	<pre>plt.show() heatmap_with_projection(X)</pre>
	2D Heatmap - Sample 0  20 -  40 -  80 -
	100 - 120 - 10
	40 -  60 -  80 -  100 -  120 -  120 -
	20 - 20 - 40 60 80 100 120 20 - 20 - 100 - 80 - 60 - 60 - 60 - 60 - 60 - 60 -
In [11]:	120 - 80 100 120 120 120 120 120 120 120 120 12
Out[11]:	<pre>anim = FuncAnimation(fig, update, frames=np.arange(0, 360, 2), interval=50) plt.close() return HTML(anim.to_html5_video()) animate_3d_rotation(X, sample_idx=0)</pre>
In [12]: In [13]:	<pre>def extract_nonzero_mask(images):     reshaped = images.reshape((-1, images.shape[1] * images.shape[2], 3))     return np.any(reshaped != [0., 0., 0.], axis=-1).reshape(images.shape[:3])  mask = extract_nonzero_mask(X)  def create_graph_features(masked_data):     indices, features = [], []     for img_idx, mask in enumerate(masked_data):</pre>
In [14]:	<pre>coords = np.column_stack(np.where(mask))     features.append(X[img_idx, coords[:, 0], coords[:, 1], :])     indices.append(coords)     return indices, features  indices_list, features_list = create_graph_features(mask)  def build_graph_structure(coords, k=4):     from scipy_spatial import ckDTree     from scipy_sparse import coo_matrix     tree = ckDTree(coords)     dist, indices = tree.query(coords, k=k)     sigma2 = np.mean(dist[:, -1])**2     weights = np.exp(-dist**2 / sigma2)</pre>
In [15]:	<pre>row, col = np.arange(len(coords)).repeat(k), indices.flatten() return coo_matrix((weights.flatten(), (row, col)), shape=(len(coords), len(coords)))  def create_graph_dataset(indices_list, features_list, metadata, labels, neighbors=8):     dataset = []     for i, points in enumerate(indices_list):         adjacency = build_graph_structure(points, k=neighbors)         edge_idx = torch.from_numpy(np.vstack((adjacency.row, adjacency.col))).long()         edge_weights = torch.from_numpy(adjacency.data).float().view(-1, 1)      mass, momentum = metadata[i]     mass_tensor = torch.full((features_list[i].shape[0], 1), mass, dtype=torch.float32)     momentum_tensor = torch.full((features_list[i].shape[0], 1), momentum, dtype=torch.float32)      node_features = torch.from_numpy(features_list[i]).float()     node_features = torch.cat((node_features, mass_tensor, momentum_tensor), dim=1)      label = torch.tensor([int(labels[i])], dtype=torch.long)     graph = Data(x=node_features, edge_index=edge_idx, edge_attr=edge_weights, y=label)     dataset.append(graph)</pre>
In [16]: In [17]:	<pre>return dataset  graph_dataset = create_graph_dataset(indices_list, features_list, metadata, y, neighbors=8)  G = nx.Graph() data = graph_dataset[0] edge_tensor = data.edge_index edge_list = [(edge_tensor[0, i].item(), edge_tensor[1, i].item()) for i in range(edge_tensor.shape[1])] G.add_edges_from(edge_list) pos = nx.spring_layout(G, iterations=15, seed=1721) fig, ax = plt.subplots(figsize=(15, 9)) ax.axis("off") nx.draw_networkx(G, pos=pos, ax=ax, node_size=10, with_labels=False, width=0.05) plt.show()  print(f'Number of graphs to work upon : {len(graph_dataset)}') print(f'Type of each graph entity data object: {type(data)}') print(f'Number of nodes: {data.num_nodes}') print(f'Number of node features: {data.num_odes}') print(f'Number of node features: {data.num_ode_features}')</pre>
	<pre>print(f'Number of edges features; {data.num_edge_features}')</pre>
	Number of graphs to work upon: 10000 For the FIRST graph in the graph dataset: Type of each graph entity data object: <class 'torch_geometric.data.data.data'=""> Number of nodes: 1530 Number of edges: 12240 Number of node features: 5 Number of edges features: 1</class>
In [18]:	<pre>import torch import torch.nn as nn import torch.nn.functional as F from torch_geometric.nn import GCNConv, global_mean_pool  class GraphEncoder (nn.Module):     definit(self, point_dim=3, metadata_dim=2, hidden_dim=128, out_dim=64):         super()init()         self.point_encoder = nn.Sequential(</pre>
	<pre>self.conv1 = GCNConv(hidden_dim, hidden_dim) self.conv2 = GCNConv(hidden_dim, hidden_dim) self.conv3 = GCNConv(hidden_dim, out_dim)  def forward(self, data):     point_features = data.x[:, :3]     metadata_features = data.x[:, 3:]      point_emb = self.point_encoder(point_features)     metadata_emb = self.metadata_encoder(metadata_features)  x = torch.cat([point_emb, metadata_emb], dim=1)  x = F.relu(self.conv1(x, data.edge_index)) x = F.relu(self.conv2(x, data.edge_index)) x = self.conv3(x, data.edge_index)</pre>
In [19]:	<pre>import torch.nn as nn import torch.nn.functional as F  class Model(nn.Module):     definit(self, encoder, projection_dim=32):         super()init()         self.encoder = encoder          self.projector = nn.Sequential(</pre>
In [20]:	<pre>embedding = self.encoder(graph)     projected = self.projector(embedding)     return F.normalize(projected, dim=1)  import torch import torch.nn as nn import torch.nn.functional as F  class Loss(nn.Module):     definit(self, temperature=0.1, hard_neg_weight=0.5):         super()init()         self.temp = temperature         self.hard_neg_weight = hard_neg_weight  def forward(self, features, labels):         features = F.normalize(features, dim=1)</pre>
	<pre>sim_matrix = torch.matmul(features, features.T) / self.temp  mask = torch.eq(labels.unsqueeze(1), labels.unsqueeze(0)).float()  exp_sim = torch.exp(sim_matrix)  hard_neg_mask = (1 - mask) * (sim_matrix &gt; 0.5).float()  log_prob = sim_matrix - torch.log(exp_sim.sum(dim=1, keepdim=True))  weighted_log_prob = log_prob * (mask + self.hard_neg_weight * hard_neg_mask)  mean_log_prob = weighted_log_prob.sum(1) / (mask.sum(1) + self.hard_neg_weight * hard_neg_mask.sum(1))  return -mean_log_prob.mean()</pre>
	<pre>def train(model, train_loader, val_loader, optimizer, criterion, schedular, num_epocha=50, device="cuda"):     model.co(invice)     % Failister ZBM ance     knn = KNeighborsUlassifier(n_neighbors=5)     train_losses = []     train_accuration = []     val_accuration = []     val_accuration = []     val_accuration = []     train_inhedistors = []     for mpoch in range(num_epochs):         model.train()         loadel.train()         loadel.train()         loadel.train()         portion = model (batch)         inse = batch.to(device)         optimizer.rec_grad()         projections = model(batch)         loas = nrilerios(projections, batch.y.view(-1))         loade = model.core(projections, batch.y.view(-1))         loade = model.core(projections, batch.y.view(-1))         loade = model.core(projections)         train_accuration(projections)         val_accuration(projections)         val_accu</pre>
In [22]:	<pre>f"Val Acc: {val_acc:.4f}   "     f"Val ROC-AUC: {val_auc:.4f}")  # Print best validation accuracy print(f"\n' Best Validation Accuracy: {best_val_acc:.4f}")  return train_losses, train_accuracies, val_accuracies  import torch import numpy as np  def evaluate(model, loader, knn, device="cuda"):     model.eval()     embeddings = []     labels = []  with torch.no_grad():     for batch in loader:     batch = batch.to(device)     emb = model.encoder(batch).cpu()     embeddings.append(emb)     labels.append(batch.y.view(-1).cpu())</pre>
	<pre>if not embeddings:     return 0.0  embeddings = torch.cat(embeddings).numpy() labels = torch.cat(labels).numpy()  val_acc = knn.score(embeddings, labels)  probs = knn.predict_proba(embeddings)[:, 1] val_auc = roc_auc_score(labels, probs) if len(np.unique(labels)) &gt; 1 else 0.0  fpr, tpr, _ = roc_curve(labels, probs) if len(np.unique(labels)) &gt; 1 else ([], [], [])  return val_acc, val_auc, fpr, tpr</pre>
In [23]:	<pre>import torch from torch.utils.data import random_split from torch_geometric.loader import DataLoader from sklearn.neighbors import KNeighborsClassifier from sklearn.metrics import roc_auc_score, roc_curve  device = torch.device("cuda" if torch.cuda.is_available() else "cpu")  ifname == "main":     train_size = int(0.8 * len(graph_dataset))     val_size = len(graph_dataset) - train_size     train_set, val_set = random_split(graph_dataset, [train_size, val_size], generator=torch.Generator().manual_seed(4 2))  train_loader = DataLoader(train_set, batch_size=16, shuffle=True) val_loader = DataLoader(val_set, batch_size=16)  encoder = GraphEncoder(point_dim=3, metadata_dim=2).to(device) model = Model(encoder).to(device) optimizer = torch.optim.Adam(model.parameters(), lr=le=3) scheduler = torch.optim.lr_scheduler.CosineAnnealingLR(optimizer, T_max=50, eta_min=le-5) criterion = Loss()</pre>
	<pre>train_losses, train_accuracies, val_accuracies= train(     model, train_loader, val_loader, optimizer, criterion, scheduler, num_epochs=50, device=device )  knn = KNeighborsClassifier(n_neighbors=5) train_embeddings, train_labels = [], [] model.eval() with torch.no_grad():     for batch in train_loader:         batch = batch.to(device)         emb = model.encoder(batch).cpu()         train_embeddings.append(emb)         train_labels.append(batch.y.cpu())  train_labels = torch.cat(train_embeddings).numpy() train_labels = torch.cat(train_labels).numpy() knn.fit(train_embeddings, train_labels)</pre>
	test_acc, test_auc, fpr, tpr = evaluate(model, val_loader, knn, device=device)     print(f"\n"inal Test Accuracy; {test_acc:.4f}")  Epoch 1/50   Loss: 2.7705   Train Acc: 0.7592   Val Acc: 0.6370   Val ROC-AUC: 0.6804  Epoch 2/50   Loss: 2.7698   Train Acc: 0.7700   Val Acc: 0.6660   Val ROC-AUC: 0.7037  Epoch 3/50   Loss: 2.7691   Train Acc: 0.7715   Val Acc: 0.6665   Val ROC-AUC: 0.7037  Epoch 3/50   Loss: 2.7691   Train Acc: 0.7715   Val Acc: 0.6665   Val ROC-AUC: 0.7037  Epoch 5/50   Loss: 2.7681   Train Acc: 0.7710   Val Acc: 0.6950   Val ROC-AUC: 0.7237  Epoch 5/50   Loss: 2.7688   Train Acc: 0.7738   Val Acc: 0.6950   Val ROC-AUC: 0.7385  Epoch 6/50   Loss: 2.7686   Train Acc: 0.7661   Val Acc: 0.6775   Val ROC-AUC: 0.7281  Epoch 7/50   Loss: 2.7685   Train Acc: 0.7786   Val Acc: 0.6780   Val ROC-AUC: 0.7281  Epoch 7/50   Loss: 2.7685   Train Acc: 0.7736   Val Acc: 0.6595   Val ROC-AUC: 0.7014  Epoch 9/50   Loss: 2.7685   Train Acc: 0.7746   Val Acc: 0.6595   Val ROC-AUC: 0.7017  Epoch 10/50   Loss: 2.7683   Train Acc: 0.7746   Val Acc: 0.6895   Val ROC-AUC: 0.7017  Epoch 10/50   Loss: 2.7683   Train Acc: 0.7741   Val Acc: 0.6895   Val ROC-AUC: 0.7284  Epoch 12/50   Loss: 2.7683   Train Acc: 0.7741   Val Acc: 0.6895   Val ROC-AUC: 0.7280  Epoch 12/50   Loss: 2.7683   Train Acc: 0.7741   Val Acc: 0.6680   Val ROC-AUC: 0.7280  Epoch 12/50   Loss: 2.7680   Train Acc: 0.7796   Val Acc: 0.6680   Val ROC-AUC: 0.7188  Epoch 12/50   Loss: 2.7680   Train Acc: 0.7756   Val Acc: 0.6680   Val ROC-AUC: 0.7385  Epoch 13/50   Loss: 2.7680   Train Acc: 0.7756   Val Acc: 0.6690   Val ROC-AUC: 0.7385  Epoch 15/50   Loss: 2.7680   Train Acc: 0.7750   Val Acc: 0.6690   Val ROC-AUC: 0.7345  Epoch 15/50   Loss: 2.7680   Train Acc: 0.7750   Val Acc: 0.6690   Val ROC-AUC: 0.7345  Epoch 15/50   Loss: 2.7677   Train Acc: 0.7750   Val Acc: 0.6690   Val ROC-AUC: 0.7345  Epoch 15/50   Loss: 2.7678   Train Acc: 0.7750   Val Acc: 0.6945   Val ROC-AUC: 0.7341  Epoch 25/50   Loss: 2.7677   Train Acc: 0.7750   Val Acc: 0.6995   Val ROC-A
	Epoch 30/50   Loss: 2.7672   Train Acc: 0.7799   Val Acc: 0.6945   Val ROC-AUC: 0.7385   Epoch 31/50   Loss: 2.7671   Train Acc: 0.7826   Val Acc: 0.6835   Val ROC-AUC: 0.7374   Epoch 32/50   Loss: 2.7672   Train Acc: 0.7834   Val Acc: 0.6895   Val ROC-AUC: 0.7345   Epoch 33/50   Loss: 2.7669   Train Acc: 0.7837   Val Acc: 0.6915   Val ROC-AUC: 0.7364   Epoch 34/50   Loss: 2.7669   Train Acc: 0.7817   Val Acc: 0.6905   Val ROC-AUC: 0.7400   Epoch 35/50   Loss: 2.7669   Train Acc: 0.7889   Val Acc: 0.6905   Val ROC-AUC: 0.7379   Epoch 36/50   Loss: 2.7669   Train Acc: 0.7889   Val Acc: 0.6965   Val ROC-AUC: 0.7379   Epoch 36/50   Loss: 2.7669   Train Acc: 0.7913   Val Acc: 0.6965   Val ROC-AUC: 0.7434   Epoch 37/50   Loss: 2.7667   Train Acc: 0.7887   Val Acc: 0.6965   Val ROC-AUC: 0.7403   Epoch 38/50   Loss: 2.7668   Train Acc: 0.7887   Val Acc: 0.6995   Val ROC-AUC: 0.7395   Epoch 39/50   Loss: 2.7668   Train Acc: 0.7827   Val Acc: 0.6905   Val ROC-AUC: 0.7395   Epoch 40/50   Loss: 2.7667   Train Acc: 0.7839   Val Acc: 0.6905   Val ROC-AUC: 0.7484   Epoch 41/50   Loss: 2.7666   Train Acc: 0.7833   Val Acc: 0.6905   Val ROC-AUC: 0.7444   Epoch 43/50   Loss: 2.7666   Train Acc: 0.7876   Val Acc: 0.6995   Val ROC-AUC: 0.7444   Epoch 43/50   Loss: 2.7665   Train Acc: 0.7876   Val Acc: 0.6995   Val ROC-AUC: 0.7453   Epoch 45/50   Loss: 2.7665   Train Acc: 0.7866   Val Acc: 0.6995   Val ROC-AUC: 0.7453   Epoch 46/50   Loss: 2.7666   Train Acc: 0.7866   Val Acc: 0.7020   Val ROC-AUC: 0.7386   Epoch 46/50   Loss: 2.7666   Train Acc: 0.7866   Val Acc: 0.7020   Val ROC-AUC: 0.7386   Epoch 47/50   Loss: 2.7666   Train Acc: 0.7850   Val Acc: 0.7030   Val ROC-AUC: 0.7383   Epoch 47/50   Loss: 2.7666   Train Acc: 0.7850   Val Acc: 0.7030   Val ROC-AUC: 0.7368   Epoch 48/50   Loss: 2.7667   Train Acc: 0.7850   Val Acc: 0.7030   Val ROC-AUC: 0.7368   Epoch 48/50   Loss: 2.7667   Train Acc: 0.7850   Val Acc: 0.7035   Val ROC-AUC: 0.7468   Epoch 48/50   Loss: 2.7667   Train Acc: 0.7850   Val Acc: 0.7035   Val ROC-AUC: 0.7468
In [24]:	Epoch 49/50   Loss: 2.7664   Train Acc: 0.7847   Val Acc: 0.7015   Val ROC-AUC: 0.7441  Epoch 50/50   Loss: 2.7665   Train Acc: 0.7861   Val Acc: 0.7090   Val ROC-AUC: 0.7439  Best Validation Accuracy: 0.7090  Final Test Accuracy: 0.7040  Final Test ROC-AUC: 0.7462  plt.figure(figsize=(15, 8)) plt.plot(train_accuracies, marker='o', linestyle='-', label='Training Accuracy', color='violet') plt.plot(val_accuracies, marker='x', linestyle='', label='Validation Accuracy', color='blue')  plt.xlabel("Epochs") plt.ylabel("Accuracy") plt.title("Training vs Validation Accuracy") plt.grid(True, linestyle='', alpha=0.6) plt.legend() plt.show()
	Training vs Validation Accuracy  O.78  O.70  O.70  O.68  O.66
In [25]:	plt.figure(figsize=(15, 8)) plt.plot(train_losses, marker='o', linestyle='-', label='Training Loss', color='blue')  plt.xlabel("Epochs") plt.ylabel("Loss") plt.title("Training Loss") plt.grid(True, linestyle='', alpha=0.6) plt.legend() plt.show()
	2.768 2.767 2.767  Description of the content of th
In [26]:	<pre>plt.figure(figsize=(8, 6)) plt.plot(fpr, tpr, label=f'ROC Curve (AUC = {test_auc:.4f})', color='blue') plt.plot([0, 1], [0, 1], linestyle='', color='gray') plt.xlabel('False Positive Rate') plt.ylabel('True Positive Rate') plt.title('Receiver Operating Characteristic (ROC) Curve') plt.legend() plt.grid() plt.grid() plt.show()</pre> Receiver Operating Characteristic (ROC) Curve
	1.0 ROC Curve (AUC = 0.7462)  0.8  0.6  0.7  0.9
	0.2 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

Specific\_Task\_01

Collecting torch-geometric

In [1]: pip install torch-geometric

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torch-geometric) (1.2.0)

import numpy as np

import torch.nn as nn

import networkx as nx

import torch.optim as optim
import matplotlib.pyplot as plt

from torch.optim import Adam
import pytorch\_lightning as pl
import torch.nn.functional as F
from torch.nn import Linear

from mpl\_toolkits.mplot3d import Axes3D

with h5py.File(file, "r") as f:

Keys in dataset: ['X\_jets', 'm0', 'pt', 'y']

with h5py.File(file\_name, 'r') as f:

X, y, metadata = load\_data(file\_path, 10000)

from skimage.transform import resize
# Resize to 128x128 and normalize

return (metadata - mean) / std

metadata = normalize\_metadata(metadata)

for idx in range(num\_samples):

# 2D Heatmap

# 3D Projection

plt.tight\_layout()

In [10]: def heatmap\_with\_projection(images, num\_samples=3):

plt.colorbar(heatmap, ax=ax1)

Dataset keys: ['X\_jets', 'm0', 'pt', 'y']

print("Dataset keys:", list(f.keys()))
print("Total images:", len(f['X\_jets']))

X = np.array(f['X\_jets'][:sample\_size])

label\_counts = np.bincount(labels.astype(np.int64))

mean, std = np.mean(processed), np.std(processed)
return np.clip((processed - mean) / std, 0, None)

fig = plt.figure(figsize=(18, 6 \* num\_samples))

ax1 = fig.add\_subplot(num\_samples, 2, 2\*idx + 1)
combined\_data = np.sum(images[idx], axis=-1)

ax2.plot\_surface(X, Y, combined\_data, cmap='viridis')

ax2.set\_title(f'3D Projection - Sample {idx}')

ax1.set\_title(f'2D Heatmap - Sample {idx}')

heatmap = ax1.imshow(combined\_data, cmap='hot', interpolation='nearest')

X, Y = np.meshgrid(np.arange(combined\_data.shape[1]), np.arange(combined\_data.shape[0]))

ax2 = fig.add\_subplot(num\_samples, 2, 2\*idx + 2, projection='3d')

return {str(i): count for i, count in enumerate(label\_counts)}

mean, std = np.mean(metadata, axis=0), np.std(metadata, axis=0)

for key in f.keys():

Shape of X\_jets: (139306, 125, 125, 3)

In [6]: def load\_data(file\_name, sample\_size):

return X, y, metadata

Image dimensions: (125, 125, 3)

Total images: 139306

In [7]: def count\_labels(labels):

print(count\_labels(y))

{'0': 4994, '1': 5006}

In [8]: def preprocess\_images(images):

X = preprocess\_images(X)

In [9]: def normalize\_metadata(metadata):

from sklearn.metrics import roc\_curve, auc
from torch\_geometric.data import Data, Batch
from torch\_geometric.loader import DataLoader

from sklearn.model\_selection import train\_test\_split

In [3]: device = torch.device("cuda" if torch.cuda.is\_available() else "cpu")

print("Keys in dataset:", list(f.keys()))

print(f"Shape of {key}: {f[key].shape}")

print("Image dimensions:", f['X\_jets'].shape[1:])

y = np.array(f['y'][:sample\_size], dtype=np.int64)

metadata = np.column\_stack((f['m0'][:sample\_size], f['pt'][:sample\_size]))

processed = np.array([resize(img, (128, 128), anti\_aliasing=True) for img in images], dtype=np.float32)

file\_path = "/kaggle/input/autoencoder-data/quark-gluon\_data-set\_n139306.hdf5"

import torch

torch-geometric) (2024.2.0)

0, >=4.5-aiohttp->torch-geometric) (4.12.2)

enmp>=2024->mkl->numpy->torch-geometric) (2024.2.0)

Installing collected packages: torch-geometric
Successfully installed torch-geometric-2.6.1

Downloading torch\_geometric-2.6.1-py3-none-any.whl (1.1 MB)

Note: you may need to restart the kernel to use updated packages.

1.1)

In [2]: import h5py

In [4]: print(device)

cuda

In [5]: def explore\_hdf5(file):

explore\_hdf5(file\_path)

Shape of m0: (139306,) Shape of pt: (139306,) Shape of y: (139306,)

quark/gluon Classification using Contrastive Loss

Downloading torch\_geometric-2.6.1-py3-none-any.whl.metadata (63 kB)

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Requirement already satisfied: mkl\_random in /usr/local/lib/python3.10/dist-packages (from numpy->torch-geometric)

Requirement already satisfied: pyparsing in /usr/local/lib/python3.10/dist-packages (from torch-geometric) (3.2.0)
Requirement already satisfied: requests in /usr/local/lib/python3.10/dist-packages (from torch-geometric) (2.32.3)
Requirement already satisfied: tqdm in /usr/local/lib/python3.10/dist-packages (from torch-geometric) (4.67.1)

- 63.1/63.1 kB 4.6 MB/s eta 0:00:00