```
# Install required packages.
import os
import torch
os.environ['TORCH'] = torch.__version__
print(torch.__version__)
print('CUDA available:', torch.cuda.is_available())
```

```
2.1.2.post303
CUDA available: True
```

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from matplotlib.pyplot import cm

from tqdm import tqdm

import torch.nn.functional as F
from torch.nn import Sequential, Linear, ReLU, BatchNorm1d, Identity, Dropout, Softmax
from torch_geometric.nn import EdgeConv, GCNConv, GraphConv
from torch_geometric.nn import global_mean_pool
from torch_geometric.data import Data
from torch_geometric.loader import DataLoader
from torch_geometric.utils import from_networkx

from torch.utils.tensorboard import SummaryWriter
```

```
/home/karthik/anaconda3/lib/python3.10/site-packages/torch_geometric/typing.py:73: UserWarning: An issue occurred while
  warnings.warn(f"An issue occurred while importing 'torch-scatter'. "
/home/karthik/anaconda3/lib/python3.10/site-packages/torch_geometric/typing.py:111: UserWarning: An issue occurred while
  warnings.warn(f"An issue occurred while importing 'torch-sparse'. "
```

```
data = np.load('./task2Datasets/QG_jets_withbc_1.npz')
print(data)

print(data.files)
X = data['X']
y = data['y']
print(X.shape, y.shape, sep='\n')
```

```
<numpy.lib.npyio.NpzFile object at 0x79673bd6080>
['X', 'y']
(100000, 137, 4)
(100000,)
```

Utility functions

```
# arr is a 2d array
# function returns a 1d array consisting each row's (jet's) multiplicity

def get_multiplicities(arr):
    nonzeros = (arr != 0).astype(int)
    return np.sum(nonzeros, axis=1)

def plot_jets(jet_index, jet_etas, jet_phis):
    if jet_index < 0:
        raise Excetion('Error, Jet index should be between 0 and 99999')

    eta = X[jet_index, :, 1]
    phi = X[jet_index, :, 2]

    # remove zero paddings,
    nonzero_mask = X[jet_index, :, 1] != 0
    eta = X[jet_index, nonzero_mask, 1] - jet_etas[jet_index]
    phi = X[jet_index, nonzero_mask, 2] - jet_phis[jet_index]

    # check multiplicities
    print(eta.shape, phi.shape)
    print(get_multiplicities(X[:, :, 1])[jet_index])

    # plot
    plt.figure(figsize=(8, 3))

    plt.subplot(1, 2, 1)
    plt.hist2d(eta, phi, cmap='viridis', range=[[-2, 2], [-2, 2]], bins =100)

    plt.subplot(1, 2, 2)
    plt.scatter(eta, phi)
    ax = plt.gca()
    ax.set_xlim([-5, 5])
    ax.set_ylim([-5, 5])

    plt.show()
```

Feature Engineering

```
print(X.shape)
```

```
(100000, 137, 4)
```

```
# checking bounds of dataset
print(f'transverse momentum bounds: min={np.min(X[:,:, 0])}, max={np.max(X[:,:, 0])}, mean={np.mean(X[:,:, 0])}')
print(f'pseudo-rapidity bounds: min={np.min(X[:,:, 1])}, max={np.max(X[:,:, 1])}, mean={np.mean(X[:,:, 1])}')
print(f'azimuthal angle bounds: min={np.min(X[:,:, 2])}, max={np.max(X[:,:, 2])}, mean={np.mean(X[:,:, 2])}')
```

```
transverse momentum bounds: min=0.0, max=548.415807621, mean=3.8235925586685777
pseudo-rapidity bounds: min=-2.10354644796, max=2.1094042875, mean=0.0017309813976636966
azimuthal angle bounds: min=-0.462937251085, max=6.75555673857, mean=0.9957003344113187
```

The bounds indicate that they have to be normalized

After getting the jet pT, rapidiy and azimuthal angles, we plot the jets to see if we are getting the correct jet centered images

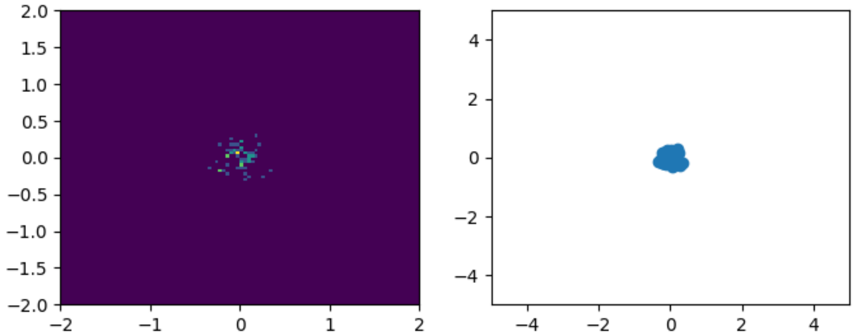
```
# creating jet-centered features - step-1

# derive jet pT, rapidity and azimuthal angles

# assuming jet momentum is the sum of the momenta of all particles
jet_pTs = np.sum(X[:, :, 0], axis=1)
print(jet_pTs.shape)
print(jet_pTs.min(), jet_pTs.max(), jet_pTs.mean())

# mean rapidity of all particles is taken as jet rapididty
jet_etas = np.sum(X[:, :, 1], axis=1) / get_multiplicities(X[:, :, 1])
print(jet_etas.shape)
print(jet_etas.min(), jet_etas.max(), jet_etas.mean())

# mean of azimuthal angles of all particles is jet azimuthal angle
jet_phis = np.sum(X[:, :, 2], axis=1) / get_multiplicities(X[:, :, 2])
print(jet_phis.shape)
print(jet_phis.min(), jet_phis.max(), jet_phis.mean())
```

```
(100000,)
500.0463140266235 561.457792111489 523.8321805375957
(100000,)
```

```
-1.7755351646578785 1.7951616238948889 0.005324459752633116
(100000,)
-0.09567027409355122 6.526761820212942 3.1443253285741286
```

```
# run this function below with a random jet index to see its jet structure plotted on eta-phi plane
plot_jets(6950, jet_etas, jet_phis)
```

```
(67,) (67,)
67
```



The images are centered around the origin for all the jets that are checked, so we can proceed creating derived features

```
# step 2. Create arrays with respective operations

# take only non-padded elements
particle_mask = (X[:, :, 0] != 0).astype(int)
padding_mask = (X[:, :, 0] == 0).astype(int)

# delta eta, delta phi features
rel_eta_arr = X[:, :, 1] - (particle_mask * jet_etas[:, None])
rel_phi_arr = X[:, :, 2] - (particle_mask * jet_phis[:, None])


# log(pT) feature
log_pT_arr = X[:, :, 0] + (padding_mask * np.ones(X[:, :, 0].shape))
log_pT_arr = np.log(log_pT_arr)

# log(pT/pT_jet) feature
pT_div_pTjet = X[:, :, 0] / (jet_pTs[:, None])
log_pT_pTjet_arr = pT_div_pTjet + (padding_mask * np.ones(X[:, :, 0].shape))
log_pT_pTjet_arr = np.log(log_pT_pTjet_arr)

# delta R feature
delta_r_arr = np.sqrt(np.square(rel_eta_arr) + np.square(rel_phi_arr))
```

The last feature array is left out, Now extracting its details,

```
pdgid = np.abs(X[:, :, 3])

pdgid_list = np.ravel(pdgid)
print(np.unique(pdgid_list))
```

```
[   0.    11.    13.    22.   130.   211.   321. 2112. 2212.]
```

This output array tells us the pdgid's of all particles encountered in the jets,
so that we can create an exhaustive classification of particles as features

output: [0. 11. 13. 22. 130. 211. 321. 2112. 2212.]

Note: This output is consistent across whole dataset, ie., across 2M jets

0 -> no data
11 -> electron (charge = -1)
13 -> muon (charge = -1)
22 -> photon (charge = 0)
130 -> K_L^0 (charge = 0)
211 -> $\pi^+ Meson$ (charge = +1) 321 -> $K^+ Meson$ (charge = +1)
2112 -> n (charge = 0) in hadron scheme
2212 -> p (charge = +1)

We use this data to create additional feature arrays

```
# creating new 2d arrays binning particles into respective categories

is_electron_arr = (pdgid == 11).astype(int) # e- is the only particle with pdgid 11
is_muon_arr = (pdgid == 13).astype(int) # muon is the only particle with pdgid 13
is_photon_arr = (pdgid == 22).astype(int) # photon is the only particle with pdgid 22
is_charged_hadron_arr = ((pdgid == 211).astype(int)) + ((pdgid == 2212).astype(int)) # pi meson and protons are charged hadr
is_neutral_hadron_arr = ((pdgid == 130).astype(int)) + ((pdgid == 2112).astype(int)) # pi meson and protons are charged hadr

charge_arr = (is_electron_arr*-1) + (is_muon_arr*-1) + (is_charged_hadron_arr*+1)


# now create the data array with all created feature arrays
Xnew = np.dstack([rel_eta_arr, rel_phi_arr, log_pT_arr, log_pT_pTjet_arr, delta_r_arr,
                 charge_arr, is_electron_arr, is_muon_arr, is_charged_hadron_arr, is_neutral_hadron_arr, is_photon_arr])

print(Xnew.shape)
```

```
(100000, 137, 11)
```

```
df = pd.DataFrame(Xnew[:,:,0])
df

# save this curated dataset into numpy file
np.save('./task2Datasets/curated_data', Xnew)
np.save('./task2Datasets/labels', y)
```

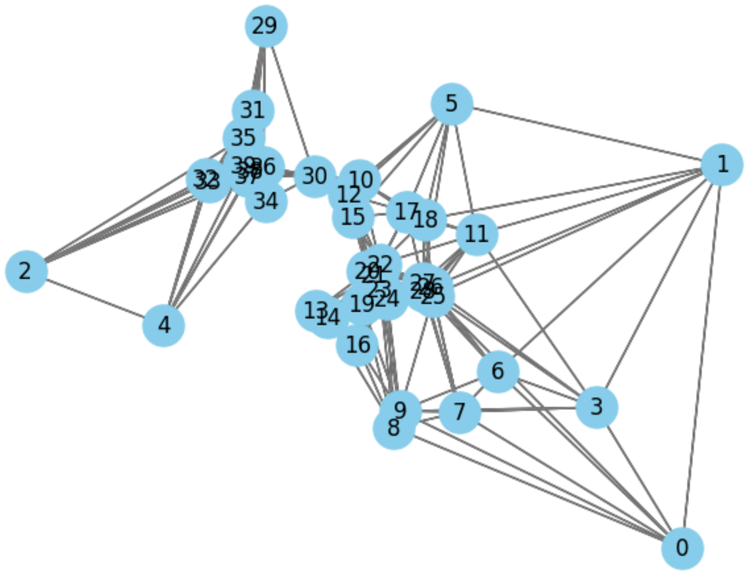
TODO Describe the feature set

Edge-Conv Model

```
# generate edge list of k-nearest neighbors of a node using given coordinates

def knn_particle_graph(positions, k):
  # Calculate pairwise distances between nodes
  n_nodes = positions.shape[0]
  distance_matrix = np.linalg.norm(positions[:, None] - positions[None, :], axis=2)

  # Extract top k nearest neighbors for each node (excluding itself)
  edge_list = []
  for i in range(n_nodes):
    # Sort distances in ascending order and get indices
    sorted_indices = np.argsort(distance_matrix[i])
    # Select top k neighbors (excluding itself)
    neighbors = sorted_indices[1: k + 1]
    # Create edges between the node and its neighbors
    for neighbor in neighbors:
      edge_list.append((i, neighbor))

  return edge_list
```

```
import networkx as nx

# function to visualize jet data as graphs
def visualize_jet_graph(jet_index):
    mask = Xnew[jet_index, :, 0] != 0
    pos = Xnew[jet_index, mask, 0:2]
    node_indices = list(range(len(pos)))
    edges = knn_particle_graph(pos, 7)

    G = nx.Graph()

    node_positions = {}

    for i in node_indices:
        node_positions.update({i:pos[i]})

    G.add_nodes_from(node_positions.keys())
    nx.set_node_attributes(G, node_positions, 'pos')
    G.add_edges_from(edges)

    # visualize
    plot_pos = nx.get_node_attributes(G, 'pos')
    nx.draw(G, plot_pos, with_labels=True, node_size=500, node_color='skyblue', font_size=12)
    nx.draw_networkx_edges(G, plot_pos, edge_color='gray')
    plt.show()
```

```
# sample graph representation for a jet indexed 25
visualize_jet_graph(15000)
```



Dataloading into Pytorch

```
from torch_geometric.data import Dataset
from torch_geometric.data import Data

class JetGraphDataset(Dataset):
    def __init__(self, root, filename, test=False, transform=None, pre_transform=None, pre_filter=None):
        # root (where dataset is stored) -> raw_dir = we put in original dataset file
        #                                -> processed_dir = pytorch fills up intermediate/processed datasets

        self.test = test
        self.filename = filename
        super(JetGraphDataset, self).__init__(root, transform, pre_transform, pre_filter)

    @property
    def raw_file_names(self):
        # file name of dataset, should return a string
        # if pytorch finds files with this name, no download will be triggered
        return self.filename

    @property
    def processed_file_names(self):
        # names of files pytorch should give to processed datafiles
        # if these files are found, process() function will not be triggered
        if self.test:
            return ['data_test.pt']
        else:
            return ['data.pt']

    def download(self):
        pass

    def process(self):
        # create the graph and pass it to the model as data obj
        self.data = np.load(self.raw_paths[0])
        labels = np.load('./task2Datasets/labels.npy')

        for jet_index in tqdm(range(self.data.shape[0])):
            k = 7
            # constuct graph for each jet
            mask = self.data[jet_index, :, 0] != 0
            pos = self.data[jet_index, mask, 0:2]
            node_indices = list(range(len(pos)))
            edges = knn_particle_graph(pos, k)

            # create the graph object in networkx
            G = nx.Graph()
            node_positions = {}
            for i in node_indices:
                node_positions.update({i:pos[i]})
            G.add_nodes_from(node_positions.keys())
            nx.set_node_attributes(G, node_positions, 'pos')
            G.add_edges_from(edges)


            # extract required data from graph object
            node_features = torch.tensor(self.data[jet_index, mask, :], dtype=torch.float)

            edge_index_no_duplicates = G.edges()
            edge_indices = []
            for edge in edge_index_no_duplicates:
                i = edge[0]
                j = edge[1]
                edge_indices += [[i, j], [j, i]]
            edge_indices = torch.tensor(edge_indices)
            edge_indices = edge_indices.t().to(torch.long).view(2, -1)

            edge_features = torch.tensor(self._get_edge_features(edges, pos, jet_index), dtype=torch.float)

            label = torch.tensor(np.asarray([labels[jet_index]]), dtype=torch.int64)

            data = Data(x = node_features,
                        edge_index = edge_indices,
                        edge_attr = edge_features,
                        y = label,
                        jet_index = torch.tensor(jet_index, dtype=torch.int64))

            if self.test:
                torch.save(data,
                    os.path.join(self.processed_dir,
                                 f'data_test_{jet_index}.pt'))
            else:
                torch.save(data,
                    os.path.join(self.processed_dir,
```

```
                                     f'data_{jet_index}.pt'))

    def _get_edge_features(self, edge_list, pos, jet_index):
        edge_lengths = []
        same_particle = []
        for p_id1, p_id2 in edge_list:
            edge_length = np.sqrt((pos[p_id1, 0]-pos[p_id2, 0])**2 + (pos[p_id1, 1]-pos[p_id2, 1])**2)
            edge_lengths.append(edge_length)

            if all(self.data[jet_index, p_id1, 6:11] == self.data[jet_index, p_id2, 6:11]):
                same_particle.append(1)
            else:
                same_particle.append(0)

        return np.vstack([edge_lengths, same_particle]).T


    def len(self):
        return self.data.shape[0]

    def get(self, idx):
        if self.test:
            data = torch.load(os.path.join(self.processed_dir,
                                     f'data_test_{idx}.pt'))
        else:
            data = torch.load(os.path.join(self.processed_dir,
                                     f'data_{idx}.pt'))
        return data


dataset = JetGraphDataset(root='./task2Datasets/', filename='curated_data.npy')

# Train/test split (80-20)
train_share = int(len(dataset) * 0.8)

train_dataset = dataset[:train_share]
test_dataset = dataset[train_share:]
```

```
Processing...
100%|██████████████████████████████████| 100000/100000 [02:33<00:00, 650.00it/s]
Done!
```

Model - 1

Definition

```
class EdgeConvNetwork1(torch.nn.Module):
    def __init__(self, hidden_channels):
        super().__init__()

        self.hidden_channels2 = 2 * hidden_channels
        self.hidden_channels3 = 4 * hidden_channels

        # Initialize MLPs used by EdgeConv layers
        self.mlp1 = Sequential(Linear(2 * dataset.num_node_features, hidden_channels),
                               BatchNorm1d(hidden_channels),
                               ReLU(),
                               Linear(hidden_channels, hidden_channels),
                               BatchNorm1d(hidden_channels),
                               ReLU(),
                               Linear(hidden_channels, hidden_channels),
                               BatchNorm1d(hidden_channels),
                               ReLU(),
                               )
        self.mlp2 = Sequential(Linear(2* hidden_channels, self.hidden_channels2),
                               BatchNorm1d(self.hidden_channels2),
                               ReLU(),
                               Linear(self.hidden_channels2, self.hidden_channels2),
                               BatchNorm1d(self.hidden_channels2),
                               ReLU(),
                               Linear(self.hidden_channels2, self.hidden_channels2),
                               BatchNorm1d(self.hidden_channels2),
                               ReLU(),
                               )

        self.conv1 = EdgeConv(self.mlp1, aggr='mean')
        self.conv2 = EdgeConv(self.mlp2, aggr='mean')

        # Shortcut connections
        self.shortcut1 = Linear(dataset.num_node_features, hidden_channels)
        self.shortcut2 = Linear(hidden_channels, self.hidden_channels2)

        # Fully connected layer with dropout
        self.fc1 = Sequential(
            Linear(in_features=self.hidden_channels2, out_features=self.hidden_channels3),
            ReLU(),
            Dropout(p=0.1)
        )
        # second fully connected layer
        self.fc2 = Sequential(
            Linear(in_features=self.hidden_channels3, out_features=2),
        )

    def forward(self, data):
        x, edge_index, batch = data.x, data.edge_index, data.batch

        # 1st edge convolution block
        out = self.conv1(x, edge_index)
        out = out + self.shortcut1(x)
        out = F.relu(out)
        out1 = out.detach().clone()
        # 2nd edge convolution block - uses the learned feature vectors as inputs
        out = self.conv2(out, edge_index)
        out = out + self.shortcut2(out1)
        out = F.relu(out)
        # global average pooling
        out = global_mean_pool(out, batch)
        # fully-connected-1
        out = self.fc1(out)
        # fully-connected-2
        out = self.fc2(out)

        out = F.softmax(out, dim=0)

        return out


# instantiate model and print summary

def count_parameters(model):
    return sum(p.numel() for p in model.parameters() if p.requires_grad)

model = EdgeConvNetwork1(64)
print(model)

print('Num parameters: ', count_parameters(model))
```

```
EdgeConvNetwork1(
  (mlp1): Sequential(
```

```
      (0): Linear(in_features=22, out_features=64, bias=True)
      (1): BatchNorm1d(64, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (2): ReLU()
      (3): Linear(in_features=64, out_features=64, bias=True)
      (4): BatchNorm1d(64, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (5): ReLU()
      (6): Linear(in_features=64, out_features=64, bias=True)
      (7): BatchNorm1d(64, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (8): ReLU()
    )
    (mlp2): Sequential(
      (0): Linear(in_features=128, out_features=128, bias=True)
      (1): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (2): ReLU()
      (3): Linear(in_features=128, out_features=128, bias=True)
      (4): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (5): ReLU()
      (6): Linear(in_features=128, out_features=128, bias=True)
      (7): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (8): ReLU()
    )
    (conv1): EdgeConv(nn=Sequential(
      (0): Linear(in_features=22, out_features=64, bias=True)
      (1): BatchNorm1d(64, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (2): ReLU()
      (3): Linear(in_features=64, out_features=64, bias=True)
      (4): BatchNorm1d(64, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (5): ReLU()
      (6): Linear(in_features=64, out_features=64, bias=True)
      (7): BatchNorm1d(64, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (8): ReLU()
    ))
    (conv2): EdgeConv(nn=Sequential(
      (0): Linear(in_features=128, out_features=128, bias=True)
      (1): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (2): ReLU()
      (3): Linear(in_features=128, out_features=128, bias=True)
      (4): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (5): ReLU()
      (6): Linear(in_features=128, out_features=128, bias=True)
      (7): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
      (8): ReLU()
    ))
    (shortcut1): Linear(in_features=11, out_features=64, bias=True)
    (shortcut2): Linear(in_features=64, out_features=128, bias=True)
    (fc1): Sequential(
      (0): Linear(in_features=128, out_features=256, bias=True)
      (1): ReLU()
      (2): Dropout(p=0.1, inplace=False)
    )
    (fc2): Sequential(
      (0): Linear(in_features=256, out_features=2, bias=True)
    )
  )
  Num parameters:  103106
```

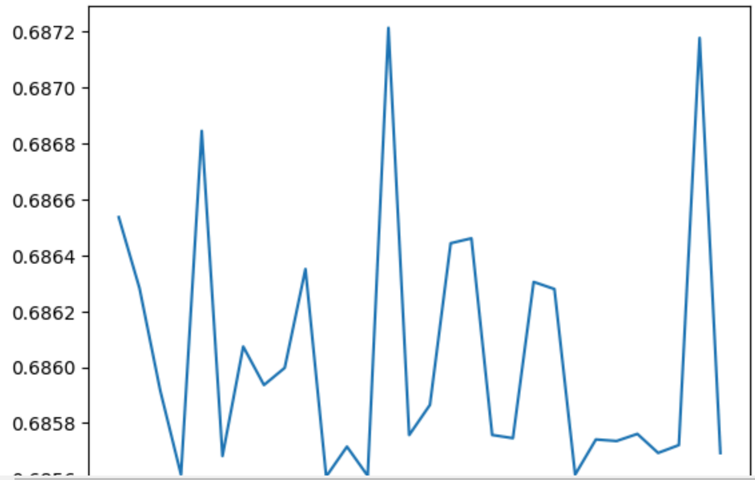
Training and Evaluation function definitions

```
def train(model, loss_fn, device, data_loader, optimizer):
    """ Performs an epoch of model training.

    Parameters:
    model (nn.Module): Model to be trained.
    loss_fn (nn.Module): Loss function for training.
    device (torch.Device): Device used for training.
    data_loader (torch.utils.data.DataLoader): Data loader containing all batches.
    optimizer (torch.optim.Optimizer): Optimizer used to update model.

    Returns:
    float: Total loss for epoch.
    """
    model.train()
    loss = 0

    for batch in tqdm(data_loader):
        batch = batch.to(device)

        optimizer.zero_grad()
        out = model(batch)

        loss = loss_fn(out, batch.y)

        loss.backward()
        optimizer.step()

    return loss.item()

def eval(model, device, loader):
    """ Calculate accuracy for all examples in a DataLoader.

    Parameters:
    model (nn.Module): Model to be evaluated.
    device (torch.Device): Device used for training.
    loader (torch.utils.data.DataLoader): DataLoader containing examples to test.
    """
    model.eval()
    cor = 0
    tot = 0

    for batch in loader:
        batch = batch.to(device)

        with torch.no_grad():
            pred = torch.argmax(model(batch), 1)

        y = batch.y
        cor += (pred == y).sum()
        tot += pred.shape[0]

    return cor / tot
```

Training and Model Evaulation

```
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")

model = EdgeConvNetwork1(128).to(device)


optimizer1 = torch.optim.AdamW(model.parameters(), lr=3e-5, weight_decay=0.0001)

train_loader = DataLoader(train_dataset, batch_size=128, shuffle=True)
test_loader = DataLoader(test_dataset, batch_size=128, shuffle=False)

loss_fn = torch.nn.CrossEntropyLoss()
losses = []

for epoch in range(0, 30):
    # variable learning rates
    if epoch < 8:
        l_r = 0.0005 + ((0.005-0.0005) * (epoch+1) / 8)
    if (epoch >= 8) and (epoch < 16):
        l_r = 0.005 + ((0.0005-0.005) * (epoch-7) / 8)
    if epoch >= 16:
        l_r = 0.0005/(5**(epoch-15))

    optimizer = torch.optim.AdamW(model.parameters(), lr=l_r, weight_decay=0.0001)

    loss = train(model, loss_fn, device, train_loader, optimizer1)
    train_result = eval(model, device, train_loader)
    test_result = eval(model, device, test_loader)

    losses.append(loss)

    print(f'Epoch: {epoch + 1:02d}, '
          f'LR: {l_r:.2E}, '
          f'Loss: {loss:.4f}, '
          f'Train: {100 * train_result:.2f}%, '
          f'Test: {100 * test_result:.2f}%')

plt.plot(losses)
plt.show()
```

```
100%|██████████| 625/625 [00:28<00:00, 21.65
Epoch: 01, LR: 1.06E-03, Loss: 0.6865, Train: 76.78%, Test: 76.71%
100%|██████████| 625/625 [00:28<00:00, 21.61
Epoch: 02, LR: 1.63E-03, Loss: 0.6863, Train: 77.43%, Test: 77.27%
100%|██████████| 625/625 [00:29<00:00, 21.53
Epoch: 03, LR: 2.19E-03, Loss: 0.6859, Train: 77.71%, Test: 77.61%
100%|██████████| 625/625 [00:29<00:00, 21.49
Epoch: 04, LR: 2.75E-03, Loss: 0.6856, Train: 77.99%, Test: 77.90%
100%|██████████| 625/625 [00:29<00:00, 21.50
Epoch: 05, LR: 3.31E-03, Loss: 0.6868, Train: 77.50%, Test: 77.31%
100%|██████████| 625/625 [00:29<00:00, 21.48
Epoch: 06, LR: 3.88E-03, Loss: 0.6857, Train: 78.16%, Test: 78.27%
100%|██████████| 625/625 [00:29<00:00, 21.49
Epoch: 07, LR: 4.44E-03, Loss: 0.6861, Train: 77.80%, Test: 77.88%
100%|██████████| 625/625 [00:29<00:00, 21.45
Epoch: 08, LR: 5.00E-03, Loss: 0.6859, Train: 77.85%, Test: 77.78%
100%|██████████| 625/625 [00:29<00:00, 21.45
Epoch: 09, LR: 4.44E-03, Loss: 0.6860, Train: 78.04%, Test: 78.07%
100%|██████████| 625/625 [00:29<00:00, 21.44
Epoch: 10, LR: 3.87E-03, Loss: 0.6864, Train: 77.96%, Test: 78.01%
100%|██████████| 625/625 [00:29<00:00, 21.45
Epoch: 11, LR: 3.31E-03, Loss: 0.6856, Train: 78.00%, Test: 77.97%
100%|██████████| 625/625 [00:29<00:00, 21.45
Epoch: 12, LR: 2.75E-03, Loss: 0.6857, Train: 77.63%, Test: 77.44%
100%|██████████| 625/625 [00:29<00:00, 21.44
Epoch: 13, LR: 2.19E-03, Loss: 0.6856, Train: 78.06%, Test: 77.87%
100%|██████████| 625/625 [00:29<00:00, 21.43
Epoch: 14, LR: 1.62E-03, Loss: 0.6872, Train: 77.93%, Test: 77.69%
100%|██████████| 625/625 [00:29<00:00, 21.45
Epoch: 15, LR: 1.06E-03, Loss: 0.6858, Train: 77.56%, Test: 77.42%
100%|██████████| 625/625 [00:29<00:00, 21.44
Epoch: 16, LR: 5.00E-04, Loss: 0.6859, Train: 77.83%, Test: 77.65%
100%|██████████| 625/625 [00:29<00:00, 21.43
Epoch: 17, LR: 1.00E-04, Loss: 0.6864, Train: 77.86%, Test: 77.73%
100%|██████████| 625/625 [00:29<00:00, 21.43
Epoch: 18, LR: 2.00E-05, Loss: 0.6865, Train: 78.03%, Test: 78.17%
100%|██████████| 625/625 [00:29<00:00, 21.42
Epoch: 19, LR: 4.00E-06, Loss: 0.6858, Train: 78.54%, Test: 78.53%
100%|██████████| 625/625 [00:29<00:00, 21.40
Epoch: 20, LR: 8.00E-07, Loss: 0.6857, Train: 77.98%, Test: 77.89%
100%|██████████| 625/625 [00:29<00:00, 21.37
Epoch: 21, LR: 1.60E-07, Loss: 0.6863, Train: 78.33%, Test: 78.40%
100%|██████████| 625/625 [00:29<00:00, 21.41
Epoch: 22, LR: 3.20E-08, Loss: 0.6863, Train: 77.97%, Test: 77.98%
100%|██████████| 625/625 [00:29<00:00, 21.40
Epoch: 23, LR: 6.40E-09, Loss: 0.6856, Train: 78.62%, Test: 78.40%
100%|██████████| 625/625 [00:29<00:00, 21.40
Epoch: 24, LR: 1.28E-09, Loss: 0.6857, Train: 77.30%, Test: 77.03%
100%|██████████| 625/625 [00:29<00:00, 21.40
Epoch: 25, LR: 2.56E-10, Loss: 0.6857, Train: 76.76%, Test: 76.38%
100%|██████████| 625/625 [00:29<00:00, 21.43
Epoch: 26, LR: 5.12E-11, Loss: 0.6858, Train: 77.71%, Test: 77.58%
100%|██████████| 625/625 [00:29<00:00, 21.43
Epoch: 27, LR: 1.02E-11, Loss: 0.6857, Train: 77.18%, Test: 76.83%
100%|██████████| 625/625 [00:29<00:00, 21.34
Epoch: 28, LR: 2.05E-12, Loss: 0.6857, Train: 78.16%, Test: 77.97%
100%|██████████| 625/625 [00:29<00:00, 21.42
Epoch: 29, LR: 4.10E-13, Loss: 0.6872, Train: 77.11%, Test: 76.80%
100%|██████████| 625/625 [00:29<00:00, 21.41
Epoch: 30, LR: 8.19E-14, Loss: 0.6857, Train: 77.26%, Test: 77.06%
```



Model 2

Definition

```
class EdgeConvNetwork2(torch.nn.Module):
    def __init__(self, hidden_channels):
        super().__init__()

        self.hidden_channels2 = 2 * hidden_channels
        self.hidden_channels3 = 4 * hidden_channels

        # Initialize MLPs used by EdgeConv layers
        self.mlp1 = Sequential(Linear(2 * dataset.num_node_features, hidden_channels),
                               BatchNorm1d(hidden_channels),
                               ReLU(),
                               Linear(hidden_channels, hidden_channels),
```

Instantiation and Model Summary

```
                               BatchNorm1d(hidden_channels)
```

```
model = EdgeConvNetwork2(128)
print(model)

print('Num parameters: ', count_parameters(model))
```

```
EdgeConvNetwork2(
  (mlp1): Sequential(
    (0): Linear(in_features=22, out_features=128, bias=True)
    (1): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
    (2): ReLU()
    (3): Linear(in_features=128, out_features=128, bias=True)
    (4): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
    (5): ReLU()
    (6): Linear(in_features=128, out_features=128, bias=True)
    (7): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
    (8): ReLU()
  )
  (mlp2): Sequential(
    (0): Linear(in_features=256, out_features=256, bias=True)
    (1): BatchNorm1d(256, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
```