diffusion_gsoc

March 21, 2023

[ ]:
```
import h5py
import matplotlib.pyplot as plt

import torch
import torch.nn as nn
from torch.nn import functional as F
import torch.utils.data as data_utils
from torch.utils.data import Dataset, DataLoader, Subset
import torch.optim as optim
from torch.nn.functional import interpolate
```

[ ]:
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from torchvision.transforms import transforms
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```
# CONFIG

DEVICE = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")
BATCH_SIZE = 8
NUM_WORKERS = 4
PATH = "/content/drive/MyDrive/gsoc/quark-gluon_data-set_n139306.hdf5"
epochs = 10
lr = 1e-3
```

[ ]:
```
from google.colab import drive
drive.mount('/content/drive')
```

```
Mounted at /content/drive
```

[ ]:
```
class HDF5Dataset(Dataset):
    def __init__(self, file_path):
        self.file = h5py.File(file_path, 'r')
        self.data = self.file['X_jets']
        self.m0 = self.file['m0']
        self.pt = self.file['pt']
        self.y = self.file['y']

    def __len__(self):
        return self.data.shape[0]
```

```
    def __getitem__(self, idx):
        # Load X_jets in shape (125, 125, 3) from HDF5 file
        x_jets = self.data[idx]
        # Transpose the array to shape (3, 125, 125)
        x_jets = torch.tensor(x_jets.transpose(2, 0, 1)).detach().clone()
        return interpolate(x_jets.unsqueeze(0), size=(64,64), mode='bilinear',␣
↪align_corners=False).squeeze(0)
```

[32]:

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dataset = HDF5Dataset(PATH)

indices = torch.arange(100)
train_dataset = Subset(dataset, indices)
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[ ]:

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train_dataset.__getitem__(0).shape
```

[ ]:

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torch.Size([3, 64, 64])
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from tqdm import tqdm
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[31]:

```
class Diffusion:
    def __init__(self, noise_steps=100, beta_start=1e-4, beta_end=0.02,␣
↪img_size=256, device="cuda"):
        self.noise_steps = noise_steps
        self.beta_start = beta_start
        self.beta_end = beta_end
        self.img_size = img_size
        self.device = device

        self.beta = self.prepare_noise_schedule().to(device)
        self.alpha = 1. - self.beta
        self.alpha_hat = torch.cumprod(self.alpha, dim=0)

    def prepare_noise_schedule(self):
        return torch.linspace(self.beta_start, self.beta_end, self.noise_steps)

    def noise_images(self, x, t):
        sqrt_alpha_hat = torch.sqrt(self.alpha_hat[t])[:, None, None, None]
        sqrt_one_minus_alpha_hat = torch.sqrt(1 - self.alpha_hat[t])[:, None,␣
↪None, None]
          = torch.randn_like(x)
        return sqrt_alpha_hat * x + sqrt_one_minus_alpha_hat *  , 

    def sample_timesteps(self, n):
        return torch.randint(low=1, high=self.noise_steps, size=(n,))

    def sample(self, model, n):
        model.eval()
```

```
        with torch.no_grad():
            x = torch.randn((n, 1, self.img_size, self.img_size)).to(self.
↪device)
            for i in reversed(range(1, self.noise_steps)):
                t = (torch.ones(n) * i).long().to(self.device)
                predicted_noise = model(x, t)
                alpha = self.alpha[t][:, None, None, None]
                alpha_hat = self.alpha_hat[t][:, None, None, None]
                beta = self.beta[t][:, None, None, None]
                if i > 1:
                    noise = torch.randn_like(x)
                else:
                    noise = torch.zeros_like(x)
                x = 1 / torch.sqrt(alpha) * (x - ((1 - alpha) / (torch.sqrt(1 -␣
↪alpha_hat))) * predicted_noise) + torch.sqrt(beta) * noise
        model.train()
        x = (x.clamp(-1, 1) + 1) / 2
        x = (x * 255).type(torch.uint8)
        return x
```

[ ]:
```
class SelfAttention(nn.Module):
    def __init__(self, channels, size):
        super(SelfAttention, self).__init__()
        self.channels = channels
        self.size = size
        self.mha = nn.MultiheadAttention(channels, 4, batch_first=True)
        self.ln = nn.LayerNorm([channels])
        self.ff_self = nn.Sequential(
            nn.LayerNorm([channels]),
            nn.Linear(channels, channels),
            nn.GELU(),
            nn.Linear(channels, channels),
        )

    def forward(self, x):
        x = x.view(-1, self.channels, self.size * self.size).swapaxes(1, 2)
        x_ln = self.ln(x)
        attention_value, _ = self.mha(x_ln, x_ln, x_ln)
        attention_value = attention_value + x
        attention_value = self.ff_self(attention_value) + attention_value
        return attention_value.swapaxes(2, 1).view(-1, self.channels, self.
↪size, self.size)


class DoubleConv(nn.Module):
    def __init__(self, in_channels, out_channels, mid_channels=None,␣
↪residual=False):
```

```
        super().__init__()
        self.residual = residual
        if not mid_channels:
            mid_channels = out_channels
        self.double_conv = nn.Sequential(
            nn.Conv2d(in_channels, mid_channels, kernel_size=3, padding=1,␣
 ↪bias=False),
            nn.GroupNorm(1, mid_channels),
            nn.GELU(),
            nn.Conv2d(mid_channels, out_channels, kernel_size=3, padding=1,␣
 ↪bias=False),
            nn.GroupNorm(1, out_channels),
        )

    def forward(self, x):
        if self.residual:
            return F.gelu(x + self.double_conv(x))
        else:
            return self.double_conv(x)
```

[ ]:

```
class Down(nn.Module):
    def __init__(self, in_channels, out_channels, emb_dim=256):
        super().__init__()
        self.maxpool_conv = nn.Sequential(
            nn.MaxPool2d(2),
            DoubleConv(in_channels, in_channels, residual=True),
            DoubleConv(in_channels, out_channels),
        )

        self.emb_layer = nn.Sequential(
            nn.SiLU(),
            nn.Linear(
                emb_dim,
                out_channels
            ),
        )

    def forward(self, x, t):
        x = self.maxpool_conv(x)
        emb = self.emb_layer(t)[:, :, None, None].repeat(1, 1, x.shape[-2], x.
 ↪shape[-1])
        return x + emb


class Up(nn.Module):
    def __init__(self, in_channels, out_channels, emb_dim=256):
        super().__init__()
```

```
        self.up = nn.Upsample(scale_factor=2, mode="bilinear",␣
↪align_corners=True)
        self.conv = nn.Sequential(
            DoubleConv(in_channels, in_channels, residual=True),
            DoubleConv(in_channels, out_channels, in_channels // 2),
        )

        self.emb_layer = nn.Sequential(
            nn.SiLU(),
            nn.Linear(
                emb_dim,
                out_channels
            ),
        )

    def forward(self, x, skip_x, t):
        x = self.up(x)
        x = torch.cat([skip_x, x], dim=1)
        x = self.conv(x)
        emb = self.emb_layer(t)[:, :, None, None].repeat(1, 1, x.shape[-2], x.
↪shape[-1])
        return x + emb
```

[ ]:
```
class UNet(nn.Module):
    def __init__(self, c_in=3, c_out=3, time_dim=256, device="cuda"):
        super().__init__()
        self.device = device
        self.time_dim = time_dim
        self.inc = DoubleConv(c_in, 64)
        self.down1 = Down(64, 128)
        self.sa1 = SelfAttention(128, 32)
        self.down2 = Down(128, 256)
        self.sa2 = SelfAttention(256, 16)
        self.down3 = Down(256, 256)
        self.sa3 = SelfAttention(256, 8)

        self.bot1 = DoubleConv(256, 512)
        self.bot2 = DoubleConv(512, 512)
        self.bot3 = DoubleConv(512, 256)

        self.up1 = Up(512, 128)
        self.sa4 = SelfAttention(128, 16)
        self.up2 = Up(256, 64)
        self.sa5 = SelfAttention(64, 32)
        self.up3 = Up(128, 64)
        self.sa6 = SelfAttention(64, 64)
```

```
        self.outc = nn.Conv2d(64, c_out, kernel_size=1)

    def pos_encoding(self, t, channels):
        inv_freq = 1.0 / (
            10000
            ** (torch.arange(0, channels, 2, device=self.device).float() /␣
↪channels)
        )
        pos_enc_a = torch.sin(t.repeat(1, channels // 2) * inv_freq)
        pos_enc_b = torch.cos(t.repeat(1, channels // 2) * inv_freq)
        pos_enc = torch.cat([pos_enc_a, pos_enc_b], dim=-1)
        return pos_enc

    def forward(self, x, t):
        t = t.unsqueeze(-1).type(torch.float)
        t = self.pos_encoding(t, self.time_dim)

        x1 = self.inc(x)
        x2 = self.down1(x1, t)
        x2 = self.sa1(x2)
        x3 = self.down2(x2, t)
        x3 = self.sa2(x3)
        x4 = self.down3(x3, t)
        x4 = self.sa3(x4)

        x4 = self.bot1(x4)
        x4 = self.bot2(x4)
        x4 = self.bot3(x4)

        x = self.up1(x4, x3, t)
        x = self.sa4(x)
        x = self.up2(x, x2, t)
        x = self.sa5(x)
        x = self.up3(x, x1, t)
        x = self.sa6(x)
        output = self.outc(x)
        return output
```

[ ]:
```
import torchvision
```

[29]:
```
def display_images(input_image, output_image, display=1):
    titles = ['Tracker', 'ECAL', 'HCAL']

    for d in range(display):
        # plot input images
        input_image_numpy = input_image.detach().cpu().numpy()
        plt.figure(figsize=(18,6))
```

```
        plt.suptitle('Original images // Reconstructed images', fontsize=20)

        # plot 4 images
        for i in range(len(titles)):
            plt.subplot(1, 3, i+1)

            plt.imshow(input_image_numpy[0][i], cmap='jet', vmin=0, vmax=0.01)
            plt.colorbar()
            plt.title(titles[i])
            plt.axis(False)

        plt.show()

        # plot output images
        output_image_numpy = output_image.detach().cpu().numpy()
        plt.figure(figsize=(18,6))

        # plot 4 images
        for i in range(len(titles)):
            plt.subplot(1, 3, i+1)

            plt.imshow(output_image_numpy[0][i], cmap='jet', vmin=0, vmax=0.01)
            plt.colorbar()
            plt.title(titles[i])
            plt.axis(False)

        plt.show()
```

[ ]:
```
device = DEVICE
dataloader = DataLoader(train_dataset, shuffle=True, num_workers=NUM_WORKERS)
model = UNet(c_in=1, c_out=1).to(device)
optimizer = optim.AdamW(model.parameters(), lr=lr)
mse = nn.MSELoss()
diffusion = Diffusion(img_size=64, device=device)
l = len(dataloader)

for epoch in range(epochs):
    for i, images in enumerate(tqdm(dataloader)):
        images = images.to(device)
        outputs_list = []

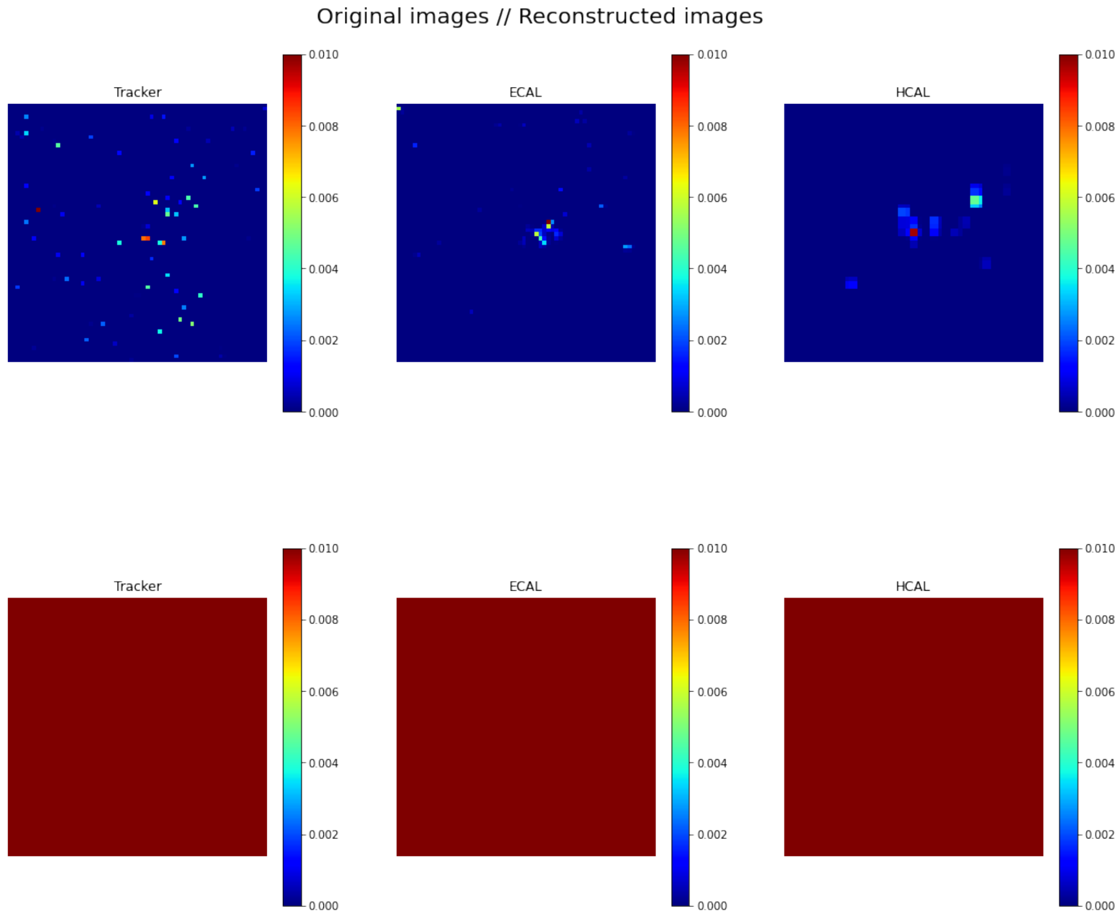
        for channel in range(3):
          data_channel = images[:, channel].unsqueeze(1)
          t = diffusion.sample_timesteps(data_channel.shape[0]).to(device)
          x_t, noise = diffusion.noise_images(data_channel, t)
          predicted_noise = model(x_t, t)
          loss = mse(noise, predicted_noise)
```

```
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

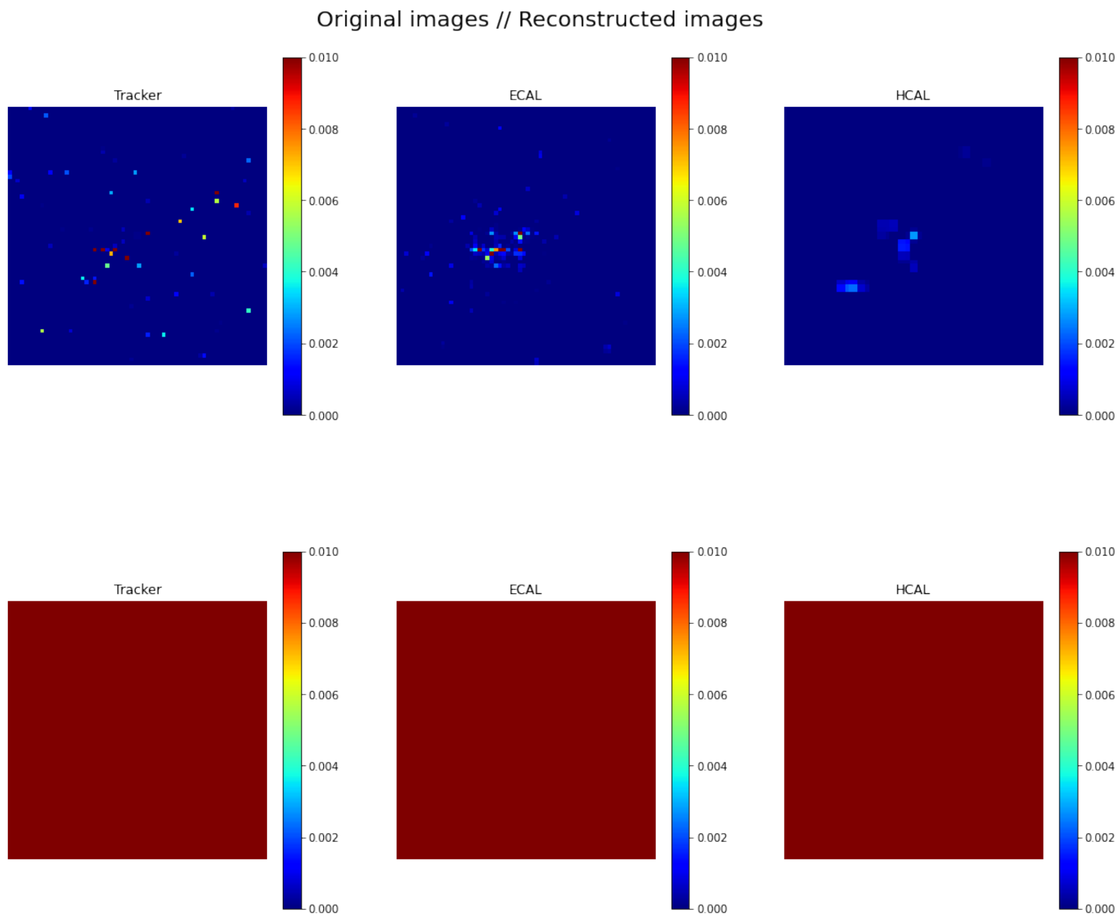
        outputs_list.append(diffusion.sample(model, n=data_channel.shape[0]))

    outputs_list = torch.cat(outputs_list, dim=1) # concatenate Tracker, ECAL,␣
↪HCAL images
    display_images(images, outputs_list)
    print("Loss: ",mse(images,outputs_list).item())
```

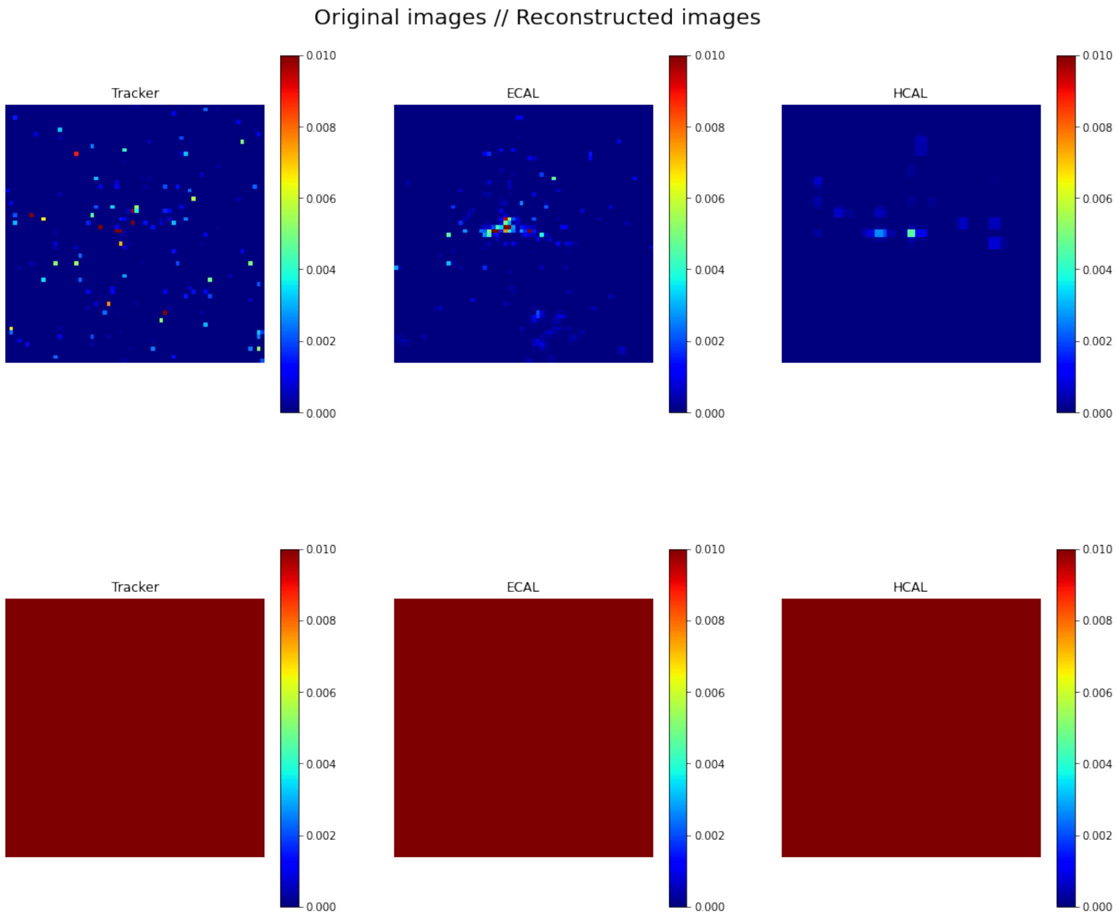
```
/usr/local/lib/python3.9/dist-packages/torch/utils/data/dataloader.py:554:
UserWarning: This DataLoader will create 4 worker processes in total. Our
suggested max number of worker in current system is 2, which is smaller than
what this DataLoader is going to create. Please be aware that excessive worker
creation might get DataLoader running slow or even freeze, lower the worker
number to avoid potential slowness/freeze if necessary.
  warnings.warn(_create_warning_msg(
100%|      | 100/100 [11:48<00:00,  7.09s/it]
```



```
Loss:  17353.5234375
100%|      | 100/100 [11:39<00:00,  7.00s/it]
```




```
Loss:  17054.701171875
100%|      | 100/100 [11:41<00:00,  7.01s/it]
```




```
Loss:  19161.09765625
  3%|          | 3/100 [00:30<14:42,  9.10s/it]
```