In [ ]:
```
!pip install torch_geometric
```

```
Collecting torch_geometric
  Downloading torch_geometric-2.6.1-py3-none-any.whl.metadata (63 kB)
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kages (from requests->torch_geometric) (3.10)
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hon3.10/dist-packages (from intel-openmp>=2024->mkl->numpy->torch_geometric) (202
4.2.0)
Downloading torch_geometric-2.6.1-py3-none-any.whl (1.1 MB)
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0:01
Installing collected packages: torch_geometric
Successfully installed torch_geometric-2.6.1
```

In [ ]:
```python
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim
from torch.utils.data import DataLoader, TensorDataset, Subset
from torchvision import transforms

import torch_geometric
import torch_geometric.nn as pyg_nn
from torch_geometric.data import Data, Dataset, DataLoader as PyGDataLoader
from torch_geometric.utils import to_networkx
from sklearn.neighbors import kneighbors_graph
import scipy.sparse

import h5py
import numpy as np
import matplotlib.pyplot as plt
import networkx as nx
import os
import time
from tqdm.notebook import tqdm

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

```
Using device: cuda
```

In [ ]:
```python
SEED = 42
SUBSET_SIZE = 15000
VALIDATION_SPLIT = 0.2
BATCH_SIZE = 64
RESIZE_DIM = 128

GAE_LATENT_DIM = 128
GAE_HIDDEN_DIM = 128
LEARNING_RATE_GAE = 1e-3
NUM_EPOCHS_GAE = 30
K_NEIGHBORS = 8

DATA_PATH = '/kaggle/input/falcon/quark-gluon_data-set_n139306.hdf5'
VAE_WEIGHTS_PATH = '/kaggle/input/vae/pytorch/default/1/best_vae_model_weights-m
GAE_SAVE_PATH = './best_gae_model_weights.pth'

VAE_LATENT_DIM = 128
```

```python
VAE_BASE_FILTERS = 32
VAE_INPUT_CHANNELS = 3

torch.manual_seed(SEED)
np.random.seed(SEED)
if torch.cuda.is_available():
    torch.cuda.manual_seed_all(SEED)
    torch.backends.cudnn.deterministic = True
    torch.backends.cudnn.benchmark = False

print(f"Configuration:")
print(f"  SEED: {SEED}")
print(f"  SUBSET_SIZE: {SUBSET_SIZE}")
print(f"  BATCH_SIZE: {BATCH_SIZE}")
print(f"  GAE_LATENT_DIM: {GAE_LATENT_DIM}")
print(f"  GAE_HIDDEN_DIM: {GAE_HIDDEN_DIM}")
print(f"  LEARNING_RATE_GAE: {LEARNING_RATE_GAE}")
print(f"  NUM_EPOCHS_GAE: {NUM_EPOCHS_GAE}")
print(f"  K_NEIGHBORS: {K_NEIGHBORS}")
print(f"  DATA_PATH: {DATA_PATH}")
print(f"  VAE_WEIGHTS_PATH: {VAE_WEIGHTS_PATH}")
print(f"  GAE_SAVE_PATH: {GAE_SAVE_PATH}")
```

```
Configuration:
  SEED: 42
  SUBSET_SIZE: 15000
  BATCH_SIZE: 64
  GAE_LATENT_DIM: 128
  GAE_HIDDEN_DIM: 128
  LEARNING_RATE_GAE: 0.001
  NUM_EPOCHS_GAE: 30
  K_NEIGHBORS: 8
  DATA_PATH: /kaggle/input/falcon/quark-gluon_data-set_n139306.hdf5
  VAE_WEIGHTS_PATH: /kaggle/input/vae/pytorch/default/1/best_vae_model_weights-ma
in.pth
  GAE_SAVE_PATH: ./best_gae_model_weights.pth
```

In [ ]:

```python
def load_hdf5_data_raw(file_path, image_key='X_jets', label_key='y', subset_size
    print(f"Loading raw data from: {file_path}")
    try:
        with h5py.File(file_path, 'r') as f:
            print("Keys in HDF5 file:", list(f.keys()))

            if image_key not in f:
                raise KeyError(f"Image key '{image_key}' not found in HDF5 file.
            else:
                 labels_raw = f[label_key]

            images_raw = f[image_key]
            num_samples = images_raw.shape[0]
            print(f"Found {num_samples} total samples.")

            if subset_size is not None and subset_size > 0 and subset_size < num
                print(f"Selecting a random subset of {subset_size} samples.")
                np.random.seed(SEED)
                indices = np.random.choice(num_samples, subset_size, replace=Fal
                indices = np.sort(indices)
                images_loaded = images_raw[indices]
                if labels_raw is not None:
                    labels_loaded = labels_raw[indices]
```

```
                else:
                    labels_loaded = np.zeros(subset_size)
            else:
                print(f"Using all {num_samples} available samples.")
                images_loaded = images_raw[:]
                if labels_raw is not None:
                     labels_loaded = labels_raw[:]
                else:
                     labels_loaded = np.zeros(num_samples)

            print(f"Loaded raw images shape: {images_loaded.shape}")
            print(f"Loaded labels shape: {labels_loaded.shape}")

            if images_loaded.ndim == 4 and images_loaded.shape[3] == VAE_INPUT_C
                images_tensor = torch.tensor(images_loaded, dtype=torch.float32)
                print(f"Converted to tensor shape: {images_tensor.shape}")
            else:
                 raise ValueError(f"Unexpected raw image dimensions: {images_loa

            labels_tensor = torch.tensor(labels_loaded, dtype=torch.long)

            del images_loaded

    except Exception as e:
        print(f"Error loading HDF5 data: {e}")
        raise

    return images_tensor, labels_tensor
raw_images_tensor, labels_tensor = load_hdf5_data_raw(DATA_PATH, image_key='X_je

print(f"\nRaw images tensor shape: {raw_images_tensor.shape}")
print(f"Labels tensor shape: {labels_tensor.shape}")
```

```
Loading raw data from: /kaggle/input/falcon/quark-gluon_data-set_n139306.hdf5
Keys in HDF5 file: ['X_jets', 'm0', 'pt', 'y']
Found 139306 total samples.
Selecting a random subset of 15000 samples.
Loaded raw images shape: (15000, 125, 125, 3)
Loaded labels shape: (15000,)
Converted to tensor shape: torch.Size([15000, 3, 125, 125])

Raw images tensor shape: torch.Size([15000, 3, 125, 125])
Labels tensor shape: torch.Size([15000])
```

In [ ]:

```
if raw_images_tensor.shape[-2:] != (RESIZE_DIM, RESIZE_DIM):
    print(f"\nResizing images from {raw_images_tensor.shape[-2:]} to ({RESIZE_DI
    images_resized = F.interpolate(raw_images_tensor, size=(RESIZE_DIM, RESIZE_D
else:
    print("\nImages already at target size.")
    images_resized = raw_images_tensor
print(f"Resized images tensor shape: {images_resized.shape}")
del raw_images_tensor

n_total = len(images_resized)
n_val = int(VALIDATION_SPLIT * n_total)
n_train = n_total - n_val

indices = torch.randperm(n_total, generator=torch.Generator().manual_seed(SEED))
train_indices = indices[:n_train]
val_indices = indices[n_train:]
```

```
print(f"\nSplitting resized data into {n_train} training and {n_val} validation

print("Calculating normalization statistics on the training set split...")
train_data_for_norm = images_resized[train_indices]

channel_means = train_data_for_norm.mean(dim=[0, 2, 3], keepdim=True) # Shape: (
channel_stds = train_data_for_norm.std(dim=[0, 2, 3], keepdim=True)   # Shape: (


epsilon_norm = 1e-6 #to preven 0 division
channel_stds[channel_stds < epsilon_norm] = epsilon_norm

print(f"Channel Means: {channel_means.squeeze().tolist()}")
print(f"Channel Stds: {channel_stds.squeeze().tolist()}")

print("Applying normalization to the entire dataset...")
original_images_tensor = (images_resized - channel_means) / channel_stds
del images_resized

print(f"Standardized images tensor shape: {original_images_tensor.shape}")

sample_train_idx_in_original = train_indices[0]
print(f"Sample normalized train image (mean): {original_images_tensor[sample_tra
      f"(std): {original_images_tensor[sample_train_idx_in_original].std():.4f}
sample_val_idx_in_original = val_indices[0]
print(f"Sample normalized val image (mean): {original_images_tensor[sample_val_i
      f"(std): {original_images_tensor[sample_val_idx_in_original].std():.4f}")
print(f"\nCreated train_indices (len {len(train_indices)}) and val_indices (len
normalization_means = channel_means
normalization_stds = channel_stds
print("Stored normalization_means and normalization_stds for later use.")
```

```
Resizing images from torch.Size([125, 125]) to (128, 128)...
Resized images tensor shape: torch.Size([15000, 3, 128, 128])

Splitting resized data into 12000 training and 3000 validation samples.
Calculating normalization statistics on the training set split...
Channel Means: [8.004522533155978e-05, 5.1089864427922294e-05, 3.035522240679711e
-05]
Channel Stds: [0.005717707797884941, 0.001339102745987475, 0.0004247160104569047
7]
Applying normalization to the entire dataset...
Standardized images tensor shape: torch.Size([15000, 3, 128, 128])
Sample normalized train image (mean): -0.0059, (std): 0.4596 (Note: std per image
!= 1)
Sample normalized val image (mean): -0.0052, (std): 0.5615

Created train_indices (len 12000) and val_indices (len 3000)
Stored normalization_means and normalization_stds for later use.
```

This function is similar to the graph creation in the GNN notebook but adapted for the GAE task. No edge features are used in this GAE implementation. It stores the original pixel coordinates (graph_data.coords) and image dimensions (height, width) within the Data object, which will be needed later to map the reconstructed node features back onto an image grid.

In [ ]:
```
def create_graph_from_image(image_tensor, label, k_neighbors, include_coords=Tru
    channels, height, width = image_tensor.shape
```

```
    image_tensor_cpu = image_tensor.cpu()

    energy_threshold = 1e-6
    mask = torch.sum(image_tensor_cpu, dim=0) > energy_threshold
    non_zero_coords = torch.nonzero(mask, as_tuple=False) # shape (num_points, 2

    num_points = non_zero_coords.shape[0]
    if num_points == 0:
        return None
    point_features = image_tensor[:, non_zero_coords[:, 0], non_zero_coords[:, 1

    coords_norm = non_zero_coords.float() / torch.tensor([height - 1, width - 1]

    if include_coords:
        node_features = torch.cat([point_features, coords_norm], dim=1)
    else:
        node_features = point_features
    edge_index = None
    if num_points > 1:
        coords_np = coords_norm.cpu().numpy()
        actual_k = min(k_neighbors, num_points - 1)

        if actual_k > 0:
            A = kneighbors_graph(coords_np, n_neighbors=actual_k, mode='connecti
            coo = A.tocoo()
            row = torch.from_numpy(coo.row).to(torch.long)
            col = torch.from_numpy(coo.col).to(torch.long)
            edge_index = torch.stack([row, col], dim=0)
        else:
             edge_index = torch.empty((2, 0), dtype=torch.long)

    else:
        edge_index = torch.empty((2, 0), dtype=torch.long)
    graph_data = Data(x=node_features.to(image_tensor.device),
                      edge_index=edge_index.to(image_tensor.device),
                      y=label.to(image_tensor.device))
    graph_data.num_nodes = num_points
    graph_data.height = height
    graph_data.width = width
    graph_data.coords = non_zero_coords.to(image_tensor.device)

    return graph_data
graph_list = []
print(f"Converting {original_images_tensor.shape[0]} images to graphs (using skl
for i in tqdm(range(original_images_tensor.shape[0])):
    graph = create_graph_from_image(
        original_images_tensor[i],
        labels_tensor[i],
        k_neighbors=K_NEIGHBORS,
        include_coords=True
    )
    if graph is not None:
        graph_list.append(graph)

print(f"Successfully converted {len(graph_list)} images into graphs.")
if len(graph_list) < original_images_tensor.shape[0]:
    print(f"Skipped {original_images_tensor.shape[0] - len(graph_list)} images w
```

```
Converting 15000 images to graphs (using sklearn KNN)...
```

```
  0%|          | 0/15000 [00:00<?, ?it/s]
Successfully converted 15000 images into graphs.
```

In [ ]:

```python
from torch.utils.data import random_split

class JetGraphDataset(Dataset):
    def __init__(self, data_list):
        super().__init__(None)
        self.data_list = data_list

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

    def get(self, idx):
        return self.data_list[idx]

full_dataset = JetGraphDataset(graph_list)

num_graphs = len(full_dataset)
num_val = int(num_graphs * VALIDATION_SPLIT)
num_train = num_graphs - num_val

print(f"Total graphs: {num_graphs}")
print(f"Splitting into {num_train} training and {num_val} validation graphs.")

train_dataset, val_dataset = random_split(full_dataset, [num_train, num_val],
                                          generator=torch.Generator().manual_see

train_loader = PyGDataLoader(train_dataset, batch_size=BATCH_SIZE, shuffle=True,
val_loader = PyGDataLoader(val_dataset, batch_size=BATCH_SIZE, shuffle=False, nu

print(f"Created DataLoaders:")
print(f"  Train batches: {len(train_loader)}")
print(f"  Validation batches: {len(val_loader)}")

try:
    first_batch = next(iter(train_loader))
    print("\n--- Sample Batch Info ---")
    print(first_batch)
    print(f"Number of graphs in batch: {first_batch.num_graphs}")
    print(f"Node features shape: {first_batch.x.shape}")
    print(f"Edge index shape: {first_batch.edge_index.shape}")
    print(f"Batch vector shape: {first_batch.batch.shape}")
    print(f"Labels shape: {first_batch.y.shape}")
    node_feature_dim = first_batch.num_node_features
    print(f"Detected Node Feature Dimension: {node_feature_dim}")
except StopIteration:
    print("Could not retrieve a batch, check dataset/loader.")
    node_feature_dim = VAE_INPUT_CHANNELS + 2
    print(f"Manually setting Node Feature Dimension: {node_feature_dim}")
```

```
Total graphs: 15000
Splitting into 12000 training and 3000 validation graphs.
Created DataLoaders:
  Train batches: 188
  Validation batches: 47
```

```
/usr/local/lib/python3.10/dist-packages/torch_geometric/deprecation.py:26: UserWa
rning: 'data.DataLoader' is deprecated, use 'loader.DataLoader' instead
  warnings.warn(out)
```

```
--- Sample Batch Info ---
DataBatch(x=[62031, 5], edge_index=[2, 496248], y=[64], num_nodes=62031, height=
[64], width=[64], coords=[62031, 2], batch=[62031], ptr=[65])
Number of graphs in batch: 64
Node features shape: torch.Size([62031, 5])
Edge index shape: torch.Size([2, 496248])
Batch vector shape: torch.Size([62031])
Labels shape: torch.Size([64])
Detected Node Feature Dimension: 5
```

GAE_Encoder: Takes node features (x) and graph structure (edge_index) and encodes each node into a latent representation (z) using two GCN layers with batch normalization. FeatureDecoder: A simple MLP that takes the latent embedding (z) of a single node and decodes it back to the original node feature dimension (5D in this case: ECAL, HCAL, Tracks, coord_y, coord_x). GraphAutoencoder: Combines the encoder and decoder. The goal is for recon_x (reconstructed node features) to be as close as possible to the original x (input node features).

In [ ]:
```python
class GAE_Encoder(nn.Module):
    def __init__(self, in_channels, hidden_channels, out_channels):
        super().__init__()
        self.conv1 = pyg_nn.GCNConv(in_channels, hidden_channels)
        self.bn1 = nn.BatchNorm1d(hidden_channels)
        self.conv2 = pyg_nn.GCNConv(hidden_channels, out_channels)

    def forward(self, x, edge_index):
        x = self.conv1(x, edge_index)
        x = self.bn1(x)
        x = F.relu(x)
        # x = F.dropout(x, p=0.5, training=self.training)
        z = self.conv2(x, edge_index)
        return z

class FeatureDecoder(nn.Module):
    def __init__(self, latent_channels, hidden_channels, out_channels):
        super().__init__()

        self.fc1 = nn.Linear(latent_channels, hidden_channels)
        self.fc2 = nn.Linear(hidden_channels, out_channels)


    def forward(self, z):
        z = F.relu(self.fc1(z))
        recon_features = self.fc2(z)
        return recon_features

class GraphAutoencoder(nn.Module):
    def __init__(self, node_feature_dim, gae_hidden_dim, gae_latent_dim):
        super().__init__()
        self.encoder = GAE_Encoder(node_feature_dim, gae_hidden_dim, gae_latent_
        self.decoder = FeatureDecoder(gae_latent_dim, gae_hidden_dim, node_featu
        self.node_feature_dim = node_feature_dim
    def forward(self, data):
        x, edge_index = data.x, data.edge_index
        z = self.encoder(x, edge_index)
        recon_x = self.decoder(z)
        return recon_x
```

```
    def encode(self, data):
        x, edge_index = data.x, data.edge_index
        return self.encoder(x, edge_index)

    def decode(self, z):
        return self.decoder(z)

gae_model = GraphAutoencoder(
    node_feature_dim=node_feature_dim,
    gae_hidden_dim=GAE_HIDDEN_DIM,
    gae_latent_dim=GAE_LATENT_DIM
).to(device)

print(gae_model)
num_params_gae = sum(p.numel() for p in gae_model.parameters() if p.requires_gra
print(f"\nNumber of trainable parameters in GAE: {num_params_gae:,}")
```

```
GraphAutoencoder(
  (encoder): GAE_Encoder(
    (conv1): GCNConv(5, 128)
    (bn1): BatchNorm1d(128, eps=1e-05, momentum=0.1, affine=True, track_running_s
tats=True)
    (conv2): GCNConv(128, 128)
  )
  (decoder): FeatureDecoder(
    (fc1): Linear(in_features=128, out_features=128, bias=True)
    (fc2): Linear(in_features=128, out_features=5, bias=True)
  )
)

Number of trainable parameters in GAE: 34,693
```

In [ ]:

```
reconstruction_criterion = nn.MSELoss()
optimizer = optim.Adam(gae_model.parameters(), lr=LEARNING_RATE_GAE)
scheduler = optim.lr_scheduler.ReduceLROnPlateau(optimizer, 'min', factor=0.5, p
print("Setup complete: Loss function (MSE), Optimizer (Adam), LR Scheduler (Redu
```

```
Setup complete: Loss function (MSE), Optimizer (Adam), LR Scheduler (ReduceLROnPl
ateau)
/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(
```

In [ ]:

```
def train_gae_epoch(model, loader, optimizer, criterion, device):
    model.train()
    total_loss = 0.0
    for batch in tqdm(loader, desc="Training", leave=False):
        batch = batch.to(device)
        optimizer.zero_grad()

        if not batch.x.dtype == torch.float32:
            batch.x = batch.x.float()

        recon_x = model(batch)

        target_x = batch.x
        if recon_x.shape != target_x.shape:
            raise ValueError(f"Shape mismatch: recon_x {recon_x.shape}, target_
        if recon_x.dtype != target_x.dtype:
```

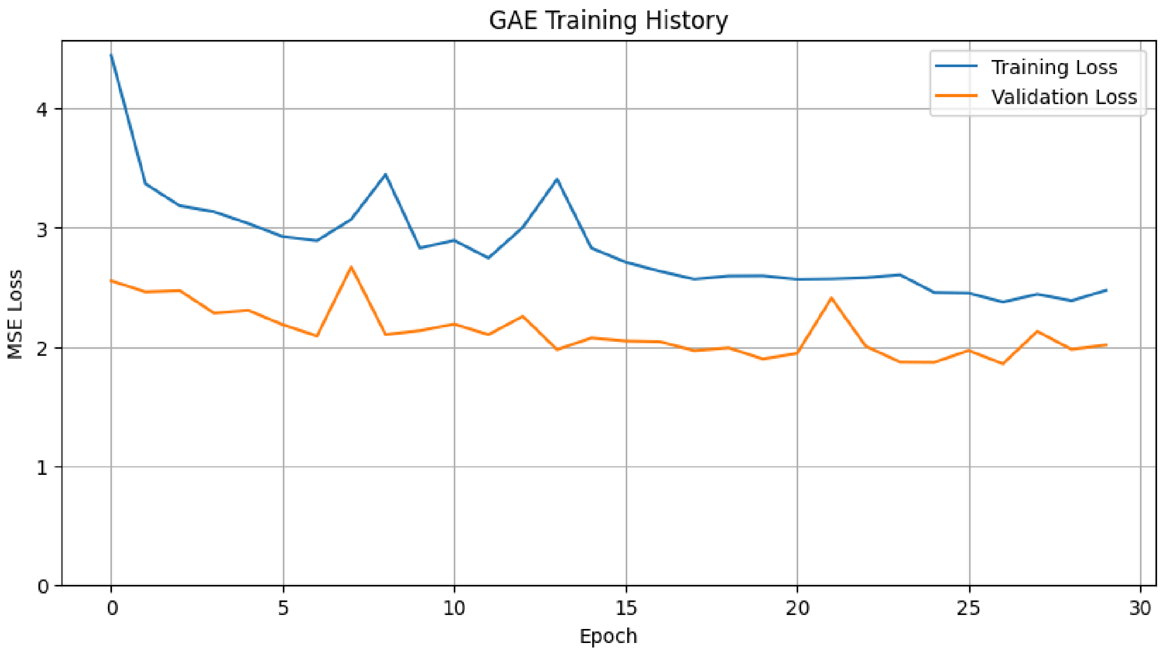
```
            target_x = target_x.to(recon_x.dtype)
        loss = criterion(recon_x, target_x)
        loss.backward()
        optimizer.step()
        total_loss += loss.item() * batch.num_graphs

    return total_loss / len(loader.dataset)

def evaluate_gae(model, loader, criterion, device):
    model.eval()
    total_loss = 0.0
    with torch.no_grad():
        for batch in tqdm(loader, desc="Validation", leave=False):
            batch = batch.to(device)

            if not batch.x.dtype == torch.float32:
                batch.x = batch.x.float()

            recon_x = model(batch)
            target_x = batch.x

            if recon_x.shape != target_x.shape:
                 raise ValueError(f"Shape mismatch during eval: recon_x {recon_x
            if recon_x.dtype != target_x.dtype:
                 target_x = target_x.to(recon_x.dtype)

            loss = criterion(recon_x, target_x)
            total_loss += loss.item() * batch.num_graphs

    return total_loss / len(loader.dataset)

history = {'train_loss': [], 'val_loss': []}
best_val_loss = float('inf')

print(f"Starting GAE training for {NUM_EPOCHS_GAE} epochs...")
start_time = time.time()

for epoch in range(NUM_EPOCHS_GAE):
    epoch_start_time = time.time()

    train_loss = train_gae_epoch(gae_model, train_loader, optimizer, reconstruct
    val_loss = evaluate_gae(gae_model, val_loader, reconstruction_criterion, dev

    history['train_loss'].append(train_loss)
    history['val_loss'].append(val_loss)

    # Update LR scheduler
    scheduler.step(val_loss)

    epoch_duration = time.time() - epoch_start_time
    print(f"Epoch {epoch+1}/{NUM_EPOCHS_GAE} | Duration: {epoch_duration:.2f}s |
          f"Train Loss: {train_loss:.6f} | Val Loss: {val_loss:.6f} | "
          f"LR: {optimizer.param_groups[0]['lr']:.1e}")
    if val_loss < best_val_loss:
        best_val_loss = val_loss
        torch.save(gae_model.state_dict(), GAE_SAVE_PATH)
        print(f"  -> New best validation loss. Saved model to {GAE_SAVE_PATH}")

total_training_time = time.time() - start_time
print(f"\nTraining finished. Total time: {total_training_time:.2f}s")
```

```
print(f"Best Validation Loss: {best_val_loss:.6f}")

plt.figure(figsize=(10, 5))
plt.plot(history['train_loss'], label='Training Loss')
plt.plot(history['val_loss'], label='Validation Loss')
plt.title('GAE Training History')
plt.xlabel('Epoch')
plt.ylabel('MSE Loss')
plt.legend()
plt.grid(True)
plt.ylim(bottom=0)
plt.show()
```

```
Starting GAE training for 30 epochs...
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 1/30 | Duration: 10.00s | Train Loss: 4.448260 | Val Loss: 2.552393 | LR: 1.0e-03
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 2/30 | Duration: 9.03s | Train Loss: 3.368642 | Val Loss: 2.460250 | LR: 1.0e-03
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 3/30 | Duration: 9.16s | Train Loss: 3.183380 | Val Loss: 2.470559 | LR: 1.0e-03
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 4/30 | Duration: 9.11s | Train Loss: 3.133199 | Val Loss: 2.281798 | LR: 1.0e-03
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 5/30 | Duration: 9.11s | Train Loss: 3.034451 | Val Loss: 2.305137 | LR: 1.0e-03
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 6/30 | Duration: 9.27s | Train Loss: 2.925105 | Val Loss: 2.184428 | LR: 1.0e-03
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 7/30 | Duration: 9.36s | Train Loss: 2.890876 | Val Loss: 2.088793 | LR: 1.0e-03
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 8/30 | Duration: 9.40s | Train Loss: 3.069419 | Val Loss: 2.670711 | LR: 1.0e-03
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 9/30 | Duration: 9.47s | Train Loss: 3.447002 | Val Loss: 2.100807 | LR: 1.0e-03
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 10/30 | Duration: 9.75s | Train Loss: 2.828446 | Val Loss: 2.133715 | LR: 1.0e-03
Training:   0%|          | 0/188 [00:00<?, ?it/s]
```

```
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 11/30 | Duration: 9.71s | Train Loss: 2.892537 | Val Loss: 2.188827 | LR:
1.0e-03
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 12/30 | Duration: 9.91s | Train Loss: 2.744199 | Val Loss: 2.100046 | LR:
1.0e-03
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 13/30 | Duration: 10.19s | Train Loss: 3.002478 | Val Loss: 2.254872 | LR:
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 14/30 | Duration: 10.51s | Train Loss: 3.407017 | Val Loss: 1.975073 | LR:
5.0e-04
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 15/30 | Duration: 10.29s | Train Loss: 2.828110 | Val Loss: 2.072748 | LR:
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 16/30 | Duration: 9.98s | Train Loss: 2.709533 | Val Loss: 2.047180 | LR:
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 17/30 | Duration: 9.93s | Train Loss: 2.633288 | Val Loss: 2.041359 | LR:
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 18/30 | Duration: 9.86s | Train Loss: 2.567058 | Val Loss: 1.966380 | LR:
5.0e-04
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 19/30 | Duration: 9.82s | Train Loss: 2.593664 | Val Loss: 1.989683 | LR:
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 20/30 | Duration: 9.95s | Train Loss: 2.595291 | Val Loss: 1.896369 | LR:
5.0e-04
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 21/30 | Duration: 10.04s | Train Loss: 2.565751 | Val Loss: 1.943587 | LR:
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 22/30 | Duration: 10.04s | Train Loss: 2.569338 | Val Loss: 2.408308 | LR:
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 23/30 | Duration: 10.08s | Train Loss: 2.579423 | Val Loss: 2.003237 | LR:
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 24/30 | Duration: 9.98s | Train Loss: 2.603769 | Val Loss: 1.870689 | LR:
5.0e-04
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
```

```
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 25/30 | Duration: 9.97s | Train Loss: 2.454317 | Val Loss: 1.868670 | LR: 
5.0e-04
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 26/30 | Duration: 9.97s | Train Loss: 2.449681 | Val Loss: 1.967380 | LR: 
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 27/30 | Duration: 9.89s | Train Loss: 2.374568 | Val Loss: 1.855656 | LR: 
5.0e-04
  -> New best validation loss. Saved model to ./best_gae_model_weights.pth
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 28/30 | Duration: 9.92s | Train Loss: 2.440413 | Val Loss: 2.128210 | LR: 
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 29/30 | Duration: 10.17s | Train Loss: 2.386061 | Val Loss: 1.977127 | LR: 
5.0e-04
Training:   0%|          | 0/188 [00:00<?, ?it/s]
Validation:   0%|          | 0/47 [00:00<?, ?it/s]
Epoch 30/30 | Duration: 9.97s | Train Loss: 2.472310 | Val Loss: 2.013710 | LR: 
5.0e-04

Training finished. Total time: 293.85s
Best Validation Loss: 1.855656
```



This is the same architecture used for VAE for the commin task. This is used for loading the VAE model and for comparisons

In [ ]:
```
RESIZE_DIM = RESIZE_DIM
LATENT_DIM = VAE_LATENT_DIM

class Encoder(nn.Module):
    def __init__(self, latent_dim, input_channels=3, base_filters=32):
        super(Encoder, self).__init__()
        self.conv1 = nn.Conv2d(input_channels, base_filters, kernel_size=3, stri
        self.bn1 = nn.BatchNorm2d(base_filters)
```

```
        self.conv2 = nn.Conv2d(base_filters, base_filters*2, kernel_size=3, stri
        self.bn2 = nn.BatchNorm2d(base_filters*2)
        self.conv3 = nn.Conv2d(base_filters*2, base_filters*4, kernel_size=3, st
        self.bn3 = nn.BatchNorm2d(base_filters*4)
        self.conv4 = nn.Conv2d(base_filters*4, base_filters*8, kernel_size=3, st
        self.bn4 = nn.BatchNorm2d(base_filters*8)

        self.flatten = nn.Flatten()
        flattened_size = base_filters*8 * (RESIZE_DIM // 16) * (RESIZE_DIM // 16
        self.fc1 = nn.Linear(flattened_size, 1024)
        self.fc_mu = nn.Linear(1024, latent_dim)
        self.fc_logvar = nn.Linear(1024, latent_dim)

    def forward(self, x):
        x = F.relu(self.bn1(self.conv1(x)))
        x = F.relu(self.bn2(self.conv2(x)))
        x = F.relu(self.bn3(self.conv3(x)))
        x = F.relu(self.bn4(self.conv4(x)))
        x = self.flatten(x)
        x = F.relu(self.fc1(x))
        mu = self.fc_mu(x)
        logvar = self.fc_logvar(x)
        return mu, logvar

class Decoder(nn.Module):
    def __init__(self, latent_dim, output_channels=3, base_filters=32):
        super(Decoder, self).__init__()
        self.latent_dim = latent_dim
        self.base_filters = base_filters
        self.unflatten_dim = base_filters*8
        self.unflatten_size = RESIZE_DIM // 16

        self.fc = nn.Linear(latent_dim, self.unflatten_dim * self.unflatten_size

        self.deconv1 = nn.ConvTranspose2d(self.unflatten_dim, base_filters*4, ke
        self.bn1 = nn.BatchNorm2d(base_filters*4)
        self.deconv2 = nn.ConvTranspose2d(base_filters*4, base_filters*2, kernel
        self.bn2 = nn.BatchNorm2d(base_filters*2)
        self.deconv3 = nn.ConvTranspose2d(base_filters*2, base_filters, kernel_s
        self.bn3 = nn.BatchNorm2d(base_filters)
        self.deconv4 = nn.ConvTranspose2d(base_filters, output_channels, kernel_


    def forward(self, z):
        x = F.relu(self.fc(z))
        x = x.view(-1, self.unflatten_dim, self.unflatten_size, self.unflatten_s
        x = F.relu(self.bn1(self.deconv1(x)))
        x = F.relu(self.bn2(self.deconv2(x)))
        x = F.relu(self.bn3(self.deconv3(x)))
        x = self.deconv4(x)
        return x

class VAE(nn.Module):
    def __init__(self, latent_dim, input_channels=3, base_filters=32):
        super(VAE, self).__init__()
        self.encoder = Encoder(latent_dim, input_channels, base_filters)
        self.decoder = Decoder(latent_dim, input_channels, base_filters)

    def reparameterize(self, mu, logvar):
        std = torch.exp(0.5 * logvar)
```

```
        eps = torch.randn_like(std)
        return mu + eps * std # Sample z

    def forward(self, x):
        mu, logvar = self.encoder(x)
        z = self.reparameterize(mu, logvar)
        recon = self.decoder(z)
        return recon, mu, logvar

    def reconstruct(self, x):
         mu, logvar = self.encoder(x)
         z = mu #  for deterministic reconstruction
         recon = self.decoder(z)
         return recon

def load_vae_model(weights_path, latent_dim, input_channels, base_filters, devic
    print(f"Loading VAE model structure...")
    model = VAE(latent_dim=latent_dim, input_channels=input_channels, base_filte
    print(f"Loading VAE weights from: {weights_path}")
    try:
        state_dict = torch.load(weights_path, map_location=device)

        if list(state_dict.keys())[0].startswith('module.'):
             state_dict = {k[len("module."):]: v for k, v in state_dict.items()}
             print("  Adjusted state_dict keys (removed 'module.' prefix).")

        model.load_state_dict(state_dict)
        print("  Successfully loaded VAE weights.")
    except FileNotFoundError:
        print(f"  Error: VAE weights file not found at {weights_path}")
        return None
    except Exception as e:
        print(f"  Error loading VAE weights: {e}")
        return None

    model.to(device)
    model.eval()
    return model
vae_model = load_vae_model(
    VAE_WEIGHTS_PATH,
    latent_dim=VAE_LATENT_DIM,
    input_channels=VAE_INPUT_CHANNELS,
    base_filters=VAE_BASE_FILTERS,
    device=device
)

if vae_model:
    print("Pre-trained VAE model loaded successfully.")
else:
    print("Could not load VAE model. Comparison plots will not include VAE.")
```

```
Loading VAE model structure...
Loading VAE weights from: /kaggle/input/vae/pytorch/default/1/best_vae_model_weig
hts-main.pth
```

```
<ipython-input-11-6adc695100b7>:89: 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.
  state_dict = torch.load(weights_path, map_location=device)
  Successfully loaded VAE weights.
Pre-trained VAE model loaded successfully.
```

This function takes the reconstructed node features (recon_x) from the GAE and maps them back onto a 2D image grid. It retrieves the original pixel coordinates (coords) and image dimensions (height, width) that were saved in the graph_data object during graph creation. It extracts only the first 3 dimensions from the reconstructed node features (recon_x) This uses the original coords to place these reconstructed energy values onto the correct pixel locations in the recon_image. The denormalize_image function (similar to VAE notebook) is used later to convert the normalized reconstructed image back to the original data scale for visualization.

In [ ]:
```
def graph_recon_to_image(recon_x, graph_data, include_coords=True):

    if recon_x is None or graph_data is None:
        return None

    coords = graph_data.coords.long()
    height = graph_data.height
    width = graph_data.width
    num_channels = VAE_INPUT_CHANNELS

    recon_image = torch.zeros((num_channels, height, width), device=recon_x.devi

    if include_coords:
         if recon_x.shape[1] < num_channels:
              print(f"Warning: recon_x has fewer features ({recon_x.shape[1]}) t
              return None
         recon_energy = recon_x[:, :num_channels]
    else:
         recon_energy = recon_x
    valid_mask = (coords[:, 0] >= 0) & (coords[:, 0] < height) & \
                 (coords[:, 1] >= 0) & (coords[:, 1] < width)

    if not torch.all(valid_mask):
         print("Warning: Some coordinates out of bounds.")
         coords = coords[valid_mask]
         recon_energy = recon_energy[valid_mask]
    recon_image[:, coords[:, 0], coords[:, 1]] = recon_energy.T
    return recon_image

def denormalize_image(img_tensor, means, stds):

    if img_tensor is None:
```

```
        return None

    means = torch.as_tensor(means, dtype=img_tensor.dtype, device=img_tensor.dev
    stds = torch.as_tensor(stds, dtype=img_tensor.dtype, device=img_tensor.devic

    if means.ndim == 1:
        means = means[:, None, None]
    if stds.ndim == 1:
        stds = stds[:, None, None]


    # X_original = X_normalized * std + mean
    return img_tensor * stds + means


def visualize_reconstructions(original_img_norm, vae_recon_norm, gae_recon_norm,
    original_img = denormalize_image(original_img_norm, norm_means, norm_stds)
    vae_recon = denormalize_image(vae_recon_norm, norm_means, norm_stds)
    gae_recon = denormalize_image(gae_recon_norm, norm_means, norm_stds)

    original_img_np = original_img.cpu().numpy().transpose(1, 2, 0) if original_
    vae_recon_np = vae_recon.cpu().numpy().transpose(1, 2, 0) if vae_recon is no
    gae_recon_np = gae_recon.cpu().numpy().transpose(1, 2, 0) if gae_recon is no

    if original_img_np is None:
        print("Error: Original image is None, cannot visualize.")
        return

    positive_pixels = original_img_np[original_img_np > 0]
    if positive_pixels.size > 0:
         clim_max = np.percentile(positive_pixels, 99.9)
    else:
         clim_max = 1.0
    clim_min = 0
    clim_max = max(clim_max, 1e-3)

    num_plots = 1 + (1 if vae_recon_np is not None else 0) + (1 if gae_recon_np
    fig, axes = plt.subplots(1, num_plots, figsize=(5 * num_plots, 5))
    if num_plots == 1: axes = [axes]
    fig.suptitle(f"Event {sample_idx} - Label: {'Quark' if label == 0 else 'Gluc

    plot_idx = 0

    ax = axes[plot_idx]

    img_display_orig = np.sum(original_img_np, axis=2)
    im = ax.imshow(img_display_orig, cmap='magma', vmin=clim_min, vmax=clim_max)
    ax.set_title("Original (Denormalized)")
    ax.set_xticks([])
    ax.set_yticks([])
    fig.colorbar(im, ax=ax, fraction=0.046, pad=0.04)
    plot_idx += 1


    if vae_recon_np is not None:
        ax = axes[plot_idx]
        img_display_vae = np.sum(vae_recon_np, axis=2)
        im = ax.imshow(img_display_vae, cmap='magma', vmin=clim_min, vmax=clim_m
        ax.set_title("VAE Recon (Denormalized)")
        ax.set_xticks([])
```

```
        ax.set_yticks([])
        fig.colorbar(im, ax=ax, fraction=0.046, pad=0.04)
        plot_idx += 1
    elif vae_model is not None:
         ax = axes[plot_idx]
         ax.set_title("VAE Recon (Failed/None)")
         ax.set_xticks([]); ax.set_yticks([])
         plot_idx += 1


    if gae_recon_np is not None:
        ax = axes[plot_idx]
        img_display_gae = np.sum(gae_recon_np, axis=2)
        im = ax.imshow(img_display_gae, cmap='magma', vmin=clim_min, vmax=clim_m
        ax.set_title("GAE Recon (Denormalized)")
        ax.set_xticks([])
        ax.set_yticks([])
        fig.colorbar(im, ax=ax, fraction=0.046, pad=0.04)
        plot_idx += 1
    elif gae_model_eval is not None:
         ax = axes[plot_idx]
         ax.set_title("GAE Recon (Failed/None)")
         ax.set_xticks([]); ax.set_yticks([])
         plot_idx += 1


    plt.tight_layout(rect=[0, 0.03, 1, 0.95])
    plt.show()

def calculate_mse(img1_norm, img2_norm):
    if img1_norm is None or img2_norm is None:
        return float('nan')
    if img1_norm.shape != img2_norm.shape:
        print(f"Warning: Image shape mismatch for MSE: {img1_norm.shape} vs {img
        return float('nan')
#??
    img1_norm = img1_norm.to(device)
    img2_norm = img2_norm.to(device)
    return F.mse_loss(img1_norm, img2_norm).item()
```

In [ ]:

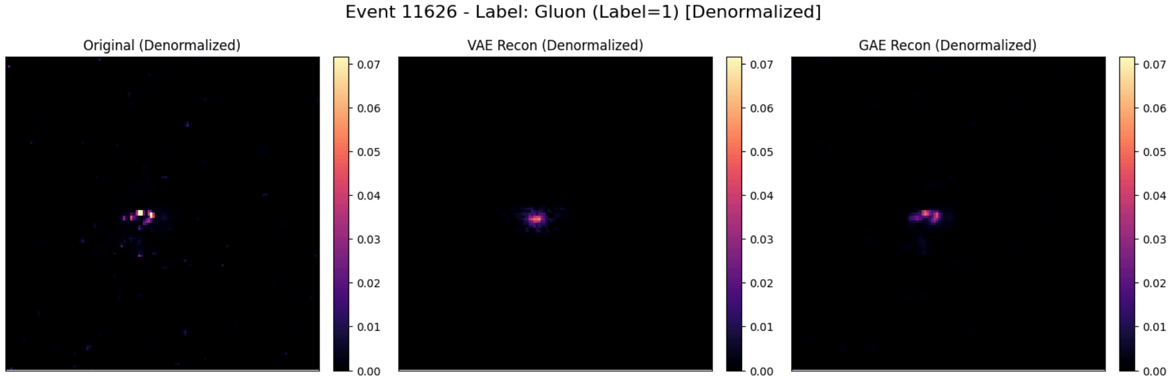
```
print("Loading best trained GAE model...")

gae_model_eval = GraphAutoencoder(
    node_feature_dim=node_feature_dim,
    gae_hidden_dim=GAE_HIDDEN_DIM,
    gae_latent_dim=GAE_LATENT_DIM
)
try:
    gae_model_eval.load_state_dict(torch.load(GAE_SAVE_PATH, map_location=device
    gae_model_eval.to(device)
    gae_model_eval.eval()
    print(f"Successfully loaded GAE model from {GAE_SAVE_PATH}")
except FileNotFoundError:
    print(f"Error: Saved GAE model not found at {GAE_SAVE_PATH}. Cannot perform
    gae_model_eval = None
except Exception as e:
    print(f"Error loading saved GAE model: {e}")
    gae_model_eval = None

num_samples_to_show = 5
```

```
vis_indices = np.random.choice(len(val_dataset), num_samples_to_show, replace=Fa


original_val_indices = val_dataset.indices

print(f"\n--- Generating Reconstructions for {num_samples_to_show} Samples ---")

vae_mses = []
gae_mses = []

val_graphs_subset = val_dataset

for i in range(num_samples_to_show):

    subset_idx = vis_indices[i]
    original_idx = val_indices[subset_idx]

    print(f"\nProcessing Sample {i+1} (Subset Idx: {subset_idx}, Original Idx: {

    original_image_norm = original_images_tensor[original_idx].to(device) # Shap
    label = labels_tensor[original_idx].to(device)

    graph_data_sample = val_graphs_subset[subset_idx]

    graph_data_sample = graph_data_sample.to(device)


    vae_recon_norm = None
    vae_mse = float('nan')
    if vae_model:
        vae_model.eval()
        with torch.no_grad():

            vae_input = original_image_norm.unsqueeze(0).to(device)
            vae_recon_norm = vae_model.reconstruct(vae_input).squeeze(0)

            vae_mse = calculate_mse(original_image_norm, vae_recon_norm)
            vae_mses.append(vae_mse)
            print(f"  VAE Reconstruction MSE (normalized): {vae_mse:.6f}")
    else:
        print("  VAE model not loaded, skipping VAE reconstruction.")

    gae_recon_image_norm = None
    gae_mse = float('nan')
    if gae_model_eval:
        gae_model_eval.eval()
        with torch.no_grad():
            if not graph_data_sample.x.dtype == torch.float32:
                graph_data_sample.x = graph_data_sample.x.float()

            recon_x_gae = gae_model_eval(graph_data_sample)

            gae_recon_image_norm = graph_recon_to_image(recon_x_gae, graph_data_

            if gae_recon_image_norm is not None:

                gae_mse = calculate_mse(original_image_norm, gae_recon_image_no
                gae_mses.append(gae_mse)
                print(f"  GAE Reconstruction MSE (normalized): {gae_mse:.6f}")
            else:
```

```
                print("  GAE reconstruction failed (likely no nodes or feature
    else:
        print("  GAE model not loaded, skipping GAE reconstruction.")



    visualize_reconstructions(
        original_image_norm,
        vae_recon_norm,
        gae_recon_image_norm,
        original_idx,
        label,
        normalization_means,
        normalization_stds
    )


if vae_mses:
    avg_vae_mse = np.nanmean(vae_mses)
    print(f"\nAverage VAE Reconstruction MSE (normalized) over {len(vae_mses)} s
if gae_mses:
    avg_gae_mse = np.nanmean(gae_mses)
    print(f"Average GAE Reconstruction MSE (normalized) over {len(gae_mses)} sam

print("\nEvaluation Complete.")
```

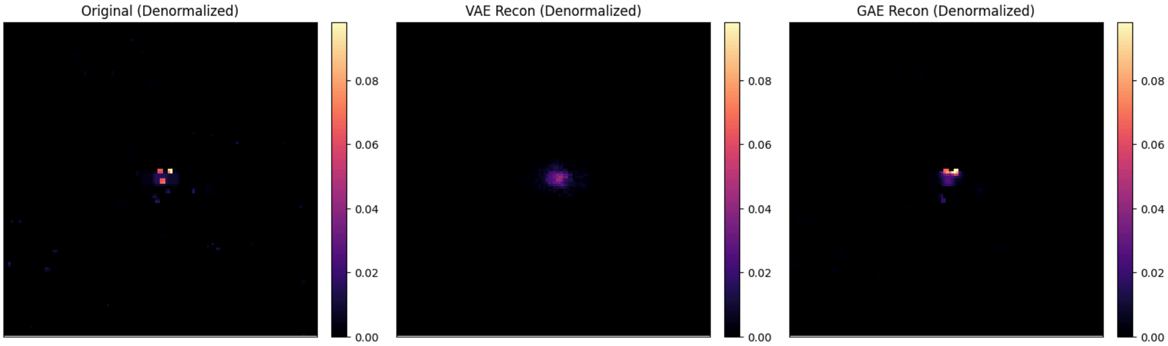
```
Loading best trained GAE model...
Successfully loaded GAE model from ./best_gae_model_weights.pth

--- Generating Reconstructions for 5 Samples ---

Processing Sample 1 (Subset Idx: 1586, Original Idx: 11626)...
  VAE Reconstruction MSE (normalized): 0.209582
  GAE Reconstruction MSE (normalized): 0.048463
```

```
<ipython-input-19-e72a1e720cca>:9: FutureWarning: You are using `torch.load` with
`weights_only=False` (the current default value), which uses the default pickle m
odule implicitly. It is possible to construct malicious pickle data which will ex
ecute arbitrary code during unpickling (See https://github.com/pytorch/pytorch/bl
ob/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.
  gae_model_eval.load_state_dict(torch.load(GAE_SAVE_PATH, map_location=device))
```



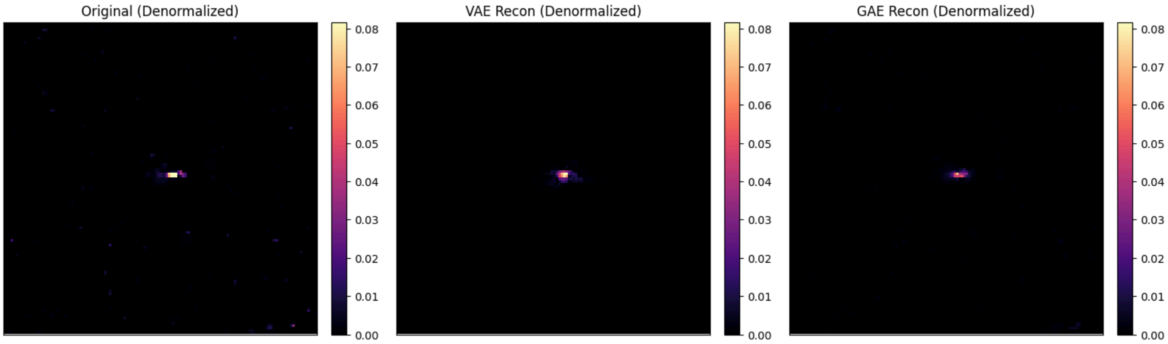
```
Processing Sample 2 (Subset Idx: 349, Original Idx: 4515)...
  VAE Reconstruction MSE (normalized): 0.177157
  GAE Reconstruction MSE (normalized): 0.071388
```

Event 4515 - Label: Gluon (Label=1) [Denormalized]



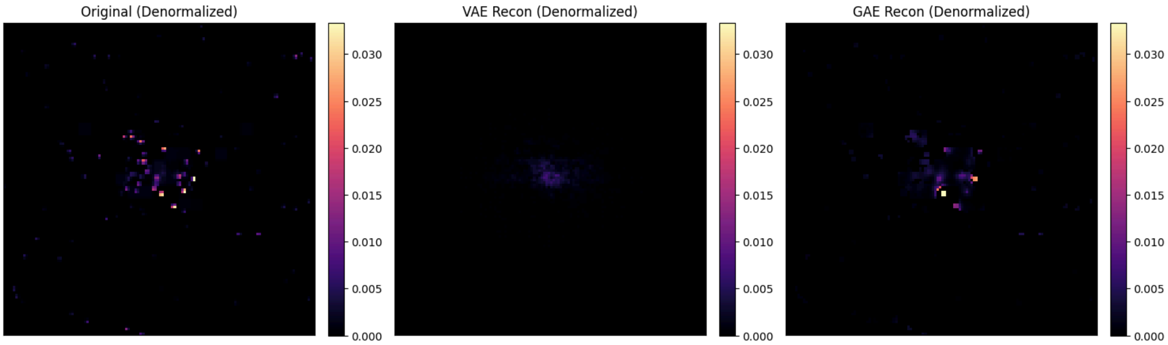

```
Processing Sample 3 (Subset Idx: 2567, Original Idx: 10712)...
  VAE Reconstruction MSE (normalized): 0.217396
  GAE Reconstruction MSE (normalized): 0.145806
```

Event 10712 - Label: Gluon (Label=1) [Denormalized]



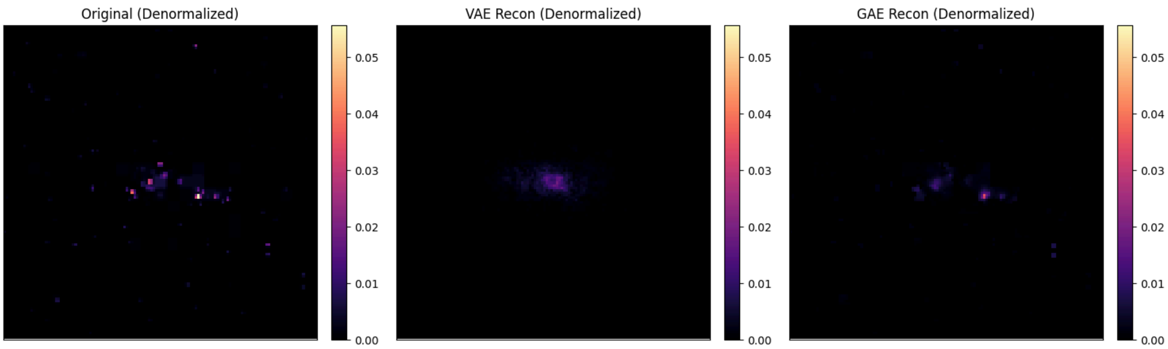

```
Processing Sample 4 (Subset Idx: 2469, Original Idx: 1217)...
  VAE Reconstruction MSE (normalized): 0.070197
  GAE Reconstruction MSE (normalized): 0.024947
```

Event 1217 - Label: Quark (Label=0) [Denormalized]




```
Processing Sample 5 (Subset Idx: 2816, Original Idx: 3647)...
  VAE Reconstruction MSE (normalized): 0.180200
  GAE Reconstruction MSE (normalized): 0.047784
```

Event 3647 - Label: Gluon (Label=1) [Denormalized]

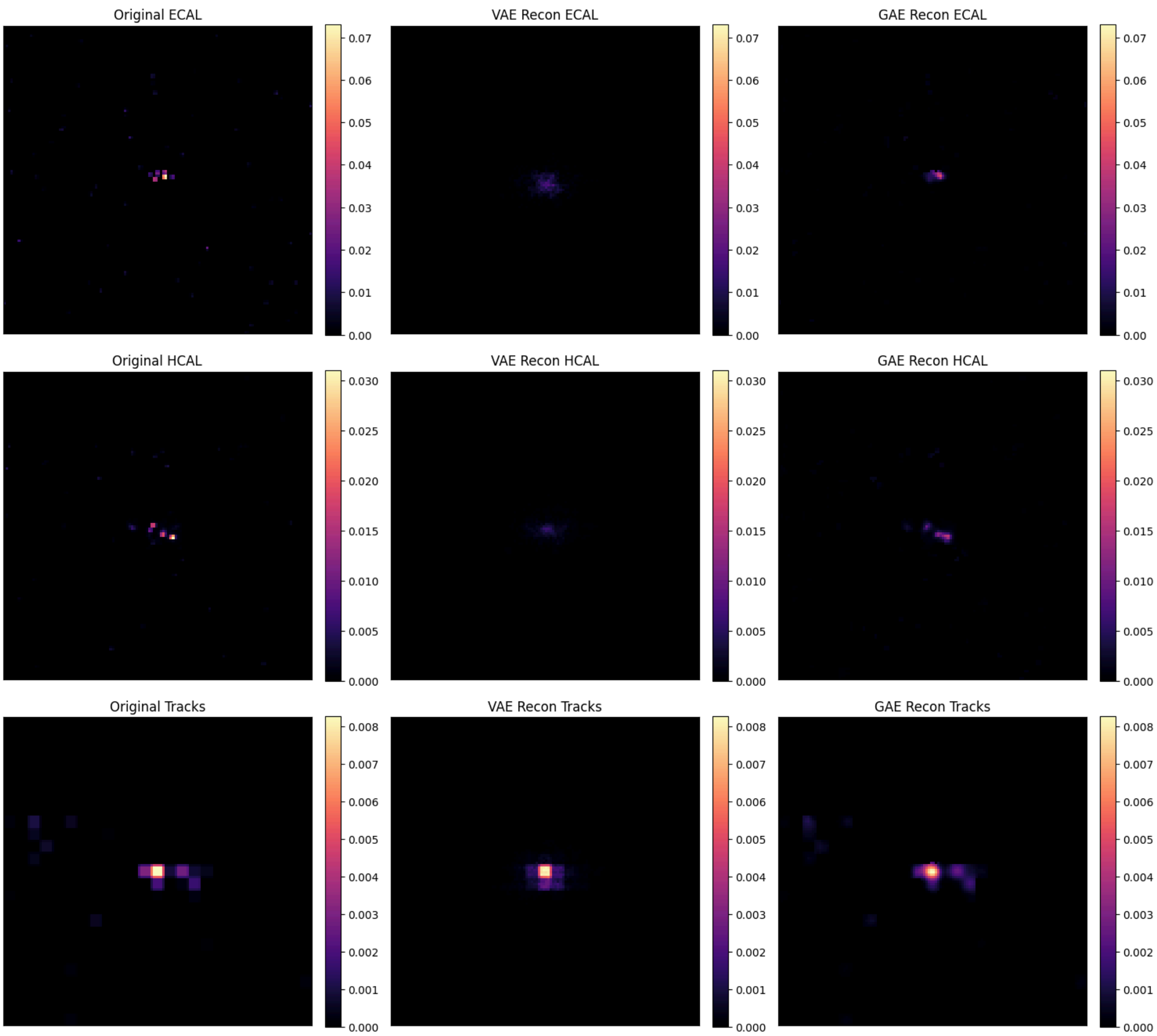


```
Average VAE Reconstruction MSE (normalized) over 5 samples: 0.170906
Average GAE Reconstruction MSE (normalized) over 5 samples: 0.067678

Evaluation Complete.
```

In [ ]:
```python
import matplotlib.pyplot as plt
import numpy as np
import torch


def visualize_reconstructions_per_channel(original_img_norm, vae_recon_norm, gae


    channels = ['ECAL', 'HCAL', 'Tracks']
    num_channels = len(channels)
    original_img = denormalize_image(original_img_norm, norm_means, norm_stds)
    vae_recon = denormalize_image(vae_recon_norm, norm_means, norm_stds)
    gae_recon = denormalize_image(gae_recon_norm, norm_means, norm_stds)

    if original_img is None:
        print(f"Error: Cannot plot Event {sample_idx}, original image is None.")
        return

    fig, axes = plt.subplots(num_channels, 3, figsize=(15, 5 * num_channels)) #
    fig.suptitle(f"Event {sample_idx} - Label: {'Quark' if label == 0 else 'Gluc


    original_np = original_img.cpu().numpy()
    vae_np = vae_recon.cpu().numpy() if vae_recon is not None else None
    gae_np = gae_recon.cpu().numpy() if gae_recon is not None else None

    for i, channel_name in enumerate(channels):

        orig_channel_data = original_np[i, :, :]
        positive_pixels = orig_channel_data[orig_channel_data > 1e-6]
        if positive_pixels.size > 0:

             clim_max = np.percentile(positive_pixels, 99.9)
        else:
             clim_max = 1e-3
        clim_min = 0
        clim_max = max(clim_max, 1e-3)

        ax = axes[i, 0]
        im = ax.imshow(orig_channel_data, cmap='magma', vmin=clim_min, vmax=clim
        ax.set_title(f"Original {channel_name}")
        ax.set_xticks([])
        ax.set_yticks([])
        fig.colorbar(im, ax=ax, fraction=0.046, pad=0.04)

        ax = axes[i, 1]
        if vae_np is not None:
            im = ax.imshow(vae_np[i, :, :], cmap='magma', vmin=clim_min, vmax=cl
            ax.set_title(f"VAE Recon {channel_name}")
            fig.colorbar(im, ax=ax, fraction=0.046, pad=0.04)
        else:
            ax.set_title(f"VAE Recon {channel_name} (N/A)")
        ax.set_xticks([])
        ax.set_yticks([])
```

```
        ax = axes[i, 2]
        if gae_np is not None:
            im = ax.imshow(gae_np[i, :, :], cmap='magma', vmin=clim_min, vmax=cl
            ax.set_title(f"GAE Recon {channel_name}")
            fig.colorbar(im, ax=ax, fraction=0.046, pad=0.04)
        else:
            ax.set_title(f"GAE Recon {channel_name} (N/A)")
        ax.set_xticks([])
        ax.set_yticks([])


    plt.tight_layout(rect=[0, 0.03, 1, 0.95])
    plt.show()

visualize_reconstructions_per_channel(
     original_image_norm,
     vae_recon_norm,
     gae_recon_image_norm,
     original_idx,
     label,
     normalization_means,
     normalization_stds
 )
```

Event 9288 - Label: Gluon [Per Channel, Denormalized]



In [ ]:
```
def calculate_all_mses(vae_model, gae_model, pyg_loader, full_image_tensor, subs
    vae_model.eval() if vae_model else None
    gae_model.eval() if gae_model else None

    all_vae_mses = []
    all_gae_mses = []
    processed_indices = []


    print(f"Calculating MSEs for {len(pyg_loader.dataset)} validation samples...

    if len(subset_indices) != len(pyg_loader.dataset):
         if len(pyg_loader.dataset) < len(subset_indices):
              print("Assuming loader uses indices 0..N-1 relative to subset. Map
         else:
              print("Cannot reliably map loader index to original index. Abortin
              return [], [], []


    with torch.no_grad():
        batch_num = 0
        for i, graph_data_sample in enumerate(tqdm(pyg_loader.dataset, desc="Cal

            original_idx = subset_indices[i]
            processed_indices.append(original_idx)

            original_image_norm = full_image_tensor[original_idx].to(device)

            vae_mse = float('nan')
            if vae_model:
                vae_input = original_image_norm.unsqueeze(0).to(device)
                vae_recon_norm = vae_model.reconstruct(vae_input).squeeze(0)
                vae_mse = calculate_mse(original_image_norm, vae_recon_norm)
            all_vae_mses.append(vae_mse)

            gae_mse = float('nan')
            if gae_model:
                graph_data_sample = graph_data_sample.to(device)
                if not graph_data_sample.x.dtype == torch.float32:
                    graph_data_sample.x = graph_data_sample.x.float()
                recon_x_gae = gae_model(graph_data_sample)
                gae_recon_image_norm = graph_recon_to_image(recon_x_gae, graph_d
                if gae_recon_image_norm is not None:
                    gae_mse = calculate_mse(original_image_norm, gae_recon_image
            all_gae_mses.append(gae_mse)


    valid_indices = [idx for idx, gae_mse in enumerate(all_gae_mses) if not np.i
    filtered_vae_mses = [all_vae_mses[i] for i in valid_indices if not np.isnan(
    filtered_gae_mses = [all_gae_mses[i] for i in valid_indices]
    filtered_processed_indices = [processed_indices[i] for i in valid_indices]


    print(f"Calculated {len(filtered_gae_mses)} valid MSE pairs.")
    if vae_model:
         print(f"  Avg VAE MSE (Eval Set): {np.mean(filtered_vae_mses):.6f}")
    if gae_model:
         print(f"  Avg GAE MSE (Eval Set): {np.mean(filtered_gae_mses):.6f}")
```

```
    return filtered_vae_mses, filtered_gae_mses, filtered_processed_indices


all_vae_mses, all_gae_mses, val_original_indices_used = calculate_all_mses(
    vae_model,
    gae_model_eval,
    val_loader,
    original_images_tensor,
    val_indices,
    device
)
```

```
Calculating MSEs for 3000 validation samples...
Calculating MSEs:   0%|          | 0/3000 [00:00<?, ?it/s]
Calculated 3000 valid MSE pairs.
  Avg VAE MSE (Eval Set): 0.516744
  Avg GAE MSE (Eval Set): 0.184959
```

In [ ]: