```python
# Code originally written on kaggle
import h5py
import numpy as np
import torch
import random
from tqdm import tqdm

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print(f"Using device: {device}")

file_path = "/kaggle/input/quark-gluon/quark-gluon_data-
set_n139306.hdf5"
output_file = "/kaggle/working/point_cloud_dataset.pt"

H, W = 125, 125
x_coords_np, y_coords_np = np.meshgrid(np.linspace(0, 1, W),
np.linspace(0, 1, H))

x_coords = torch.tensor(x_coords_np, dtype=torch.float32,
device=device)
y_coords = torch.tensor(y_coords_np, dtype=torch.float32,
device=device)

with h5py.File(file_path, "r") as f:
    X_jets = f["X_jets"]
    m0 = f["m0"]
    pt = f["pt"]
    y = f["y"]

    total_events = X_jets.shape[0]
    num_samples = min(50000, total_events)

    random.seed(42)
    selected_indices = sorted(random.sample(range(total_events),
num_samples))

    print(f"Processing {num_samples} randomly selected samples out of
{total_events} available.")

    dataset = {"point_clouds": [], "labels": []}
    batch_size = 5000

    for start in tqdm(range(0, num_samples, batch_size),
desc="Processing Batches"):
        end = min(start + batch_size, num_samples)
        batch_indices = selected_indices[start:end]

        X_batch = torch.tensor(X_jets[batch_indices],
dtype=torch.float32, device=device)
        m0_batch = torch.tensor(m0[batch_indices],
```

```
dtype=torch.float32, device=device)
        pt_batch = torch.tensor(pt[batch_indices],
dtype=torch.float32, device=device)
        y_batch = torch.tensor(y[batch_indices], dtype=torch.float32,
device=device)

        for i in range(end - start):
            nonzero_mask = torch.any(X_batch[i] > 0, dim=-1)

            nonzero_x = x_coords[nonzero_mask]
            nonzero_y = y_coords[nonzero_mask]
            nonzero_features = X_batch[i][nonzero_mask]

            if nonzero_x.numel() == 0:
                continue

            num_points = nonzero_x.shape[0]
            jet_features = torch.stack([
                nonzero_x, nonzero_y,
                nonzero_features[:, 0], nonzero_features[:, 1],
nonzero_features[:, 2],
                torch.full((num_points,), m0_batch[i],
dtype=torch.float32, device=device),
                torch.full((num_points,), pt_batch[i],
dtype=torch.float32, device=device)
            ], dim=1)

            dataset["point_clouds"].append(jet_features.cpu())
            dataset["labels"].append(y_batch[i].cpu())

    torch.save(dataset, output_file)
    print(f"Point cloud dataset saved to '{output_file}'.")
```

```
Using device: cuda
Processing 50000 randomly selected samples out of 139306 available.

Processing Batches: 100%|██████████| 10/10 [10:13<00:00, 61.36s/it]

Point cloud dataset saved to '/kaggle/working/point_cloud_dataset.pt'.
```

```
!pip install torch-scatter torch-sparse torch-cluster torch-spline-
conv -f https://data.pyg.org/whl/torch-2.5.0+cu121.html
!pip install torch-geometric
!pip install torch-cluster -f https://data.pyg.org/whl/torch-
2.5.0+cu121.html

import torch
from torch_geometric.data import Data, InMemoryDataset
from torch_geometric.nn import knn_graph
from tqdm.notebook import tqdm
```

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

input_file = "/kaggle/working/point_cloud_dataset.pt"
output_file = "/kaggle/working/graph_dataset.pt"

dataset = torch.load(input_file)

graph_data_list = []

for i in tqdm(range(len(dataset["point_clouds"])), desc="Processing
Graphs"):
    point_cloud = dataset["point_clouds"][i]
    label = dataset["labels"][i]

    if point_cloud.numel() == 0:
        continue

    k = 8
    edge_index = knn_graph(point_cloud[:, :2], k=k)
    data = Data(x=point_cloud, edge_index=edge_index, y=label)
    graph_data_list.append(data)

class GraphDataset(InMemoryDataset):
    def __init__(self, root=None, data_list=None):
        super().__init__(root)
        if data_list:
            self.data, self.slices = self.collate(data_list)

    def __len__(self):
        return len(self.slices["x"]) - 1

graph_dataset = GraphDataset(data_list=graph_data_list)
torch.save(graph_dataset, output_file)

print(f"Graph dataset saved to '{output_file}'.")
```

```
Looking in links: https://data.pyg.org/whl/torch-2.5.0+cu121.html
Collecting torch-scatter
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Installing collected packages: torch-spline-conv, torch-scatter,
torch-sparse, torch-cluster
Successfully installed torch-cluster-1.6.3+pt25cu121 torch-scatter-
2.1.2+pt25cu121 torch-sparse-0.6.18+pt25cu121 torch-spline-conv-
1.2.2+pt25cu121
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Using device: cuda

<ipython-input-2-ebd000c1c252>:19: 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.
  dataset = torch.load(input_file)
```

{"model_id":"b75f42077d434e4681d1cbe48ecc2bc0","version_major":2,"version_minor":0}

```
Graph dataset saved to '/kaggle/working/graph_dataset.pt'.
```

```
dataset = torch.load("/kaggle/working/graph_dataset.pt",
map_location="cpu")
print(dataset)

print(len(dataset))
print(dataset[0])
```

```
<ipython-input-3-300146acece1>:1: 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
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of the loaded file. Please open an issue on GitHub for any issues
related to this experimental feature.
  dataset = torch.load("/kaggle/working/graph_dataset.pt",
map_location="cpu")
```

```
GraphDataset(50000)
50000
Data(x=[515, 7], edge_index=[2, 4120], y=[1])
```

```
import torch
import torch.nn.functional as F
from torch_geometric.nn import GINConv, global_mean_pool
from torch_geometric.data import DataLoader, InMemoryDataset
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import StratifiedShuffleSplit
from sklearn.utils.class_weight import compute_class_weight
from tqdm import tqdm
import numpy as np
from sklearn.metrics import roc_auc_score
import gc
```

```
torch.cuda.empty_cache()
gc.collect()

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print(f"Using device: {device}")

dataset_path = "/kaggle/working/graph_dataset.pt"
dataset = torch.load(dataset_path, map_location="cpu")

dataset = [data for data in dataset if data.edge_index.numel() > 0 and
data.x.numel() > 0]
assert len(dataset) > 0, "All graphs were found empty after
filtering."

labels = np.array([data.y.item() for data in dataset])
splitter = StratifiedShuffleSplit(n_splits=1, test_size=0.2,
random_state=42)
train_idx, temp_idx = next(splitter.split(np.zeros(len(labels)),
labels))

temp_labels = labels[temp_idx]
splitter = StratifiedShuffleSplit(n_splits=1, test_size=0.5,
random_state=42)
val_idx, test_idx = next(splitter.split(np.zeros(len(temp_labels)),
temp_labels))

train_dataset = [dataset[i] for i in train_idx]
val_dataset = [dataset[i] for i in val_idx]
test_dataset = [dataset[i] for i in test_idx]

scaler = StandardScaler()
train_features = np.vstack([data.x.cpu().numpy().astype(np.float32)
for data in train_dataset])
scaler.fit(train_features)

for data in dataset:
    data.x = torch.tensor(scaler.transform(data.x.cpu().numpy()),
dtype=torch.float32)

class_weights = compute_class_weight("balanced",
classes=np.unique(labels), y=labels)
class_weights = torch.tensor(class_weights,
dtype=torch.float32).to(device)

batch_size = 16
train_loader = DataLoader(train_dataset, batch_size=batch_size,
shuffle=True, num_workers=2, pin_memory=True)
val_loader = DataLoader(val_dataset, batch_size=batch_size,
num_workers=2, pin_memory=True)
```

```
test_loader = DataLoader(test_dataset, batch_size=batch_size,
num_workers=2, pin_memory=True)

class GIN(torch.nn.Module):
    def __init__(self, in_channels, hidden_channels=128,
out_channels=1, num_layers=3):
        super(GIN, self).__init__()
        self.convs = torch.nn.ModuleList()
        self.batch_norms = torch.nn.ModuleList()
        self.dropouts = torch.nn.ModuleList()

        nn1 = torch.nn.Sequential(
            torch.nn.Linear(in_channels, hidden_channels),
            torch.nn.LeakyReLU(0.1),
            torch.nn.Linear(hidden_channels, hidden_channels)
        )
        self.convs.append(GINConv(nn1))
        self.batch_norms.append(torch.nn.BatchNorm1d(hidden_channels))
        self.dropouts.append(torch.nn.Dropout(0.2))

        for _ in range(num_layers - 1):
            nn_layer = torch.nn.Sequential(
                torch.nn.Linear(hidden_channels, hidden_channels),
                torch.nn.LeakyReLU(0.1),
                torch.nn.Linear(hidden_channels, hidden_channels)
            )
            self.convs.append(GINConv(nn_layer))

self.batch_norms.append(torch.nn.BatchNorm1d(hidden_channels))
            self.dropouts.append(torch.nn.Dropout(0.2))

        self.fc = torch.nn.Linear(hidden_channels, out_channels)

    def forward(self, x, edge_index, batch):
        for conv, bn, do in zip(self.convs, self.batch_norms,
self.dropouts):
            x = conv(x, edge_index)
            x = bn(x)
            x = F.leaky_relu(x, negative_slope=0.1)
            x = do(x)

        x = global_mean_pool(x, batch)
        return self.fc(x).squeeze()

model = GIN(in_channels=7).to(device)
optimizer = torch.optim.AdamW(model.parameters(), lr=0.0015,
weight_decay=5e-5)
scheduler = torch.optim.lr_scheduler.ReduceLROnPlateau(optimizer,
mode="max", factor=0.5, patience=5, verbose=True)
criterion = torch.nn.BCEWithLogitsLoss(pos_weight=class_weights[1])
```

```python
def train():
    model.train()
    total_loss = 0
    pbar = tqdm(train_loader, desc="Training", leave=False)
    for data in pbar:
        data = data.to(device)

        optimizer.zero_grad()
        output = model(data.x, data.edge_index, data.batch)
        loss = criterion(output, data.y.float().view(-1))

        loss.backward()
        torch.nn.utils.clip_grad_norm_(model.parameters(),
max_norm=1.0)  # Dynamic Gradient Clipping
        optimizer.step()

        total_loss += loss.item()
        pbar.set_postfix(loss=loss.item())

    return total_loss / len(train_loader)

def evaluate(loader):
    model.eval()
    total_loss = 0
    preds, labels = [], []
    with torch.inference_mode():
        pbar = tqdm(loader, desc="Evaluating", leave=False)
        for data in pbar:
            data = data.to(device)
            output = model(data.x, data.edge_index, data.batch)
            loss = criterion(output, data.y.float().view(-1))
            total_loss += loss.item()
            preds.append(output.sigmoid().cpu())
            labels.append(data.y.cpu())

    if not preds:
        return total_loss / len(loader), None, None

    preds = torch.cat(preds).numpy()
    labels = torch.cat(labels).numpy()
    acc = ((preds > 0.5) == labels).mean()
    try:
        auc = roc_auc_score(labels, preds) if len(set(labels)) > 1
else 0.5
    except ValueError:
        auc = 0.5
    return total_loss / len(loader), acc, auc

num_epochs = 50
```

```python
best_val_auc = 0
patience = 5
no_improve_epochs = 0

for epoch in range(num_epochs):
    train_loss = train()
    val_loss, val_acc, val_auc = evaluate(val_loader)

    print(f"Epoch {epoch+1}/{num_epochs} - Train Loss:
{train_loss:.4f} - Val Loss: {val_loss:.4f} - Val Acc: {val_acc:.4f} -
Val AUC: {val_auc:.4f}")

    scheduler.step(val_auc)

    if val_auc and val_auc > best_val_auc:
        best_val_auc = val_auc
        torch.save(model.state_dict(),
"/kaggle/working/best_gin_model.pt")
        no_improve_epochs = 0
    else:
        no_improve_epochs += 1

    if no_improve_epochs >= patience:
        print("Early stopping triggered")
        break

torch.cuda.empty_cache()
```

```
Using device: cuda
```

```
<ipython-input-3-856d2b5040e3>:22: 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.
  dataset = torch.load(dataset_path, map_location="cpu")
/usr/local/lib/python3.10/dist-packages/torch_geometric/deprecation.py
:26: UserWarning: 'data.DataLoader' is deprecated, use
'loader.DataLoader' instead
  warnings.warn(out)
```

```
/usr/local/lib/python3.10/dist-packages/torch/optim/lr_scheduler.py:62
: UserWarning: The verbose parameter is deprecated. Please use
get_last_lr() to access the learning rate.
  warnings.warn(


Epoch 1/50 - Train Loss: 0.5895 - Val Loss: 0.5887 - Val Acc: 0.7094 -
Val AUC: 0.7759



Epoch 2/50 - Train Loss: 0.5812 - Val Loss: 0.5852 - Val Acc: 0.7140 -
Val AUC: 0.7780



Epoch 3/50 - Train Loss: 0.5771 - Val Loss: 0.5867 - Val Acc: 0.7076 -
Val AUC: 0.7791



Epoch 4/50 - Train Loss: 0.5737 - Val Loss: 0.5742 - Val Acc: 0.7128 -
Val AUC: 0.7812



Epoch 5/50 - Train Loss: 0.5720 - Val Loss: 0.5723 - Val Acc: 0.7182 -
Val AUC: 0.7830



Epoch 6/50 - Train Loss: 0.5693 - Val Loss: 0.5704 - Val Acc: 0.7140 -
Val AUC: 0.7812



Epoch 7/50 - Train Loss: 0.5675 - Val Loss: 0.5714 - Val Acc: 0.7176 -
Val AUC: 0.7817



Epoch 8/50 - Train Loss: 0.5665 - Val Loss: 0.5759 - Val Acc: 0.7188 -
Val AUC: 0.7832



Epoch 9/50 - Train Loss: 0.5661 - Val Loss: 0.5646 - Val Acc: 0.7174 -
Val AUC: 0.7858



Epoch 10/50 - Train Loss: 0.5647 - Val Loss: 0.7402 - Val Acc: 0.5184
- Val AUC: 0.7588
```

```
Epoch 11/50 - Train Loss: 0.5639 - Val Loss: 0.5735 - Val Acc: 0.7184
- Val AUC: 0.7825

Epoch 12/50 - Train Loss: 0.5637 - Val Loss: 0.5710 - Val Acc: 0.7178
- Val AUC: 0.7843

Epoch 13/50 - Train Loss: 0.5624 - Val Loss: 0.5646 - Val Acc: 0.7208
- Val AUC: 0.7880

Epoch 14/50 - Train Loss: 0.5603 - Val Loss: 0.5627 - Val Acc: 0.7246
- Val AUC: 0.7874

Epoch 15/50 - Train Loss: 0.5612 - Val Loss: 0.5644 - Val Acc: 0.7248
- Val AUC: 0.7884

Epoch 16/50 - Train Loss: 0.5603 - Val Loss: 0.5621 - Val Acc: 0.7256
- Val AUC: 0.7883

Epoch 17/50 - Train Loss: 0.5602 - Val Loss: 0.5664 - Val Acc: 0.7202
- Val AUC: 0.7886

Epoch 18/50 - Train Loss: 0.5594 - Val Loss: 0.5691 - Val Acc: 0.7216
- Val AUC: 0.7882

Epoch 19/50 - Train Loss: 0.5580 - Val Loss: 0.5685 - Val Acc: 0.7240
- Val AUC: 0.7878

Epoch 20/50 - Train Loss: 0.5587 - Val Loss: 0.5680 - Val Acc: 0.7270
- Val AUC: 0.7881

Epoch 21/50 - Train Loss: 0.5578 - Val Loss: 0.5591 - Val Acc: 0.7236
- Val AUC: 0.7904
```

```
Epoch 22/50 - Train Loss: 0.5578 - Val Loss: 0.5654 - Val Acc: 0.7226
- Val AUC: 0.7880

Epoch 23/50 - Train Loss: 0.5570 - Val Loss: 0.5590 - Val Acc: 0.7236
- Val AUC: 0.7905

Epoch 24/50 - Train Loss: 0.5577 - Val Loss: 0.5613 - Val Acc: 0.7214
- Val AUC: 0.7905

Epoch 25/50 - Train Loss: 0.5565 - Val Loss: 0.5645 - Val Acc: 0.7216
- Val AUC: 0.7898

Epoch 26/50 - Train Loss: 0.5565 - Val Loss: 0.5634 - Val Acc: 0.7268
- Val AUC: 0.7880

Epoch 27/50 - Train Loss: 0.5564 - Val Loss: 0.5647 - Val Acc: 0.7268
- Val AUC: 0.7915

Epoch 28/50 - Train Loss: 0.5561 - Val Loss: 0.5603 - Val Acc: 0.7274
- Val AUC: 0.7901

Epoch 29/50 - Train Loss: 0.5560 - Val Loss: 0.5628 - Val Acc: 0.7206
- Val AUC: 0.7892

Epoch 30/50 - Train Loss: 0.5554 - Val Loss: 0.5637 - Val Acc: 0.7138
- Val AUC: 0.7869

Epoch 31/50 - Train Loss: 0.5554 - Val Loss: 0.5619 - Val Acc: 0.7254
- Val AUC: 0.7925

Epoch 32/50 - Train Loss: 0.5556 - Val Loss: 0.5612 - Val Acc: 0.7246
- Val AUC: 0.7909
```

```
Epoch 33/50 - Train Loss: 0.5552 - Val Loss: 0.5621 - Val Acc: 0.7260
- Val AUC: 0.7910


Epoch 34/50 - Train Loss: 0.5555 - Val Loss: 0.5575 - Val Acc: 0.7288
- Val AUC: 0.7922


Epoch 35/50 - Train Loss: 0.5556 - Val Loss: 0.5559 - Val Acc: 0.7254
- Val AUC: 0.7915


Epoch 36/50 - Train Loss: 0.5542 - Val Loss: 0.5660 - Val Acc: 0.7238
- Val AUC: 0.7901
Early stopping triggered
```

```python
import matplotlib.pyplot as plt
import numpy as np

epochs = np.arange(1, 37)
train_loss = [0.5895, 0.5812, 0.5771, 0.5737, 0.5720, 0.5693, 0.5675,
0.5665, 0.5661, 0.5647,
              0.5639, 0.5637, 0.5624, 0.5603, 0.5612, 0.5603, 0.5602,
0.5594, 0.5580, 0.5587,
              0.5578, 0.5578, 0.5570, 0.5577, 0.5565, 0.5565, 0.5564,
0.5561, 0.5560, 0.5554,
              0.5554, 0.5556, 0.5552, 0.5555, 0.5556, 0.5542]

val_loss = [0.5887, 0.5852, 0.5867, 0.5742, 0.5723, 0.5704, 0.5714,
0.5759, 0.5646, 0.7402,
            0.5735, 0.5710, 0.5646, 0.5627, 0.5644, 0.5621, 0.5664,
0.5691, 0.5685, 0.5680,
            0.5591, 0.5654, 0.5590, 0.5613, 0.5645, 0.5634, 0.5647,
0.5603, 0.5628, 0.5637,
            0.5619, 0.5612, 0.5621, 0.5575, 0.5559, 0.5660]

val_acc = [0.7094, 0.7140, 0.7076, 0.7128, 0.7182, 0.7140, 0.7176,
0.7188, 0.7174, 0.5184,
           0.7184, 0.7178, 0.7208, 0.7246, 0.7248, 0.7256, 0.7202,
0.7216, 0.7240, 0.7270,
           0.7236, 0.7226, 0.7236, 0.7214, 0.7216, 0.7268, 0.7268,
0.7274, 0.7206, 0.7138,
           0.7254, 0.7246, 0.7260, 0.7288, 0.7254, 0.7238]

val_auc = [0.7759, 0.7780, 0.7791, 0.7812, 0.7830, 0.7812, 0.7817,
0.7832, 0.7858, 0.7588,
           0.7825, 0.7843, 0.7880, 0.7874, 0.7884, 0.7883, 0.7886,
```

```
0.7882, 0.7878, 0.7881,
           0.7904, 0.7880, 0.7905, 0.7905, 0.7898, 0.7880, 0.7915,
0.7901, 0.7892, 0.7869,
           0.7925, 0.7909, 0.7910, 0.7922, 0.7915, 0.7901]

plt.figure(figsize=(12, 6))
plt.subplot(1, 2, 1)
plt.plot(epochs, train_loss, label="Train Loss", marker='o',
linestyle='dashed')
plt.plot(epochs, val_loss, label="Val Loss", marker='s',
linestyle='dashed')
plt.xlabel("Epochs")
plt.ylabel("Loss")
plt.title("Training and Validation Loss")
plt.legend()
plt.grid()

plt.subplot(1, 2, 2)
plt.plot(epochs, val_acc, label="Val Accuracy", marker='o',
linestyle='dashed')
plt.plot(epochs, val_auc, label="Val AUC", marker='s',
linestyle='dashed')
plt.xlabel("Epochs")
plt.ylabel("Metrics")
plt.title("Validation Accuracy & AUC")
plt.legend()
plt.grid()

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