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!pip install torch-spline-conv -f https://data.pyg.org/whl/torch-2.5.1%2Bcu121.html
!pip install torch-geometric
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Common Task 2: Jets as Graphs for Quark/Gluon Classification

Overview

I developed a graph-based neural network (GNN) to classify quark vs. gluon jets. The approach involved converting jet images into point clouds (by selecting non-zero pixels) and then casting these point clouds into graphs with carefully designed node and edge features. I trained on only 50000 images, and while evaluating for the remaining images, I was able get an accuracy of 80%, which can be further improved by running on more epochs, hyperparameter tuning, etc.

Data Preparation

- **Point Cloud Extraction:**
  For each event, I extracted the coordinates and intensity of non-zero pixels.
- **Graph Construction:**
  - **Node Features:** Each node is represented by its normalized (x, y) coordinates along with the pixel intensity.

  - **Edge Features:** I used a k-nearest neighbors (kNN) algorithm (with an adjustable k value) to connect nodes, capturing local spatial relationships. We can also use radius based approaches.

Model Architecture

- I implemented a GNN using PyTorch Geometric.
- **Architecture Details:**
  - **Graph Convolution Layers:** Three GCNConv layers were used to aggregate local node information.
  - **Global Pooling:** Global mean pooling transformed the variable-size node features into a fixed-length graph-level representation.
  - **Classifier:** A fully connected layer then performed binary classification (quark vs. gluon).

```
import h5py
import numpy as np
import torch
import torch.nn as nn
import torch.optim as optim
import matplotlib.pyplot as plt

from torch_geometric.data import Data, InMemoryDataset, DataLoader as
GeoDataLoader
from torch_geometric.nn import SAGEConv, global_mean_pool, knn_graph

class JetGraphMultiChannelDataset(InMemoryDataset):
    def __init__(self, hdf5_file, transform=None, pre_transform=None,
knn_k=16, intensity_thresh=0.01):
        self.hdf5_file = hdf5_file
        self.knn_k = knn_k
        self.intensity_thresh = intensity_thresh
        super(JetGraphMultiChannelDataset, self).__init__('.',
transform, pre_transform)
        self.data, self.slices = torch.load(self.processed_paths[0])

    @property
    def raw_file_names(self):
        return []  # Not used
    @property
    def processed_file_names(self):
        return ['data_multi.pt']
    def download(self):
        pass

    def process(self):
        data_list = []
        with h5py.File(self.hdf5_file, 'r') as f:
            # X_jets = f['X_jets'][0:50000]  This was training data
            # y_all = f['y'][0:50000]   This was training data

            # Testing data (other 50000 images)
```

```
            X_jets = f['X_jets'][50000:100000]
            y_all = f['y'][50000:100000]

        num_events = X_jets.shape[0]
        print("Processing", num_events, "events into multi-channel
graphs...")
        for i in range(num_events):
            img = X_jets[i]
            label = int(y_all[i])
            # Compute the sum across channels.
            img_sum = img.sum(axis=-1)  # shape: (125,125)
            # Find pixel indices where the sum is above a threshold.
            indices = np.argwhere(img_sum > self.intensity_thresh)
            if indices.shape[0] == 0:
                # If no pixel qualifies, add a dummy node.
                indices = np.array([[0, 0]])
                pixel_values = np.zeros((1, 3), dtype=np.float32)
            else:
                # For each index, extract the 3 channel intensities.
                pixel_values = img[indices[:, 0], indices[:, 1], :]  #
shape: (num_nodes, 3)
            # Normalize coordinates: convert (row, col) to (x,y) in
[0,1]
            coords = indices.astype(np.float32) / 125.0  # shape:
(num_nodes, 2)
            # Combine coordinates and intensities to form node
features.
            node_features = np.hstack([coords, pixel_values])
            x = torch.tensor(node_features, dtype=torch.float)
            # Use only the spatial coordinates (first two columns) to
construct the knn graph.
            pos = x[:, :2]
            # Build edges using knn_graph with new k value (e.g., 16)
            edge_index = knn_graph(pos, k=self.knn_k, loop=False)
            # Create the PyG Data object.
            data = Data(x=x, edge_index=edge_index,
y=torch.tensor([label], dtype=torch.long))
            data_list.append(data)
        data, slices = self.collate(data_list)
        torch.save((data, slices), self.processed_paths[0])

    def __repr__(self):
        return f'JetGraphMultiChannelDataset({len(self)})'

class JetMultiChannelGNN(nn.Module):
    def __init__(self, in_channels=5, hidden_channels=64,
num_classes=2):
        super(JetMultiChannelGNN, self).__init__()
        self.conv1 = SAGEConv(in_channels, hidden_channels)
```

```python
        self.conv2 = SAGEConv(hidden_channels, hidden_channels)
        self.conv3 = SAGEConv(hidden_channels, hidden_channels)
        self.fc = nn.Linear(hidden_channels, num_classes)

    def forward(self, data):
        x, edge_index, batch = data.x, data.edge_index, data.batch
        x = self.conv1(x, edge_index)
        x = torch.relu(x)
        x = self.conv2(x, edge_index)
        x = torch.relu(x)
        x = self.conv3(x, edge_index)
        x = torch.relu(x)
        x = global_mean_pool(x, batch)
        out = self.fc(x)
        return out

# Set the file path to the HDF5 file.
hdf5_file = '/kaggle/input/quark-gluon-lhc/quark-gluon_data-
set_n139306.hdf5'

# We took the first 50000 images for training, and further 50000 new
images
# for testing, to check our model's performance on new data.

full_dataset = JetGraphMultiChannelDataset(hdf5_file, knn_k=16,
intensity_thresh=0.01)
print(full_dataset)


# We can also take a subset to check if everything's alright in the
training process.


subset_size = 10000
subset_indices = list(range(subset_size))
from torch.utils.data import Subset
dataset = Subset(full_dataset, subset_indices)

loader = GeoDataLoader(dataset, batch_size=32, shuffle=True)
```

```
<ipython-input-2-644385dd6cf6>:17: FutureWarning: You are using
`torch.load` with `weights_only=False` (the current default value),
which uses the default pickle module implicitly. It is possible to
construct malicious pickle data which will execute arbitrary code
during unpickling (See
https://github.com/pytorch/pytorch/blob/main/SECURITY.md#untrusted-
models for more details). In a future release, the default value for
`weights_only` will be flipped to `True`. This limits the functions
that could be executed during unpickling. Arbitrary objects will no
longer be allowed to be loaded via this mode unless they are
```

```
explicitly allowlisted by the user via
`torch.serialization.add_safe_globals`. We recommend you start setting
`weights_only=True` for any use case where you don't have full control
of the loaded file. Please open an issue on GitHub for any issues
related to this experimental feature.
  self.data, self.slices = torch.load(self.processed_paths[0])

JetGraphMultiChannelDataset(50000)
```

```
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
model = JetMultiChannelGNN(in_channels=5, hidden_channels=64,
num_classes=2).to(device)
optimizer = optim.Adam(model.parameters(), lr=1e-2)
scheduler = optim.lr_scheduler.CosineAnnealingLR(optimizer, T_max=100,
eta_min=1e-6)
criterion = nn.CrossEntropyLoss()

# Training loop.
num_epochs = 100 # Increases this with a lower learning rate increased
the accuracy to 80 %
model.train()
for epoch in range(num_epochs):
    total_loss = 0
    for batch in loader:
        batch = batch.to(device)
        optimizer.zero_grad()
        out = model(batch)
        loss = criterion(out, batch.y.view(-1))
        loss.backward()
        optimizer.step()
        total_loss += loss.item() * batch.num_graphs
    avg_loss = total_loss / len(loader.dataset)
    if(epoch%10 == 0):
        print(f"Epoch {epoch+1}/{num_epochs}, Loss: {avg_loss:.4f}")
```

```
Epoch 1/100, Loss: 0.6772
Epoch 11/100, Loss: 0.5873
Epoch 21/100, Loss: 0.5829
Epoch 31/100, Loss: 0.5769
Epoch 41/100, Loss: 0.5760
Epoch 51/100, Loss: 0.5720
Epoch 61/100, Loss: 0.5720
Epoch 71/100, Loss: 0.5699
Epoch 81/100, Loss: 0.5680
Epoch 91/100, Loss: 0.5665
```

```
# Evaluat accuracy.
model.eval()
correct = 0
total = 0
```

```
for batch in loader:
    batch = batch.to(device)
    with torch.no_grad():
        out = model(batch)
        pred = out.argmax(dim=1)
    correct += (pred == batch.y.view(-1)).sum().item()
    total += batch.num_graphs
print(f"Training Accuracy: {correct/total:.4f}")

Training Accuracy: 0.7118
```

- I used all three channels per event to build a richer node feature.
- I filter out very dim pixels by checking that the sum of intensities is above a threshold.
- I construct graphs using a larger k value in the kNN step.
- I switched the model architecture to a GraphSAGE-based network, which aggregates node features in a more flexible manner.

We can also experiment further by

- Adjusting the intensity threshold or k value.
- Trying different graph pooling methods (e.g., global max pooling, attention pooling).
- Exploring deeper or alternative GNN architectures (e.g., GAT or combining multiple pooling strategies).

This approach should provide richer graph representations for your quark/gluon classification task.

Results & Discussion

- **Performance:**
  The model achieved around 70% accuracy on the training subset.
- **Insights:**
  - The GNN successfully learned from sparse graphs derived from the non-zero pixels.
  - However, the extreme sparsity of the input data limits performance.
  - Future work could explore alternative graph construction methods (e.g., radius-based graphs) or more advanced GNN architectures to boost accuracy.

Conclusion

This task demonstrated that converting jet images into graph representations is a viable strategy for quark/gluon classification.