ax2 : X, Y ax2.; ax2.; plt.tight	<pre>plot_surface(X, Y, combined_da set_title(f'3D Projection - Sa t_layout()</pre>	<pre>ined_data.shape[1]), n ata, cmap='viridis')</pre>	<pre>tion='3d') p.arange(combined_data.shape[0]))  3D Projection - Sample 0</pre>
40 - 60 - 80 - 100 - 120 -	40 60 80 100 2D Heatmap - Sample 1	- 40 - 30 - 20 - 10	3D Projection - Sample 1
0 - 20 - 40 - 60 - 80 -		- 200 - 150 - 100	0 20 40 60 40 60
120 - 20	40 60 80 100 2D Heatmap - Sample 2	- 100 - 100 - 80 - 60 - 40	3D Projection - Sample 2
from IPython  def animate_fig = ploax = fig  combined X, Y = ng surf = as  def updata ax.v. retus	lib.animation import FuncAnima .display import HTML  3d_rotation(images, sample_ids t.figure(figsize=(8, 6)) .add_subplot(111, projection=  _data = np.sum(images[sample_: p.meshgrid(np.arange(combined_ix.plot_surface(X, Y, combined_ix.plot_surface(X, Y, combined_ite(frame): iew_init(elev=20, azim=frame) rn fig, uncAnimation(fig, update, frame)	<pre>x=0): '3d') idx], axis=-1) _data.shape[1]), np.ar _data, cmap='viridis')</pre>	ange(combined_data.shape[0]))
	e() TML(anim.to_html5_video()) otation(X, sample_idx=0)		
► 0:00 / 0:0	09		
<pre>reshaped return np mask = extract  def create_graindices,    for img_return    indices_list</pre>	<pre>nonzero_mask(images):     = images.reshape((-1, images p.any(reshaped != [0., 0., 0.] ct_nonzero_mask(X)  raph_features(masked_data):     features = [], [] idx, mask in enumerate(masked_ds = np.column_stack(np.where ures.append(X[img_idx, coords ces.append(coords) ndices, features , features_list = create_graph raph_features(masked_data):</pre>	_data): (mask)) [:, 0], coords[:, 1],	ages.shape[:3])
for img_s coord feats indices_list  indices_list  def build_gra from scip from scip tree = cl dist, ind sigma2 = weights = row, col	<pre>features = [], [] idx, mask in enumerate(masked_ ds = np.column_stack(np.where ures.append(X[img_idx, coords ces.append(coords) ndices, features  , features_list = create_graph aph_structure(coords, k=4): py.spatial import cKDTree py.sparse import coo_matrix KDTree(coords) dices = tree.query(coords, k=4) np.mean(dist[:, -1])**2 = np.exp(-dist**2 / sigma2) = np.arange(len(coords)).reperoo_matrix((weights.flatten()),</pre>	<pre>(mask)) [:, 0], coords[:, 1], h_features(mask)  k) eat(k), indices.flatte</pre>	n ()
dataset for i, positive adjacedge edge mass mass mome:  node node labe graph	<pre>oints in enumerate(indices_list cency = build_graph_structure _idx = torch.from_numpy(np.vst _weights = torch.from_numpy(ac) , momentum = metadata[i] _tensor = torch.full((features) ntum_tensor = torch.full((features) _features = torch.from_numpy(s) _features = torch.cat((node_features) l = torch.tensor([int(labels[s] h = Data(x=node_features, edges) set.append(graph)</pre>	st): (points, k=neighbors) tack((adjacency.row, a djacency.data).float()  s_list[i].shape[0], 1) tures_list[i].shape[0]  features_list[i]).floa eatures, mass_tensor,  i])], dtype=torch.long	<pre>djacency.col))).long() .view(-1, 1)  , mass, dtype=torch.float32) , 1), momentum, dtype=torch.float32)  t() momentum_tensor), dim=1)</pre>
graph_datase:  G = nx.Graph data = graph edge_tensor = edge_list = G.add_edges_= pos = nx.spr fig, ax = pl: ax.axis("off nx.draw_netwo plt.show()  print(f'Numbo print(f'For print(f'Type print(f'Numbo	<pre>t = create_graph_dataset(indice ()     _dataset[0]     = data.edge_index [(edge_tensor[0, i].item(), edfrom(edge_list) ing_layout(G, iterations=15, st.subplots(figsize=(15, 9))</pre>	<pre>dge_tensor[1, i].item( seed=1721)  size=10, with_labels=F  len(graph_dataset) } ') dataset : ') ject: {type(data) } ') ')</pre>	)) <b>for</b> i <b>in</b> range(edge_tensor.shape[1])]
print(f'Numb	er of node features: {data.nurer of edges features: {data.nu	m_node_features}')	
Number of gr	aphs to work upon : 10000		
Type of each Number of noo Number of edd Number of edd Number of edd  : import torch import torch import torch from torch_gd  class GraphEdd defin_ super self	ges: 12240 de features: 5 ges features: 1	<pre>lass 'torch_geometric. lobal_mean_pool ata_dim=2, hidden_dim= 1(</pre>	
self  ))  self  )))	<pre>.metadata_encoder = nn.Sequent nn.Linear(metadata_dim, hidder nn.ReLU(), nn.Linear(hidden_dim // 4, hid .conv1 = GINConv(nn.Sequential nn.Linear(hidden_dim, hidden_d nn.ReLU(), nn.Linear(hidden_dim, hidden_d nn.Linear(hidden_dim, hidden_d nn.Linear(hidden_dim, hidden_d nn.Linear(hidden_dim, hidden_d nn.ReLU(), nn.Linear(hidden_dim, hidden_d nn.ReLU(), nn.Linear(hidden_dim, hidden_d .conv3 = GINConv(nn.Sequential</pre>	<pre>n_dim // 4), dden_dim // 2),  l( dim), dim)  l( dim), dim)</pre>	
def forward point metadox x = 1 x = 1 x = 1	nn.Linear(hidden_dim, out_dim) nn.ReLU(), nn.Linear(out_dim, out_dim)  ard(self, data): t_features = data.x[:, :3] data_features = data.x[:, 3:]  t_emb = self.point_encoder(postdata_emb = self.metadata_encodetorch.cat([point_emb, metadata])  torch.cat([point_emb, metadata]) F.relu(self.conv1(x, data.edge) F.relu(self.conv2(x, data.edge)) self.conv3(x, data.edge_index)	<pre>int_features) der(metadata_features) a_emb], dim=1) e_index)) e_index))</pre>	
<pre>import torch import torch import torch  class Model()     defin.     super     self  self  )  def forward  def forward </pre>	.nn as nn .nn.functional as F	n_dim=32):	
projection retuses:  import torch import torch import torch class Loss (not superself self self def forward features)	ected = self.projector(embedd: rn F.normalize(projected, dim= .nn as nn .nn.functional as F	<pre>ard_neg_weight=0.5): eight dim=1) s, features.T) / self.</pre>	
exp_s hard log_s weigh mean retus  import torch import numpy from sklearn def train (moden model.to	<pre>sim = torch.exp(sim_matrix) _neg_mask = (1 - mask) * (sim_ prob = sim_matrix - torch.log hted_log_prob = log_prob * (mater) _log_prob = weighted_log_prob rn -mean_log_prob.mean()  as np .neighbors import KNeighborsCl del, train_loader, val_loader,</pre>	_matrix > 0.5).float() (exp_sim.sum(dim=1, ke ask + self.hard_neg_we .sum(1) / (mask.sum(1))	epdim= <b>True</b> ))
<pre>knn = KNo  train_log train_accus val_accus best_val  for epocl    mode    tota train    train  # Tra for l</pre>	eighborsClassifier (n_neighbors  sses = [] curacies = [] racies = [] _acc = 0.0  h in range(num_epochs): l.train() l_loss = 0 n_embeddings = [] n_labels = []  aining phase batch in train_loader: batch = batch.to(device) optimizer.zero_grad()  projections = model(batch) loss = criterion(projections,		
schecurre train train	<pre>loss.backward() optimizer.step()  total_loss += loss.item()  with torch.no_grad():     emb = model.encoder(batch)     train_embeddings.append(er     train_labels.append(batch)  duler.step() ent_lr = scheduler.get_last_lr  n_embeddings = torch.cat(train_labels) fit(train_embeddings, train_labels</pre>	<pre>).cpu() mb) .y.cpu())  r()[0]  n_embeddings).numpy() bels).numpy()</pre>	
traint traint val_a  if val  print  # Print print(f"	acc, val_auc, _, _= evaluate(r n_losses.append(total_loss / I n_accuracies.append(train_acc) accuracies.append(val_acc)  al_acc > best_val_acc: best_val_acc = val_acc  t(f"Epoch {epoch+1}/{num_epoch f"Loss: {total_loss / len(train_acc:.4f) f"Val Acc: {val_acc:.4f}   ' f"Val ROC-AUC: {val_auc:.4f}  best validation accuracy n Best Validation Accuracy rain_losses, train_accuracies,	<pre>len(train_loader)) )  hs}   " rain_loader):.4f}   " }   "  }") : {best_val_acc:.4f}")</pre>	
<pre>import torch import numpy  def evaluate    model.evaluate    import numpy    import num</pre>	<pre>as np (model, loader, knn, device="( al() gs = []</pre>	cuda"):	
<pre>labels =   val_acc :   probs = !   val_auc :   fpr, tpr   return val : import torch   from torch.ut   from torch_ge   from sklearn   from sklearn</pre>	<pre>gs = torch.cat(embeddings).num torch.cat(labels).numpy()  = knn.score(embeddings, labels knn.predict_proba(embeddings) = roc_auc_score(labels, probs) , _ = roc_curve(labels, probs) al_acc, val_auc, fpr, tpr  tils.data import random_split eometric.loader import DataLoa .neighbors import KNeighborsCometrics import roc_auc_score, ch.device("cuda" if torch.cuda</pre>	s) [:, 1] ) if len(np.unique(lab ) if len(np.unique(lab  ader lassifier , roc_curve	els)) > 1 <b>else</b> ([], [], [])
train_sist val_size train_set  2))  train_loaval_loade  encoder = model = I optimize: schedule: criterion  train_loaval	<pre>ader = DataLoader(train_set, ker = DataLoader(val_set, batcher = DataLoader(point_dim=3, memodel(encoder).to(device) r = torch.optim.Adam(model.parr = torch.optim.lr_scheduler.or = Loss()</pre>	_size ph_dataset, [train_siz  batch_size=16, shuffle h_size=16)  etadata_dim=2).to(devi  rameters(), lr=1e-3)  CosineAnnealingLR(opti  ccuracies= train(	
train_eml model.eva with tore for l  train_eml train_lal knn.fit( test_acc	ch.no_grad(): batch in train_loader: batch = batch.to(device) emb = model.encoder(batch).cpu train_embeddings.append(emb) train_labels.append(batch.y.cpu beddings = torch.cat(train_embeddings = torch.cat(train_labels) train_embeddings, train_labels train_embeddings, train_labels	<pre>[] u() pu()) beddings).numpy() ).numpy() s) te(model, val_loader,</pre>	knn, device=device)
print(f") print(f") Epoch 1/50   Epoch 2/50   Epoch 3/50   Epoch 4/50   Epoch 5/50   Epoch 6/50   Epoch 6/50   Epoch 7/50   Epoch 8/50   Epoch 9/50   Epoch 10/50 Epoch 11/50 Epoch 12/50 Epoch 13/50 Epoch 14/50 Epoch 15/50 Epoch 16/50	test_auc, fpr, tpr = evaluate	acc:.4f}")  7460   Val Acc: 0.5910  7642   Val Acc: 0.6565  7632   Val Acc: 0.6765  7730   Val Acc: 0.6645  7735   Val Acc: 0.6690  7668   Val Acc: 0.6730  7694   Val Acc: 0.6740  7814   Val Acc: 0.6870  7741   Val Acc: 0.6965  .7722   Val Acc: 0.698  .7769   Val Acc: 0.698  .7721   Val Acc: 0.688  .7705   Val Acc: 0.689  .7801   Val Acc: 0.689  .7841   Val Acc: 0.692  .7841   Val Acc: 0.693	Val ROC-AUC: 0.6228   Val ROC-AUC: 0.7039   Val ROC-AUC: 0.7169   Val ROC-AUC: 0.7013   Val ROC-AUC: 0.7086   Val ROC-AUC: 0.7197   Val ROC-AUC: 0.7271   Val ROC-AUC: 0.7173   Val ROC-AUC: 0.7377 0   Val ROC-AUC: 0.7303 0   Val ROC-AUC: 0.7416 0   Val ROC-AUC: 0.7167 0   Val ROC-AUC: 0.7393 0   Val ROC-AUC: 0.7393 0   Val ROC-AUC: 0.7242 5   Val ROC-AUC: 0.7342 5   Val ROC-AUC: 0.7373
Epoch 17/50 Epoch 18/50 Epoch 19/50 Epoch 20/50 Epoch 21/50 Epoch 22/50 Epoch 23/50 Epoch 24/50 Epoch 25/50 Epoch 26/50 Epoch 26/50 Epoch 27/50 Epoch 28/50 Epoch 30/50 Epoch 30/50 Epoch 31/50 Epoch 33/50 Epoch 34/50 Epoch 35/50 Epoch 36/50	Loss: 2.7682   Train Acc: 0.0   Loss: 2.7680   Train Acc: 0.0   Loss: 2.7682   Train Acc: 0.0   Loss: 2.7680   Train Acc: 0.0   Loss: 2.7680   Train Acc: 0.0   Loss: 2.7679   Train Acc: 0.0   Loss: 2.7678   Train Acc: 0.0   Loss: 2.7677   Train Acc: 0.0   Loss: 2.7678   Train Acc: 0.0   Loss: 2.7677   Train Acc: 0.0   Loss: 2.7677   Train Acc: 0.0   Loss: 2.7674   Train Acc: 0.0   Loss: 2.7675   Train Acc: 0.0   Loss: 2.7676   Train Acc: 0.0   Loss: 2.7675   Train Acc: 0.	.7825   Val Acc: 0.686 .7774   Val Acc: 0.688 .7746   Val Acc: 0.676 .7794   Val Acc: 0.680 .7784   Val Acc: 0.689 .7792   Val Acc: 0.683 .7801   Val Acc: 0.699 .7829   Val Acc: 0.699 .7812   Val Acc: 0.697 .7851   Val Acc: 0.679 .7795   Val Acc: 0.679 .7795   Val Acc: 0.675 .7833   Val Acc: 0.685 .7815   Val Acc: 0.685 .7816   Val Acc: 0.690 .7811   Val Acc: 0.690 .7811   Val Acc: 0.692 .7809   Val Acc: 0.681 .7856   Val Acc: 0.685	5   Val ROC-AUC: 0.7304 5   Val ROC-AUC: 0.7376 5   Val ROC-AUC: 0.7299 5   Val ROC-AUC: 0.7299 0   Val ROC-AUC: 0.7318 0   Val ROC-AUC: 0.7366 5   Val ROC-AUC: 0.7436 0   Val ROC-AUC: 0.7280 0   Val ROC-AUC: 0.7280 0   Val ROC-AUC: 0.7213 5   Val ROC-AUC: 0.7213 5   Val ROC-AUC: 0.7275 5   Val ROC-AUC: 0.7214 5   Val ROC-AUC: 0.7500 5   Val ROC-AUC: 0.7310 0   Val ROC-AUC: 0.7397 0   Val ROC-AUC: 0.7327 5   Val ROC-AUC: 0.7327 5   Val ROC-AUC: 0.7327 5   Val ROC-AUC: 0.7327 5   Val ROC-AUC: 0.7316
Epoch 37/50 Epoch 38/50 Epoch 39/50 Epoch 40/50 Epoch 41/50 Epoch 42/50 Epoch 43/50 Epoch 44/50 Epoch 45/50 Epoch 46/50 Epoch 47/50 Epoch 48/50 Epoch 49/50 Epoch 50/50  Best Valid	Loss: 2.7675   Train Acc: 0.     Loss: 2.7674   Train Acc: 0.     Loss: 2.7676   Train Acc: 0.     Loss: 2.7673   Train Acc: 0.     Loss: 2.7672   Train Acc: 0.     Loss: 2.7673   Train Acc: 0.     Loss: 2.7671   Train Acc: 0.     Loss: 2.7671   Train Acc: 0.     Loss: 2.7674   Train Acc: 0.     Loss: 2.7671   Train Acc: 0.     Loss: 2.7673   Train Acc: 0.     Loss: 2.7671   Train Acc: 0.     Loss: 2.7670   Train Acc: 0.	.7784   Val Acc: 0.691 .7826   Val Acc: 0.691 .7778   Val Acc: 0.692 .7875   Val Acc: 0.689 .7837   Val Acc: 0.698 .7806   Val Acc: 0.686 .7837   Val Acc: 0.686 .7837   Val Acc: 0.689 .7895   Val Acc: 0.699 .7887   Val Acc: 0.693 .7837   Val Acc: 0.693 .7837   Val Acc: 0.695 .7885   Val Acc: 0.695	0   Val ROC-AUC: 0.7283 0   Val ROC-AUC: 0.7382 5   Val ROC-AUC: 0.7359 5   Val ROC-AUC: 0.7282 5   Val ROC-AUC: 0.7462 0   Val ROC-AUC: 0.7337 0   Val ROC-AUC: 0.7246 5   Val ROC-AUC: 0.7338 5   Val ROC-AUC: 0.7525 0   Val ROC-AUC: 0.7464 5   Val ROC-AUC: 0.7387 5   Val ROC-AUC: 0.7371 0   Val ROC-AUC: 0.7380
plt.plot(traplt.plot(val)  plt.xlabel("Toplt.ylabel("Toplt.grid(True) plt.legend() plt.show()	_accuracies, marker='x', lines Epochs")	style='', label='Val	aining Accuracy', color='violet') idation Accuracy', color='blue')  ition Accuracy
0.750		-*	
<pre>plt.figure(f. plt.plot(tra:  plt.xlabel(") plt.ylabel(") plt.title("T)</pre>		zo  Epoch  yle='-', label='Traini  Training	ng Loss', color='blue')
2.771			
<pre>plt.figure(f plt.plot(fpr plt.plot([0, plt.xlabel(') plt.ylabel(')</pre>	igsize=(8, 6)) , tpr, label=f'ROC Curve (AUC 1], [0, 1], linestyle='', of False Positive Rate') True Positive Rate') eceiver Operating Characterist	color='gray')	
<pre>plt.title( Red plt.legend() plt.grid() plt.show()</pre>			

Specific\_Task\_01

Collecting torch-geometric

In [1]: pip install torch-geometric

h-geometric) (2.4.6)

c) (25.1.0)

ometric) (6.1.0)

etric) (1.18.3)

rch-geometric) (3.4.1)

ometric) (2.3.0)

ometric) (2025.1.31)

geometric) (2024.2.0)

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

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

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):

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) (1.2.0)

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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