for _ in range(15):
            part = nn.Sequential(
                nn.Linear(6, 6),
                nn.ReLU(),
                nn.Linear(6, 6)
            )
            self.convs.append(GINConv(part))

        self.em = nn.Linear(6, 2) # Embedding layer
```

```
        self.fin = nn.Linear(2, 2)
        self.relu = nn.ReLU()

    def forward(self, x, edge_index, batch):
        for conv in self.convs:
            x = self.relu(conv(x, edge_index))
        x = global_mean_pool(x, batch)
        embedding = self.em(x) # Embedding
        out = self.fin(embedding)
        return out, embedding

model = Model2()
criterion = nn.CrossEntropyLoss()
optimizer = optim.Adam(model.parameters(), lr=0.01)

train_acc, val_acc = [], []
embeddings = []
predictions = []
true_labels = []
for epoch in range(95):
    model.train()
    for batch in train_loader:
        optimizer.zero_grad()
        outputs, embedding = model(batch.x, batch.edge_index, batch.batch)
        loss = criterion(outputs, batch.y)
        loss.backward()
        optimizer.step()

    with torch.no_grad():
        model.eval()
        # Train
        correct = 0
        total = 0
        for batch in train_loader:
            out, embedding = model(batch.x, batch.edge_index, batch.batch)
            pred = out.argmax(dim=1)
            correct += (pred == batch.y).sum().item()
            total += batch.y.size(0)
        train_acc.append(correct / total)

        # Test
        correct = 0
        total = 0
        for batch in test_loader:
            out, embedding = model(batch.x, batch.edge_index, batch.batch)
            pred = out.argmax(dim=1)

            embeddings.append(embedding)
            true_labels.append(batch.y)
            predictions.append(pred)

            correct += (pred == batch.y).sum().item()
            total += batch.y.size(0)
        val_acc.append(correct / total)

# Plot results
```

```
plt.plot(train_acc, label="Train")
plt.plot(val_acc, label="Test")
plt.xlabel("Epoch")
plt.ylabel("Accuracy")
plt.legend()
plt.show()
```



In [ ]:
```
# Lists to tensors
embeddings_tensor = torch.cat(embeddings, dim=0)
true_labels_tensor = torch.cat(true_labels, dim=0)
predictions_tensor = torch.cat(predictions, dim=0)

# Tensors to NumPy
emb_np = embeddings_tensor.numpy()
true_np = true_labels_tensor.numpy()
pred_np = predictions_tensor.numpy()

x_min, x_max = emb_np[:, 0].min() - 1, emb_np[:, 0].max() + 1
y_min, y_max = emb_np[:, 1].min() - 1, emb_np[:, 1].max() + 1
xx, yy = np.meshgrid(np.linspace(x_min, x_max, 200), np.linspace(y_min, y_max, 200)
grid_points = np.c_[xx.ravel(), yy.ravel()]
grid_tensor = torch.from_numpy(grid_points.astype(np.float32))


model.eval()
with torch.no_grad():
    grid_outputs = model.fin(grid_tensor)  # Using final classification layer
    grid_preds = torch.argmax(grid_outputs, dim=1).numpy()

grid_preds = grid_preds.reshape(xx.shape)
```

```
plt.figure(figsize=(12, 5))

plt.subplot(1, 2, 1)
plt.scatter(emb_np[:, 0], emb_np[:, 1], c=true_np, cmap="plasma", edgecolor="k", al
plt.contourf(xx, yy, grid_preds, alpha=0.2, cmap="plasma")
plt.title("Samples Colored by True Labels + Decision Boundary")
plt.xlabel("Embedding dim 1")
plt.ylabel("Embedding dim 2")

plt.subplot(1, 2, 2)
plt.scatter(emb_np[:, 0], emb_np[:, 1], c=pred_np, cmap="plasma", edgecolor="k", al
plt.contourf(xx, yy, grid_preds, alpha=0.2, cmap="plasma")
plt.title("Samples Colored by Predicted Labels + Decision Boundary")
plt.xlabel("Embedding dim 1")
plt.ylabel("Embedding dim 2")

plt.tight_layout()
plt.show()
```