The given jupyter notebook contains code for task 1 evaluation of Genie Project
Task objectives :

- Train an Auto-Encoder to learn a representation based on three images channels
  i.e. :
  - ECAL -> Electromagnetic Calorimeter
  - HCAL -> Hadronic Calorimeter
  - Tracks
- Show a side-by-side comparison of original and reconstructed events

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The Quark-Gluon hdfs dataset was in compressed format so when loading every element batch wise it was decompressing it, and then reading it which was taking up unnecessary time so, an uncompressed version with the same chunk_size of (6000,...) events per-chunk was created.

In [ ]:
```
import h5py
from tqdm import tqdm
from torch.utils.data import Dataset, DataLoader, random_split
from torchvision.transforms import transforms
import torch
# from torchmetrics.functional import structural_similarity_index_measure as ssim
import torchvision.transforms.functional as trans_F
from torch import nn, optim, functional as F
import pytorch_lightning as pl
import os
import matplotlib.pyplot as plt
import multiprocessing as mp
import torchvision
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "./saved_models/"
```

In [ ]:
```
def decompress_dataset(raw_path,  processed_path):
    with h5py.File(raw_path, 'r') as r, h5py.File(processed_path, 'w') as p:
        keys = list(r.keys())
        total_events = r[keys[0]].shape[0]
        for key in keys:
            if len(r[key].shape) > 1:
                chunk_shape = tuple([6000] + list(r[key].shape[1:]))
            else:
                chunk_shape = (6000,)
            p.create_dataset(key, shape=r[key].shape, chunks= chunk_shape)
            #iterate till we reach the last element in the dataset for that feature
            for i in tqdm(range(0, total_events, 6000)):
                stop_idx = min(i+6000, total_events)
                p[key][i:stop_idx] = r[key][i:stop_idx]
```

In [ ]:
```
raw_path = "../Data/hdf5/raw/quark-gluon_data-set_n139306.hdf5"
uncompressed_data_path = "../Data/hdf5/processed/quark-gluon-dataset.hdf5"
subset_data_path = "../Data/hdf5/processed/processed.hdf5"
```

In [ ]:
```
def subset_dataset(raw_path, processed_path, subset_len = 6000):
    with h5py.File(raw_path, 'r') as f, h5py.File(processed_path, 'w') as p:
        keys = list(f.keys())
        total_events = f[keys[1]].shape[0]
        for key in keys:
            shape = (subset_len,)
            if len(f[key].shape) > 1:
                shape = (subset_len, 125, 125, 3)
            p.create_dataset(key, shape=shape)
        quark_count = 0
        gluon_count = 0
        idx = 0
        for i in range(total_events):
            if quark_count < subset_len // 2:
                for key in keys:
                    p[key][idx] = f[key][idx]
                quark_count += 1
                idx += 1
            elif gluon_count < subset_len // 2:
                for key in keys:
                    p[key][idx] = f[key][idx]
                gluon_count += 1
                idx += 1
            elif idx >= subset_len:
                break
```

In [ ]:
```
if not os.path.exists(uncompressed_data_path):
    decompress_dataset(raw_path, uncompressed_data_path)
if not os.path.exists(subset_data_path):
    subset_dataset(uncompressed_data_path, subset_data_path)
```

Quark-Gluon Torch Dataset Class

In [ ]:

```
class QuarkGluonDataset(Dataset):
    def __init__(self, path, channel = 0, transform = None) -> None:
        super().__init__()
        self.path = path
        self.channel = channel
        self.transform = transform
        with h5py.File(self.path, 'r') as f:
            self.keys = list(f.keys())
    def __len__(self):
        with h5py.File(self.path, 'r') as f:
            return len(f[self.keys[1]])
    def __getitem__(self, index):
        with h5py.File(self.path, 'r') as f:
            x = f[self.keys[0]][index]
            x = torch.from_numpy(x)
            x = torch.permute(x, (2, 0, 1)) # convert (n, n, 3) -> (3, n, n)
            if self.transform is not None:
                x = self.transform(x)
                return x
            return x
```

Methodology

1. Divide pytorch Quark dataset into:
    - Train -> 60%
    - Validation -> 20%
    - Test -> 20%
2. Create pytorch lightning DataModule with following with train, val and test dataloaders

Bottle-Necks:

1. Dataset is too large
2. Not enough GPU VRAM to try out larger and more state of the art models

Adopted Solutions

Use only a subset of the dataset about 6K events

1. Use a lighter model for proof of concept

In [ ]:

```
def train_val_test_split(dataset, train = 0.6, val = 0.2, test = 0.2):
    train_data, val_data, test_data = random_split(dataset, [train, val, test])
    datasets = {}
    datasets['train'] = train_data
    datasets['val'] = val_data
    datasets['test'] = test_data
    return datasets

cpu_count = mp.cpu_count()

transform = transforms.Compose([
                transforms.Normalize(mean=0.5, std=1),
                ])
dataset = QuarkGluonDataset(subset_data_path, transform = transform)
dataset =  train_val_test_split(dataset)
train_data = dataset['train']
val_data = dataset['val']
test_data = dataset['test']

class QuarkGluonDataModule(pl.LightningDataModule):
    def __init__(self,dataset, batch_size = 64) -> None:
        super().__init__()
        self.batch_size = batch_size
        self.dataset = dataset
    def setup(self, stage:str):
        self.train_data = self.dataset['train']
        self.val_data = self.dataset['val']
        self.test_data = self.dataset['test']
    def get_train(self, idx):
        return self.train_data[idx][0]
    def train_dataloader(self):
        return DataLoader(self.train_data, batch_size=self.batch_size, shuffle=True,
                          num_workers=cpu_count, prefetch_factor=2* cpu_count)
    def val_dataloader(self):
        return DataLoader(self.val_data, batch_size=self.batch_size, shuffle=False,
                           num_workers=cpu_count, prefetch_factor=2* cpu_count)
    def test_dataloader(self):
        return DataLoader(self.test_data, batch_size=self.batch_size, shuffle=False,
                           num_workers=cpu_count, prefetch_factor=2* cpu_count)
```

NN layer to print the dimesions of input data

In [ ]:

```
class PrintDim(nn.Module):
    def __init__(self) -> None:
        super().__init__()
    def forward(self, x):
        print(x.shape)
        print("-" * 50)
```

```
        return x
```

Encoder layer

Architecture :

- CNN layer
- Activation Funtion -> Relu
- pooling layers -> maxpool, adaptive avg pooling
- Normalization -> BatchNorm

In [ ]:
```
class Encoder(nn.Module):

    def __init__(self,
                 num_input_channels : int,
                 base_channel_size : int,
                 latent_dim : int,
                 act_fn : object = nn.GELU):
        """
        Inputs:
            - num_input_channels : Number of input channels of the image.
              For QuarkGluon, this parameter is 3
            - base_channel_size : Number of channels we use in the first
              convolutional layers. Deeper layers might use a duplicate of it.
            - latent_dim : Dimensionality of latent representation z
            - act_fn : Activation function used throughout the encoder network
        """
        super().__init__()
        c_hid = base_channel_size
        self.net = nn.Sequential(
            nn.Conv2d(num_input_channels, c_hid, kernel_size=3, padding=1, stride=2), # 125x125 => 63x63
            act_fn(),
            nn.Conv2d(c_hid, c_hid, kernel_size=3, padding=1),
            act_fn(),
            nn.Conv2d(c_hid, 2*c_hid, kernel_size=3, padding=1, stride=2), # 63x63 => 32x32
            act_fn(),
            nn.Conv2d(2*c_hid, 2*c_hid, kernel_size=3, padding=1),
            act_fn(),
            nn.Conv2d(2*c_hid, 2*c_hid, kernel_size=3, padding=1, stride=2), # 32x32 => 16x16
            act_fn(),
            nn.Flatten(), # Image grid to single feature vector
            nn.Linear(2*16*16*c_hid, latent_dim) # input_dim => 32768 ~ 2x16x16x c_hid
        )

    def forward(self, x):
        return self.net(x)
```

Decoder Layer

Architecture :

- ConvTranspose2d layer
- Normalization -> BatchNorm

In [ ]:
```
class Decoder(nn.Module):

    def __init__(self,
                 num_input_channels : int,
                 base_channel_size : int,
                 latent_dim : int,
                 act_fn : object = nn.GELU):
        """
        Inputs:
            - num_input_channels : Number of channels of the image to reconstruct.
             For QUarkGluon, this parameter is 3
            - base_channel_size : Number of channels we use in the last
             convolutional layers. Early layers might use a duplicate of it.
            - latent_dim : Dimensionality of latent representation z
            - act_fn : Activation function used throughout the decoder network
        """
        super().__init__()
        c_hid = base_channel_size
        self.linear = nn.Sequential(
            nn.Linear(latent_dim, 2*16*16*c_hid),
            act_fn()
        )
        self.net = nn.Sequential(
            nn.ConvTranspose2d(2*c_hid, 2*c_hid, kernel_size=3, output_padding=1, padding=1, stride=2), # 16x16 => 32x32
            act_fn(),
            nn.Conv2d(2*c_hid, 2*c_hid, kernel_size=3, padding=1),
            act_fn(),
            nn.ConvTranspose2d(2*c_hid, c_hid, kernel_size=3, output_padding=0, padding=1, stride=2), # 32x32 => 63x63
            act_fn(),
            nn.Conv2d(c_hid, c_hid, kernel_size=3, padding=1),
            act_fn(),
            nn.ConvTranspose2d(c_hid, num_input_channels, kernel_size=3, output_padding=0, padding=1, stride=2), # 63x63 => 125
            nn.Tanh() # The input images is scaled between -1 and 1, hence the output has to be bounded as well
        )

    def forward(self, x):
```

```
        x = self.linear(x)
        x = x.reshape(x.shape[0], -1, 16, 16)
        x = self.net(x)
        return x
```

Encoder Decoder layer stacked to make CNN AutoEncoder

- Loss function -> structural similarity index measure
- Optimiser -> AdaGrad

In [ ]:
```
class ConvAutoEncoder(pl.LightningModule):
    def __init__(self,
                base_channel_size: int,
                latent_dim: int,
                encoder_class : object = Encoder,
                decoder_class : object = Decoder,
                num_input_channels: int = 3,
                width: int = 125,
                height: int = 125,
                lr: float = 1e-3):
        super().__init__()
        self.lr = lr
        self.save_hyperparameters()

        self.encoder = encoder_class(num_input_channels, base_channel_size, latent_dim)
        self.decoder = decoder_class(num_input_channels, base_channel_size, latent_dim)
        # Example input array needed for visualizing the graph of the network
        self.example_input_array = torch.zeros(2, num_input_channels, width, height)

    def forward(self, x):
        z = self.encoder(x)
        x_hat = self.decoder(z)
        return x_hat

    def _get_reconstruction_loss(self, batch):
        reconstructed = self.decoder(self.encoder(batch))
        loss = torch.nn.functional.mse_loss(batch, reconstructed, reduction="none")
        loss = loss.sum(dim=[1,2,3]).mean(dim=[0])
        return loss
    def configure_optimizers(self):
        optimiser = optim.Adam(self.parameters(), lr = self.lr)
        scheduler = optim.lr_scheduler.ReduceLROnPlateau(optimizer=optimiser,
                                                         mode='min',
                                                         factor=.2,
                                                         patience=20,
                                                         min_lr = 5e-5,
                                                         )
        return {
                "optimizer": optimiser,
                "lr_scheduler":scheduler,
                "monitor":"val_loss"
                }
    def training_step(self, batch, batc_idx):
        loss = self._get_reconstruction_loss(batch)
        self.log("train_loss", loss.item())
        return loss
    def validation_step(self, batch, batch_idx):
        loss = self._get_reconstruction_loss(batch)
        self.log("val_loss", loss.item())
        return loss
    def test_step(self, batch, batch_idx):
        loss = self._get_reconstruction_loss(batch)
        self.log("test_loss", loss.item())
        return loss
```

In [ ]:
```
class GenerateCallback(pl.Callback):

    def __init__(self, input_imgs, every_n_epochs=1):
        super().__init__()
        self.input_imgs = input_imgs # Images to reconstruct during training
        # Only save those images every N epochs (otherwise tensorboard gets quite large)
        self.every_n_epochs = every_n_epochs

    def on_train_epoch_end(self, trainer, pl_module):
        if trainer.current_epoch % self.every_n_epochs == 0:
            # Reconstruct images
            input_imgs = self.input_imgs.to(pl_module.device)
            with torch.no_grad():
                pl_module.eval()
                reconst_imgs = pl_module(input_imgs)
                pl_module.train()
            # Plot and add to tensorboard
            imgs = torch.stack([input_imgs, reconst_imgs], dim=1).flatten(0,1)
            grid = torchvision.utils.make_grid(imgs, nrow=2, normalize=True, range=(-1,1))
            trainer.logger.experiment.add_image("Reconstructions", grid, global_step=trainer.global_step)
            # results of reconstruction of events after
            #  2 epochs is logged and can be viewd using tensorboard
```

In [ ]:
```
transform = transforms.Compose([
    transforms.Normalize(mean=0.5, std=1),
    ])
data_module = QuarkGluonDataModule(dataset, batch_size=64) #increasing the batch size
                                                        # may cause GPU memory overflow
```

In [ ]:
```
def get_train_images(num):
    return torch.stack([dataset['train'][i] for i in range(num)])
```

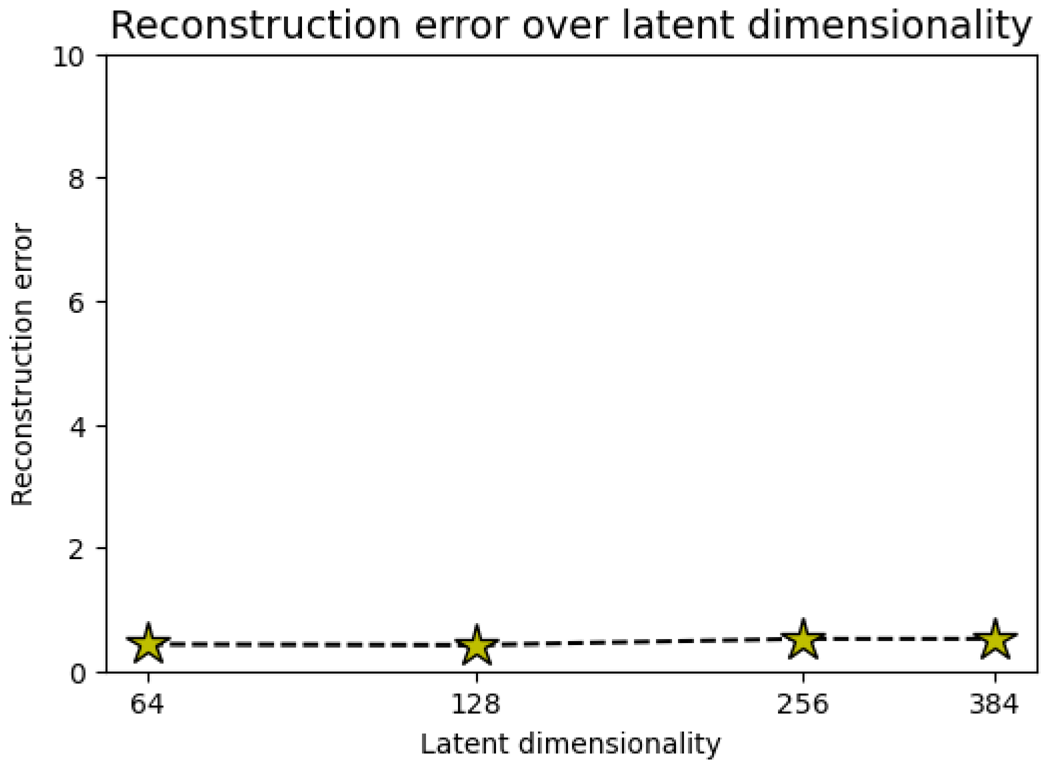
In [ ]:
```
def train_QuarkGluon(latent_dim,epochs):
    # Create a PyTorch Lightning trainer with the generation callback
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, f"QuarkGluon_{latent_dim}"),
                         accelerator="gpu",
                         devices="auto",
                         max_epochs=epochs,
                         callbacks=[ModelCheckpoint(save_weights_only=True),
                                    GenerateCallback(get_train_images(8), every_n_epochs=2),
                                    LearningRateMonitor("epoch")],
                        enable_progress_bar=False)
    trainer.logger._log_graph = True         # If True, we plot the computation graph in tensorboard
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't need


    model = ConvAutoEncoder(base_channel_size=64, latent_dim=latent_dim)
    trainer.fit(model, datamodule=data_module)
    # Test best model on validation and test set
    val_result = trainer.test(model, datamodule=data_module, verbose=False)
    test_result = trainer.test(model, datamodule=data_module, verbose=False)
    result = {"test": test_result, "val": val_result}
    return model, result
```

In [ ]:
```
model_dict = {}
for latent_dim in [64, 128, 256, 384]:
    model_ld, result_ld = train_QuarkGluon(latent_dim, 1000)
    model_dict[latent_dim] = {"model": model_ld, "result": result_ld}
```

```
GPU available: True (cuda), used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
Missing logger folder: saved_models/QuarkGluon_64/lightning_logs
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]

  | Name    | Type    | Params | In sizes         | Out sizes
-------------------------------------------------------------------------
0 | encoder | Encoder | 2.5 M  | [2, 3, 125, 125] | [2, 64]
1 | decoder | Decoder | 2.5 M  | [2, 64]          | [2, 3, 125, 125]
-------------------------------------------------------------------------
5.0 M     Trainable params
0         Non-trainable params
5.0 M     Total params
20.170    Total estimated model params size (MB)
`Trainer.fit` stopped: `max_epochs=10` reached.
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
GPU available: True (cuda), used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
Missing logger folder: saved_models/QuarkGluon_128/lightning_logs
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]

  | Name    | Type    | Params | In sizes         | Out sizes
-------------------------------------------------------------------------
0 | encoder | Encoder | 4.6 M  | [2, 3, 125, 125] | [2, 128]
1 | decoder | Decoder | 4.6 M  | [2, 128]         | [2, 3, 125, 125]
-------------------------------------------------------------------------
9.2 M     Trainable params
0         Non-trainable params
9.2 M     Total params
36.947    Total estimated model params size (MB)
`Trainer.fit` stopped: `max_epochs=10` reached.
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
GPU available: True (cuda), used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
Missing logger folder: saved_models/QuarkGluon_256/lightning_logs
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]

  | Name    | Type    | Params | In sizes         | Out sizes
-------------------------------------------------------------------------
0 | encoder | Encoder | 8.8 M  | [2, 3, 125, 125] | [2, 256]
1 | decoder | Decoder | 8.8 M  | [2, 256]         | [2, 3, 125, 125]
-------------------------------------------------------------------------
17.6 M    Trainable params
0         Non-trainable params
17.6 M    Total params
70.502    Total estimated model params size (MB)
`Trainer.fit` stopped: `max_epochs=10` reached.
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
GPU available: True (cuda), used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
Missing logger folder: saved_models/QuarkGluon_384/lightning_logs
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]

  | Name    | Type    | Params | In sizes         | Out sizes
-------------------------------------------------------------------------
0 | encoder | Encoder | 13.0 M | [2, 3, 125, 125] | [2, 384]
1 | decoder | Decoder | 13.0 M | [2, 384]         | [2, 3, 125, 125]
-------------------------------------------------------------------------
26.0 M    Trainable params
0         Non-trainable params
26.0 M    Total params
104.057   Total estimated model params size (MB)
`Trainer.fit` stopped: `max_epochs=10` reached.
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
```

In [ ]:

```
latent_dims = sorted([k for k in model_dict])
val_scores = [model_dict[k]["result"]["val"][0]["test_loss"] for k in latent_dims]

fig = plt.figure(figsize=(6,4))
plt.plot(latent_dims, val_scores, '--', color="#000", marker="*", markeredgecolor="#000",
          markerfacecolor="y", markersize=16)
plt.xscale("log")
plt.xticks(latent_dims, labels=latent_dims)
plt.title("Reconstruction error over latent dimensionality", fontsize=14)
plt.xlabel("Latent dimensionality")
plt.ylabel("Reconstruction error")
plt.minorticks_off()
plt.ylim(0,10)
plt.show()
```

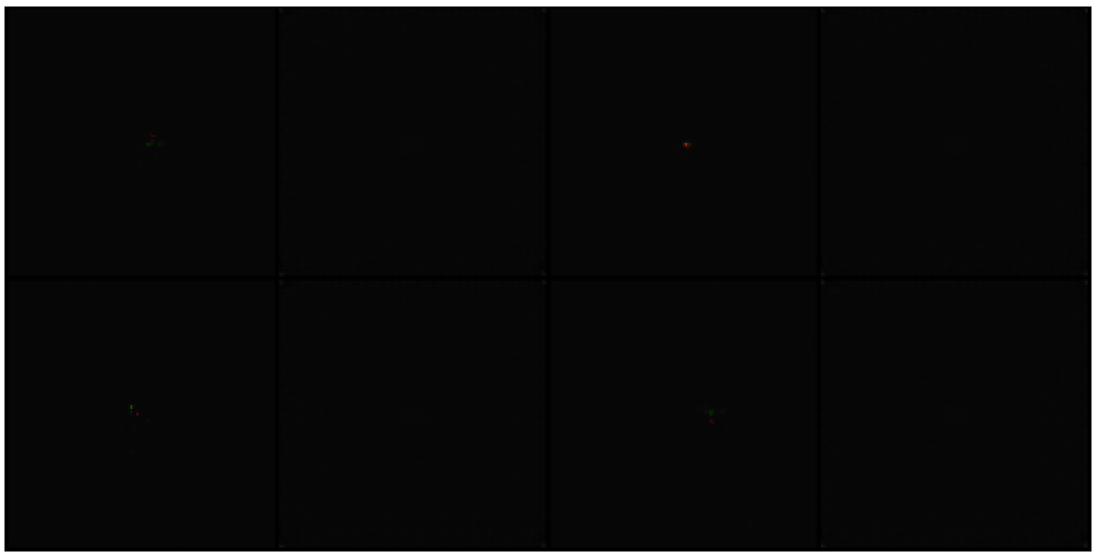


In [ ]:
```
def visualize_reconstructions(model, input_imgs):
    # Reconstruct images
    model.eval()
    with torch.no_grad():
        reconst_imgs = model(input_imgs.to(model.device))
    reconst_imgs = reconst_imgs.cpu()

    # Plotting
    imgs = torch.stack([input_imgs, reconst_imgs], dim=1).flatten(0,1)
    grid = torchvision.utils.make_grid(imgs, nrow=4, normalize=True, range=(-1,1))
    grid = grid.permute(1, 2, 0)
    plt.figure(figsize=(7,4.5))
    plt.title(f"Reconstructed from {model.hparams.latent_dim} latents")
    plt.imshow(grid)
    plt.axis('off')
    plt.show()

    return reconst_imgs
```

In [ ]:
```
input_images = get_train_images(4)
for latent_dim in model_dict:
    recon_images = visualize_reconstructions(model_dict[latent_dim]["model"], input_images)
```

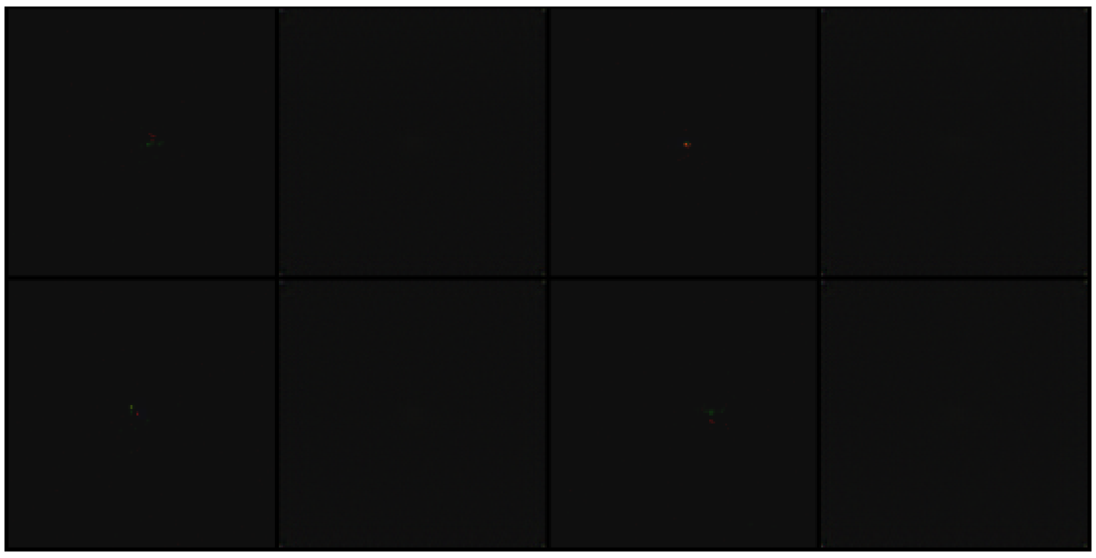
Reconstructed from 64 latents

Reconstructed from 128 latents



Reconstructed from 256 latents

Reconstructed from 384 latents



Problems with the given approach

1. The sparcity of the data is extremely high i.e. these events tend to have a very small that are none-zero so even-though the loss is low we are not able to effectively recreate the the original events.
   Possible solution:
   - Rather than using a full 125*125 image of an event we should create a possible smaller snapshot of the image to decrease the sparsity.
   - Increase the number of hidden layers and experiment with changing pooling layers and different activation functions.
   - Try different loss functions such as structural similarity index measure to effectively capture the structural information of the event.