

```
!pip install torch_geometric
!pip install torchviz
```

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/usr/local/lib/python3.10/dist-packages (2.6.1)
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Requirement already satisfied: MarkupSafe>=2.0 in
/usr/local/lib/python3.10/dist-packages (from jinja2->torch->torchviz)
(3.0.2)

```
import numpy as np
import torch
import torch_geometric
import h5py
import matplotlib.pyplot as plt

from torch_geometric.data import Data, Batch
from torch_geometric.loader import DataLoader
from sklearn.neighbors import kneighbors_graph
from sklearn.model_selection import train_test_split

import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim

from torch_geometric.nn import global_mean_pool
from torch.nn import Linear

Data_Path = '/kaggle/input/paraquet-df/quark-gluon_data-
set_n139306.hdf5'
```

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Data_Size = 40000
k = 8

import h5py
import numpy as np
import torch
from torch_geometric.data import Data
from sklearn.neighbors import kneighbors_graph

def load_data(k=8, max_nodes=800, activation_threshold=1e-3):
    # Adding coordinates to the features.
    data = h5py.File(Data_Path, "r")
    images = data['X_jets'][0:Data_Size]
    coords = np.indices((125, 125))
    coords = np.moveaxis(coords, 1, -1).T
    coords = np.expand_dims(coords, axis=0)
    coords = coords.astype(np.float32) / 125.
    coords = np.repeat(coords, Data_Size, axis=0)

    # Suppressing smaller activations
    images[images < activation_threshold] = 0.0
    images_with_coords = np.concatenate((images, coords), axis=-1)

    del coords
    del images
    del data

    data = images_with_coords.reshape((-1, images_with_coords.shape[1]
* images_with_coords.shape[2], 5))
    node_list = []
    for i, x in enumerate(data):
        mask = np.any(x[..., :3] != [0., 0., 0.], axis=-1)
        filtered_nodes = x[mask]
        # canonical ordering of nodes. (sorted positions)
        sorted_nodes = filtered_nodes[np.lexsort((filtered_nodes[:,
4], filtered_nodes[:, 3]))]

        if sorted_nodes.shape[0] > max_nodes:
            sorted_nodes = sorted_nodes[:max_nodes]

        node_list.append(sorted_nodes)

    dataset = []
    for i, nodes in enumerate(node_list):
        edges = kneighbors_graph(nodes[:, :3], k,
mode='connectivity', include_self=True)
        c = edges.tocoo()
        edge_list = torch.from_numpy(np.vstack((c.row,
c.col))).type(torch.long)
        edge_weight = torch.from_numpy(c.data.reshape(-1, 1))

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        data = Data(x=torch.from_numpy(nodes), edge_index=edge_list,
edge_attr=edge_weight)
        dataset.append(data)

    return dataset

#dataset = load_data()
train_loader = DataLoader(dataset[:36000], batch_size=64,
shuffle=True)
test_loader = DataLoader(dataset[36000:36500], batch_size=1,
shuffle=False)

from torch_geometric.nn import SAGEConv, GATConv

# Graph level latent Graph Auto Encoder
class GAE(torch.nn.Module):
    def __init__(self, input_embed_dim : int, latent_dim = None,
max_nodes : int = 800):
        super(GAE, self).__init__()

        self.node_dim = input_embed_dim
        if latent_dim is None:
            self.latent_dim = self.node_dim
        else:
            self.latent_dim = latent_dim
        self.max_nodes = max_nodes
        self.output_size = self.max_nodes * self.node_dim

        self.Conv1 = GATConv(self.node_dim, self.latent_dim, heads=1,
concat=False)
        self.Conv2 = GATConv(self.latent_dim, 2*self.latent_dim, heads=1,
concat=False)
        self.Conv3 = GATConv(2*self.latent_dim, 4*self.latent_dim,
heads=1, concat=False)
        self.Conv4 = GATConv(4*self.latent_dim, 8*self.latent_dim,
heads=1, concat=False)
        self.lin1 = torch.nn.Linear(8*self.latent_dim, 16*self.latent_dim)
        self.lin2 = torch.nn.Linear(16*self.latent_dim,
32*self.latent_dim)
        self.lin3 = torch.nn.Linear(32*self.latent_dim,
int(self.output_size / 2))
        self.lin4 = torch.nn.Linear(int(self.output_size / 2),
self.output_size)
        self.p5 = nn.Dropout(p=0.5)
        self.p3 = nn.Dropout(p=0.3)
        self.p1 = nn.Dropout(p=0.1)

    def forward(self, x, edge_index, batch):

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    # Encoder.
    x = F.relu(self.Conv1(x, edge_index))
    x = F.relu(self.Conv2(x, edge_index))
    x = F.relu(self.Conv3(x, edge_index))
    x = F.relu(self.Conv4(x, edge_index))

    # mask generation and pooling.
    x, mask = torch_geometric.utils.to_dense_batch(x, batch,
fill_value=0)
    x = torch.mean(x, dim=1)

    # Decoder
    x = F.relu(self.lin1(x))
    x = self.pl(x)
    x = F.relu(self.lin2(x))
    x = self.pl(x)
    x = F.relu(self.lin3(x))
    x = self.lin4(x)
    x = torch.reshape(x, (-1, self.max_nodes, self.node_dim))
    new_mask = torch.zeros(mask.shape[0], self.max_nodes,
dtype=torch.bool)
    new_mask[:, :mask.shape[1]] = mask
    mask = new_mask

    return x, mask

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")

import torch
import torch.nn.functional as F
from torchvision import transforms
from torchvision.transforms import functional as TF
from torchmetrics.image import StructuralSimilarityIndexMeasure

ssim_metric = StructuralSimilarityIndexMeasure(data_range=1.0)

def reconstruct_image(features):
    x_coords = (features[:, -2] * 125).cpu().numpy().astype(int)
    y_coords = (features[:, -1] * 125).cpu().numpy().astype(int)
    tracks_act = features[:, 0].cpu().numpy()
    ecal_act = features[:, 1].cpu().numpy()
    hcal_act = features[:, 2].cpu().numpy()

    img_tracks = np.zeros((125, 125))
    img_ecal = np.zeros((125, 125))
    img_hcal = np.zeros((125, 125))

    for i in range(len(x_coords)):
        if 0 <= x_coords[i] < 125 and 0 <= y_coords[i] < 125:

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        img_tracks[y_coords[i], x_coords[i]] = tracks_act[i]
        img_ecal[y_coords[i], x_coords[i]] = ecal_act[i]
        img_hcal[y_coords[i], x_coords[i]] = hcal_act[i]

    # Stack the channels to get a 3-channel image
    image = np.stack([img_tracks, img_ecal, img_hcal], axis=0)
    return torch.tensor(image, dtype=torch.float32).unsqueeze(0) /
np.max(image)

def calculate_ssim(data, x):
    original_image = reconstruct_image(data)
    reconstructed_image = reconstruct_image(x)

    # Ensure both images are in the correct format
    original_image = original_image.clamp(0, 1)
    reconstructed_image = reconstructed_image.clamp(0, 1)

    ssim_score = ssim_metric(reconstructed_image, original_image)
    return ssim_score.item()

# Graph features based reconstruction loss.
def weighted_mse_loss(output, target, mask):
    weights = torch.tensor([1.0, 1.0, 1.0], device=output.device)
    squared_error = (output - target) ** 2
    for i in range(0, 3):
        squared_error[:, :, i] = squared_error[:, :, i] * weights[i]
    # Apply mask to the loss
    masked_error = squared_error * mask.unsqueeze(-1).to(device)
    loss = masked_error.sum() / ((mask.sum() * 5) + 1e-8) # Prevent
division by zero
    return loss

def visualize(data):
    x = data[:, 3]
    y = data[:, 4]
    tracks_act = data[:, 0]
    hcal_act = data[:, 2]
    ecal_act = data[:, 1]
    fig, axs = plt.subplots(1, 3, figsize=(18, 6))
    axs[0].set_xlim(0, 1) # Force x-axis to show 0-1 range
    axs[0].set_ylim(0, 1)
    # Plot tracks_act
    axs[0].scatter(x, y, c=tracks_act, s= torch.abs(tracks_act) * 500,
cmap='inferno', alpha=0.5)
    axs[0].set_title('Tracks Activity')
    axs[0].set_xlabel('X')
    axs[0].set_ylabel('Y')

    axs[1].set_xlim(0, 1) # Force x-axis to show 0-1 range
    axs[1].set_ylim(0, 1)

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    # Plot ecal_act
    axs[1].scatter(x, y, c=ecal_act, s= torch.abs(ecal_act) * 500,
cmap='inferno', alpha=0.5)
    axs[1].set_title('Ecal Activity')
    axs[1].set_xlabel('X')
    axs[1].set_ylabel('Y')

    axs[2].set_xlim(0, 1) # Force x-axis to show 0-1 range
    axs[2].set_ylim(0, 1)
    # Plot hcal_act
    axs[2].scatter(x, y, c=hcal_act, s= torch.abs(hcal_act) * 500,
cmap='inferno', alpha=0.5)
    axs[2].set_title('Hcal Activity')
    axs[2].set_xlabel('X')
    axs[2].set_ylabel('Y')

plt.tight_layout()
plt.show()

from tqdm import tqdm
# Training loop.
def train():
    model.train()
    total_loss = 0

    with tqdm(train_loader, desc="Training", leave=False) as t:
        temp_loss = 0
        for data in t:
            data = data.to(device)
            out, mask = model(data.x, data.edge_index, data.batch)
            x,_ = torch_geometric.utils.to_dense_batch(data.x,
data.batch, fill_value=0)
            # Mask padding and loss calculation.
            pad_size = model.max_nodes - x.shape[1]
            if (pad_size > 0):
                x = F.pad(x, (0, 0, 0, pad_size, 0, 0))
            loss = weighted_mse_loss(out, x, mask)
            loss.backward()
            optimizer.step()
            optimizer.zero_grad()
            total_loss += loss.item()
            t.set_postfix(loss=loss.item())
        total_loss += temp_loss / 64. # batch_size
    return total_loss / len(train_loader) # number of batches

# Inference and validation loop.
def inference(model, data_loader, device, vis = False):
    model.eval()
    loss = 0.

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```

with torch.no_grad():
    with tqdm(data_loader, desc="Inference", leave=False) as t:
        for data in t:
            data = data.to(device)
            out, mask = model(data.x, data.edge_index, data.batch)
            # Convert input to dense and pad if necessary
            x, _ = torch_geometric.utils.to_dense_batch(data.x,
data.batch, fill_value=0)
            # Generate visualizations.
            if (vis):
                visualize(x[0].cpu())
                visualize(out[0][:data.x.shape[0]].cpu())
                ssim_score = calculate_ssim(data.x, out[0]
[:data.x.shape[0]])
                print(f"SSIM Score: {ssim_score}")
                pad_size = model.max_nodes - x.shape[1]
                if (pad_size > 0):
                    x = F.pad(x, (0, 0, 0, pad_size, 0, 0))
                loss += weighted_mse_loss(out, x, mask).item()

    return loss / len(data_loader)

model = GAE(5, 8)
#model = nn.DataParallel(model)
model.to(device)
optimizer = torch.optim.Adam(model.parameters(), lr=0.001)
train_losses = []
val_losses = []
for epoch in range(50):
    train_loss = train()
    train_losses.append(train_loss)
    if (epoch + 1) % 10 == 0:
        val_loss = inference(model, test_loader, device, True)
    else :
        val_loss = inference(model, test_loader, device)
    val_losses.append(val_loss)
    print("Epoch : ", epoch + 1, " Train Loss : ", train_loss, " Val
Loss : ", val_loss)

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Epoch : 1 Train Loss : 0.011057700763322532 Val Loss :
0.011028019478544593

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Epoch : 2 Train Loss : 0.009681786243434909 Val Loss :
0.013218925567343831

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Epoch : 3 Train Loss : 0.009481961878602183 Val Loss : 0.009621655801311135

Epoch : 4 Train Loss : 0.00945135609281529 Val Loss : 0.011157069820910692

Epoch : 5 Train Loss : 0.009359213483038475 Val Loss : 0.010025429306551814

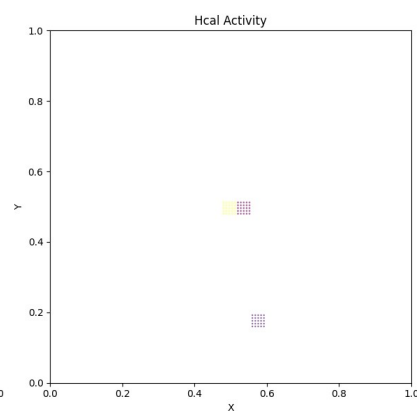
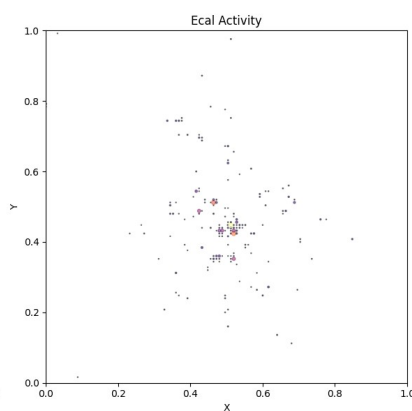
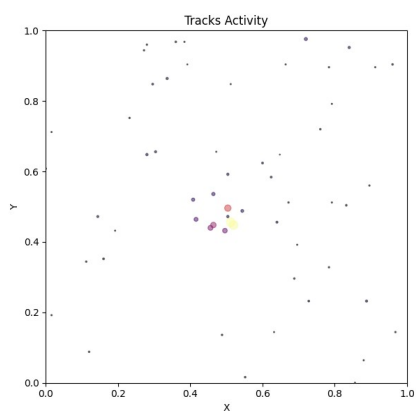
Epoch : 6 Train Loss : 0.009265957575549452 Val Loss : 0.010447329841554165

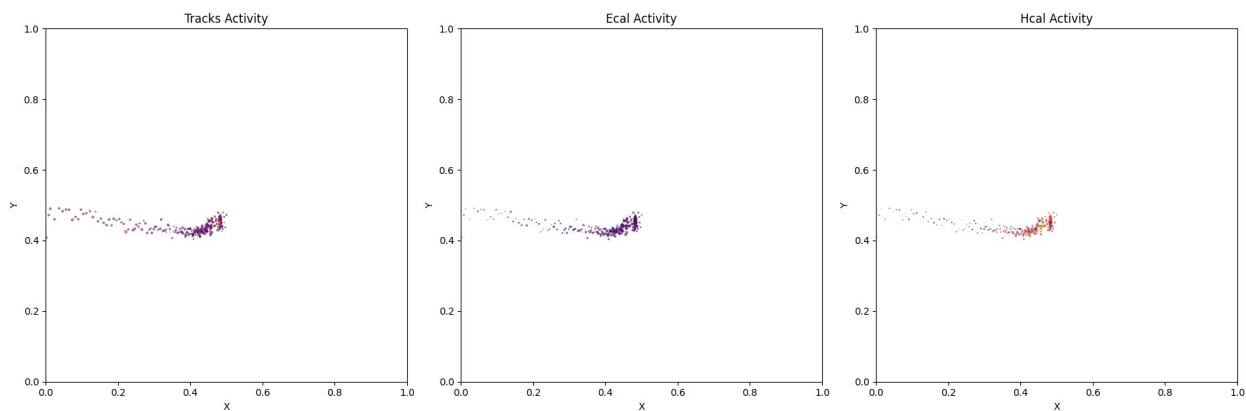
Epoch : 7 Train Loss : 0.009272608742263452 Val Loss : 0.009542359854094684

Epoch : 8 Train Loss : 0.009084289726432326 Val Loss : 0.009346499224193394

Epoch : 9 Train Loss : 0.009021497163656921 Val Loss : 0.009343842626549304

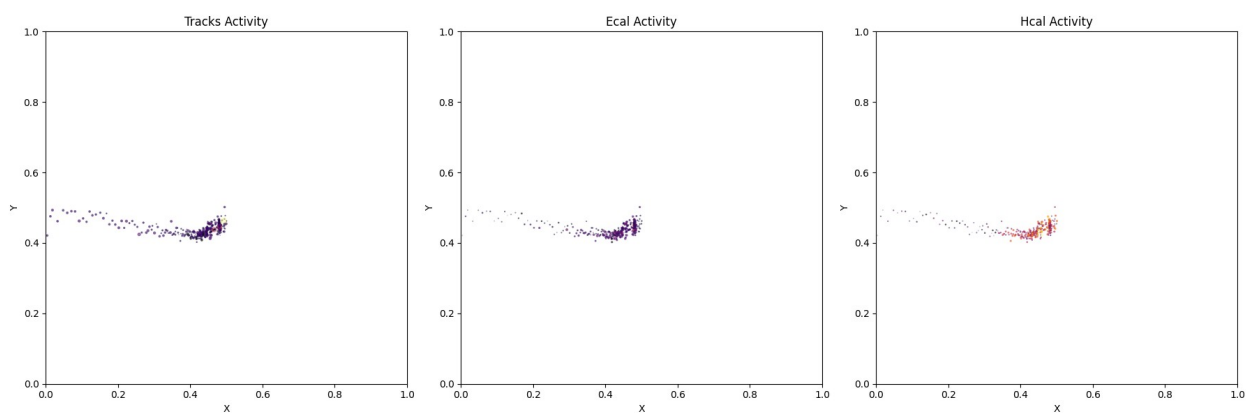
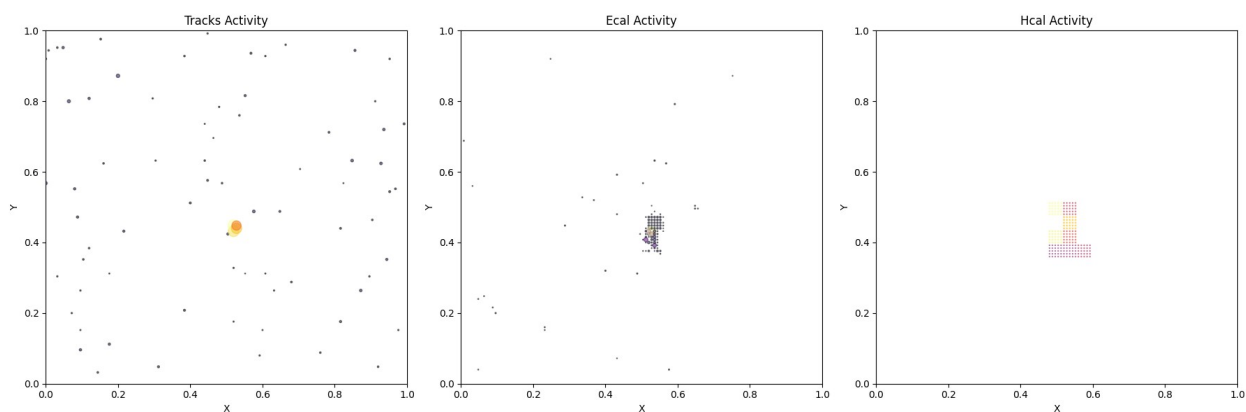
Inference: 0%| | 0/4 [00:00<?, ?it/s]





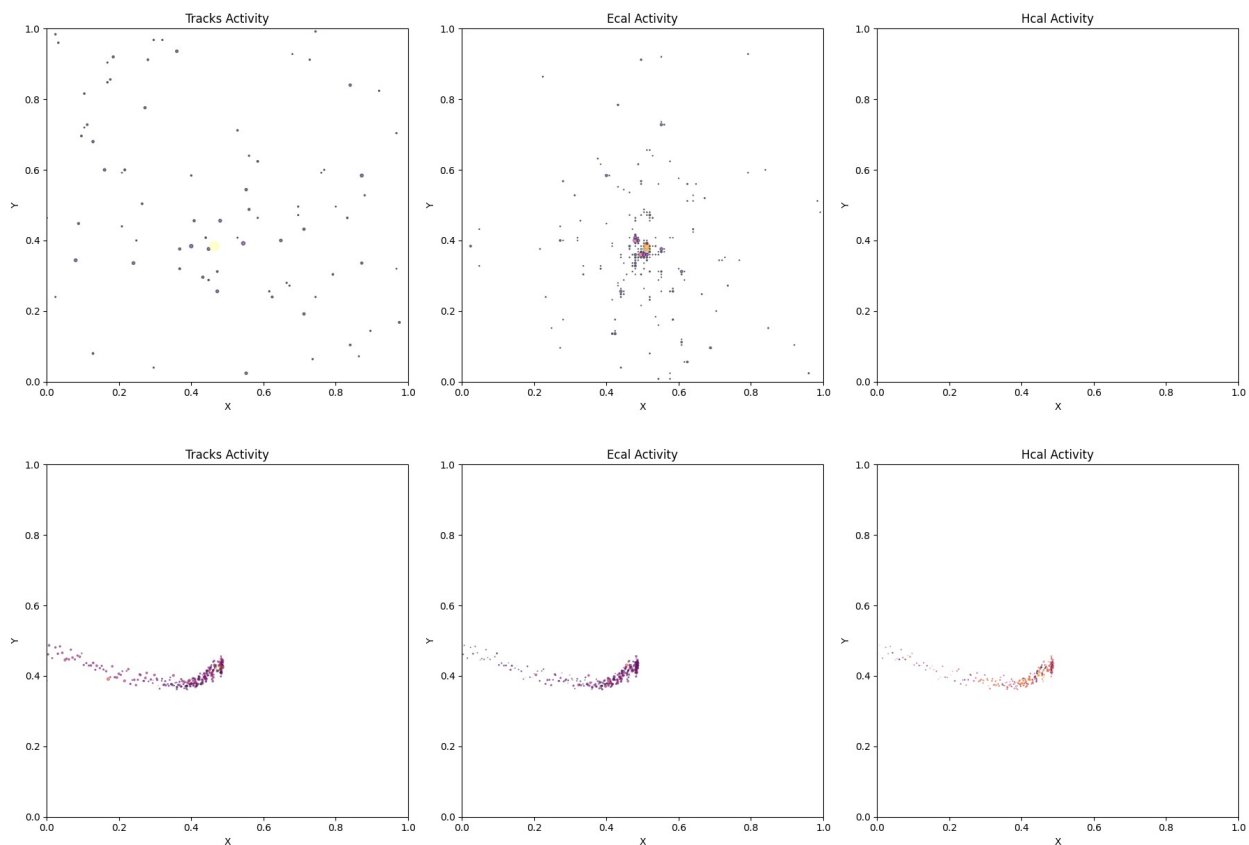
Inference: 25% | ████████ | 1/4 [00:01<00:03, 1.05s/it]

SSIM Score: 0.9599383473396301



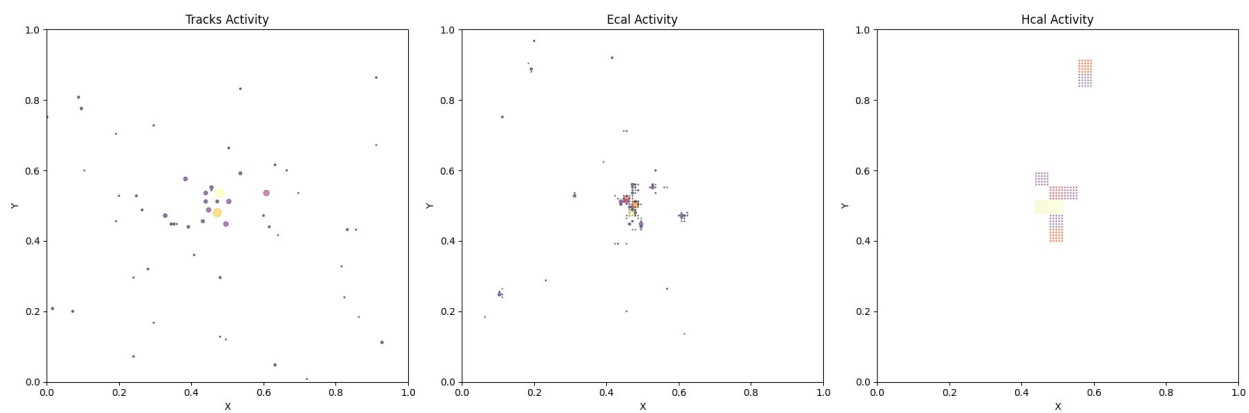
Inference: 50% | ████████ | 2/4 [00:02<00:02, 1.03s/it]

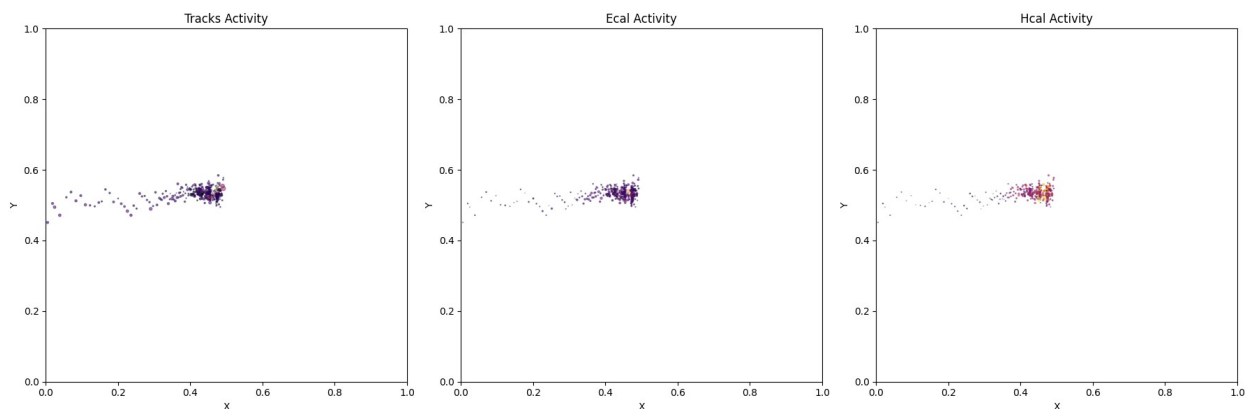
SSIM Score: 0.9795094132423401



Inference: 75% | ██████████ | 3/4 [00:03<00:01, 1.23s/it]

SSIM Score: 0.9687685966491699





SSIM Score: 0.9654818177223206

Epoch : 10 Train Loss : 0.008994988630629983 Val Loss : 0.010450502159073949

Epoch : 11 Train Loss : 0.008929351400120803 Val Loss : 0.010678368853405118

Epoch : 12 Train Loss : 0.008901529056293026 Val Loss : 0.01010836276691407

Epoch : 13 Train Loss : 0.008906047820191347 Val Loss : 0.009127994417212903

Epoch : 14 Train Loss : 0.008947819495345358 Val Loss : 0.00971486559137702

Epoch : 15 Train Loss : 0.00887957946719936 Val Loss : 0.009875562856905162

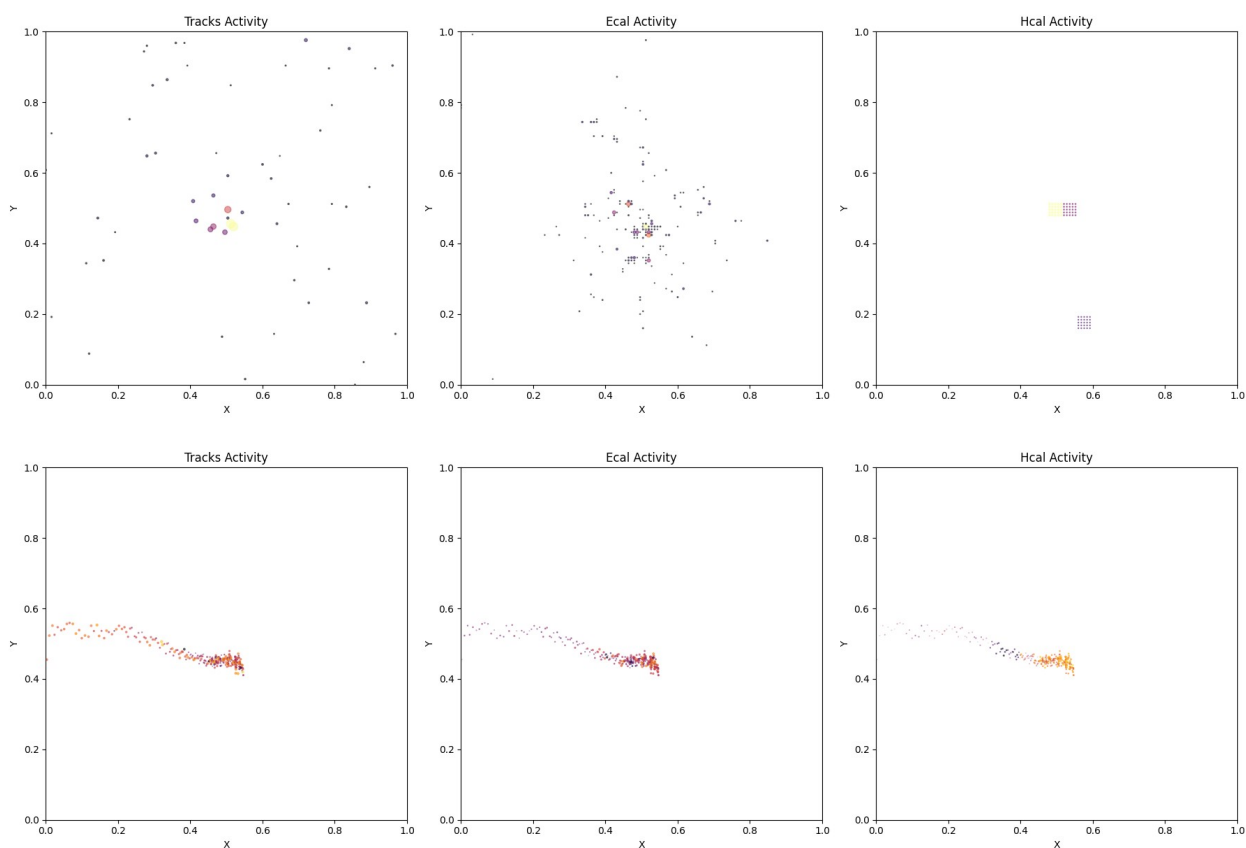
Epoch : 16 Train Loss : 0.008787396745210377 Val Loss : 0.009927683626301587

Epoch : 17 Train Loss : 0.008780649725883723 Val Loss : 0.009619026212021708

Epoch : 18 Train Loss : 0.008720445104247724 Val Loss : 0.009117868961766362

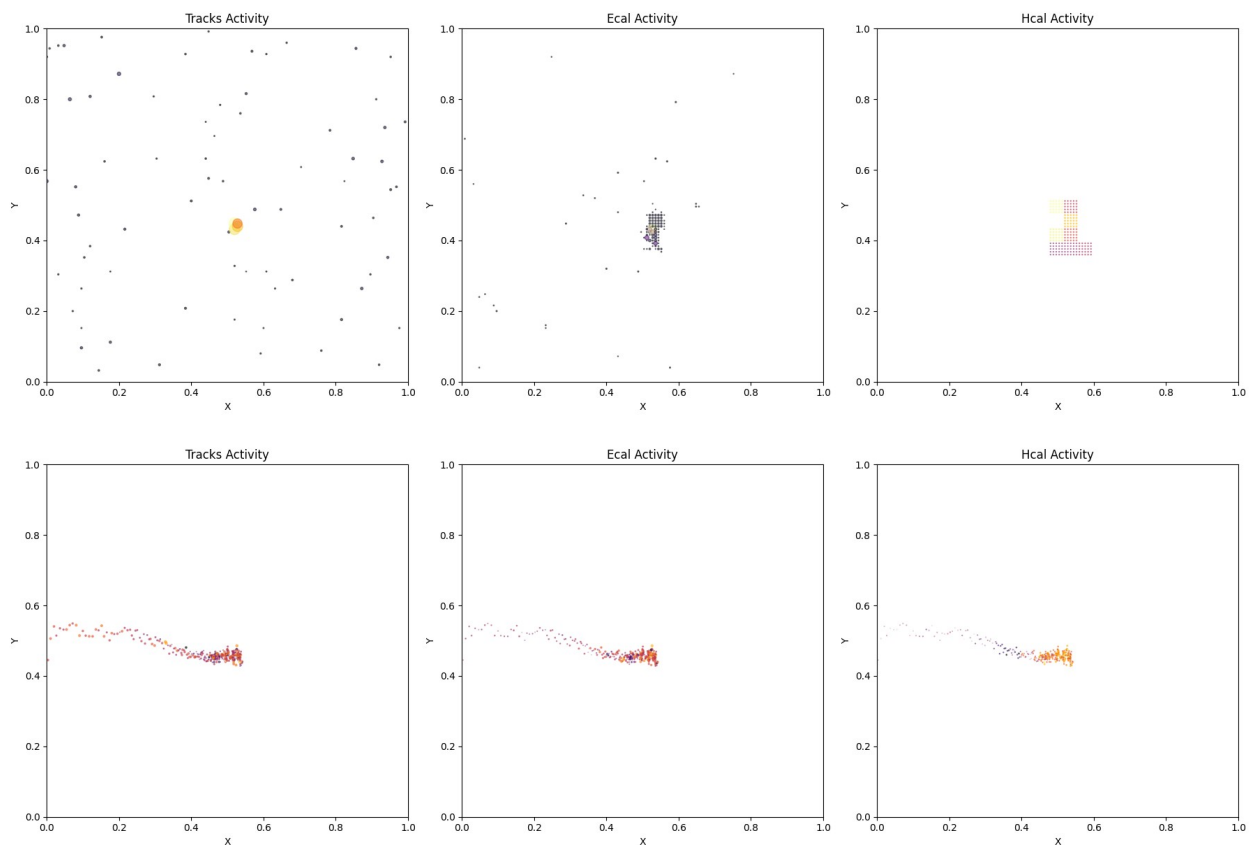
Epoch : 19 Train Loss : 0.008744694974081554 Val Loss : 0.009707177756354213

Inference: 0%| | 0/4 [00:00<?, ?it/s]



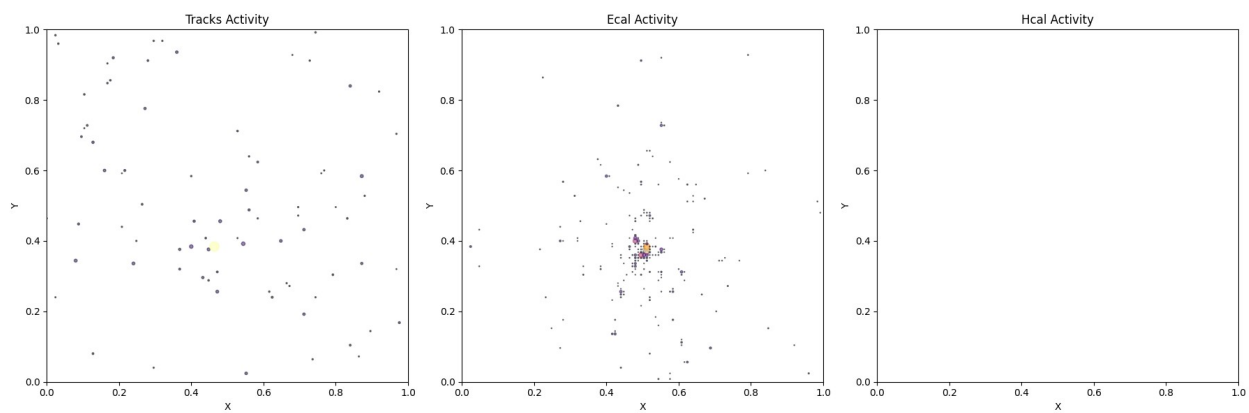
Inference: 25%| | 1/4 [00:01<00:03, 1.04s/it]

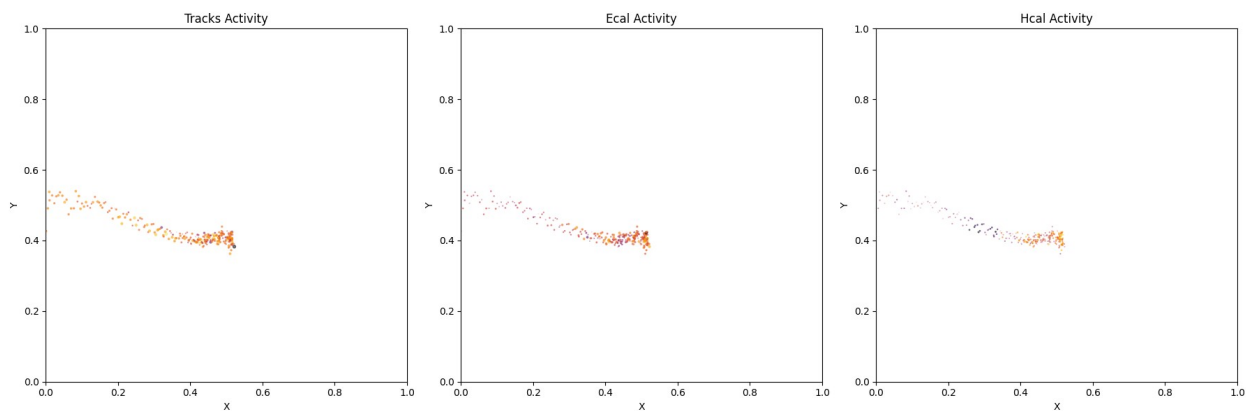
SSIM Score: 0.9573631882667542



Inference: 50% | ████████ | 2/4 [00:02<00:02, 1.03s/it]

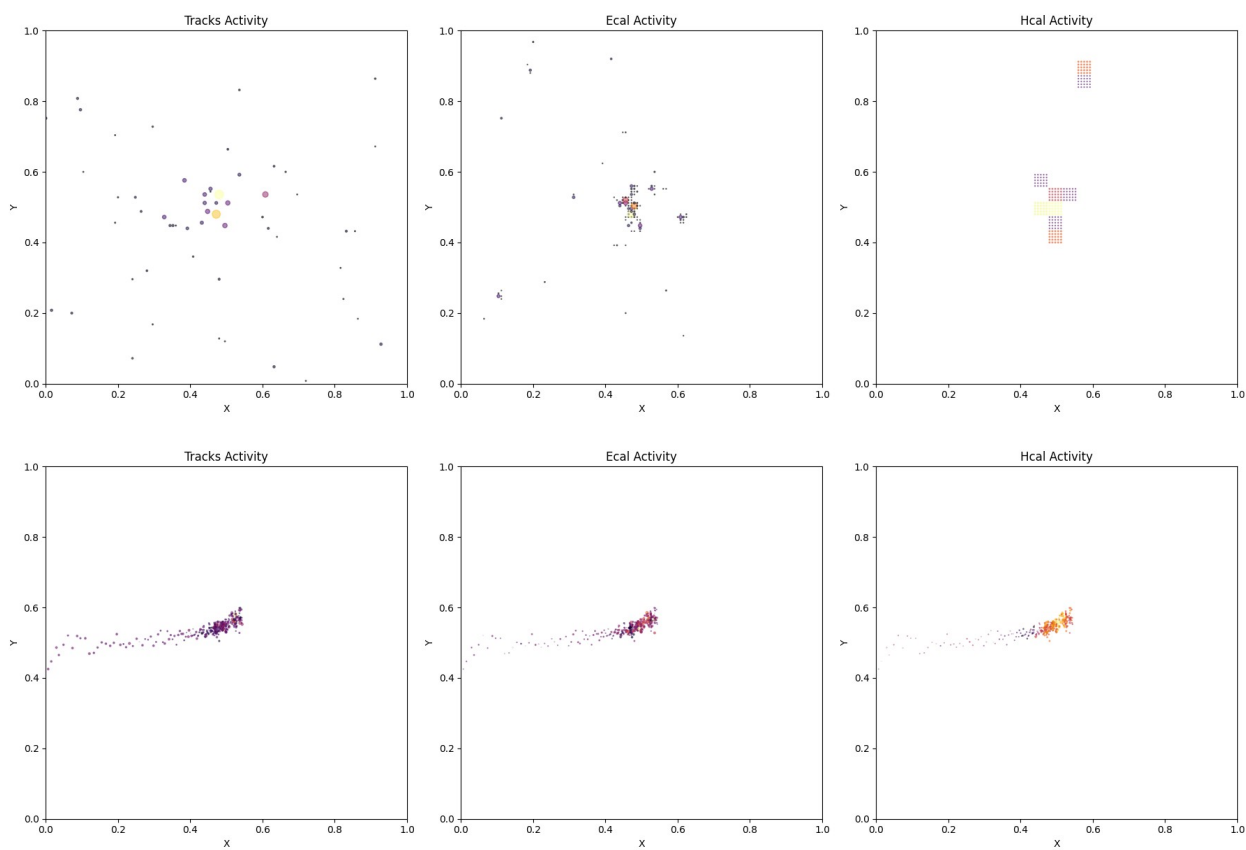
SSIM Score: 0.96088707447052





Inference: 75% | ██████████ | 3/4 [00:03<00:01, 1.00s/it]

SSIM Score: 0.9580322504043579



SSIM Score: 0.9638659358024597

Epoch : 20 Train Loss : 0.008736778385639455 Val Loss : 0.00918939197435975

Epoch : 21 Train Loss : 0.008692319047526452 Val Loss :
0.009900415199808776

Epoch : 22 Train Loss : 0.008650521112549686 Val Loss :
0.009183650487102568

Epoch : 23 Train Loss : 0.008670025537382699 Val Loss :
0.009176626452244818

Epoch : 24 Train Loss : 0.008634347900364474 Val Loss :
0.009426713455468416

Epoch : 25 Train Loss : 0.008688366285411121 Val Loss :
0.008845760952681303

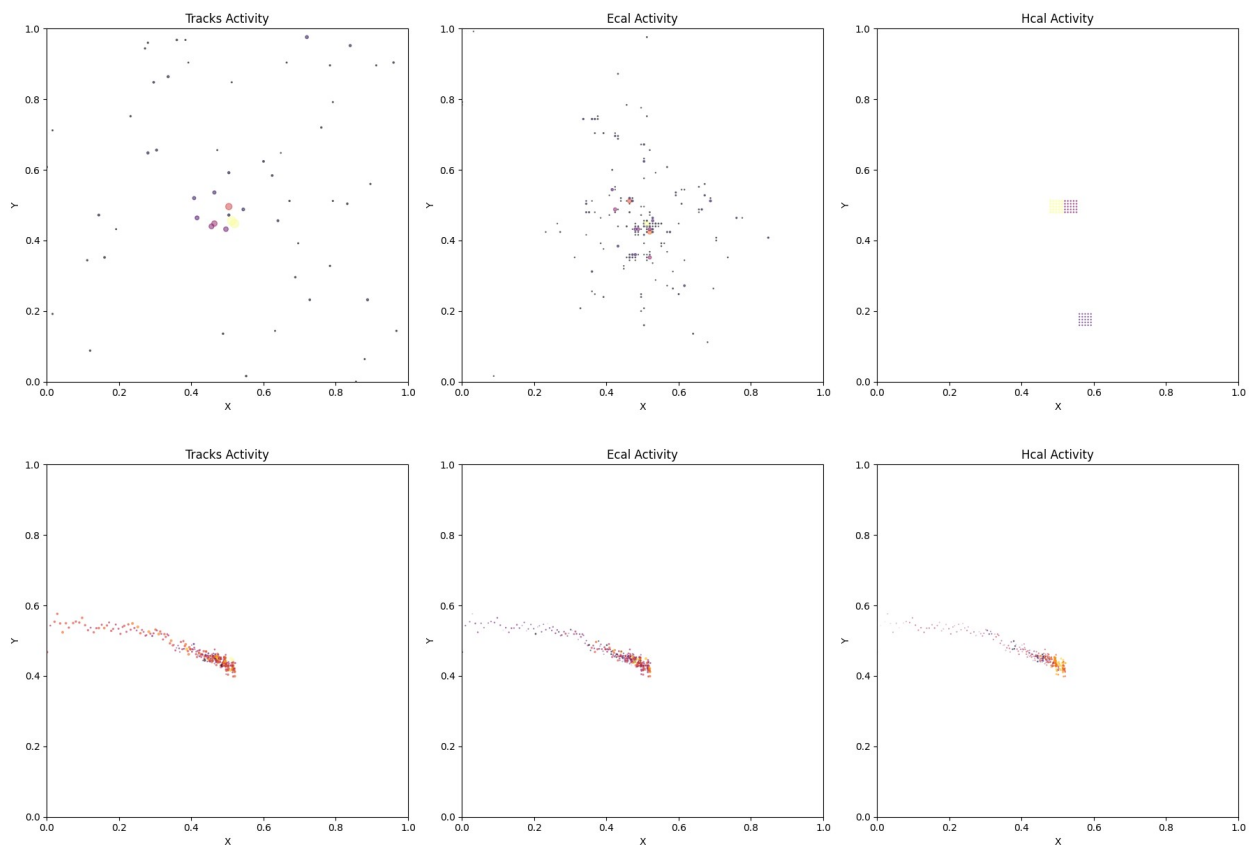
Epoch : 26 Train Loss : 0.008635075004410733 Val Loss :
0.008883912465535104

Epoch : 27 Train Loss : 0.008611272770719566 Val Loss :
0.00970402848906815

Epoch : 28 Train Loss : 0.008589943334109566 Val Loss :
0.010046445298939943

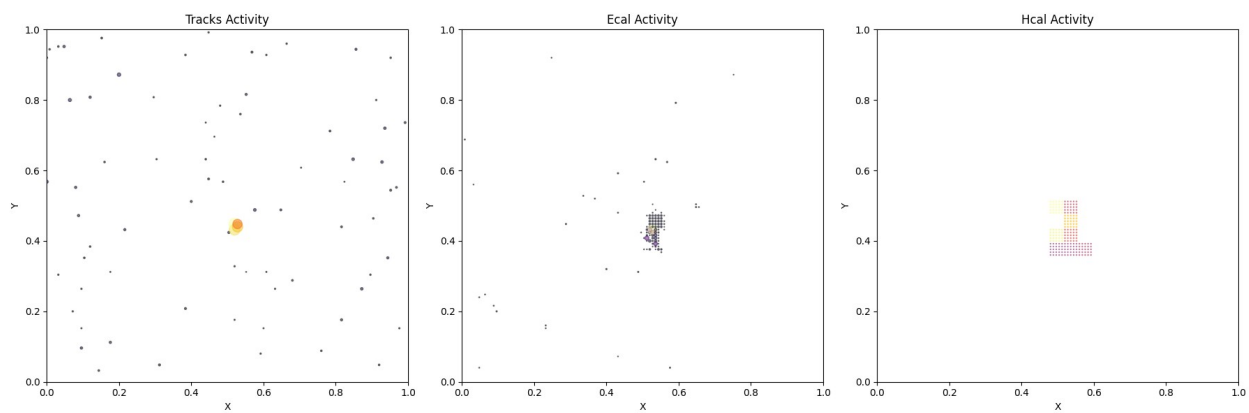
Epoch : 29 Train Loss : 0.008601670426384381 Val Loss :
0.008998936624266207

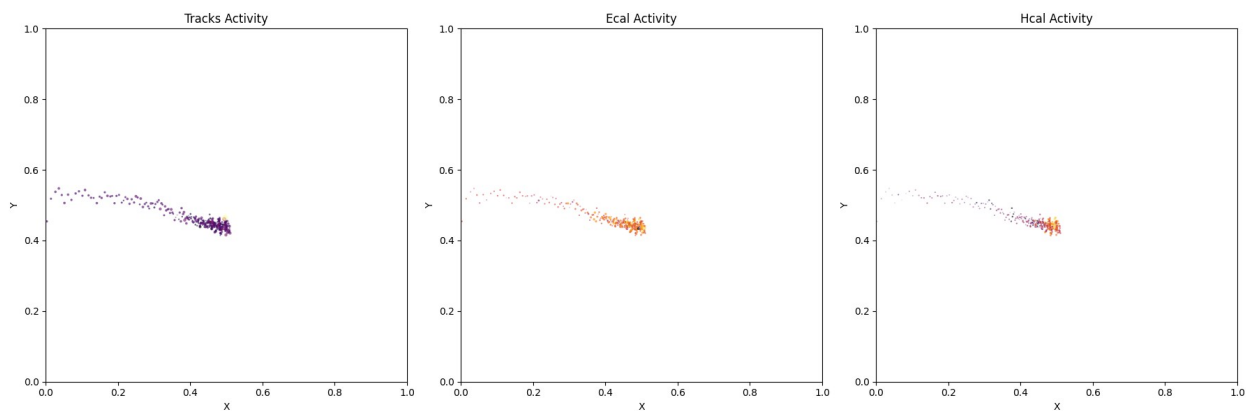
Inference: 0%| | 0/4 [00:00<?, ?it/s]



Inference: 25% | ██████████ | 1/4 [00:01<00:03, 1.03s/it]

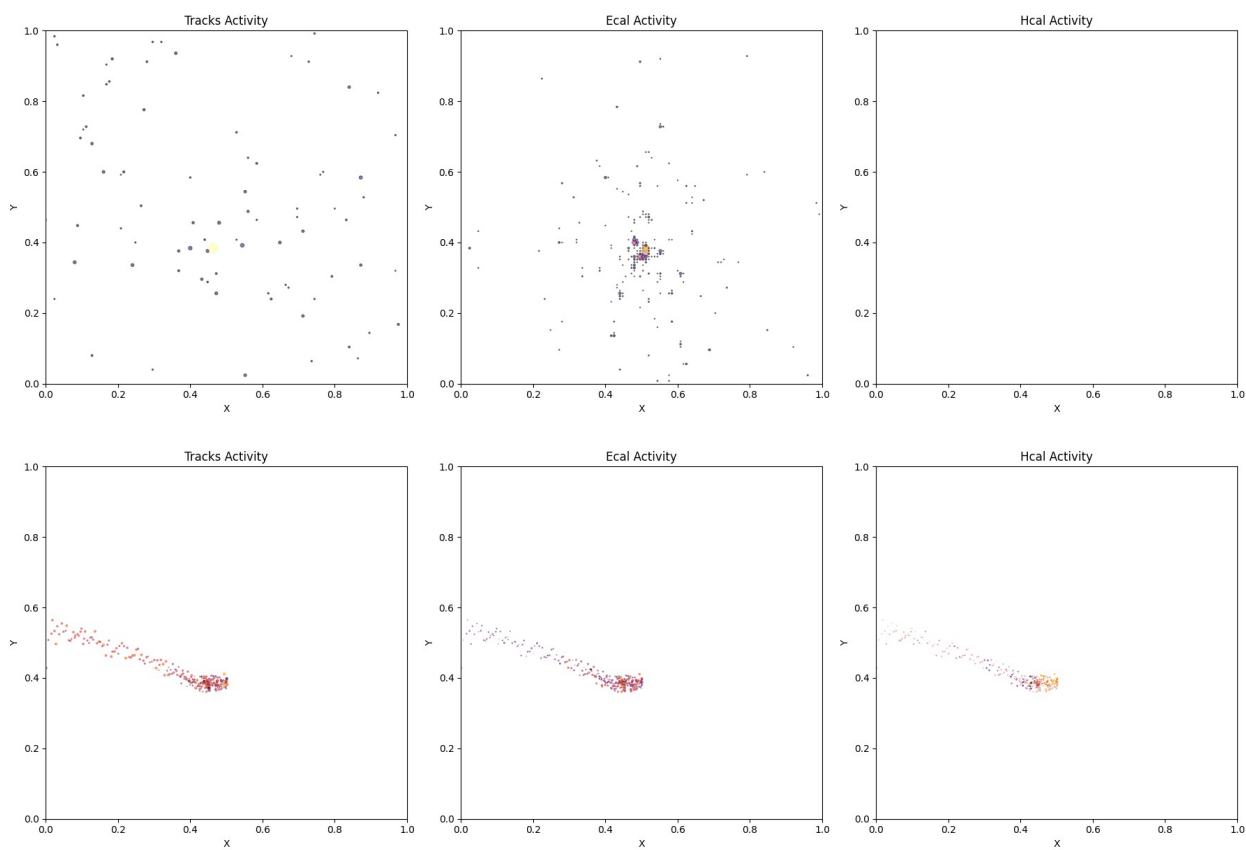
SSIM Score: 0.9595366716384888





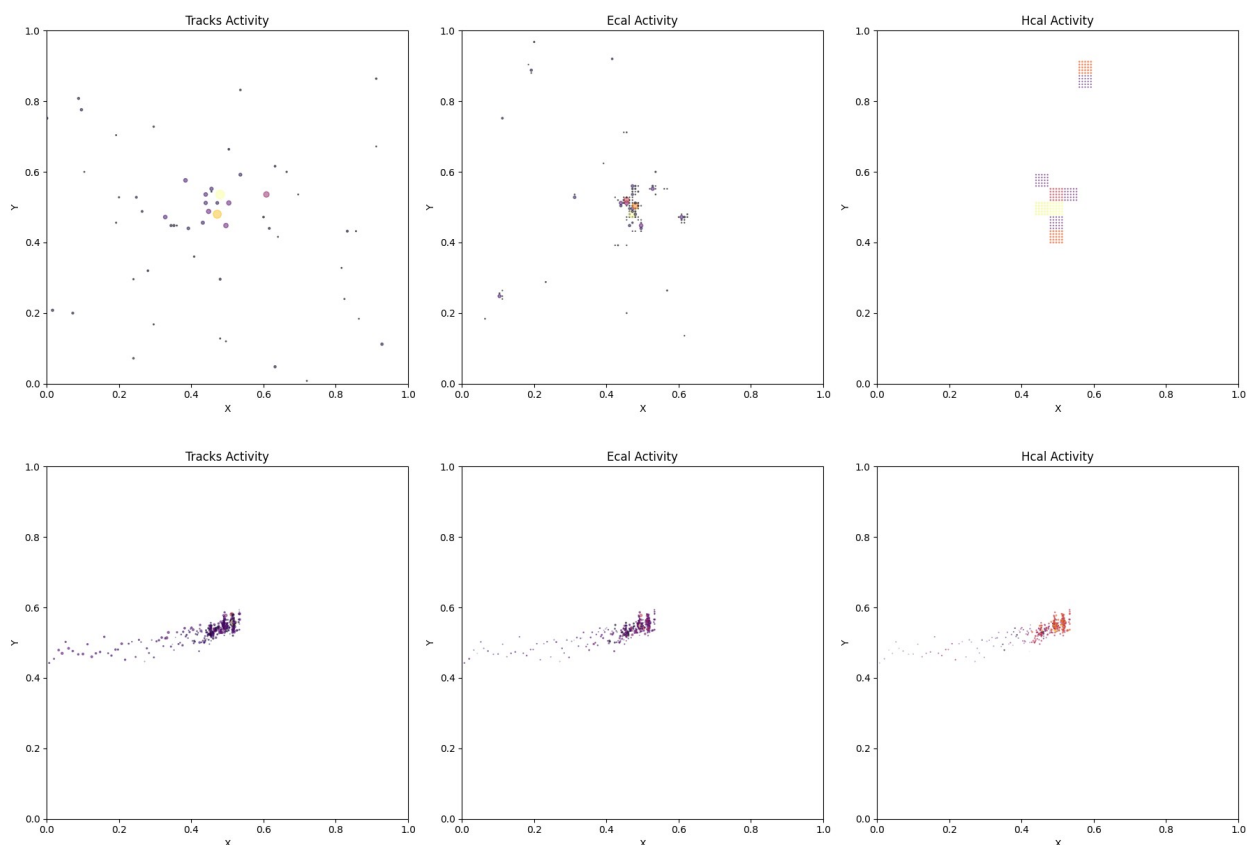
Inference: 50% | ████████ | 2/4 [00:02<00:02, 1.02s/it]

SSIM Score: 0.9767847657203674



Inference: 75% | ████████ | 3/4 [00:03<00:01, 1.02s/it]

SSIM Score: 0.9558960199356079



SSIM Score: 0.9662761092185974

Epoch : 30 Train Loss : 0.008628227656167893 Val Loss : 0.009777276078239083

Epoch : 31 Train Loss : 0.008558325271815274 Val Loss : 0.009466765564866364

Epoch : 32 Train Loss : 0.008548969789168286 Val Loss : 0.008939487277530134

Epoch : 33 Train Loss : 0.008526289833918028 Val Loss : 0.009354538982734084

Epoch : 34 Train Loss : 0.008546243548280763 Val Loss : 0.009495973004959524

Epoch : 35 Train Loss : 0.008523650654321983 Val Loss : 0.00925806793384254

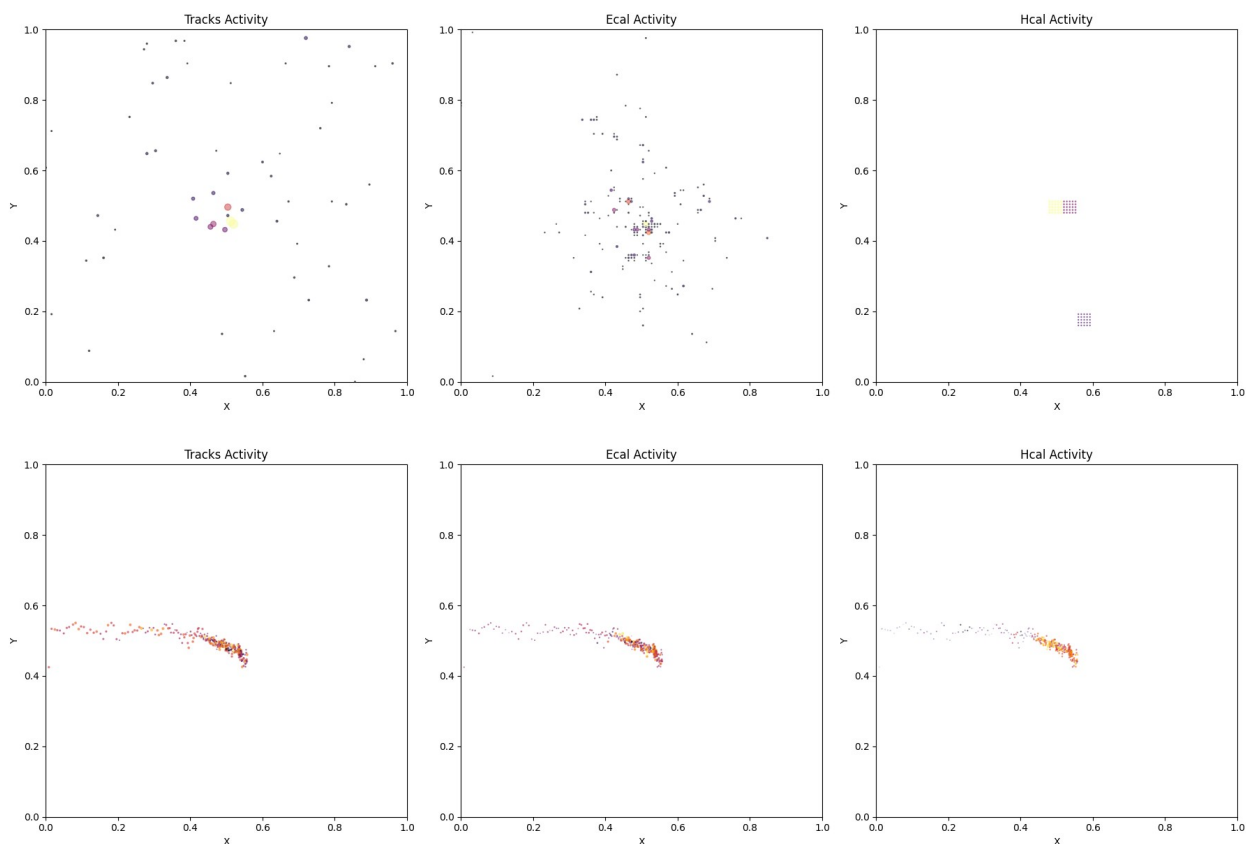
Epoch : 36 Train Loss : 0.008536117230781865 Val Loss : 0.010088531067594886

Epoch : 37 Train Loss : 0.008526687841154436 Val Loss : 0.00907885329797864

Epoch : 38 Train Loss : 0.008466630610000494 Val Loss : 0.008832145831547678

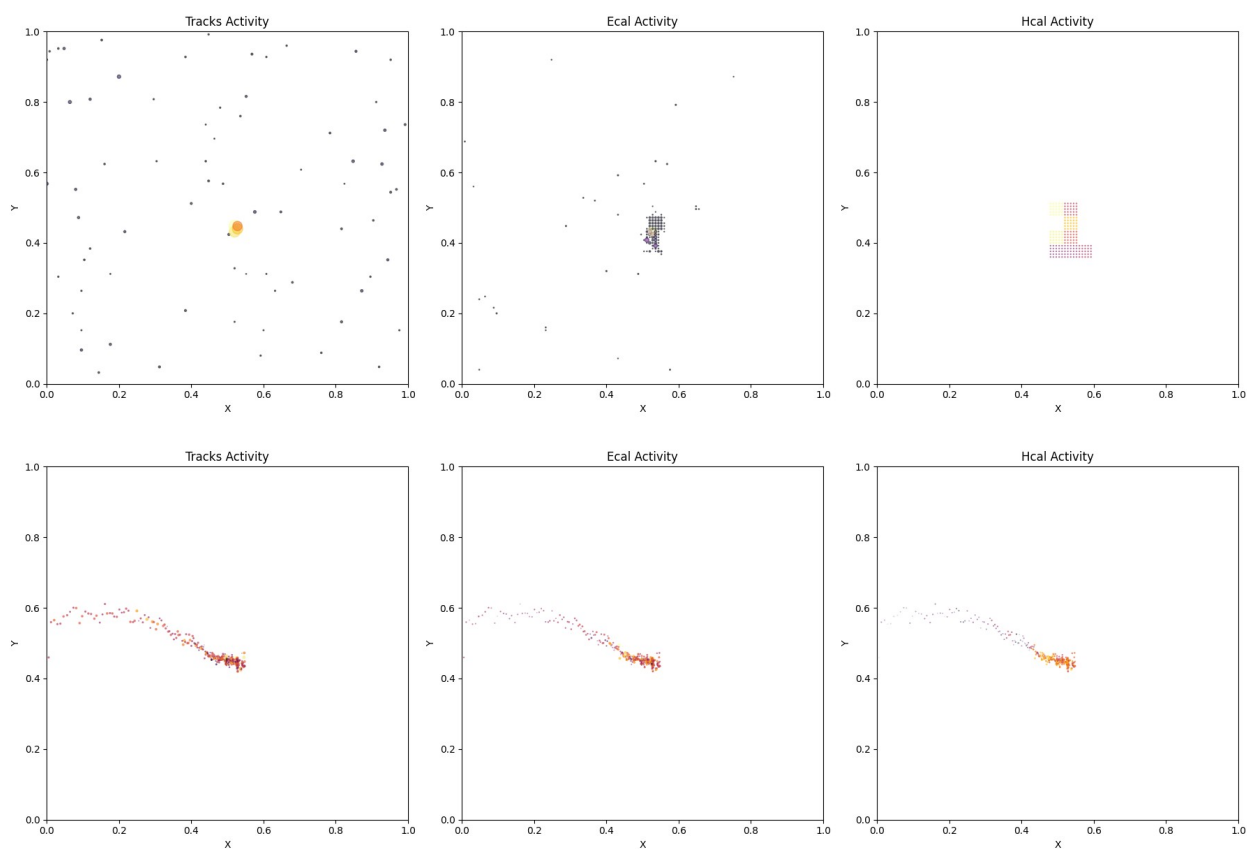
Epoch : 39 Train Loss : 0.008485055593095495 Val Loss : 0.00974288396537304

Inference: 0%| | 0/4 [00:00<?, ?it/s]



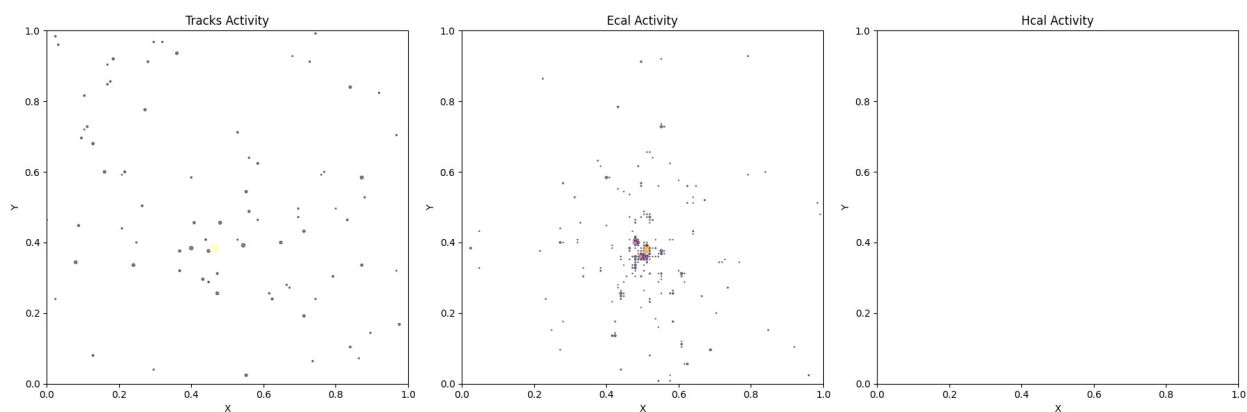
Inference: 25%|■ | 1/4 [00:01<00:03, 1.01s/it]

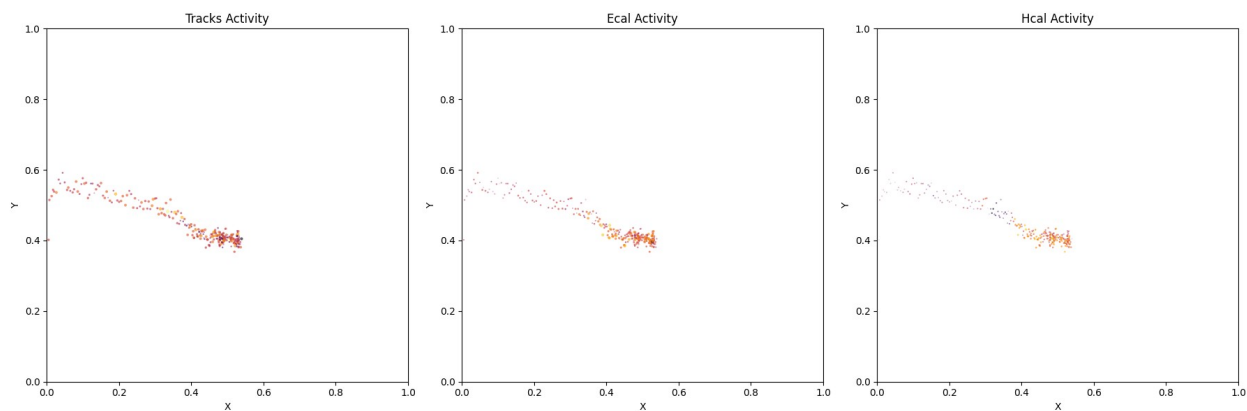
SSIM Score: 0.9556882381439209



Inference: 50% | ████████ | 2/4 [00:02<00:02, 1.03s/it]

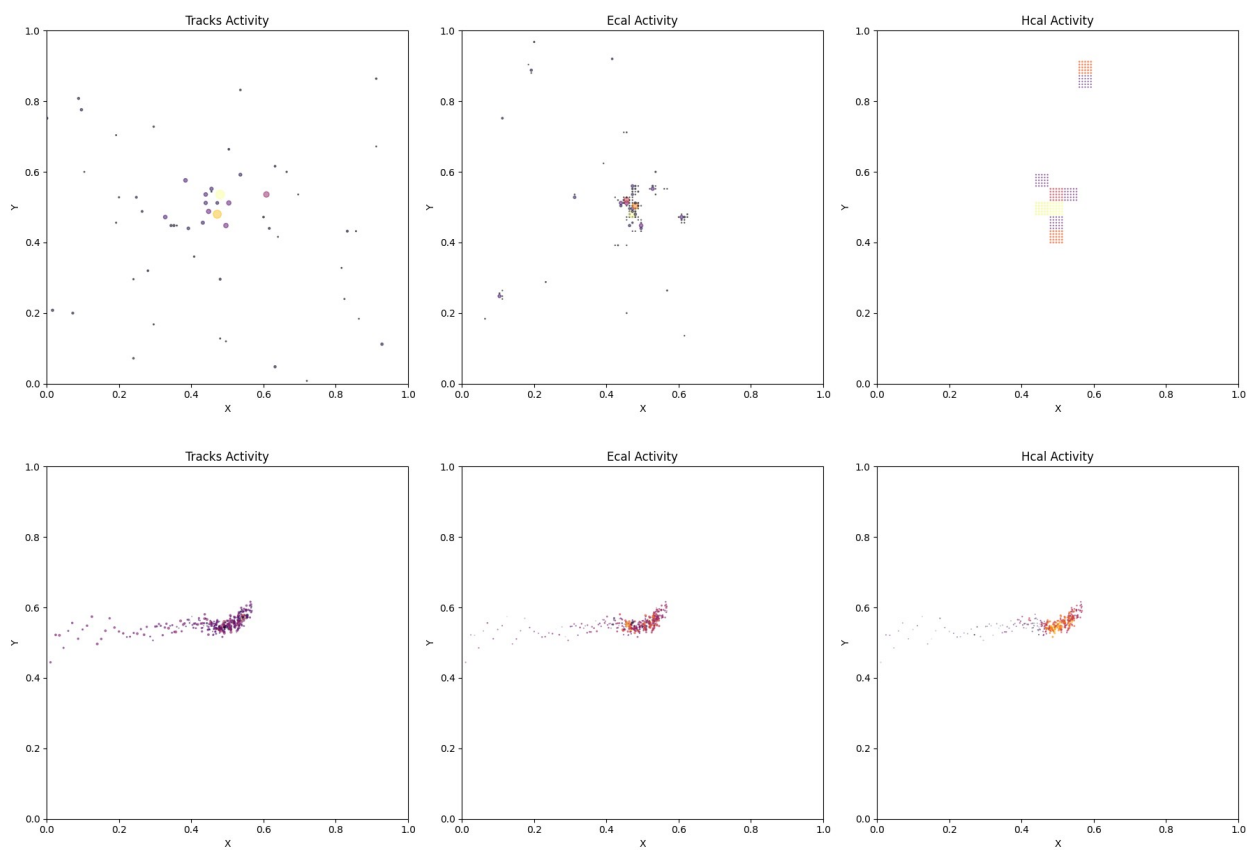
SSIM Score: 0.9610778093338013





Inference: 75% | ██████████ | 3/4 [00:03<00:01, 1.21s/it]

SSIM Score: 0.9533557295799255



SSIM Score: 0.9513310194015503

Epoch : 40 Train Loss : 0.0084461042174464 Val Loss : 0.009159923996776342

```
Epoch : 41 Train Loss : 0.008466531698745849 Val Loss :  
0.00942206708714366
```

```
Epoch : 42 Train Loss : 0.008449674049660325 Val Loss :  
0.009602669510059059
```

```
Epoch : 43 Train Loss : 0.008426422557626483 Val Loss :  
0.009184606606140733
```

```
Epoch : 44 Train Loss : 0.00840988868953359 Val Loss :  
0.00945672660600394
```

```
Epoch : 45 Train Loss : 0.008444719004145364 Val Loss :  
0.009671390289440751
```

```
Epoch : 46 Train Loss : 0.008448507139694151 Val Loss :  
0.009033823967911303
```

```
Training: 51%|██████████| 285/563 [00:06<00:06, 42.27it/s,  
loss=0.00944]
```

```
val_losses[-1] # previously recorded mse loss on validation set  
0.009607707150280476
```

```
# training and validation curves
```

```
epochs = np.arange(1, 51)  
plt.plot(epochs, train_losses, label="Training Loss", marker="o",  
linestyle="-")  
plt.plot(epochs, val_losses, label="Validation Loss", marker="o",  
linestyle="-")
```

```
plt.xlabel("Epochs")  
plt.ylabel("Loss")  
plt.title("Training vs Validation Loss")  
plt.legend()
```

```
# Show the plot  
plt.show()
```


Training vs Validation Loss

