In [1]:
```
!pip install torch_geometric umap-learn
```

```
Collecting torch_geometric
  Downloading torch_geometric-2.6.1-py3-none-any.whl.metadata (63 kB)
     ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 63.1/63.1 kB 1.6 MB/s eta 0:00:00
Collecting umap-learn
  Downloading umap_learn-0.5.7-py3-none-any.whl.metadata (21 kB)
Requirement already satisfied: aiohttp in /usr/local/lib/python3.10/dist-packages (from torch_geometric) (3.11.12)
Requirement already satisfied: fsspec in /usr/local/lib/python3.10/dist-packages (from torch_geometric) (2024.12.0)
Requirement already satisfied: jinja2 in /usr/local/lib/python3.10/dist-packages (from torch_geometric) (3.1.4)
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Requirement already satisfied: scipy>=1.3.1 in /usr/local/lib/python3.10/dist-packages (from umap-learn) (1.13.1)
Requirement already satisfied: scikit-learn>=0.22 in /usr/local/lib/python3.10/dist-packages (from umap-learn) (1.2.2)
Requirement already satisfied: numba>=0.51.2 in /usr/local/lib/python3.10/dist-packages (from umap-learn) (0.60.0)
Collecting pynndescent>=0.5 (from umap-learn)
  Downloading pynndescent-0.5.13-py3-none-any.whl.metadata (6.8 kB)
Requirement already satisfied: llvmlite<0.44,>=0.43.0dev0 in /usr/local/lib/python3.10/dist-packages (from numba>=0.51.2->umap-learn) (0.43.0)
Requirement already satisfied: mkl_fft in /usr/local/lib/python3.10/dist-packages (from numpy->torch_geometric) (1.3.8)
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Requirement already satisfied: frozenlist>=1.1.1 in /usr/local/lib/python3.10/dist-packages (from aiohttp->torch_geometric) (1.5.0)
Requirement already satisfied: multidict<7.0,>=4.5 in /usr/local/lib/python3.10/dist-packages (from aiohttp->torch_geometric) (6.1.0)
Requirement already satisfied: propcache>=0.2.0 in /usr/local/lib/python3.10/dist
```

```
-packages (from aiohttp->torch_geometric) (0.2.1)
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t-packages (from aiohttp->torch_geometric) (1.18.3)
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packages (from jinja2->torch_geometric) (3.0.2)
Requirement already satisfied: charset-normalizer<4,>=2 in /usr/local/lib/python
3.10/dist-packages (from requests->torch_geometric) (3.4.1)
Requirement already satisfied: idna<4,>=2.5 in /usr/local/lib/python3.10/dist-pac
kages (from requests->torch_geometric) (3.10)
Requirement already satisfied: urllib3<3,>=1.21.1 in /usr/local/lib/python3.10/di
st-packages (from requests->torch_geometric) (2.3.0)
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.10/di
st-packages (from requests->torch_geometric) (2025.1.31)
Requirement already satisfied: typing-extensions>=4.1.0 in /usr/local/lib/python
3.10/dist-packages (from multidict<7.0,>=4.5->aiohttp->torch_geometric) (4.12.2)
Requirement already satisfied: intel-openmp>=2024 in /usr/local/lib/python3.10/di
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4.2.0)
Downloading torch_geometric-2.6.1-py3-none-any.whl (1.1 MB)
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0:01
Downloading umap_learn-0.5.7-py3-none-any.whl (88 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 88.8/88.8 kB 4.3 MB/s eta 0:00:00
Downloading pynndescent-0.5.13-py3-none-any.whl (56 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 56.9/56.9 kB 2.8 MB/s eta 0:00:00
Installing collected packages: pynndescent, umap-learn, torch_geometric
Successfully installed pynndescent-0.5.13 torch_geometric-2.6.1 umap-learn-0.5.7
```

In [2]:

```python
import os
import h5py
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.neighbors import NearestNeighbors
from sklearn.metrics import confusion_matrix, classification_report, ConfusionMa
from tqdm.notebook import tqdm
import umap
import copy

import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim
from torch.utils.data import Dataset

from torch_geometric.data import Data
from torch_geometric.loader import DataLoader as PyGDataLoader
from torch_geometric.nn import GATv2Conv, GraphNorm, global_mean_pool, global_ma
from torch_geometric import warnings as pyg_warnings

SEED = 42
torch.manual_seed(SEED)
```

```
np.random.seed(SEED)
if torch.cuda.is_available():
    torch.cuda.manual_seed(SEED)
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print(f"Using device: {device}")

pyg_warnings.filterwarnings("ignore", message=".*scatter.*")
```

```
Using device: cuda
```

Below I am loading, resizing, and normalizing the image data similarly to the VAE notebook, but while keeping it as NumPy arrays.

In [ ]:
```
N_SAMPLES = 15000
VAL_SPLIT = 0.2
RESIZE_DIM = 64

try:
    data_path = "/kaggle/input/falcon/quark-gluon_data-set_n139306.hdf5"
    with h5py.File(data_path, 'r') as f:
        print(f"Keys in dataset: {list(f.keys())}")
        X_jets_raw = f['X_jets'][:N_SAMPLES] # (N, 125, 125, 3)
        y_raw = f['y'][:N_SAMPLES]           # (N,)
except FileNotFoundError:
    print("Kaggle path not found, trying local path './quark-gluon_data-set_n139
    data_path = "./quark-gluon_data-set_n139306.hdf5"
    try:
        with h5py.File(data_path, 'r') as f:
            print(f"Keys in dataset: {list(f.keys())}")
            X_jets_raw = f['X_jets'][:N_SAMPLES] # (N, 125, 125, 3)
            y_raw = f['y'][:N_SAMPLES]           # (N,)
    except FileNotFoundError:
        print(f"ERROR: Dataset not found at {data_path}. Please check the path."
        X_jets_raw, y_raw = None, None

if X_jets_raw is not None:
    print(f"Loaded X_jets shape: {X_jets_raw.shape}")
    print(f"Loaded y shape: {y_raw.shape}")
    X_jets = torch.tensor(X_jets_raw, dtype=torch.float32).permute(0, 3, 1, 2)

    if RESIZE_DIM != 125:
        print(f"Resizing images to {RESIZE_DIM}x{RESIZE_DIM}...")
        X_jets = F.interpolate(X_jets, size=(RESIZE_DIM, RESIZE_DIM), mode='bili

    print("Normalizing images per channel...")
    for i in tqdm(range(X_jets.shape[0]), desc="Normalizing"):
        for c in range(X_jets.shape[1]):
            channel = X_jets[i, c]
            min_val, max_val = channel.min(), channel.max()
            if max_val > min_val:
                X_jets[i, c] = (channel - min_val) / (max_val - min_val)
            else:
                X_jets[i, c] = torch.zeros_like(channel)
    X_jets = X_jets.numpy()
    y = y_raw.astype(np.int64)

    n_total = len(X_jets)
    n_val = int(VAL_SPLIT * n_total)
    n_train = n_total - n_val
```

```
    indices = np.arange(n_total)
    np.random.shuffle(indices)
    train_indices = indices[:n_train]
    val_indices = indices[n_train:]

    X_train, X_val = X_jets[train_indices], X_jets[val_indices]
    y_train, y_val = y[train_indices], y[val_indices]

    print(f"\nTotal samples: {n_total}")
    print(f"Training set: {X_train.shape[0]} samples")
    print(f"Validation set: {X_val.shape[0]} samples")
    print(f"Image shape (CHW): {X_train.shape[1:]}")
else:
    print("Skipping further processing due to missing data.")
```

```
Keys in dataset: ['X_jets', 'm0', 'pt', 'y']
Loaded X_jets shape: (15000, 125, 125, 3)
Loaded y shape: (15000,)
Resizing images to 64x64...
Normalizing images per channel...
Normalizing:   0%|          | 0/15000 [00:00<?, ?it/s]
Total samples: 15000
Training set: 12000 samples
Validation set: 3000 samples
Image shape (CHW): (3, 64, 64)
```

This cell converts a 3-channel image into a point cloud by selecting only pixels whose combined intensity across channels exceeds a threshold and extracting the y,x coords of those selected pixels. The channel features are then extracted from them. An additional two new features are added as well(radial distance and polar angle). So the resultant points has 5 features

A graph is then created by using a knn to find the k nearest neighbours for each node based on their coords positions. Then the edges are added between each node and its k neighbours. The normalized euclidean distance between connected nodes is calculated and stored as an edge feature as well

In [4]:

```
K_NEIGHBORS = 8
POINT_THRESHOLD = 0.01

def image_to_pointcloud(image_3d, threshold=0.01):
    image_hwc = image_3d.transpose(1, 2, 0)
    h, w, c = image_hwc.shape

    grid_y, grid_x = np.indices((h, w))
    mask = np.sum(image_hwc, axis=-1) > threshold
    coords_yx = np.stack([grid_y[mask], grid_x[mask]], axis=-1)
    feats_3chan = image_hwc[mask]

    if coords_yx.shape[0] == 0:
        return np.empty((0, 2)), np.empty((0, 5))

    center = np.array([h / 2.0, w / 2.0])
    offsets = coords_yx - center
    r = np.linalg.norm(offsets, axis=1, keepdims=True) / h
    theta = np.arctan2(offsets[:, 1], offsets[:, 0] + 1e-8)
    theta = (theta / (2 * np.pi)) + 0.5
    theta = theta.reshape(-1, 1)
```

```
    enhanced_feats = np.concatenate([feats_3chan, r, theta], axis=1)

    return coords_yx, enhanced_feats


class JetGraphDataset(Dataset):

    def __init__(self, X_array, y_array, k=8, threshold=0.01, name="train"):
        self.X_array = X_array
        self.y_array = y_array
        self.k = k
        self.threshold = threshold
        self.name = name
        self.valid_indices = []
        print(f"\nProcessing {self.name} dataset to create graphs...")
        for idx in tqdm(range(len(X_array)), desc=f"Filtering {name} samples"):

            coords_yx, _ = image_to_pointcloud(X_array[idx], threshold)

            if coords_yx.shape[0] > 1: # min(self.k + 1, 2):
                self.valid_indices.append(idx)

        print(f"Filtered {self.name} set: {len(self.valid_indices)} / {len(X_arr
        if len(self.valid_indices) == 0:
             warnings.warn("Warning: No valid samples found after filtering!")


    def __len__(self):
        return len(self.valid_indices)

    def __getitem__(self, idx):

        actual_idx = self.valid_indices[idx]
        image = self.X_array[actual_idx]
        label = self.y_array[actual_idx]

        coords_yx, node_features = image_to_pointcloud(image, self.threshold)
        num_nodes = node_features.shape[0]

        data = Data(
            x=torch.tensor(node_features, dtype=torch.float),
            y=torch.tensor([label], dtype=torch.long),
            pos=torch.tensor(coords_yx, dtype=torch.float)
        )


        if num_nodes > 1:

            current_k = min(self.k, num_nodes - 1)

            if current_k > 0:
                 nbrs = NearestNeighbors(n_neighbors=current_k + 1, algorithm='b
                 distances, indices = nbrs.kneighbors(coords_yx)

                 edge_list = []
                 edge_attrs = []
                 img_size = image.shape[1]

                 for i in range(num_nodes):
                     for j_idx in range(1, current_k + 1):
```

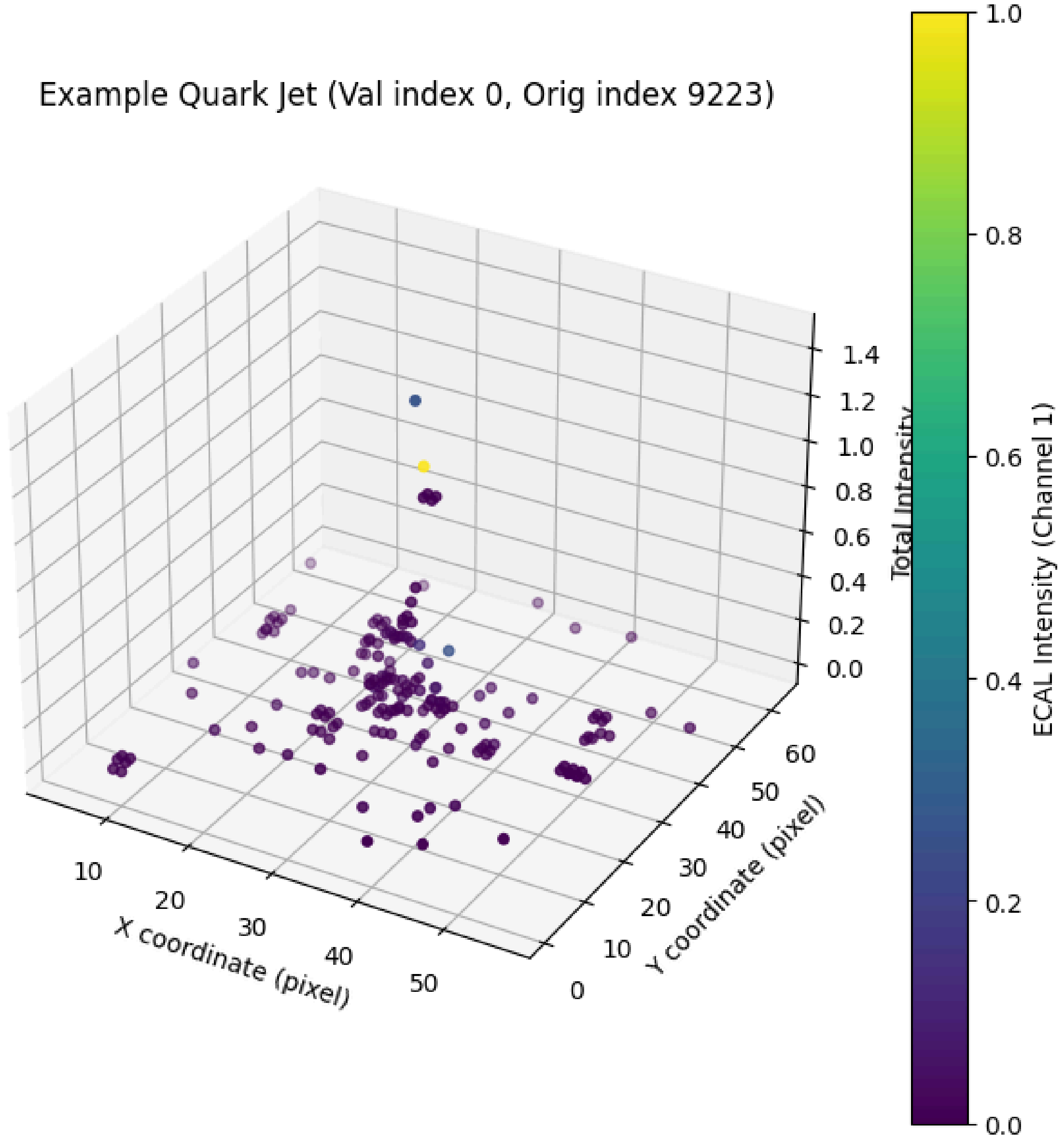
```
                        neighbor_node_idx = indices[i, j_idx]
                        edge_list.append([i, neighbor_node_idx])

                        dist = distances[i, j_idx]
                        normalized_dist = dist / img_size
                        edge_attr = [normalized_dist]

                        edge_attrs.append(edge_attr)

                data.edge_index = torch.tensor(edge_list, dtype=torch.long).t()
                data.edge_attr = torch.tensor(edge_attrs, dtype=torch.float)

        if not hasattr(data, 'edge_index'):
            data.edge_index = torch.empty((2, 0), dtype=torch.long)
            data.edge_attr = torch.empty((0, 1), dtype=torch.float)

        return data


def visualize_point_cloud_3d(coords, features, title="Jet Point Cloud"):
    if coords.shape[0] == 0:
        print(f"Skipping visualization for '{title}': No points found.")
        return

    fig = plt.figure(figsize=(8, 8))
    ax = fig.add_subplot(111, projection='3d')
    x = coords[:, 1]
    y = coords[:, 0]
    z = features[:, 0] + features[:, 1] + features[:, 2]
    colors = features[:, 1]

    scatter = ax.scatter(x, y, z, c=colors, cmap='viridis', marker='o', s=15)

    ax.set_xlabel("X coordinate (pixel)")
    ax.set_ylabel("Y coordinate (pixel)")
    ax.set_zlabel("Total Intensity")
    ax.set_title(title)
    fig.colorbar(scatter, label='ECAL Intensity (Channel 1)')
    plt.show()
```

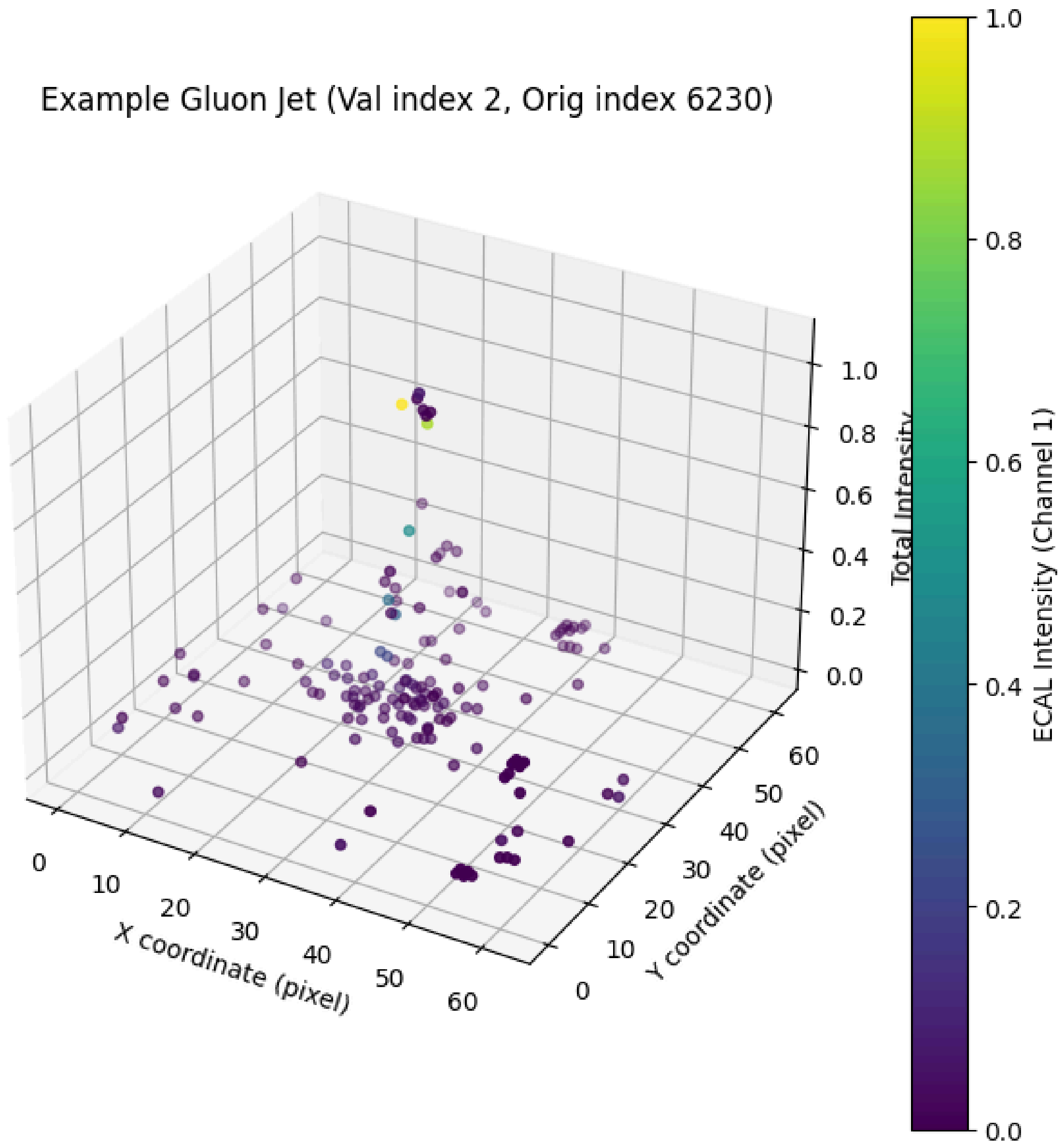
In [5]:

```
if 'X_train' in locals():
    train_dataset_pyg = JetGraphDataset(X_train, y_train, k=K_NEIGHBORS, threshc
    val_dataset_pyg = JetGraphDataset(X_val, y_val, k=K_NEIGHBORS, threshold=POI
    print("\nVisualizing example point clouds...")
    val_indices_original = np.where(np.isin(np.arange(len(y_raw)), val_indices))
    quark_example_idx_orig = -1
    gluon_example_idx_orig = -1




    for i, orig_idx in enumerate(val_indices):
        if y_raw[orig_idx] == 0 and quark_example_idx_orig == -1:
            quark_example_idx_orig = orig_idx
            quark_example_idx_val = i
        if y_raw[orig_idx] == 1 and gluon_example_idx_orig == -1:
            gluon_example_idx_orig = orig_idx
            gluon_example_idx_val = i
        if quark_example_idx_orig != -1 and gluon_example_idx_orig != -1:
            break
```

```
    if quark_example_idx_orig != -1:
        coords_q, feats_q = image_to_pointcloud(X_val[quark_example_idx_val], t
        visualize_point_cloud_3d(coords_q, feats_q, title=f"Example Quark Jet (
    else:
        print("Could not find a quark jet example in validation set for visuali

    if gluon_example_idx_orig != -1:
        coords_g, feats_g = image_to_pointcloud(X_val[gluon_example_idx_val], t
        visualize_point_cloud_3d(coords_g, feats_g, title=f"Example Gluon Jet (
    else:
        print("Could not find a gluon jet example in validation set for visuali

    EDGE_DIM = 1
else:
    print("Skipping dataset creation and visualization as X_train is not defined
    train_dataset_pyg, val_dataset_pyg = None, None
    EDGE_DIM = 1
```

```
Processing train dataset to create graphs...
Filtering train samples:   0%|          | 0/12000 [00:00<?, ?it/s]
Filtered train set: 12000 / 12000 samples have > 1 point.

Processing val dataset to create graphs...
Filtering val samples:   0%|          | 0/3000 [00:00<?, ?it/s]
Filtered val set: 3000 / 3000 samples have > 1 point.

Visualizing example point clouds...
```


Example Quark Jet (Val index 0, Orig index 9223)
X coordinate (pixel)
Y coordinate (pixel)
Total Intensity
ECAL Intensity (Channel 1)
10
20
30
40
50
0
10
20
30
40
50
60
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0.0
0.2
0.4
0.6
0.8
1.0



THis cell defines the model architecture. It consists of three GATv2 layers, each followed by GraphNorm and ELU activation. Dropout is applied after the first two layers. GATv2 allows the model to learn attention weights for edges based on both node and edge features (normalized distance in this case). Multiple attention heads are used in the first two layers for stability.An MLP (Multi-Layer Perceptron) takes the graph embedding and produces the final classification logits for the two classes (Quark/Gluon). The forward pass processes the graph data through the GAT layers, pools the resulting node embeddings, and classifies the pooled graph embedding.

In [6]:
```
class JetGNN(nn.Module):
    def __init__(self, in_dim=5, edge_dim=1, hidden_dim=128, out_dim=2, heads=4,
        super().__init__()
        self.heads = heads
        self.dropout = dropout

        self.conv1 = GATv2Conv(in_dim, hidden_dim, edge_dim=edge_dim, heads=head
        self.norm1 = GraphNorm(hidden_dim * heads)

        self.conv2 = GATv2Conv(hidden_dim * heads, hidden_dim, edge_dim=edge_dim
        self.norm2 = GraphNorm(hidden_dim * heads)
```

```
        self.conv3 = GATv2Conv(hidden_dim * heads, hidden_dim, edge_dim=edge_dim
        self.norm3 = GraphNorm(hidden_dim)

        self.pool_method = "mean_max"

        mlp_in_dim = hidden_dim * 2 if self.pool_method == "mean_max" else hidde

        self.mlp = nn.Sequential(
            nn.Linear(mlp_in_dim, hidden_dim),
            nn.ELU(),
            nn.Dropout(self.dropout),
            nn.Linear(hidden_dim, hidden_dim // 2),
            nn.ELU(),
            nn.Dropout(self.dropout),
            nn.Linear(hidden_dim // 2, out_dim)
        )

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

        x = self.conv1(x, edge_index, edge_attr)
        x = self.norm1(x)
        x = F.elu(x)
        x = F.dropout(x, p=self.dropout, training=self.training)

        x = self.conv2(x, edge_index, edge_attr)
        x = self.norm2(x)
        x = F.elu(x)
        x = F.dropout(x, p=self.dropout, training=self.training)

        x = self.conv3(x, edge_index, edge_attr)
        x = self.norm3(x)
        embeddings = F.elu(x)


        if self.pool_method == "mean":
            pooled_x = global_mean_pool(embeddings, batch)
        elif self.pool_method == "max":
            pooled_x = global_max_pool(embeddings, batch)
        elif self.pool_method == "mean_max":
            x_mean = global_mean_pool(embeddings, batch)
            x_max = global_max_pool(embeddings, batch)
            pooled_x = torch.cat([x_mean, x_max], dim=1)
        else:
            raise ValueError(f"Unsupported pool_method: {self.pool_method}")


        out = self.mlp(pooled_x)


        return out, embeddings


NODE_FEATURES_DIM = 5
model = JetGNN(in_dim=NODE_FEATURES_DIM, edge_dim=EDGE_DIM, hidden_dim=128, out_

print("\nGNN Model Architecture:")
print(model)
```

```
GNN Model Architecture:
JetGNN(
  (conv1): GATv2Conv(5, 128, heads=4)
  (norm1): GraphNorm(512)
  (conv2): GATv2Conv(512, 128, heads=4)
  (norm2): GraphNorm(512)
  (conv3): GATv2Conv(512, 128, heads=1)
  (norm3): GraphNorm(128)
  (mlp): Sequential(
    (0): Linear(in_features=256, out_features=128, bias=True)
    (1): ELU(alpha=1.0)
    (2): Dropout(p=0.5, inplace=False)
    (3): Linear(in_features=128, out_features=64, bias=True)
    (4): ELU(alpha=1.0)
    (5): Dropout(p=0.5, inplace=False)
    (6): Linear(in_features=64, out_features=2, bias=True)
  )
)
```

In [7]:

```
print("\n--- Inspecting Example Graph Statistics ---")

if 'train_dataset_pyg' in locals() and len(train_dataset_pyg) > 0:

    example_data = train_dataset_pyg[0]

    print("Statistics for the first graph in the training dataset:")
    print(f"  Number of nodes: {example_data.num_nodes}")
    print(f"  Number of edges: {example_data.num_edges}")
    print(f"  Number of node features: {example_data.num_node_features}")
    print(f"  Number of edge features: {example_data.num_edge_features}")

    if example_data.num_node_features != NODE_FEATURES_DIM:
        print(f"  WARNING: Node feature mismatch! Graph has {example_data.num_nc
    if example_data.num_edge_features != EDGE_DIM:
        print(f"  WARNING: Edge feature mismatch! Graph has {example_data.num_ed

else:
    print("Training dataset ('train_dataset_pyg') not available or empty, cannot
```

```
--- Inspecting Example Graph Statistics ---
Statistics for the first graph in the training dataset:
  Number of nodes: 349
  Number of edges: 2792
  Number of node features: 5
  Number of edge features: 1
```

In [8]:

```
class Trainer:
    def __init__(self, model, train_loader, val_loader, device, learning_rate=1e
        self.model = model.to(device)
        self.train_loader = train_loader
        self.val_loader = val_loader
        self.device = device
        self.optimizer = optim.AdamW(model.parameters(), lr=learning_rate, weigh

        self.scheduler = optim.lr_scheduler.ReduceLROnPlateau(self.optimizer, mc
        self.criterion = nn.CrossEntropyLoss()

        self.early_stopping_patience = early_stopping_patience
        self.best_val_acc = 0.0
        self.best_epoch = 0
```

```
        self.epochs_no_improve = 0
        self.best_model_state = None


        self.history = {'train_loss': [], 'val_loss': [], 'val_acc': [], 'lr': [

    def train_epoch(self):
        self.model.train()
        epoch_loss = 0
        num_batches = len(self.train_loader)
        pbar = tqdm(self.train_loader, desc="Training", leave=False, total=num_b
        for data in pbar:
            data = data.to(self.device)
            self.optimizer.zero_grad()
            logits, _ = self.model(data)
            target = data.y
            if target.ndim > 1:
                 target = target.squeeze()
            loss = self.criterion(logits, target)
            loss.backward()

            nn.utils.clip_grad_norm_(self.model.parameters(), max_norm=1.0)
            self.optimizer.step()

            epoch_loss += loss.item()
            pbar.set_postfix({'loss': loss.item()})

        avg_loss = epoch_loss / num_batches if num_batches > 0 else 0
        return avg_loss

    def validate(self):
        self.model.eval()
        total_loss = 0
        correct = 0
        total_samples = 0
        all_preds = []
        all_labels = []
        num_batches = len(self.val_loader)

        with torch.no_grad():
            pbar = tqdm(self.val_loader, desc="Validation", leave=False, total=n
            for data in pbar:
                data = data.to(self.device)
                logits, _ = self.model(data)
                target = data.y
                if target.ndim > 1:
                    target = target.squeeze()
                loss = self.criterion(logits, target)
                total_loss += loss.item()

                preds = logits.argmax(dim=1)
                correct += preds.eq(target).sum().item()
                total_samples += target.size(0)

                all_preds.extend(preds.cpu().numpy())
                all_labels.extend(target.cpu().numpy())
                pbar.set_postfix({'acc': correct / total_samples if total_sample

        avg_loss = total_loss / num_batches if num_batches > 0 else 0
        acc = correct / total_samples if total_samples > 0 else 0
```

```
        return avg_loss, acc, np.array(all_labels), np.array(all_preds)

    def train(self, epochs=50):
        print(f"\nStarting training for {epochs} epochs...")
        for epoch in range(1, epochs + 1):
            train_loss = self.train_epoch()
            val_loss, val_acc, _, _ = self.validate()

            current_lr = self.optimizer.param_groups[0]['lr']
            self.history['train_loss'].append(train_loss)
            self.history['val_loss'].append(val_loss)
            self.history['val_acc'].append(val_acc)
            self.history['lr'].append(current_lr)

            print(f"Epoch {epoch:03d}/{epochs:03d} | Train Loss: {train_loss:.4f

            self.scheduler.step(val_acc)


            if val_acc > self.best_val_acc:
                self.best_val_acc = val_acc
                self.best_epoch = epoch
                self.epochs_no_improve = 0

                self.best_model_state = copy.deepcopy(self.model.state_dict())
                print(f"New best validation accuracy: {self.best_val_acc:.4f} at

            else:
                self.epochs_no_improve += 1
                print(f"Validation accuracy did not improve for {self.epochs_no_

            if self.epochs_no_improve >= self.early_stopping_patience:
                print(f"\n Early stopping triggered after {epoch} epochs.")
                print(f"Best validation accuracy was {self.best_val_acc:.4f} at
                break

        print("\nTraining finished.")


        if self.best_model_state:
            print(f"Loading best model state from epoch {self.best_epoch} with a
            self.model.load_state_dict(self.best_model_state)


            torch.save(self.best_model_state, "best_model_final.pth")
            print("Best model saved to 'best_model_final.pth'")
        else:
            print("Warning: No improvement detected during training, using the m



        self.plot_metrics()
        return self.best_val_acc

    def plot_metrics(self):
        epochs_ran = range(1, len(self.history['train_loss']) + 1)

        plt.figure(figsize=(15, 5))
```

```
        plt.subplot(1, 3, 1)
        plt.plot(epochs_ran, self.history['train_loss'], label='Train Loss', mar
        plt.plot(epochs_ran, self.history['val_loss'], label='Validation Loss',
        if self.best_epoch > 0:
            plt.axvline(self.best_epoch, linestyle='--', color='r', label=f'Best
        plt.xlabel('Epoch')
        plt.ylabel('Loss')
        plt.title('Training & Validation Loss')
        plt.legend()
        plt.grid(True)


        plt.subplot(1, 3, 2)
        plt.plot(epochs_ran, self.history['val_acc'], label='Validation Accuracy
        if self.best_epoch > 0:
            plt.axvline(self.best_epoch, linestyle='--', color='r', label=f'Best
            plt.plot(self.best_epoch, self.best_val_acc, 'ro', markersize=8, lab
        plt.xlabel('Epoch')
        plt.ylabel('Accuracy')
        plt.title('Validation Accuracy')
        plt.legend()
        plt.grid(True)

        plt.subplot(1, 3, 3)
        plt.plot(epochs_ran, self.history['lr'], label='Learning Rate', marker='
        plt.xlabel('Epoch')
        plt.ylabel('Learning Rate')
        plt.title('Learning Rate Schedule')
        plt.legend()
        plt.grid(True)
        plt.yscale('log')

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

In [13]:

```
BATCH_SIZE = 64
LEARNING_RATE = 3e-4
WEIGHT_DECAY = 1e-5
EPOCHS = 30
SCHEDULER_PATIENCE = 5
EARLY_STOPPING_PATIENCE = 10


if train_dataset_pyg and val_dataset_pyg:

    train_loader = PyGDataLoader(train_dataset_pyg, batch_size=BATCH_SIZE, shuff
    val_loader = PyGDataLoader(val_dataset_pyg, batch_size=BATCH_SIZE*2, shuffle

    print(f"\nCreated DataLoaders:")
    print(f"Train batches: {len(train_loader)}, Val batches: {len(val_loader)}")

    model = JetGNN(in_dim=NODE_FEATURES_DIM, edge_dim=EDGE_DIM, hidden_dim=128,
    print(f"\nRe-initialized Model on {device}")


    trainer = Trainer(
        model=model,
        train_loader=train_loader,
        val_loader=val_loader,
        device=device,
```

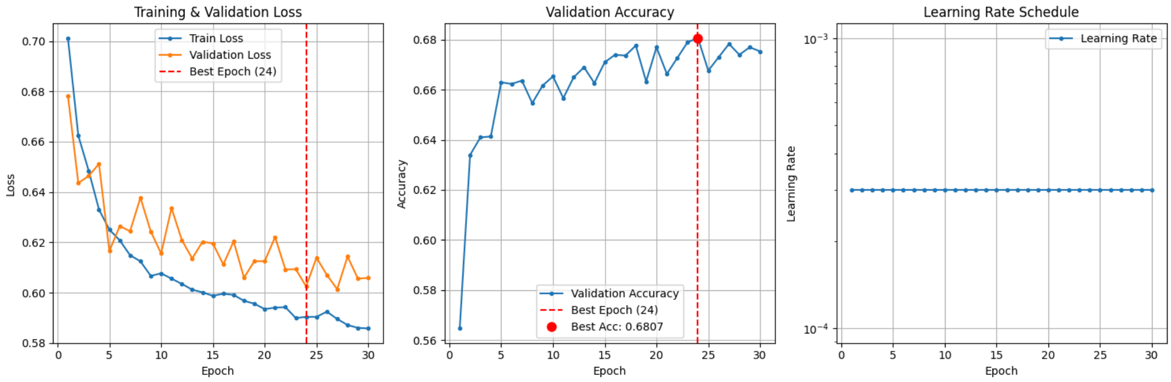
```
        learning_rate=LEARNING_RATE,
        weight_decay=WEIGHT_DECAY,
        scheduler_patience=SCHEDULER_PATIENCE,
        early_stopping_patience=EARLY_STOPPING_PATIENCE
    )


    best_accuracy = trainer.train(epochs=EPOCHS)

    print(f"\n--- Training Complete ---")
    print(f"Best Validation Accuracy achieved: {best_accuracy:.4f}")

else:
    print("Skipping training execution as datasets are not available.")
    best_accuracy = 0.0
```

```
Created DataLoaders:
Train batches: 188, Val batches: 24

Re-initialized Model on cuda

Starting training for 30 epochs...
/usr/local/lib/python3.10/dist-packages/torch/optim/lr_scheduler.py:62: UserWarni
ng: The verbose parameter is deprecated. Please use get_last_lr() to access the l
earning rate.
  warnings.warn(
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 001/030 | Train Loss: 0.7012 | Val Loss: 0.6783 | Val Acc: 0.5647 | LR: 3.0
0e-04
New best validation accuracy: 0.5647 at epoch 1
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 002/030 | Train Loss: 0.6624 | Val Loss: 0.6436 | Val Acc: 0.6340 | LR: 3.0
0e-04
New best validation accuracy: 0.6340 at epoch 2
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 003/030 | Train Loss: 0.6485 | Val Loss: 0.6464 | Val Acc: 0.6410 | LR: 3.0
0e-04
New best validation accuracy: 0.6410 at epoch 3
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 004/030 | Train Loss: 0.6330 | Val Loss: 0.6512 | Val Acc: 0.6413 | LR: 3.0
0e-04
New best validation accuracy: 0.6413 at epoch 4
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 005/030 | Train Loss: 0.6250 | Val Loss: 0.6165 | Val Acc: 0.6630 | LR: 3.0
0e-04
New best validation accuracy: 0.6630 at epoch 5
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 006/030 | Train Loss: 0.6208 | Val Loss: 0.6264 | Val Acc: 0.6623 | LR: 3.0
0e-04
Validation accuracy did not improve for 1 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
```

```
Epoch 007/030 | Train Loss: 0.6149 | Val Loss: 0.6244 | Val Acc: 0.6637 | LR: 3.0
0e-04
New best validation accuracy: 0.6637 at epoch 7
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 008/030 | Train Loss: 0.6124 | Val Loss: 0.6378 | Val Acc: 0.6547 | LR: 3.0
0e-04
Validation accuracy did not improve for 1 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 009/030 | Train Loss: 0.6067 | Val Loss: 0.6243 | Val Acc: 0.6617 | LR: 3.0
0e-04
Validation accuracy did not improve for 2 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 010/030 | Train Loss: 0.6077 | Val Loss: 0.6156 | Val Acc: 0.6653 | LR: 3.0
0e-04
New best validation accuracy: 0.6653 at epoch 10
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 011/030 | Train Loss: 0.6056 | Val Loss: 0.6336 | Val Acc: 0.6567 | LR: 3.0
0e-04
Validation accuracy did not improve for 1 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 012/030 | Train Loss: 0.6034 | Val Loss: 0.6209 | Val Acc: 0.6650 | LR: 3.0
0e-04
Validation accuracy did not improve for 2 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 013/030 | Train Loss: 0.6012 | Val Loss: 0.6136 | Val Acc: 0.6690 | LR: 3.0
0e-04
New best validation accuracy: 0.6690 at epoch 13
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 014/030 | Train Loss: 0.6001 | Val Loss: 0.6202 | Val Acc: 0.6627 | LR: 3.0
0e-04
Validation accuracy did not improve for 1 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 015/030 | Train Loss: 0.5987 | Val Loss: 0.6195 | Val Acc: 0.6710 | LR: 3.0
0e-04
New best validation accuracy: 0.6710 at epoch 15
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 016/030 | Train Loss: 0.5996 | Val Loss: 0.6112 | Val Acc: 0.6740 | LR: 3.0
0e-04
New best validation accuracy: 0.6740 at epoch 16
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 017/030 | Train Loss: 0.5991 | Val Loss: 0.6204 | Val Acc: 0.6737 | LR: 3.0
0e-04
Validation accuracy did not improve for 1 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 018/030 | Train Loss: 0.5967 | Val Loss: 0.6059 | Val Acc: 0.6777 | LR: 3.0
0e-04
New best validation accuracy: 0.6777 at epoch 18
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
```

```
Epoch 019/030 | Train Loss: 0.5956 | Val Loss: 0.6125 | Val Acc: 0.6633 | LR: 3.0
0e-04
Validation accuracy did not improve for 1 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 020/030 | Train Loss: 0.5934 | Val Loss: 0.6125 | Val Acc: 0.6770 | LR: 3.0
0e-04
Validation accuracy did not improve for 2 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 021/030 | Train Loss: 0.5940 | Val Loss: 0.6221 | Val Acc: 0.6663 | LR: 3.0
0e-04
Validation accuracy did not improve for 3 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 022/030 | Train Loss: 0.5942 | Val Loss: 0.6092 | Val Acc: 0.6727 | LR: 3.0
0e-04
Validation accuracy did not improve for 4 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 023/030 | Train Loss: 0.5899 | Val Loss: 0.6093 | Val Acc: 0.6790 | LR: 3.0
0e-04
New best validation accuracy: 0.6790 at epoch 23
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 024/030 | Train Loss: 0.5903 | Val Loss: 0.6025 | Val Acc: 0.6807 | LR: 3.0
0e-04
New best validation accuracy: 0.6807 at epoch 24
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Epoch 025/030 | Train Loss: 0.5903 | Val Loss: 0.6139 | Val Acc: 0.6677 | LR: 3.0
0e-04
Validation accuracy did not improve for 1 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 026/030 | Train Loss: 0.5924 | Val Loss: 0.6071 | Val Acc: 0.6730 | LR: 3.0
0e-04
Validation accuracy did not improve for 2 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 027/030 | Train Loss: 0.5895 | Val Loss: 0.6013 | Val Acc: 0.6783 | LR: 3.0
0e-04
Validation accuracy did not improve for 3 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 028/030 | Train Loss: 0.5871 | Val Loss: 0.6143 | Val Acc: 0.6740 | LR: 3.0
0e-04
Validation accuracy did not improve for 4 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Epoch 029/030 | Train Loss: 0.5860 | Val Loss: 0.6056 | Val Acc: 0.6770 | LR: 3.0
0e-04
Validation accuracy did not improve for 5 epoch(s).
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
```

```
Epoch 030/030 | Train Loss: 0.5858 | Val Loss: 0.6059 | Val Acc: 0.6753 | LR: 3.0
0e-04
Validation accuracy did not improve for 6 epoch(s).

Training finished.
Loading best model state from epoch 24 with accuracy 0.6807
Best model saved to 'best_model_final.pth'
```

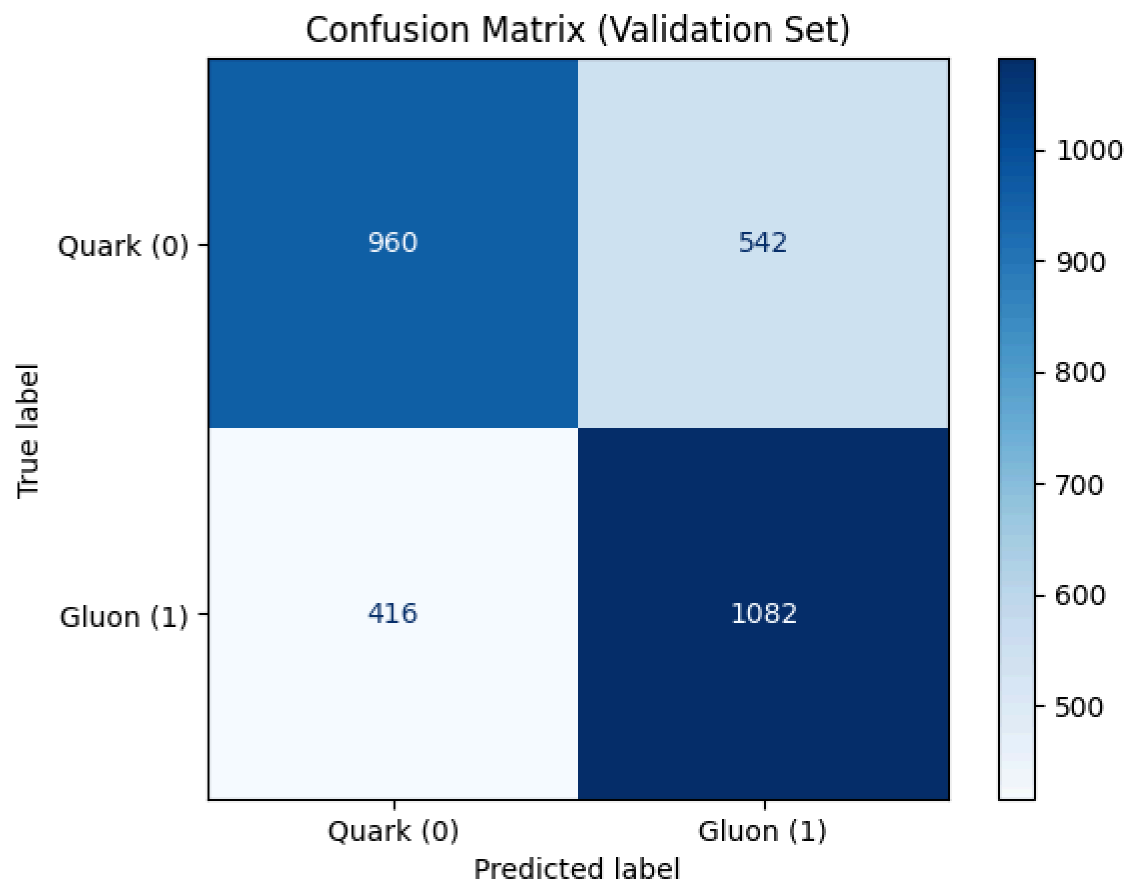



```
--- Training Complete ---
Best Validation Accuracy achieved: 0.6807
```

In [14]:
```
import umap.umap_ as umap

if 'trainer' in locals() and best_accuracy > 0:
    print("\n--- Evaluating Best Model on Validation Set ---")

    best_model_path = "best_model_final.pth"
    if os.path.exists(best_model_path):
        print(f"Loading best model from {best_model_path}")
        eval_model = JetGNN(in_dim=NODE_FEATURES_DIM, edge_dim=EDGE_DIM, hidden_
        eval_model.load_state_dict(torch.load(best_model_path, map_location=devi
        eval_model.eval()

        val_loss, val_acc, all_labels, all_preds = trainer.validate()

        print(f"\nBest Model Performance on Validation Set:")
        print(f"Validation Loss: {val_loss:.4f}")
        print(f"Validation Accuracy: {val_acc:.4f}")

        print("\nGenerating Confusion Matrix...")
        cm = confusion_matrix(all_labels, all_preds)
        disp = ConfusionMatrixDisplay(confusion_matrix=cm, display_labels=['Quar
        disp.plot(cmap=plt.cm.Blues)
        plt.title("Confusion Matrix (Validation Set)")
        plt.show()

        print("\nClassification Report (Validation Set):")
        report = classification_report(all_labels, all_preds, target_names=['Qua
        print(report)

        print("\nGenerating UMAP visualization of graph embeddings...")
        all_embeddings = []
        all_batch_labels = []
        eval_model.eval()
        with torch.no_grad():
            pbar = tqdm(val_loader, desc="Extracting Embeddings", leave=False)
            for data in pbar:
                data = data.to(device)
                _, embeddings = eval_model(data)
```

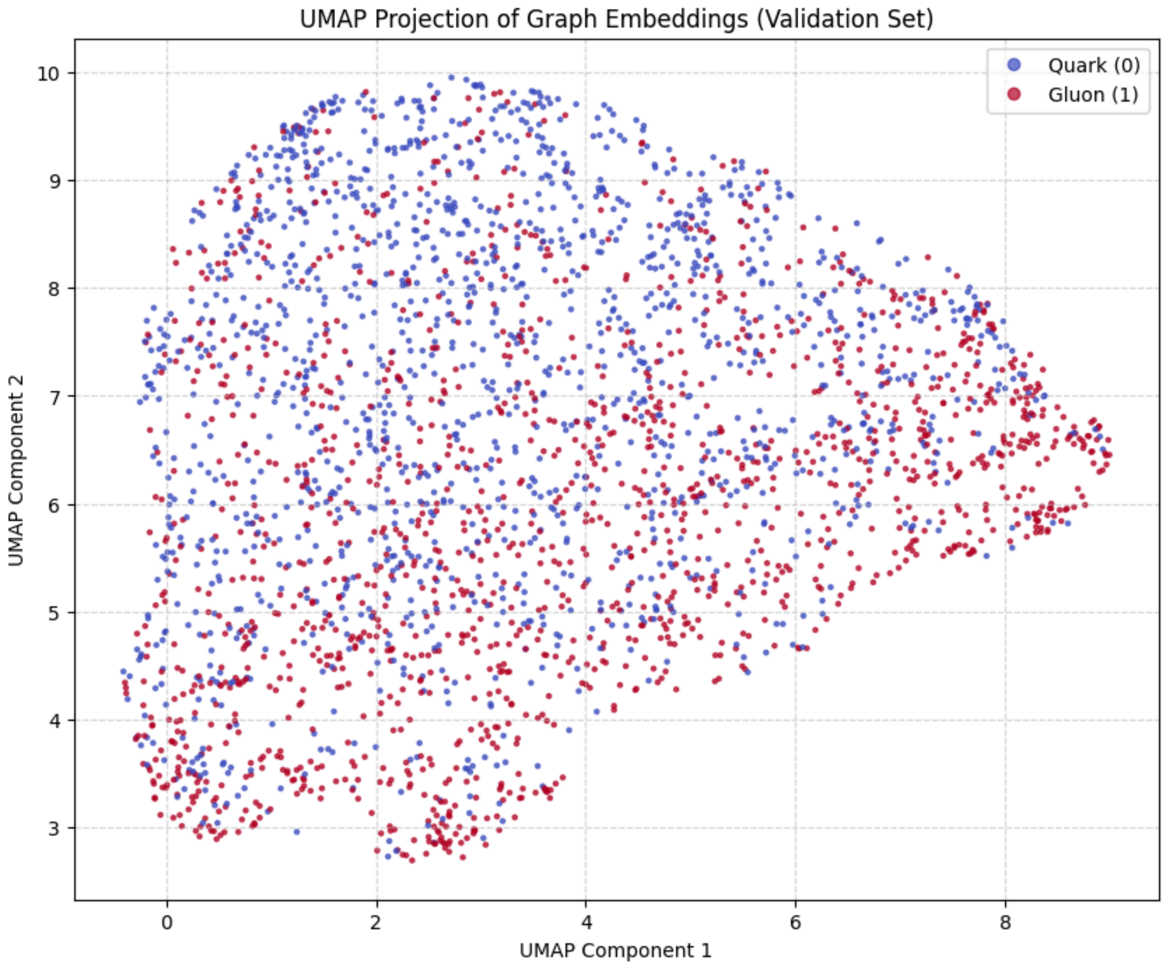
```
                pooled_embeddings = global_mean_pool(embeddings, data.batch).cpu
                all_embeddings.append(pooled_embeddings)
                all_batch_labels.append(data.y.cpu().numpy())

        if all_embeddings:
            all_embeddings = np.concatenate(all_embeddings, axis=0)
            all_batch_labels = np.concatenate(all_batch_labels, axis=0).flatten(
            print(f"Total embeddings extracted: {all_embeddings.shape[0]}")

            reducer = umap.UMAP(n_neighbors=30, min_dist=0.1, n_components=2, ra
            print("Fitting UMAP...")
            embedding_2d = reducer.fit_transform(all_embeddings)

            plt.figure(figsize=(10, 8))
            scatter = plt.scatter(embedding_2d[:, 0], embedding_2d[:, 1], c=all_
            plt.title('UMAP Projection of Graph Embeddings (Validation Set)')
            plt.xlabel('UMAP Component 1')
            plt.ylabel('UMAP Component 2')
            plt.legend(handles=scatter.legend_elements()[0], labels=['Quark (0)'
            plt.grid(True, linestyle='--', alpha=0.5)
            plt.show()
        else:
            print("Could not extract embeddings for UMAP.")

    else:
        print(f"Error: Best model file '{best_model_path}' not found. Cannot eva
else:
    print("\nSkipping final evaluation as training did not complete successfully
```

```
--- Evaluating Best Model on Validation Set ---
Loading best model from best_model_final.pth
<ipython-input-14-3ee90de41758>:10: FutureWarning: You are using `torch.load` wit
h `weights_only=False` (the current default value), which uses the default pickle
module implicitly. It is possible to construct malicious pickle data which will e
xecute arbitrary code during unpickling (See https://github.com/pytorch/pytorch/b
lob/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 funct
ions that could be executed during unpickling. Arbitrary objects will no longer b
e allowed to be loaded via this mode unless they are explicitly allowlisted by th
e 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 loa
ded file. Please open an issue on GitHub for any issues related to this experimen
tal feature.
  eval_model.load_state_dict(torch.load(best_model_path, map_location=device))
Validation:   0%|          | 0/24 [00:00<?, ?it/s]
Best Model Performance on Validation Set:
Validation Loss: 0.6025
Validation Accuracy: 0.6807

Generating Confusion Matrix...
```




```
Classification Report (Validation Set):
              precision    recall  f1-score   support

   Quark (0)       0.70      0.64      0.67      1502
   Gluon (1)       0.67      0.72      0.69      1498

    accuracy                           0.68      3000
   macro avg       0.68      0.68      0.68      3000
weighted avg       0.68      0.68      0.68      3000


Generating UMAP visualization of graph embeddings...
Extracting Embeddings:   0%|          | 0/24 [00:00<?, ?it/s]
Total embeddings extracted: 3000
Fitting UMAP...
```

```
/usr/local/lib/python3.10/dist-packages/umap/umap_.py:1952: UserWarning: n_jobs v
alue 1 overridden to 1 by setting random_state. Use no seed for parallelism.
  warn(
```


UMAP Projection of Graph Embeddings (Validation Set)
Quark (0)
Gluon (1)
UMAP Component 2
UMAP Component 1
10
9
8
7
6
5
4
3
0
2
4
6
8

In [ ]: