Installing and Importing the neccessary dependencies

```
import torch
import os
os.environ['TORCH'] = torch.__version__
print(torch.__version__)

!pip install -q torch-scatter -f https://data.pyg.org/whl/torch-$
{TORCH}.html
!pip install -q torch-sparse -f https://data.pyg.org/whl/torch-$
{TORCH}.html
!pip install -q git+https://github.com/pyg-team/pytorch_geometric.git
```

```
2.2.1+cu121
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(pyproject.toml) ...
```

```
import numpy as np
import h5py
import matplotlib.pyplot as plt
from sklearn.neighbors import kneighbors_graph

import torch.nn.functional as F
from torch.nn import Linear

from torch_geometric.data import Data
from torch_geometric.loader import DataLoader
from torch_geometric.nn import global_mean_pool
from torch_geometric.nn import GCNConv, GATConv, SAGEConv
```

Mounting and Loading the data

```
from google.colab import drive
drive.mount('/content/drive')
```

```
Mounted at /content/drive
```

```
path = "/content/drive/MyDrive/quark-gluon_data-set_n139306.hdf5"
#Path to the dataset on my google drive

with h5py.File(path, 'r') as f:
```

```
  X_jets = f['X_jets'][0:5000] # Working with only a subset of data
due to computational limits
  y = f['y'][0:5000]
  print(f"X_jets shape : {X_jets.shape}, y : {y.shape}") # printing
the shape of the images and amount
```

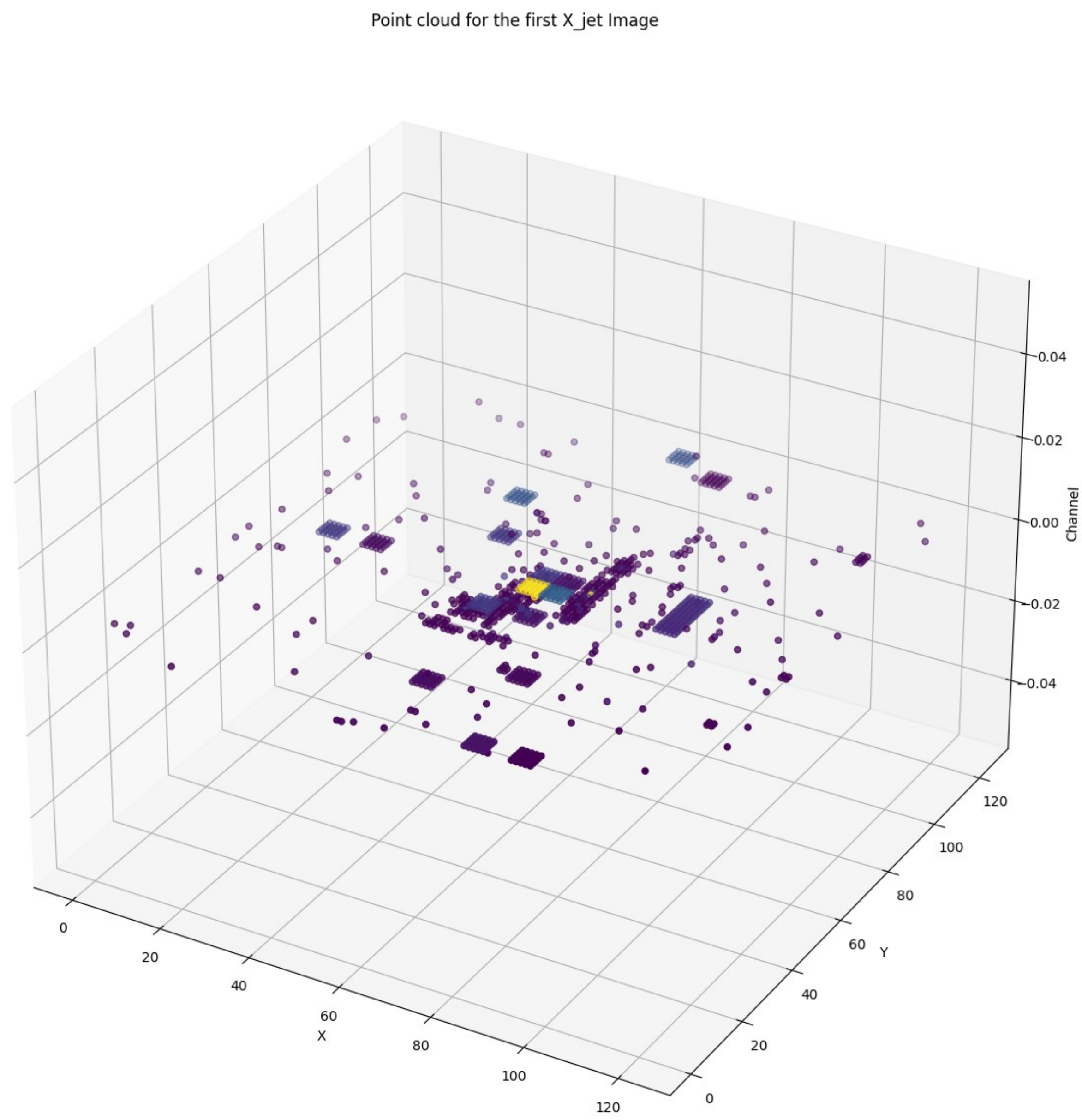
```
X_jets shape : (5000, 125, 125, 3), y : (5000,)
```

```
X_jets = np.array(X_jets)
y = np.array(y)
```

Creating the point cloud from the dataset

```
size = X_jets.shape[0]
cloud = []
for i in range(size):
  #Selecting only the nonzero points
  nonzero_Track = np.nonzero(X_jets[i,:,:,0])
  nonzero_ECAL = np.nonzero(X_jets[i,:,:,1])
  nonzero_HCAL = np.nonzero(X_jets[i,:,:,2])

  #Getting the values of the respective channels
  valuesTrack = X_jets[i,nonzero_Track[0],nonzero_Track[1],0]
  valuesECAL = X_jets[i,nonzero_ECAL[0],nonzero_ECAL[1],1]
  valuesHCAL = X_jets[i,nonzero_HCAL[0],nonzero_HCAL[1],2]

  #Getting the co-ordinates of the respective channels
  coord_Track = np.hstack((np.column_stack(nonzero_Track),
np.zeros((np.column_stack(nonzero_Track).shape[0],1))))
  coord_ECAL = np.hstack((np.column_stack(nonzero_ECAL),
np.zeros((np.column_stack(nonzero_ECAL).shape[0],1))))
  coord_HCAL = np.hstack((np.column_stack(nonzero_HCAL),
np.zeros((np.column_stack(nonzero_HCAL).shape[0],1))))


  cloud.append({"Track":(coord_Track, valuesTrack), "ECAL":
(coord_ECAL, valuesECAL), "HCAL":(coord_HCAL, valuesHCAL)})


sample_cloud = cloud[0]

ax = plt.figure(figsize=(15,15)).add_subplot(111,projection='3d')

ax.scatter(sample_cloud["Track"][0][:,0],sample_cloud["Track"][0]
[:,1],sample_cloud["Track"][0][:,2],c=sample_cloud["Track"][1])
ax.scatter(sample_cloud["ECAL"][0][:,0],sample_cloud["ECAL"][0]
[:,1],sample_cloud["ECAL"][0][:,2],c=sample_cloud["ECAL"][1])
ax.scatter(sample_cloud["HCAL"][0][:,0],sample_cloud["HCAL"][0]
[:,1],sample_cloud["HCAL"][0][:,2],c=sample_cloud["HCAL"][1])
```

```
# sample_cloud['Track'

ax.set_xlabel('X')
ax.set_ylabel('Y')
ax.set_zlabel("Channel")
ax.set_title("Point cloud for the first X_jet Image")

plt.show()
```



Converting the dataset to a graph format

```
dataset = []

for i, x in enumerate(X_jets):
  flattened = x.reshape(-1,3)
  non_zero = np.any(flattened != (0,0,0), axis = -1)
  node = flattened[non_zero]
  edges = kneighbors_graph(node, 4, mode = 'connectivity',include_self
= True)
  edges = edges.tocoo()
  data = Data(x=torch.from_numpy(node),
edge_index=torch.from_numpy(np.vstack((edges.row,edges.col))).type(tor
ch.long), edge_attr=torch.from_numpy(edges.data.reshape(-1,1)),
y=torch.tensor([int(y[i])]))
  dataset.append(data)


print(f'Number of graphs: {len(dataset)}')
print(f'Number of nodes: {dataset[0].num_nodes}')
print(f'Number of edges: {dataset[0].num_edges}')
print(f'Number of node features: {dataset[0].num_node_features}')
print(f'Number of edges features: {dataset[0].num_edge_features}')
print(dataset[0])
```

```
Number of graphs: 5000
Number of nodes: 884
Number of edges: 3536
Number of node features: 3
Number of edges features: 1
Data(x=[884, 3], edge_index=[2, 3536], edge_attr=[3536, 1], y=[1])
```

Splitting the dataset to train, test and validation split

```
train_loader = DataLoader(dataset[:4000], batch_size=32, shuffle=True)
test_loader = DataLoader(dataset[3000:4000], batch_size=32,
shuffle=False)
val_loader = DataLoader(dataset[4000:], batch_size = 32, shuffle =
False)
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
```

Defining the traing and evaluation functions

```
def train(model,loader,optimizer,criterion):
    model.train()
    correct = 0
    for data in loader:  # Iterate in batches over the training 
dataset.

         data = data.to(device)
         out = model(data.x, data.edge_index, data.batch)  # Perform a 
single forward pass.
         loss = criterion(out, data.y) # Compute the loss.
         loss.backward()  # Derive gradients.
         optimizer.step()  # Update parameters based on gradients.
         optimizer.zero_grad()  # Clear gradients.
         pred = out.argmax(dim=1)  # Use the class with highest 
probability.
         correct += int((pred == data.y).sum())  # Check against 
ground-truth labels.
    return loss, correct / len(loader.dataset)
def val(model,loader,optimizer,criterion):
  model.eval()
  correct = 0
  with torch.no_grad():
    for data in loader:
      data = data.to(device)
      out = model(data.x, data.edge_index, data.batch)
      loss = criterion(out, data.y) # Compute the loss.
      pred = out.argmax(dim=1)  # Use the class with highest 
probability.
      correct += int((pred == data.y).sum())  # Check against ground-
truth labels.
    return loss, correct / len(loader.dataset)
```

Defining and traing Model 1

This model is based on Graph Convolution.

```
class GCN(torch.nn.Module):
  def __init__(self, hidden_channels):
    super(GCN, self).__init__()
    torch.manual_seed(42)
    self.conv1 = GCNConv(dataset[0].num_node_features, 
hidden_channels)
    self.conv2 = GCNConv(hidden_channels, 2*hidden_channels)
    self.lin = Linear(2*hidden_channels, 2)
```

```
  def forward(self, x, edge_index, batch):
    x = self.conv1(x, edge_index)
    x = x.relu()
    x = self.conv2(x, edge_index)
    x = global_mean_pool(x, batch)

    x = F.dropout(x, p = 0.5, training = self.training)
    x = self.lin(x)

    return x

model = GCN(hidden_channels = 32).to(device)
print(model)
```

```
GCN(
  (conv1): GCNConv(3, 32)
  (conv2): GCNConv(32, 64)
  (lin): Linear(in_features=64, out_features=2, bias=True)
)
```

```
optimizer = torch.optim.Adam(model.parameters(), lr=0.001)
criterion = torch.nn.CrossEntropyLoss().to(device)
best_valid_loss = float('inf')

for epoch in range(1, 31):
    train_loss, train_acc =
train(model,train_loader,optimizer,criterion)
    val_loss, val_acc = val(model,val_loader,optimizer,criterion)
    if val_loss < best_valid_loss:
        best_valid_loss = val_loss
        torch.save(model.state_dict(), 'gcn-model.pt')
    print(f'Epoch: {epoch:03d},Train Loss: {train_loss:.4f}, Train
Acc: {train_acc:.4f}, Val Loss: {val_loss:.4f} Val Acc :
{val_acc:.4f}')
```

```
Epoch: 001,Train Loss: 0.7006, Train Acc: 0.4915, Val Loss: 0.6971 Val
Acc : 0.5120
Epoch: 002,Train Loss: 0.6908, Train Acc: 0.5252, Val Loss: 0.6942 Val
Acc : 0.5230
Epoch: 003,Train Loss: 0.6893, Train Acc: 0.5423, Val Loss: 0.6731 Val
Acc : 0.4880
Epoch: 004,Train Loss: 0.6773, Train Acc: 0.5555, Val Loss: 0.6725 Val
Acc : 0.6650
Epoch: 005,Train Loss: 0.6609, Train Acc: 0.6222, Val Loss: 0.6335 Val
Acc : 0.7020
Epoch: 006,Train Loss: 0.6578, Train Acc: 0.6538, Val Loss: 0.5882 Val
Acc : 0.7070
Epoch: 007,Train Loss: 0.5705, Train Acc: 0.6610, Val Loss: 0.5452 Val
Acc : 0.7050
Epoch: 008,Train Loss: 0.6157, Train Acc: 0.6690, Val Loss: 0.5288 Val
```

```
Acc : 0.6970
Epoch: 009,Train Loss: 0.6256, Train Acc: 0.6715, Val Loss: 0.5256 Val
Acc : 0.6840
Epoch: 010,Train Loss: 0.5839, Train Acc: 0.6730, Val Loss: 0.5009 Val
Acc : 0.7010
Epoch: 011,Train Loss: 0.5880, Train Acc: 0.6753, Val Loss: 0.4981 Val
Acc : 0.7010
Epoch: 012,Train Loss: 0.7440, Train Acc: 0.6675, Val Loss: 0.4930 Val
Acc : 0.7020
Epoch: 013,Train Loss: 0.6542, Train Acc: 0.6710, Val Loss: 0.4878 Val
Acc : 0.7070
Epoch: 014,Train Loss: 0.7517, Train Acc: 0.6750, Val Loss: 0.4953 Val
Acc : 0.6990
Epoch: 015,Train Loss: 0.6512, Train Acc: 0.6715, Val Loss: 0.4832 Val
Acc : 0.7090
Epoch: 016,Train Loss: 0.6724, Train Acc: 0.6707, Val Loss: 0.4897 Val
Acc : 0.7040
Epoch: 017,Train Loss: 0.5903, Train Acc: 0.6740, Val Loss: 0.4839 Val
Acc : 0.7050
Epoch: 018,Train Loss: 0.5905, Train Acc: 0.6735, Val Loss: 0.4811 Val
Acc : 0.7060
Epoch: 019,Train Loss: 0.5423, Train Acc: 0.6807, Val Loss: 0.4973 Val
Acc : 0.6950
Epoch: 020,Train Loss: 0.5777, Train Acc: 0.6743, Val Loss: 0.5105 Val
Acc : 0.6780
Epoch: 021,Train Loss: 0.7218, Train Acc: 0.6757, Val Loss: 0.4826 Val
Acc : 0.7060
Epoch: 022,Train Loss: 0.5787, Train Acc: 0.6775, Val Loss: 0.4716 Val
Acc : 0.7110
Epoch: 023,Train Loss: 0.5953, Train Acc: 0.6710, Val Loss: 0.4789 Val
Acc : 0.7100
Epoch: 024,Train Loss: 0.7579, Train Acc: 0.6755, Val Loss: 0.4879 Val
Acc : 0.7030
Epoch: 025,Train Loss: 0.5673, Train Acc: 0.6727, Val Loss: 0.4801 Val
Acc : 0.7070
Epoch: 026,Train Loss: 0.5082, Train Acc: 0.6783, Val Loss: 0.4796 Val
Acc : 0.7080
Epoch: 027,Train Loss: 0.7786, Train Acc: 0.6777, Val Loss: 0.4940 Val
Acc : 0.6940
Epoch: 028,Train Loss: 0.5185, Train Acc: 0.6743, Val Loss: 0.4701 Val
Acc : 0.7100
Epoch: 029,Train Loss: 0.6405, Train Acc: 0.6720, Val Loss: 0.4912 Val
Acc : 0.6960
Epoch: 030,Train Loss: 0.6003, Train Acc: 0.6720, Val Loss: 0.4770 Val
Acc : 0.7140
```

```
model.load_state_dict(torch.load('gcn-model.pt'))

test_loss, test_acc = val(model,test_loader,optimizer,criterion)
print(f'Test Loss: {test_loss:.3f} | Test Acc: {test_acc:.4f}')
```

```
Test Loss: 0.446 | Test Acc: 0.6880
```

Defining and traing Model 2

This model is based on Graph Attention.

```
class GAT(torch.nn.Module):
  def __init__(self, hidden_channels):
    super(GAT, self).__init__()
    torch.manual_seed(42)
    self.conv1 = GATConv(dataset[0].num_node_features,
hidden_channels)
    self.conv2 = GATConv(hidden_channels, 2*hidden_channels)
    self.lin = Linear(2*hidden_channels, 2)

  def forward(self, x, edge_index, batch):
    x = self.conv1(x, edge_index)
    x = F.elu(x)
    x = self.conv2(x, edge_index)
    x = global_mean_pool(x, batch)

    x = F.dropout(x, p = 0.5, training = self.training)
    x = self.lin(x)

    return F.log_softmax(x, dim = 1)

model_2 = GAT(hidden_channels = 32).to(device)
print(model_2)

GAT(
  (conv1): GATConv(3, 32, heads=1)
  (conv2): GATConv(32, 64, heads=1)
  (lin): Linear(in_features=64, out_features=2, bias=True)
)

optimizer = torch.optim.Adam(model_2.parameters(), lr=0.001)
criterion = torch.nn.CrossEntropyLoss().to(device)
best_valid_loss = float('inf')

for epoch in range(1, 31):
    train_loss, train_acc =
train(model_2,train_loader,optimizer,criterion)
    val_loss, val_acc = val(model_2,val_loader,optimizer,criterion)
    if val_loss < best_valid_loss:
        best_valid_loss = val_loss
        torch.save(model_2.state_dict(), 'gat-model.pt')
    print(f'Epoch: {epoch:03d},Train Loss: {train_loss:.4f}, Train
```

```
Acc: {train_acc:.4f}, Val Loss: {val_loss:.4f} Val Acc :
{val_acc:.4f}')
```

```
Epoch: 001,Train Loss: 0.6944, Train Acc: 0.4948, Val Loss: 0.6968 Val
Acc : 0.5120
Epoch: 002,Train Loss: 0.6935, Train Acc: 0.4983, Val Loss: 0.6944 Val
Acc : 0.5120
Epoch: 003,Train Loss: 0.6937, Train Acc: 0.4985, Val Loss: 0.6923 Val
Acc : 0.4880
Epoch: 004,Train Loss: 0.6923, Train Acc: 0.5082, Val Loss: 0.6905 Val
Acc : 0.4880
Epoch: 005,Train Loss: 0.6894, Train Acc: 0.5065, Val Loss: 0.6905 Val
Acc : 0.4880
Epoch: 006,Train Loss: 0.6945, Train Acc: 0.5088, Val Loss: 0.6908 Val
Acc : 0.4880
Epoch: 007,Train Loss: 0.6926, Train Acc: 0.5140, Val Loss: 0.6919 Val
Acc : 0.5170
Epoch: 008,Train Loss: 0.6954, Train Acc: 0.5045, Val Loss: 0.6891 Val
Acc : 0.4880
Epoch: 009,Train Loss: 0.6940, Train Acc: 0.5232, Val Loss: 0.6863 Val
Acc : 0.4880
Epoch: 010,Train Loss: 0.6931, Train Acc: 0.5268, Val Loss: 0.6919 Val
Acc : 0.5520
Epoch: 011,Train Loss: 0.6897, Train Acc: 0.5523, Val Loss: 0.6877 Val
Acc : 0.5810
Epoch: 012,Train Loss: 0.6929, Train Acc: 0.5515, Val Loss: 0.6657 Val
Acc : 0.4880
Epoch: 013,Train Loss: 0.6767, Train Acc: 0.5893, Val Loss: 0.6518 Val
Acc : 0.6970
Epoch: 014,Train Loss: 0.6489, Train Acc: 0.6012, Val Loss: 0.6112 Val
Acc : 0.7050
Epoch: 015,Train Loss: 0.6272, Train Acc: 0.6418, Val Loss: 0.5962 Val
Acc : 0.6480
Epoch: 016,Train Loss: 0.5246, Train Acc: 0.6428, Val Loss: 0.5956 Val
Acc : 0.6180
Epoch: 017,Train Loss: 0.6363, Train Acc: 0.6520, Val Loss: 0.5011 Val
Acc : 0.5590
Epoch: 018,Train Loss: 0.6048, Train Acc: 0.6475, Val Loss: 0.5123 Val
Acc : 0.6930
Epoch: 019,Train Loss: 0.6044, Train Acc: 0.6687, Val Loss: 0.4900 Val
Acc : 0.7050
Epoch: 020,Train Loss: 0.5652, Train Acc: 0.6567, Val Loss: 0.4938 Val
Acc : 0.7020
Epoch: 021,Train Loss: 0.5309, Train Acc: 0.6677, Val Loss: 0.4803 Val
Acc : 0.7050
Epoch: 022,Train Loss: 0.6795, Train Acc: 0.6630, Val Loss: 0.5228 Val
Acc : 0.6650
Epoch: 023,Train Loss: 0.6739, Train Acc: 0.6643, Val Loss: 0.4725 Val
Acc : 0.6850
Epoch: 024,Train Loss: 0.6455, Train Acc: 0.6600, Val Loss: 0.4921 Val
```

```
Acc : 0.6960
Epoch: 025,Train Loss: 0.7643, Train Acc: 0.6653, Val Loss: 0.5414 Val
Acc : 0.6500
Epoch: 026,Train Loss: 0.6586, Train Acc: 0.6647, Val Loss: 0.4779 Val
Acc : 0.7120
Epoch: 027,Train Loss: 0.6634, Train Acc: 0.6590, Val Loss: 0.5033 Val
Acc : 0.6760
Epoch: 028,Train Loss: 0.5862, Train Acc: 0.6675, Val Loss: 0.4750 Val
Acc : 0.7060
Epoch: 029,Train Loss: 0.7920, Train Acc: 0.6597, Val Loss: 0.4847 Val
Acc : 0.7040
Epoch: 030,Train Loss: 0.7898, Train Acc: 0.6647, Val Loss: 0.4830 Val
Acc : 0.7080
```

```
model_2.load_state_dict(torch.load('gat-model.pt'))

test_loss, test_acc = val(model_2,test_loader,optimizer,criterion)
print(f'Test Loss: {test_loss:.3f} | Test Acc: {test_acc:.4f}')
```

```
Test Loss: 0.484 | Test Acc: 0.6700
```

Defining and traing Model 3 (Selected model)

This model is based on Graph Sage.

```
class GSage(torch.nn.Module):
  def __init__(self, hidden_channels):
    super(GSage, self).__init__()
    torch.manual_seed(42)
    self.conv1 = SAGEConv(3, hidden_channels)
    self.conv2 = SAGEConv(hidden_channels, 2*hidden_channels)
    self.lin = Linear(2*hidden_channels, 2)

  def forward(self, x, edge_index, batch):
    x = self.conv1(x, edge_index)
    x = F.relu(x)
    x = self.conv2(x, edge_index)
    x = global_mean_pool(x, batch)

    x = F.dropout(x, p = 0.5, training = self.training)
    x = self.lin(x)

    return x
model_3 = GSage(hidden_channels = 32).to(device)
print(model_3)
```

```
GSage(
  (conv1): SAGEConv(3, 32, aggr=mean)
```

```
  (conv2): SAGEConv(32, 64, aggr=mean)
  (lin): Linear(in_features=64, out_features=2, bias=True)
)

optimizer = torch.optim.Adam(model_3.parameters(), lr=0.001)
criterion = torch.nn.CrossEntropyLoss().to(device)
best_valid_loss = float('inf')

for epoch in range(1, 31):
    train_loss, train_acc = 
train(model_3,train_loader,optimizer,criterion)
    val_loss, val_acc = val(model_3,val_loader,optimizer,criterion)
    if val_loss < best_valid_loss:
        best_valid_loss = val_loss
        torch.save(model_3.state_dict(), 'sage-model.pt')
    print(f'Epoch: {epoch:03d},Train Loss: {train_loss:.4f}, Train 
Acc: {train_acc:.4f}, Val Loss: {val_loss:.4f} Val Acc : 
{val_acc:.4f}')

Epoch: 001,Train Loss: 0.6937, Train Acc: 0.5140, Val Loss: 0.6966 Val 
Acc : 0.5380
Epoch: 002,Train Loss: 0.6898, Train Acc: 0.5260, Val Loss: 0.7064 Val 
Acc : 0.5150
Epoch: 003,Train Loss: 0.6738, Train Acc: 0.5317, Val Loss: 0.6845 Val 
Acc : 0.6100
Epoch: 004,Train Loss: 0.6840, Train Acc: 0.5635, Val Loss: 0.6637 Val 
Acc : 0.6460
Epoch: 005,Train Loss: 0.6556, Train Acc: 0.6185, Val Loss: 0.6435 Val 
Acc : 0.6470
Epoch: 006,Train Loss: 0.6409, Train Acc: 0.6300, Val Loss: 0.6360 Val 
Acc : 0.6360
Epoch: 007,Train Loss: 0.6852, Train Acc: 0.6558, Val Loss: 0.5494 Val 
Acc : 0.6910
Epoch: 008,Train Loss: 0.6403, Train Acc: 0.6657, Val Loss: 0.5370 Val 
Acc : 0.6980
Epoch: 009,Train Loss: 0.5904, Train Acc: 0.6660, Val Loss: 0.5196 Val 
Acc : 0.7020
Epoch: 010,Train Loss: 0.6256, Train Acc: 0.6663, Val Loss: 0.4917 Val 
Acc : 0.7040
Epoch: 011,Train Loss: 0.5668, Train Acc: 0.6717, Val Loss: 0.4955 Val 
Acc : 0.7240
Epoch: 012,Train Loss: 0.5500, Train Acc: 0.6815, Val Loss: 0.5076 Val 
Acc : 0.7040
Epoch: 013,Train Loss: 0.4873, Train Acc: 0.6743, Val Loss: 0.4894 Val 
Acc : 0.7210
Epoch: 014,Train Loss: 0.6331, Train Acc: 0.6827, Val Loss: 0.4807 Val 
Acc : 0.7250
Epoch: 015,Train Loss: 0.6479, Train Acc: 0.6805, Val Loss: 0.4796 Val 
Acc : 0.7270
Epoch: 016,Train Loss: 0.6427, Train Acc: 0.6837, Val Loss: 0.4785 Val 
```

```
Acc : 0.7230
Epoch: 017,Train Loss: 0.6041, Train Acc: 0.6850, Val Loss: 0.4785 Val
Acc : 0.7260
Epoch: 018,Train Loss: 0.6415, Train Acc: 0.6797, Val Loss: 0.4909 Val
Acc : 0.7210
Epoch: 019,Train Loss: 0.5670, Train Acc: 0.6777, Val Loss: 0.4769 Val
Acc : 0.7270
Epoch: 020,Train Loss: 0.6566, Train Acc: 0.6823, Val Loss: 0.5128 Val
Acc : 0.6920
Epoch: 021,Train Loss: 0.5851, Train Acc: 0.6890, Val Loss: 0.4880 Val
Acc : 0.7230
Epoch: 022,Train Loss: 0.5765, Train Acc: 0.6863, Val Loss: 0.4946 Val
Acc : 0.7130
Epoch: 023,Train Loss: 0.6066, Train Acc: 0.6805, Val Loss: 0.4836 Val
Acc : 0.7230
Epoch: 024,Train Loss: 0.6982, Train Acc: 0.6795, Val Loss: 0.4779 Val
Acc : 0.7260
Epoch: 025,Train Loss: 0.5577, Train Acc: 0.6843, Val Loss: 0.4875 Val
Acc : 0.7240
Epoch: 026,Train Loss: 0.5674, Train Acc: 0.6853, Val Loss: 0.4860 Val
Acc : 0.7200
Epoch: 027,Train Loss: 0.5357, Train Acc: 0.6797, Val Loss: 0.4948 Val
Acc : 0.7120
Epoch: 028,Train Loss: 0.5392, Train Acc: 0.6830, Val Loss: 0.4712 Val
Acc : 0.7240
Epoch: 029,Train Loss: 0.6296, Train Acc: 0.6817, Val Loss: 0.4710 Val
Acc : 0.7210
Epoch: 030,Train Loss: 0.6185, Train Acc: 0.6847, Val Loss: 0.4770 Val
Acc : 0.7260
```

```
model_3.load_state_dict(torch.load('sage-model.pt'))
```

```
test_loss, test_acc = val(model_3,test_loader,optimizer,criterion)
print(f'Test Loss: {test_loss:.3f} | Test Acc: {test_acc:.4f}')
```

```
Test Loss: 0.450 | Test Acc: 0.6990
```

Method-2 : Normalizing the Jets

Here I am normalizing the jets considering only the non-zero element

```
#Reloading the data due to indexing error
with h5py.File(path, 'r') as f:
  X_jet = np.array(f['X_jets'][:5000])
  label = np.array(f['y'][:5000])

# Calculate mean and standard deviation for non-zero pixels for each
channel
```

```
mean_non_zero_track = np.mean(X_jet[X_jet[:,:,:,0] != 0])
std_non_zero_track = np.std(X_jet[X_jet[:,:,:,0] != 0])

mean_non_zero_ecal = np.mean(X_jet[X_jet[:,:,:,1] != 0])
std_non_zero_ecal = np.std(X_jet[X_jet[:,:,:,1] != 0])

mean_non_zero_hcal = np.mean(X_jet[X_jet[:,:,:,2] != 0])
std_non_zero_hcal = np.std(X_jet[X_jet[:,:,:,2] != 0])

non_zero_pixels_track = X_jet[:,:,:,0] != 0
non_zero_pixels_ecal = X_jet[:,:,:,1] != 0
non_zero_pixels_hcal = X_jet[:,:,:,2] != 0
# Normalize non-zero pixels for each channel
normalized_track = np.zeros_like(X_jet)
normalized_track[non_zero_pixels_track] =
(X_jet[non_zero_pixels_track] - mean_non_zero_track) /
std_non_zero_track

normalized_ecal = np.zeros_like(X_jet)
normalized_ecal[non_zero_pixels_ecal] = (X_jet[non_zero_pixels_ecal] -
mean_non_zero_ecal) / std_non_zero_ecal

normalized_hcal = np.zeros_like(X_jet)
normalized_hcal[non_zero_pixels_hcal] = (X_jet[non_zero_pixels_hcal] -
mean_non_zero_hcal) / std_non_zero_hcal

# Combine the normalized channels back into an image with three
channels
normalized_jets = normalized_track + normalized_ecal + normalized_hcal

dataset = []
for i, x in enumerate(normalized_jets):
  flattened = x.reshape(-1,3)
  non_zero = np.any(flattened != (0,0,0), axis = -1) # Removing any
zero element by considering only non zero ones
  node = flattened[non_zero]
  edges = kneighbors_graph(node, 4, mode = 'connectivity',include_self
= True)
  edges = edges.tocoo()
  y = torch.tensor([int(label[i])], dtype=torch.long)
  data = Data(x=torch.from_numpy(node),
edge_index=torch.from_numpy(np.vstack((edges.row,edges.col))).type(tor
ch.long), edge_attr=torch.from_numpy(edges.data.reshape(-1,1)), y=y)
  dataset.append(data)

train_loader = DataLoader(dataset[:4000], batch_size=32, shuffle=True)
test_loader = DataLoader(dataset[3000:4000], batch_size=32,
shuffle=False)
val_loader = DataLoader(dataset[4000:], batch_size = 32, shuffle =
False)
```

```
model_norm = GSage(hidden_channels = 32).to(device)
optimizer = torch.optim.Adam(model_norm.parameters(), lr=0.001)
criterion = torch.nn.CrossEntropyLoss().to(device)
best_valid_loss = float('inf')
for epoch in range(1, 31):
    train_loss, train_acc =
train(model_norm,train_loader,optimizer,criterion)
    val_loss, val_acc = val(model_norm,val_loader,optimizer,criterion)
    if val_loss < best_valid_loss:
        best_valid_loss = val_loss
        torch.save(model_norm.state_dict(), 'sage-model-norm.pt')
    print(f'Epoch: {epoch:03d},Train Loss: {train_loss:.4f}, Train
Acc: {train_acc:.4f}, Val Loss: {val_loss:.4f} Val Acc :
{val_acc:.4f}')
```

```
Epoch: 001,Train Loss: 0.6120, Train Acc: 0.6180, Val Loss: 0.5382 Val
Acc : 0.6810
Epoch: 002,Train Loss: 0.7164, Train Acc: 0.6593, Val Loss: 0.5263 Val
Acc : 0.6780
Epoch: 003,Train Loss: 0.6547, Train Acc: 0.6520, Val Loss: 0.5097 Val
Acc : 0.6920
Epoch: 004,Train Loss: 0.7080, Train Acc: 0.6645, Val Loss: 0.5027 Val
Acc : 0.6930
Epoch: 005,Train Loss: 0.6459, Train Acc: 0.6653, Val Loss: 0.5061 Val
Acc : 0.6940
Epoch: 006,Train Loss: 0.6592, Train Acc: 0.6623, Val Loss: 0.5142 Val
Acc : 0.6880
Epoch: 007,Train Loss: 0.6115, Train Acc: 0.6627, Val Loss: 0.5073 Val
Acc : 0.6920
Epoch: 008,Train Loss: 0.6398, Train Acc: 0.6695, Val Loss: 0.5068 Val
Acc : 0.6930
Epoch: 009,Train Loss: 0.6372, Train Acc: 0.6657, Val Loss: 0.4916 Val
Acc : 0.7090
Epoch: 010,Train Loss: 0.5884, Train Acc: 0.6615, Val Loss: 0.4936 Val
Acc : 0.7060
Epoch: 011,Train Loss: 0.5894, Train Acc: 0.6610, Val Loss: 0.5029 Val
Acc : 0.6990
Epoch: 012,Train Loss: 0.5404, Train Acc: 0.6663, Val Loss: 0.5140 Val
Acc : 0.6930
Epoch: 013,Train Loss: 0.5267, Train Acc: 0.6655, Val Loss: 0.5086 Val
Acc : 0.7010
Epoch: 014,Train Loss: 0.5815, Train Acc: 0.6710, Val Loss: 0.4894 Val
Acc : 0.7120
Epoch: 015,Train Loss: 0.6436, Train Acc: 0.6680, Val Loss: 0.4916 Val
Acc : 0.7120
Epoch: 016,Train Loss: 0.6301, Train Acc: 0.6695, Val Loss: 0.4889 Val
Acc : 0.7120
Epoch: 017,Train Loss: 0.6117, Train Acc: 0.6703, Val Loss: 0.4928 Val
Acc : 0.7150
Epoch: 018,Train Loss: 0.6146, Train Acc: 0.6743, Val Loss: 0.5134 Val
```

```
Acc : 0.7080
Epoch: 019,Train Loss: 0.6291, Train Acc: 0.6690, Val Loss: 0.4949 Val
Acc : 0.7140
Epoch: 020,Train Loss: 0.6275, Train Acc: 0.6695, Val Loss: 0.5528 Val
Acc : 0.6850
Epoch: 021,Train Loss: 0.5712, Train Acc: 0.6723, Val Loss: 0.5266 Val
Acc : 0.7120
Epoch: 022,Train Loss: 0.5863, Train Acc: 0.6743, Val Loss: 0.5151 Val
Acc : 0.7150
Epoch: 023,Train Loss: 0.5864, Train Acc: 0.6775, Val Loss: 0.5174 Val
Acc : 0.7160
Epoch: 024,Train Loss: 0.7502, Train Acc: 0.6725, Val Loss: 0.5055 Val
Acc : 0.7130
Epoch: 025,Train Loss: 0.5484, Train Acc: 0.6780, Val Loss: 0.5385 Val
Acc : 0.7150
Epoch: 026,Train Loss: 0.5569, Train Acc: 0.6750, Val Loss: 0.5304 Val
Acc : 0.7070
Epoch: 027,Train Loss: 0.5501, Train Acc: 0.6703, Val Loss: 0.5410 Val
Acc : 0.7030
Epoch: 028,Train Loss: 0.5643, Train Acc: 0.6727, Val Loss: 0.4964 Val
Acc : 0.7070
Epoch: 029,Train Loss: 0.5953, Train Acc: 0.6693, Val Loss: 0.4937 Val
Acc : 0.7200
Epoch: 030,Train Loss: 0.6234, Train Acc: 0.6830, Val Loss: 0.5029 Val
Acc : 0.7170
```

```
model_norm.load_state_dict(torch.load('sage-model-norm.pt'))
```

```
test_loss, test_acc = val(model_norm,test_loader,optimizer,criterion)
print(f'Test Loss: {test_loss:.3f} | Test Acc: {test_acc:.4f}')
```

```
Test Loss: 0.481 | Test Acc: 0.6820
```

Discussion

The final architecture choosen here is the Graph Sage architecture.

- Firstly, among all three architectures we experimented on Graph Sage performed just slightly better.
- From a computational point of view Graph Sage is much more efficient than the other two architectures as it samples and aggregates the features of neighbors of a node.
- Although the performance between the models is more or less the same here, it can change when we use large batches or use a bigger subset of data, or tune the -hyperparameter.

- I tried using global_mean_pool to aggregate the node features and provide a global graph vector but there are more efficient methods to do that such as using mincut pooling and more.
- Also normalizing the jets didn't improve anything. This may be because the Jets are raw sensor data in physical space and as such standard preprocessing may not be the same here as it is for an RGB image.