gcnconv-final

March 26, 2024

[1]:
```python
import torch
import numpy as np
import pandas as pd
import pyarrow.parquet as pq
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split

import torch
import torch.nn as nn
from torch.utils.data import Dataset,DataLoader, random_split
import torch.nn.functional as F
from torchvision import models

import torch.optim as optim
from tqdm import tqdm

from sklearn.metrics import roc_auc_score, confusion_matrix ,roc_curve
import seaborn as sns
```

[2]:
```
!pip install torch_geometric
!pip install networkx
```

```
Collecting torch_geometric
  Downloading torch_geometric-2.5.2-py3-none-any.whl.metadata (64 kB)
                           64.2/64.2 kB
3.7 MB/s eta 0:00:00
Requirement already satisfied: tqdm in /opt/conda/lib/python3.10/site-
packages (from torch_geometric) (4.66.1)
Requirement already satisfied: numpy in /opt/conda/lib/python3.10/site-packages
(from torch_geometric) (1.26.4)
Requirement already satisfied: scipy in /opt/conda/lib/python3.10/site-packages
(from torch_geometric) (1.11.4)
Requirement already satisfied: fsspec in /opt/conda/lib/python3.10/site-packages
(from torch_geometric) (2024.3.0)
Requirement already satisfied: jinja2 in /opt/conda/lib/python3.10/site-packages
(from torch_geometric) (3.1.2)
Requirement already satisfied: aiohttp in /opt/conda/lib/python3.10/site-
packages (from torch_geometric) (3.9.1)
```

```
Requirement already satisfied: requests in /opt/conda/lib/python3.10/site-
packages (from torch_geometric) (2.31.0)
Requirement already satisfied: pyparsing in /opt/conda/lib/python3.10/site-
packages (from torch_geometric) (3.1.1)
Requirement already satisfied: scikit-learn in /opt/conda/lib/python3.10/site-
packages (from torch_geometric) (1.2.2)
Requirement already satisfied: psutil>=5.8.0 in /opt/conda/lib/python3.10/site-
packages (from torch_geometric) (5.9.3)
Requirement already satisfied: attrs>=17.3.0 in /opt/conda/lib/python3.10/site-
packages (from aiohttp->torch_geometric) (23.2.0)
Requirement already satisfied: multidict<7.0,>=4.5 in
/opt/conda/lib/python3.10/site-packages (from aiohttp->torch_geometric) (6.0.4)
Requirement already satisfied: yarl<2.0,>=1.0 in /opt/conda/lib/python3.10/site-
packages (from aiohttp->torch_geometric) (1.9.3)
Requirement already satisfied: frozenlist>=1.1.1 in
/opt/conda/lib/python3.10/site-packages (from aiohttp->torch_geometric) (1.4.1)
Requirement already satisfied: aiosignal>=1.1.2 in
/opt/conda/lib/python3.10/site-packages (from aiohttp->torch_geometric) (1.3.1)
Requirement already satisfied: async-timeout<5.0,>=4.0 in
/opt/conda/lib/python3.10/site-packages (from aiohttp->torch_geometric) (4.0.3)
Requirement already satisfied: MarkupSafe>=2.0 in
/opt/conda/lib/python3.10/site-packages (from jinja2->torch_geometric) (2.1.3)
Requirement already satisfied: charset-normalizer<4,>=2 in
/opt/conda/lib/python3.10/site-packages (from requests->torch_geometric) (3.3.2)
Requirement already satisfied: idna<4,>=2.5 in /opt/conda/lib/python3.10/site-
packages (from requests->torch_geometric) (3.6)
Requirement already satisfied: urllib3<3,>=1.21.1 in
/opt/conda/lib/python3.10/site-packages (from requests->torch_geometric)
(1.26.18)
Requirement already satisfied: certifi>=2017.4.17 in
/opt/conda/lib/python3.10/site-packages (from requests->torch_geometric)
(2024.2.2)
Requirement already satisfied: joblib>=1.1.1 in /opt/conda/lib/python3.10/site-
packages (from scikit-learn->torch_geometric) (1.3.2)
Requirement already satisfied: threadpoolctl>=2.0.0 in
/opt/conda/lib/python3.10/site-packages (from scikit-learn->torch_geometric)
(3.2.0)
Downloading torch_geometric-2.5.2-py3-none-any.whl (1.1 MB)
                         1.1/1.1 MB
30.7 MB/s eta 0:00:00
Installing collected packages: torch_geometric
Successfully installed torch_geometric-2.5.2
Requirement already satisfied: networkx in /opt/conda/lib/python3.10/site-
packages (3.2.1)
```

[3]:
```
from torch_geometric.data import Data
from sklearn.neighbors import kneighbors_graph
```

```
from torch_geometric.data import Dataset, Data, DataLoader
from sklearn.metrics import mean_squared_error
from sklearn.neighbors import NearestNeighbors
import networkx as nx
from torch_geometric.utils import to_networkx



from torch_geometric.loader import DataLoader
from torch_geometric.nn import GCNConv, global_mean_pool
from torch.nn import Linear
import torch.nn.functional as F
from torch.utils.data import random_split
```

[4]:

```
chunk_size = 25

# List of Parquet file paths
file_paths = [
    '/kaggle/input/task2-24/QCDToGGQQ_IMGjet_RH1all_jet0_run0_n36272.test.
 ↪snappy.parquet',
    '/kaggle/input/task2-24/QCDToGGQQ_IMGjet_RH1all_jet0_run1_n47540.test.
 ↪snappy.parquet',
    '/kaggle/input/task2-24/QCDToGGQQ_IMGjet_RH1all_jet0_run2_n55494.test.
 ↪snappy.parquet'
]

# Initialize an empty list to store dataframes
dfs = []

# Loop through each file path
for file_path in file_paths:
    # Create a Parquet file reader object
    parquet_file = pq.ParquetFile(file_path)

    # Determine the total number of rows in the file
    total_rows = parquet_file.metadata.num_rows

    # Calculate the number of chunks
    num_chunks = total_rows // chunk_size + (1 if total_rows % chunk_size else␣
 ↪0)

    # Loop over the file in chunks
    for chunk_index in range(num_chunks):
        # Read a chunk of rows from the file
        chunk = parquet_file.read_row_group(chunk_index, columns=None)
        df = chunk.to_pandas()
```

```
        # Append the DataFrame to the list
        dfs.append(df)

# Concatenate all the DataFrames into a single DataFrame
data = pd.concat(dfs, ignore_index=True)
```

[5]:
```
def to_3d(arr):
    vishak=[]
    for i in range (0,3):
        vis=np.stack(np.stack(arr)[i],axis=-1)
        vishak.append(vis)
    vishak=np.array(vishak)
    return vishak
```

[6]:
```
data["X_jets"]  = data["X_jets"].apply(to_3d)
```

[7]:
```
def image_to_graph(image, patch_size=5, n_neighbors=5):
        """
        Convert an image to a graph of its 5x5 patches.

        Parameters:
        - image: A (125, 125, 3) numpy array.
        - patch_size: Size of the square patches (default 5).
        - n_neighbors: Number of neighbors for KNN (default 5).

        Returns:
        - nodes: An array of node features.
        - edges: A list of tuples (i, j, mse) representing edges and their MSE.
        """
        # Validate image shape

        assert image.shape[0] == image.shape[1], "Image must be square."

        # Number of patches along one dimension
        num_patches = image.shape[0] // patch_size

        # Initialize nodes and edges
        nodes = []
        edges = []

        # Create patches and flatten them to create node features
        for i in range(0, image.shape[0], patch_size):
            for j in range(0, image.shape[1], patch_size):
                patch = image[i:i+patch_size, j:j+patch_size, :].reshape(-1)
                nodes.append(patch)

        nodes = np.array(nodes)
```

```
        # Use KNN to find nearest neighbors for each node
        nbrs = NearestNeighbors(n_neighbors=n_neighbors+1,␣
↪algorithm='ball_tree').fit(nodes)
        distances, indices = nbrs.kneighbors(nodes)

        # Calculate MSE for each pair of neighbors and create edges
        for i in range(indices.shape[0]):
            for j in range(1, indices.shape[1]):  # Start from 1 to skip␣
↪self-connection
                mse = mean_squared_error(nodes[i], nodes[indices[i, j]])
                edges.append((i, indices[i, j], mse))

        return nodes, edges
```

[8]:
```
class QuarkGluonDataset(Dataset):

    def __init__(self, dataframe, root='', transform=None, pre_transform=None):
        """
        Custom dataset for quarks and gluons classification.

        Parameters:
        - image_list: A list of (125, 125, 3) numpy arrays.
        - labels: A list of integers (0 or 1) representing the class labels for␣
↪the images.
        """
        self.dataframe = dataframe
        super(QuarkGluonDataset, self).__init__(root, transform, pre_transform)


    def len(self):
        return len(self.dataframe)

    def get(self, idx):
        # Convert an image to graph data
        image = self.dataframe.iloc[idx]['X_jets']
        image = image.transpose(1,2,0)
        label = self.dataframe.iloc[idx]['y']
#          print(type(image))
        nodes, edges = image_to_graph(image)

        # Convert to PyTorch tensors
        x = torch.tensor(nodes, dtype=torch.float)  # Node features
        edge_index = torch.tensor([(i, j) for i, j, _ in edges], dtype=torch.
↪long).t().contiguous()  # Edge indices
        edge_attr = torch.tensor([mse for _, _, mse in edges], dtype=torch.
↪float).unsqueeze(1)  # Edge attributes
```

```
        y = torch.tensor([label], dtype=torch.long)  # Label

        return Data(x=x, edge_index=edge_index, edge_attr=edge_attr, y=y)
```

[9]:
```
dataset = QuarkGluonDataset(data)
```

[10]:
```
next(iter(dataset))
```

[10]: Data(x=[625, 75], edge_index=[2, 3125], edge_attr=[3125, 1], y=[1])

[11]:
```
len(dataset)
```

[11]: 5573

[12]:
```
dataset_size = len(dataset)
train_size = int(0.8 * dataset_size)
test_size = dataset_size - train_size

# Perform the random split
train_dataset, test_dataset = random_split(dataset, [train_size, test_size])

# Create the DataLoaders for the train and test sets
train_loader = DataLoader(train_dataset, batch_size=32, shuffle=True)
valid_loader = DataLoader(test_dataset, batch_size=32, shuffle=False)
```

[13]:
```
# next(iter(train_loader))
```

[14]:
```
from torch.nn import BatchNorm1d , Dropout,  Linear

class DeepGNN(torch.nn.Module):
    def __init__(self, num_node_features, num_classes):
        super(DeepGNN, self).__init__()
        self.conv1 = GCNConv(num_node_features, 1024)
        self.bn1 = BatchNorm1d(1024)
        self.conv2 = GCNConv(1024, 512)
        self.bn2 = BatchNorm1d(512)
        self.conv3 = GCNConv(512, 256)
        self.bn3 = BatchNorm1d(256)
        self.conv4 = GCNConv(256, 128)
        self.bn4 = BatchNorm1d(128)
        self.dropout = Dropout(0.5)
        self.lin = Linear(128, num_classes)

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

        x = F.relu(self.bn1(self.conv1(x, edge_index)))
```

```
        x = self.dropout(x)
        x = F.relu(self.bn2(self.conv2(x, edge_index)))
        x = self.dropout(x)
        x = F.relu(self.bn3(self.conv3(x, edge_index)))
        x = self.dropout(x)
        x = F.relu(self.bn4(self.conv4(x, edge_index)))

        x = global_mean_pool(x, batch)  # Pooling to use graph-level features
        x = self.dropout(x)
        x = self.lin(x)

        return x
```

1 In an other notebook had trained the model for 10 epochs and the weights saved in then used here to train for one more epoch

[15]:
```
num_node_features = 75  # Number of features per node
num_classes = 2  # Number of classes for binary classification

model = DeepGNN(num_node_features=num_node_features, num_classes=num_classes)
model.load_state_dict(torch.load("/kaggle/input/fork-of-ml4sci-24-task3-a6/
 ↪best_model.pth"))
print(model)
```

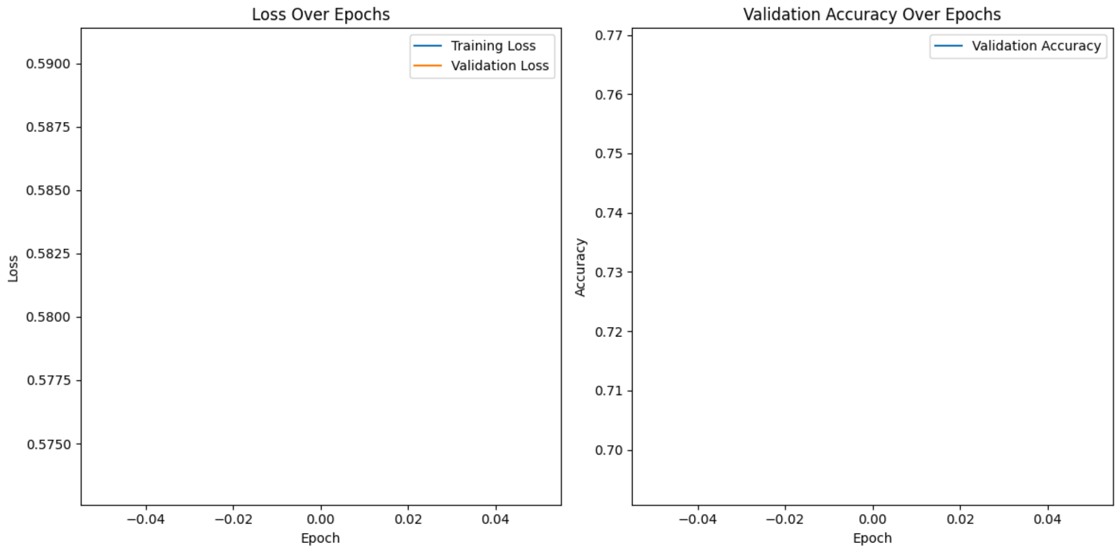
```
DeepGNN(
  (conv1): GCNConv(75, 1024)
  (bn1): BatchNorm1d(1024, eps=1e-05, momentum=0.1, affine=True,
track_running_stats=True)
  (conv2): GCNConv(1024, 512)
  (bn2): BatchNorm1d(512, eps=1e-05, momentum=0.1, affine=True,
track_running_stats=True)
  (conv3): GCNConv(512, 256)
  (bn3): BatchNorm1d(256, eps=1e-05, momentum=0.1, affine=True,
track_running_stats=True)
  (conv4): GCNConv(256, 128)
  (bn4): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True,
track_running_stats=True)
  (dropout): Dropout(p=0.5, inplace=False)
  (lin): Linear(in_features=128, out_features=2, bias=True)
)
```

[16]:
```
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print(f'Using device: {device}')

# Move the model to the chosen device
model.to(device)
```

```python
def train(model, train_loader, optimizer, criterion, device):
    model.train()
    total_loss = 0
    for data in tqdm(train_loader, desc="Training", leave=False):
        data = data.to(device)
        optimizer.zero_grad()
        out = model(data)
        loss = criterion(out, data.y)
        loss.backward()
        optimizer.step()
        total_loss += loss.item() * data.num_graphs
    return total_loss / len(train_loader.dataset)

def test(model, loader, criterion, device):
    model.eval()
    correct = 0
    total_loss = 0
    with torch.no_grad(), tqdm(loader, desc="Evaluating", leave=False) as␣
 ↪tepoch:
        for data in tepoch:
            data = data.to(device)
            out = model(data)
            loss = criterion(out, data.y)
            total_loss += loss.item() * data.num_graphs
            pred = out.argmax(dim=1)
            correct += int((pred == data.y).sum())
    accuracy = correct / len(loader.dataset)
    return accuracy, total_loss / len(loader.dataset)

optimizer = torch.optim.Adam(model.parameters(), lr=0.001)
criterion = torch.nn.CrossEntropyLoss()

train_losses = []
val_losses = []
val_accuracies = []

best_val_acc = 0.0
for epoch in range(1, 2):
    train_loss = train(model, train_loader, optimizer, criterion, device)
    val_acc, val_loss = test(model, valid_loader, criterion, device)

    train_losses.append(train_loss)
    val_losses.append(val_loss)
    val_accuracies.append(val_acc)

    if val_acc > best_val_acc:
```

```
        best_val_acc = val_acc
        torch.save(model.state_dict(), 'best_model.pth')
        print(f"Saved Best Model: Epoch {epoch}, Val. Acc.: {val_acc:.4f}")

    print(f'Epoch: {epoch:03d}, Train Loss: {train_loss:.4f}, Val. Loss:␣
 ↪{val_loss:.4f}, Val. Acc.: {val_acc:.4f}')

# Plotting the training curves
plt.figure(figsize=(12, 6))
plt.subplot(1, 2, 1)
plt.plot(train_losses, label='Training Loss')
plt.plot(val_losses, label='Validation Loss')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.title('Loss Over Epochs')
plt.legend()

plt.subplot(1, 2, 2)
plt.plot(val_accuracies, label='Validation Accuracy')
plt.xlabel('Epoch')
plt.ylabel('Accuracy')
plt.title('Validation Accuracy Over Epochs')
plt.legend()

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

```
Using device: cuda


Saved Best Model: Epoch 1, Val. Acc.: 0.7309
Epoch: 001, Train Loss: 0.5905, Val. Loss: 0.5734, Val. Acc.: 0.7309
```


Loss Over Epochs
Training Loss
Validation Loss
Loss
0.5900
0.5875
0.5850
0.5825
0.5800
0.5775
0.5750
−0.04
−0.02
0.00
0.02
0.04
Epoch
Validation Accuracy Over Epochs
Validation Accuracy
Accuracy
0.77
0.76
0.75
0.74
0.73
0.72
0.71
0.70
−0.04
−0.02
0.00
0.02
0.04
Epoch

```
[ ]:
```

```
[ ]:
```