```
import os
import pandas as pd
import numpy as np
import torch
from torch import nn
from torch.utils.data import Dataset
from torchvision.transforms import ToTensor
import matplotlib.pyplot as plt
from torch.utils.data import DataLoader, random_split
from torch.optim.lr_scheduler import LinearLR
import torchvision.transforms.functional as TF
from torch.nn import functional as F
from math import exp

# The hdf5 X_jets dataset was converted to a zip and used as a private
dataset on kaggle
class DeepFalconData(Dataset):
    def __init__(self, data_dir, transform=None, target_size=(128,
128)):
        self.data_dir = data_dir
        self.transform = transform
        self.target_size = target_size

    def __len__(self):
        return 10000 #len(os.listdir(self.data_dir))

    def __getitem__(self, idx):
        # resize and normalize each datapoint
        image = np.load(os.path.join(self.data_dir, f"{idx}.npy"))  #
(H, W, C)
        image = (image - image.min()) / (image.max() - image.min() +
1e-6)
        image = torch.tensor(image, dtype=torch.float32).permute(2, 0,
1)
        image = TF.resize(image, self.target_size, antialias=True)

        return image

batch_size = 128

dataset =
DeepFalconData(data_dir='/kaggle/input/task-1/content/sample_data/
deepfalcon_1/train_jets', transform=ToTensor())
train_len = int(len(dataset)*0.95)
train_set, test_set = random_split(dataset, [train_len, len(dataset)-
train_len])
train_dataloader = DataLoader(train_set, batch_size=batch_size,
shuffle=True)
test_dataloader = DataLoader(test_set,
batch_size=batch_size,shuffle=True)
```

```python
# Save directly to Kaggle's output folder
CHECKPOINT_DIR = "/kaggle/working"
os.makedirs(CHECKPOINT_DIR, exist_ok=True)

def save_checkpoint(model, optimizer, epoch,
filename="vae_checkpoint.pth"):
    checkpoint = {
        "epoch": epoch,
        "model_state_dict": model.state_dict(),
        "optimizer_state_dict": optimizer.state_dict(),
    }
    filepath = os.path.join(CHECKPOINT_DIR, filename)
    torch.save(checkpoint, filepath)
    print(f"Checkpoint saved at {filepath}")

# Adapted from the AntixK/PyTorch-VAE project on github

class VAE(nn.Module):

  def __init__(self, input_channels : int, latent_dim : int,
hidden_dims = [32, 64, 128, 256]):
    super(VAE, self).__init__()
    self.input_channels = input_channels
    self.latent_dim = latent_dim
    self.hidden_dims = hidden_dims
    modules = []
    for h_dim in self.hidden_dims:
      modules.append(
                nn.Sequential(
                    nn.Conv2d(input_channels, out_channels=h_dim,
                              kernel_size= 3, stride= 2, padding  =
1),
                    nn.BatchNorm2d(h_dim),
                    nn.LeakyReLU())
            )
      input_channels = h_dim
    self.encoder = nn.Sequential(*modules)
    self.mean = nn.Linear(hidden_dims[-1]*64, latent_dim)
    self.log_var = nn.Linear(hidden_dims[-1]*64, latent_dim)

    modules = []

    self.decoder_input = nn.Linear(latent_dim, hidden_dims[-1]*64)
    hidden_dims.reverse()

    for i in range(len(hidden_dims) - 1):
      modules.append(
                nn.Sequential(
                    nn.ConvTranspose2d(hidden_dims[i],
                                       hidden_dims[i + 1],
```

```
                                        kernel_size=3,
                                        stride = 2,
                                        padding=1,
                                        output_padding=1),
                        nn.BatchNorm2d(hidden_dims[i + 1]),
                        nn.LeakyReLU())
                )
        self.decoder = nn.Sequential(*modules)

        self.final_layer = nn.Sequential(
                            nn.ConvTranspose2d(hidden_dims[-1],
                                               hidden_dims[-1],
                                               kernel_size=3,
                                               stride=2,
                                               padding=1,
                                               output_padding=1),
                            nn.BatchNorm2d(hidden_dims[-1]),
                            nn.LeakyReLU(),
                            nn.Conv2d(hidden_dims[-1], out_channels= 3,
                                      kernel_size= 3, padding= 1)
                            )

    def encode(self, x):

        x = self.encoder(x)
        x = torch.flatten(x, start_dim=1)
        mean = self.mean(x)
        log_var = self.log_var(x)

        return mean, log_var

    def decode(self, x):

        x = self.decoder_input(x)
        x = x.view(-1, self.hidden_dims[0], 8, 8)
        x = self.decoder(x)
        x = self.final_layer(x)

        return x

    def reparameterize(self, mean, log_var):

        std = torch.exp(0.5 * log_var)
        eps = torch.randn_like(std)
        return eps * std + mean

    def forward(self, x):

        mean, log_var = self.encode(x)
        z = self.reparameterize(mean, log_var)
```

```
    x_reconst = self.decode(z)

    return x_reconst, mean, log_var

# The MSSIM loss can be used as component of the reconstruction loss
class MSSIM(nn.Module):

    def __init__(self,
                 in_channels: int = 3,
                 window_size: int=11,
                 size_average:bool = True) -> None:
        """
        Computes the differentiable MS-SSIM loss
        Reference:
        [1]
https://github.com/jorge-pessoa/pytorch-msssim/blob/dev/pytorch_msssim
/__init__.py
            (MIT License)

        :param in_channels: (Int)
        :param window_size: (Int)
        :param size_average: (Bool)
        """
        super(MSSIM, self).__init__()
        self.in_channels = in_channels
        self.window_size = window_size
        self.size_average = size_average

    def gaussian_window(self, window_size:int, sigma: float) ->
torch.Tensor:
        kernel = torch.tensor([exp((x - window_size // 2)**2/(2 *
sigma ** 2))
                               for x in range(window_size)])
        return kernel/kernel.sum()

    def create_window(self, window_size, in_channels):
        _1D_window = self.gaussian_window(window_size,
1.5).unsqueeze(1)
        _2D_window =
_1D_window.mm(_1D_window.t()).float().unsqueeze(0).unsqueeze(0)
        window = _2D_window.expand(in_channels, 1, window_size,
window_size).contiguous()
        return window

    def ssim(self,
             img1: torch.Tensor,
             img2: torch.Tensor,
             window_size: int,
             in_channel: int,
             size_average: bool) -> torch.Tensor:
```

```
        device = img1.device
        window = self.create_window(window_size,
in_channel).to(device)
        mu1 = F.conv2d(img1, window, padding= window_size//2,
groups=in_channel)
        mu2 = F.conv2d(img2, window, padding= window_size//2,
groups=in_channel)

        mu1_sq = mu1.pow(2)
        mu2_sq = mu2.pow(2)
        mu1_mu2 = mu1 * mu2

        sigma1_sq = F.conv2d(img1 * img1, window, padding =
window_size//2, groups=in_channel) - mu1_sq
        sigma2_sq = F.conv2d(img2 * img2, window, padding =
window_size//2, groups=in_channel) - mu2_sq
        sigma12   = F.conv2d(img1 * img2, window, padding =
window_size//2, groups=in_channel) - mu1_mu2

        img_range = 1.0 #img1.max() - img1.min() # Dynamic range
        C1 = (0.01 * img_range) ** 2
        C2 = (0.03 * img_range) ** 2

        v1 = 2.0 * sigma12 + C2
        v2 = sigma1_sq + sigma2_sq + C2
        cs = torch.mean(v1 / v2)  # contrast sensitivity

        ssim_map = ((2 * mu1_mu2 + C1) * v1) / ((mu1_sq + mu2_sq + C1)
* v2)

        if size_average:
            ret = ssim_map.mean()
        else:
            ret = ssim_map.mean(1).mean(1).mean(1)
        return ret, cs

    def forward(self, img1: torch.Tensor, img2: torch.Tensor) ->
torch.Tensor:
        device = img1.device
        weights = torch.FloatTensor([0.0448, 0.2856, 0.3001, 0.2363,
0.1333]).to(device)
        levels = weights.size()[0]
        mssim = []
        mcs = []

        for _ in range(levels):
            sim, cs = self.ssim(img1, img2,
                                self.window_size,
                                self.in_channels,
```

```
                                self.size_average)
            mssim.append(sim)
            mcs.append(cs)

            img1 = F.avg_pool2d(img1, (2, 2))
            img2 = F.avg_pool2d(img2, (2, 2))

        mssim = torch.stack(mssim)
        mcs = torch.stack(mcs)

        # # Normalize (to avoid NaNs during training unstable models, 
not compliant with original definition)
        # if normalize:
        #     mssim = (mssim + 1) / 2
        #     mcs = (mcs + 1) / 2

        pow1 = mcs ** weights
        pow2 = mssim ** weights

        output = torch.prod(pow1[:-1] * pow2[-1])
        return 1 - output

# Since each datapoint has more zeros than non-zero values a weighetd 
mse is taken applying higher weigtages to non-zero values

def weighted_mse(x_recon, x_true):

    mask_1 = (x_true > 0) * 1.
    mask_2 = (x_true == 0) * 1.
    #num of 1's
    num_pos = mask_1.sum(dim=(-1, -2, -3))
    #num of 0's
    num_neg = mask_2.sum(dim=(-1, -2, -3))
    weight_1 = num_neg / (num_pos + 1e-6)
    #weight_2 = num_pos / (num_neg + 1e-6)
    mask_1 *= weight_1[:,None,None,None]
    #mask_2 *= weight_2[:,None,None,None]
    weights = mask_2 * 6 + mask_1
    weights = weights.to(x_recon.device)
    mse = nn.MSELoss(reduction='none')(x_recon, x_true)
    weighted_mse = torch.sum((weights * mse))
    return weighted_mse

# The final beta loss of the VAE
def beta_loss(x_recon, x_true, log_var, mean, beta, epoch):

  recon_loss = weighted_mse(x_recon, x_true)
  kld = torch.mean(-0.5 * torch.sum(1 + log_var - mean ** 2 - 
log_var.exp(), dim = 1), dim = 0)
  return beta * kld  + recon_loss , recon_loss, kld
```

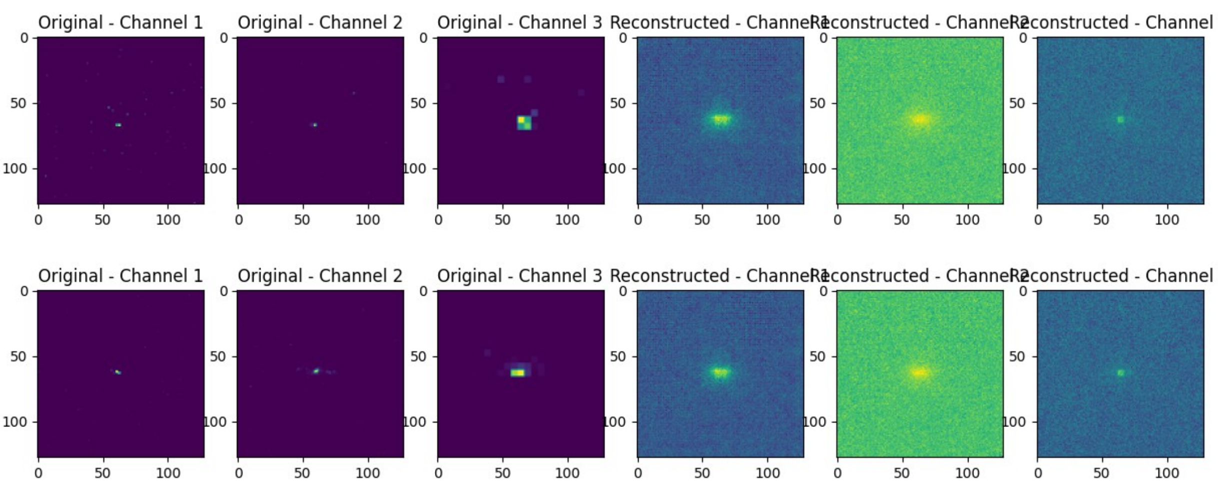
```python
# A scheduler for the beta value in beta loss function(importance of
KL Divergence term).
def kl_linear_anneal(step, total_steps):
    return min(1.0, step * 2 / (total_steps))

import torch
from torch.nn.parallel import DataParallel

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
VAE_model = VAE(3, 128).to(device)
VAE_model = DataParallel(VAE_model)
optimizer = torch.optim.Adam(VAE_model.parameters(), lr=1e-4)

from tqdm import tqdm
import torch
import matplotlib.pyplot as plt

def train_vae(VAE_model, train_dataloader, test_dataloader, optimizer,
device, epochs=20):
    beta = 0
    for epoch in range(epochs):
        epoch_loss, epoch_recon_loss, epoch_kld = 0, 0, 0

        beta = 1
        progress_bar = tqdm(train_dataloader, desc=f"Epoch
{epoch+1}/{epochs}", leave=True)

        for batch_idx, batch in enumerate(progress_bar):
            batch = batch.to(device)
            optimizer.zero_grad()

            # Forward pass
            x_recon, mean, log_var = VAE_model(batch)
            loss, recon_loss, kld= beta_loss(x_recon, batch, log_var,
mean, beta, epoch)

            loss.backward()
            optimizer.step()

            epoch_loss += loss.item()
            epoch_recon_loss += recon_loss.item()
            epoch_kld += kld.item()

            # Update progress bar
            progress_bar.set_postfix(loss=f"{loss.item():.4f}",
recon=f"{recon_loss.item():.4f}", kld=f"{kld.item():.4f}")
            #if batch_idx % 1000 == 0:
            #   validate_vae(VAE_model, test_dataloader, beta_loss,
device, epoch+1)
```

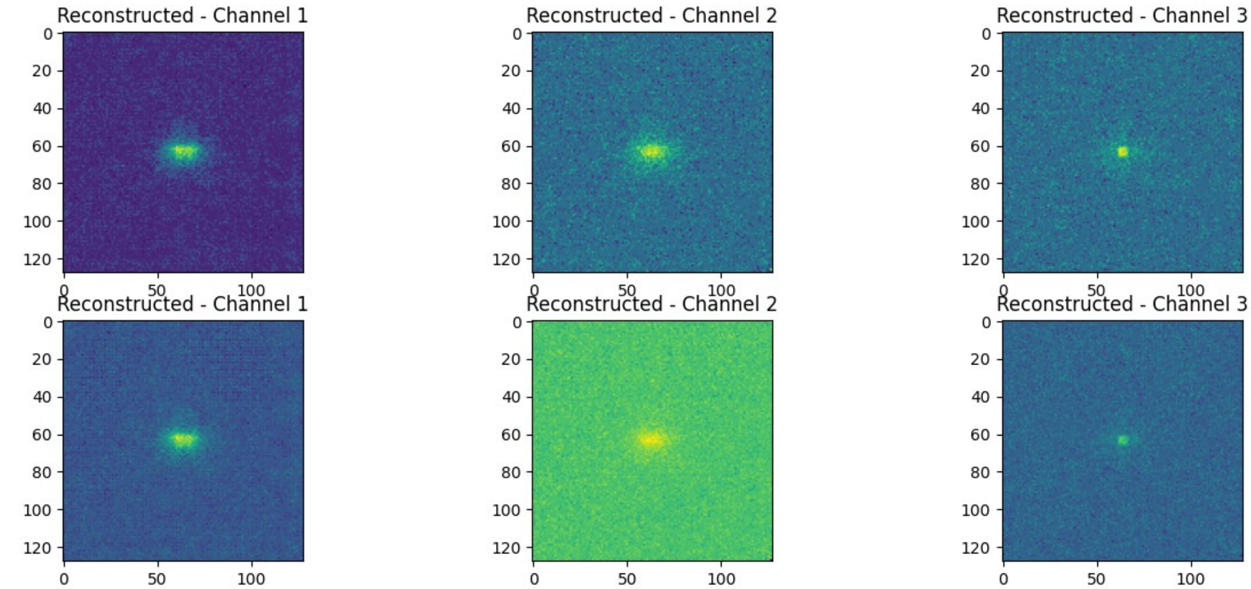
```
        # Print final epoch loss

        print(f"Epoch {epoch+1} | Loss:
{epoch_loss/len(train_dataloader):.6f} | "
              f"Recon Loss:
{epoch_recon_loss/len(train_dataloader):.6f} | "
              f"KLD: {epoch_kld/len(train_dataloader):.6f}")

        # Validation & Visualization
        if (epoch + 1) % 20 == 0:  # Run validation every 20 epochs
            validate_vae(VAE_model, test_dataloader, beta_loss,
device, epoch+1)
            save_checkpoint(VAE_model, optimizer, epoch,
filename="vae_checkpoint_" + str(epoch) + ".pth")

def validate_vae(VAE_model, test_dataloader, beta_loss, device,
epoch):

    VAE_model.eval()
    with torch.no_grad():
        for batch_idx, test_batch in enumerate(test_dataloader):
            test_batch = test_batch.to(device)
            x_recon, mean, log_var = VAE_model(test_batch)
            loss, recon_loss, kld = beta_loss(x_recon, test_batch,
log_var, mean, 1, epoch - 1)  # Use beta=1 for test

            print(f"Test Epoch {epoch} | Loss: {loss:.6f} | Recon
Loss: {recon_loss:.6f} | KLD: {kld:.6f}")

            visualize_reconstructions(test_batch, x_recon,
num_samples=2)
            if batch_idx % 5:
                break  # Only visualize once per epoch

def visualize_reconstructions(originals, reconstructions,
num_samples=4):

    num_samples = min(num_samples, originals.shape[0])
    fig, axes = plt.subplots(num_samples, 6, figsize=(15, 3 *
num_samples))

    for idx in range(num_samples):
        original = originals[idx].cpu().numpy()
        reconstructed = reconstructions[idx].cpu().numpy()

        for c in range(3):  # Loop over 3 channels
            axes[idx, c].imshow(original[c, :, :])
            axes[idx, c].set_title(f"Original - Channel {c+1}")

            axes[idx, c + 3].imshow(reconstructed[c, :, :])
```

```
            axes[idx, c + 3].set_title(f"Reconstructed - Channel
{c+1}")

    plt.show()
    fig, axes = plt.subplots(num_samples, 3, figsize=(15, 3 *
num_samples))
    for idx in range(num_samples):
        recon_mask = (reconstructed[idx] >= 0)
        reconstructed = (reconstructions[idx].cpu().numpy() *
recon_mask)

        for c in range(3):
            axes[idx, c].imshow(reconstructed[c, :, :])
            axes[idx, c].set_title(f"Reconstructed - Channel {c+1}")
    plt.show()

train_vae(VAE_model, train_dataloader, test_dataloader, optimizer,
device, 30)

Epoch 1/30: 100%|██████████| 75/75 [01:03<00:00,  1.19it/s,
kld=86.8830, loss=13084.6250, recon=12997.7422]

Epoch 1 | Loss: 677972.511458 | Recon Loss: 677921.643177 | KLD:
50.864881

Epoch 2/30: 100%|██████████| 75/75 [01:03<00:00,  1.17it/s,
kld=220.0556, loss=4851.8154, recon=4631.7598]

Epoch 2 | Loss: 34545.548242 | Recon Loss: 34388.336458 | KLD:
157.211751

Epoch 3/30: 100%|██████████| 75/75 [01:03<00:00,  1.17it/s,
kld=330.8916, loss=3385.2737, recon=3054.3821]

Epoch 3 | Loss: 16854.314443 | Recon Loss: 16584.847217 | KLD:
269.467170

Epoch 4/30: 100%|██████████| 75/75 [01:06<00:00,  1.12it/s,
kld=372.3990, loss=2851.5056, recon=2479.1067]

Epoch 4 | Loss: 11893.713786 | Recon Loss: 11554.699730 | KLD:
339.014016

Epoch 5/30: 100%|██████████| 75/75 [01:06<00:00,  1.13it/s,
kld=401.5809, loss=2371.6497, recon=1970.0687]

Epoch 5 | Loss: 9730.882673 | Recon Loss: 9352.590396 | KLD:
378.292318

Epoch 6/30: 100%|██████████| 75/75 [01:04<00:00,  1.17it/s,
kld=415.3592, loss=2062.1216, recon=1646.7625]
```

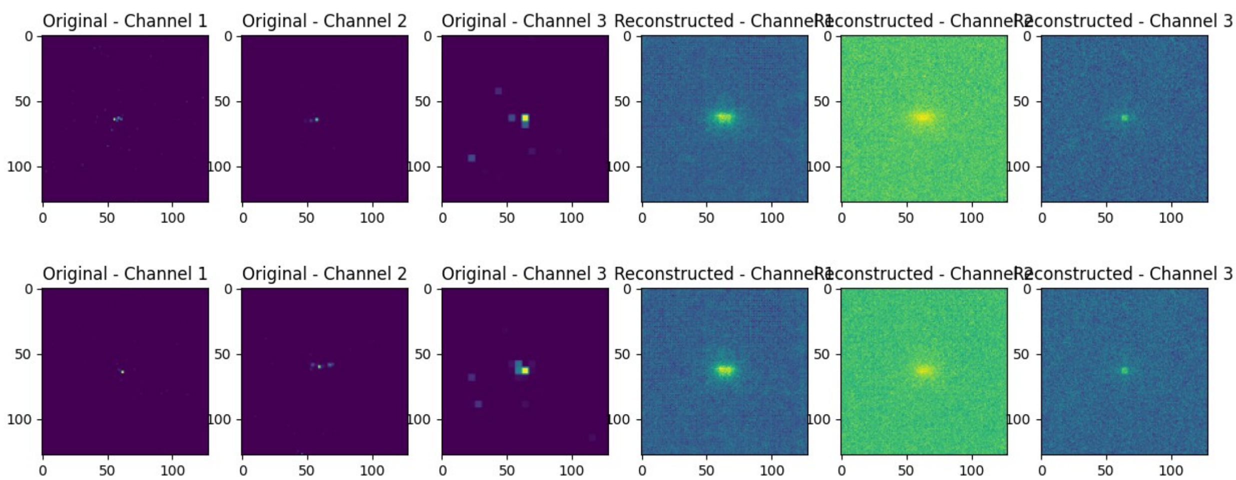
```
Epoch 6 | Loss: 8529.925273 | Recon Loss: 8131.606097 | KLD:
398.319201

Epoch 7/30: 100%|██████████| 75/75 [01:06<00:00,  1.12it/s,
kld=429.5005, loss=1921.1718, recon=1491.6713]

Epoch 7 | Loss: 7776.002889 | Recon Loss: 7370.327205 | KLD:
405.675678

Epoch 8/30: 100%|██████████| 75/75 [01:07<00:00,  1.12it/s,
kld=376.3639, loss=1874.4401, recon=1498.0762]

Epoch 8 | Loss: 7253.849657 | Recon Loss: 6850.335775 | KLD:
403.513835

Epoch 9/30: 100%|██████████| 75/75 [01:07<00:00,  1.11it/s,
kld=366.5142, loss=1648.3535, recon=1281.8394]

Epoch 9 | Loss: 6875.050605 | Recon Loss: 6480.692585 | KLD:
394.358018

Epoch 10/30: 100%|██████████| 75/75 [01:06<00:00,  1.12it/s,
kld=387.0118, loss=1610.7422, recon=1223.7303]

Epoch 10 | Loss: 6581.122318 | Recon Loss: 6198.496170 | KLD:
382.626160

Epoch 11/30: 100%|██████████| 75/75 [01:06<00:00,  1.12it/s,
kld=378.9091, loss=1604.4540, recon=1225.5449]

Epoch 11 | Loss: 6350.015773 | Recon Loss: 5980.538698 | KLD:
369.477074

Epoch 12/30: 100%|██████████| 75/75 [01:07<00:00,  1.11it/s,
kld=340.2052, loss=1562.5232, recon=1222.3180]

Epoch 12 | Loss: 6163.259919 | Recon Loss: 5807.463953 | KLD:
355.795979

Epoch 13/30: 100%|██████████| 75/75 [01:07<00:00,  1.11it/s,
kld=333.7917, loss=1703.4690, recon=1369.6772]

Epoch 13 | Loss: 6024.088857 | Recon Loss: 5681.100417 | KLD:
342.988438

Epoch 14/30: 100%|██████████| 75/75 [01:06<00:00,  1.12it/s,
kld=332.6232, loss=1360.7893, recon=1028.1660]

Epoch 14 | Loss: 5893.695264 | Recon Loss: 5563.078841 | KLD:
330.616444

Epoch 15/30: 100%|██████████| 75/75 [01:06<00:00,  1.12it/s,
kld=321.5007, loss=1356.3264, recon=1034.8257]
```

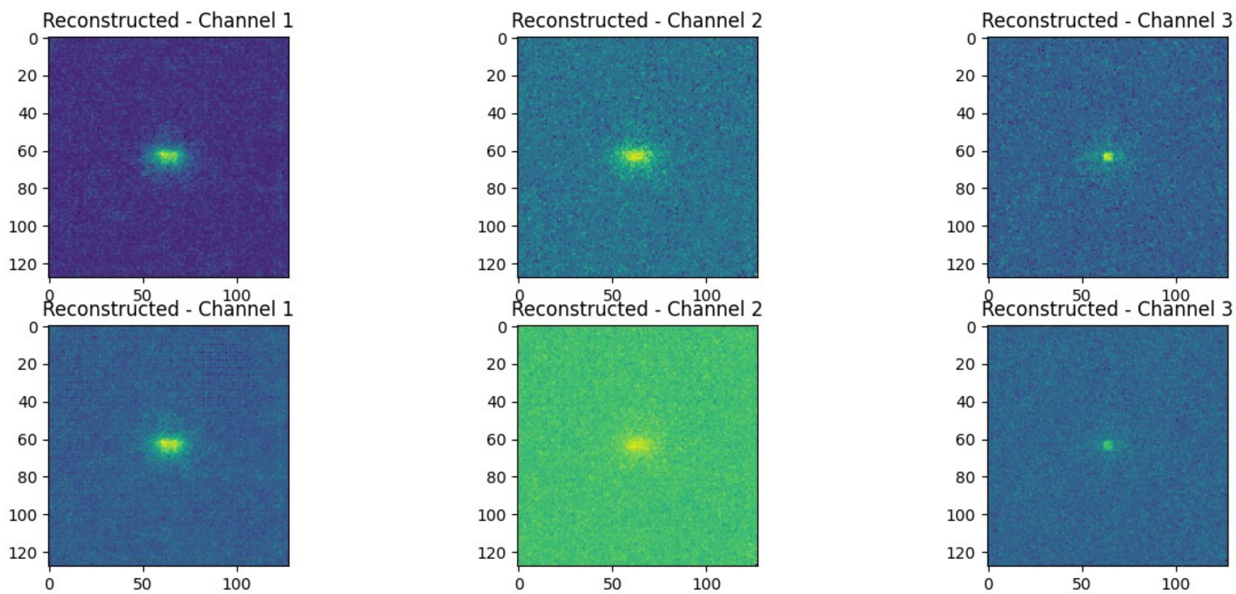
```
Epoch 15 | Loss: 5770.854867 | Recon Loss: 5450.903542 | KLD:
319.951326

Epoch 16/30: 100%|██████████| 75/75 [01:06<00:00,  1.12it/s,
kld=301.6525, loss=1585.0811, recon=1283.4286]

Epoch 16 | Loss: 5808.187272 | Recon Loss: 5499.451216 | KLD:
308.736051

Epoch 17/30: 100%|██████████| 75/75 [01:07<00:00,  1.12it/s,
kld=299.8183, loss=1425.1589, recon=1125.3407]

Epoch 17 | Loss: 5590.218760 | Recon Loss: 5291.134966 | KLD:
299.083805

Epoch 18/30: 100%|██████████| 75/75 [01:04<00:00,  1.17it/s,
kld=281.6223, loss=1429.9723, recon=1148.3500]

Epoch 18 | Loss: 5521.294305 | Recon Loss: 5230.971724 | KLD:
290.322577

Epoch 19/30: 100%|██████████| 75/75 [01:06<00:00,  1.12it/s,
kld=288.0353, loss=1579.7979, recon=1291.7626]

Epoch 19 | Loss: 5519.361289 | Recon Loss: 5237.259842 | KLD:
282.101462

Epoch 20/30: 100%|██████████| 75/75 [01:05<00:00,  1.14it/s,
kld=278.6947, loss=1684.0602, recon=1405.3655]

Epoch 20 | Loss: 5523.024604 | Recon Loss: 5248.375908 | KLD:
274.648687
Test Epoch 20 | Loss: 5277.204590 | Recon Loss: 5000.579590 | KLD:
276.625000
```






```
Test Epoch 20 | Loss: 5413.136719 | Recon Loss: 5132.890625 | KLD:
280.246246
```






```
Checkpoint saved at /kaggle/working/vae_checkpoint_19.pth

Epoch 21/30: 100%|██████████| 75/75 [01:03<00:00,  1.19it/s,
kld=191.2528, loss=1153.2883, recon=962.0355]

Epoch 21 | Loss: 6978.941624 | Recon Loss: 6846.048156 | KLD:
132.893443

Epoch 22/30: 100%|██████████| 75/75 [01:04<00:00,  1.16it/s,
kld=188.1440, loss=1314.8903, recon=1126.7463]

Epoch 22 | Loss: 5318.010907 | Recon Loss: 5131.623031 | KLD:
186.387889

Epoch 23/30: 100%|██████████| 75/75 [01:04<00:00,  1.16it/s,
kld=186.4108, loss=1271.9342, recon=1085.5234]

Epoch 23 | Loss: 5254.933791 | Recon Loss: 5068.151445 | KLD:
186.782357

Epoch 24/30: 100%|██████████| 75/75 [01:05<00:00,  1.15it/s,
kld=188.7219, loss=1251.7346, recon=1063.0127]

Epoch 24 | Loss: 5193.780251 | Recon Loss: 5006.651029 | KLD:
187.129210

Epoch 25/30: 100%|██████████| 75/75 [01:04<00:00,  1.16it/s,
kld=189.0706, loss=1201.8368, recon=1012.7662]

Epoch 25 | Loss: 5132.230799 | Recon Loss: 4943.960470 | KLD:
188.270334
```

```
Epoch 26/30: 100%|██████████| 75/75 [01:05<00:00,  1.14it/s,
kld=194.3466, loss=1574.5913, recon=1380.2446]

Epoch 26 | Loss: 5067.345046 | Recon Loss: 4878.040007 | KLD:
189.305033

Epoch 27/30: 100%|██████████| 75/75 [01:05<00:00,  1.15it/s,
kld=193.7865, loss=1317.9596, recon=1124.1731]

Epoch 27 | Loss: 5003.637521 | Recon Loss: 4813.303337 | KLD:
190.334196

Epoch 28/30: 100%|██████████| 75/75 [01:05<00:00,  1.15it/s,
kld=197.0150, loss=1215.5846, recon=1018.5696]

Epoch 28 | Loss: 4936.699292 | Recon Loss: 4745.251911 | KLD:
191.447388

Epoch 29/30: 100%|██████████| 75/75 [01:04<00:00,  1.16it/s,
kld=194.2686, loss=1045.3383, recon=851.0696]

Epoch 29 | Loss: 4870.583914 | Recon Loss: 4678.470745 | KLD:
192.113186

Epoch 30/30: 100%|██████████| 75/75 [01:05<00:00,  1.15it/s,
kld=191.8362, loss=1200.4978, recon=1008.6616]

Epoch 30 | Loss: 4806.465827 | Recon Loss: 4613.694977 | KLD:
192.770854
```

```
import gc
gc.collect()
torch.cuda.empty_cache()

def load_checkpoint(model, optimizer, filename="vae_checkpoint.pth"):
    checkpoint_path = os.path.join(CHECKPOINT_DIR, filename)

    if os.path.exists(checkpoint_path):
        checkpoint = torch.load(checkpoint_path,
map_location=torch.device('cuda' if torch.cuda.is_available() else
'cpu'))

        model.load_state_dict(checkpoint["model_state_dict"])
        optimizer.load_state_dict(checkpoint["optimizer_state_dict"])
        epoch = checkpoint["epoch"]

        print(f"Checkpoint loaded from {checkpoint_path}, resuming
from epoch {epoch}")
        return epoch
    else:
```

```
        print("No checkpoint found, starting from scratch")
        return 0  # Start from epoch 0 if no checkpoint exists

save_checkpoint(VAE_model, optimizer, 0)
```

Inferences

1. Using a weighted MSE loss resulted in better reconstructions by reducing the influence of zero-valued pixels.
2. A latent space size of 64 to 128 provided the best trade-off between reconstruction accuracy and model complexity.
3. The reconstructions tended to be noisy regardless of the loss function used, indicating a limitation of the VAE or data format. Hence it is better to shift to a graph based dataset and utilizing GNNS for the task.
4. The model often produced reconstructions that were mean representations of the input data (bright regions at the centre with noise arouund it) showing that the model was not able to learn any meaningful representation of the datapoinst regardless of any other factors(model complexity, latent size etc..).
5. A linear beta schedule did not really help in improving perfromance as the initialy the reconstruction would improve but then the model would collapse to a mean representation and the KLD would increase rapidly indicating that the latent representation being learned is not meaningful and the reconstruction loss would then plateau and remain constant.
6. Applying any activation to the final output did not create any positive effects. ReLU and LeakyReLU caused very sparse reconstructions (model was not really learning), sigmoid also did not make any major improvements to the reconstruction and KLD loss hence it was best to keep the final layer output without any activation.
7. Further tuning of the β factor(cyclic β scheduler), using advanced loss functions might help mitigate the noise and improve reconstruction quality.