var interp

June 16, 2023

1 Setup

```
[]: from pathlib import Path
     import os
     import torch
     from torch import nn
     from torch.utils.data import TensorDataset
     import numpy as np
     import pandas as pd
     import seaborn as sns
     import matplotlib.pyplot as plt
     from FUCCIDataset import FUCCIDatasetInMemory, ReferenceChannelDatasetInMemory,
      →FUCCIChannelDatasetInMemory
     from LightningModules import AutoEncoder, FUCCIDataModule
     import lightning.pytorch as pl
     from lightning.pytorch.callbacks import BasePredictionWriter
[]: samples_ct = 10
     replicates = 30
     save_path = Path("/data/ishang/nb_data/")
     data_path = Path("/data/ishang/Fucci-dataset-v3_filtered/")
     # model_path = Path("/data/ishang/fucci_vae/
      →FUCCI_reference_VAE_2023_06_07_11_56/lightning_logs/23-754918.69.ckpt")
     model_path = Path("/data/ishang/fucci_vae/FUCCI_reference_VAE_2023_06_15_08_04/
      →lightning_logs/499-380355.34.ckpt") #regularized
     channel = "reference"
     # model_path = Path("/data/ishang/fucci_vae/fucci_256_512_2023_05_24_05_47/
     → lightning_logs/epoch=434-Val_loss=0.00.ckpt")
     # channel = "fucci"
     assert channel in str(model_path)
     assert model_path.exists()
     if not data_path.exists():
         os.mkdir(data_path)
```

[]: model = AutoEncoder.load_from_checkpoint(model_path)

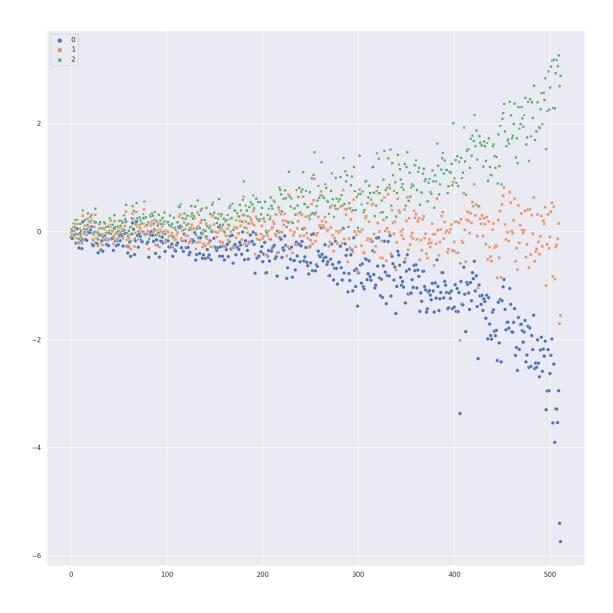
```
[]: mu_file = data_path / (channel + "_mu.pt")
     var_file = data_path / (channel + "_logvar.pt")
     indices_file = data_path / (channel + "_indices.npy")
     colors_file = data_path / "colors.npy"
[]: mu = torch.load(mu_file)
     logvar = torch.load(var file)
     print(torch.isnan(mu).sum(), torch.isnan(logvar).sum())
     print(torch.isinf(mu).sum(), torch.isinf(logvar).sum())
     print(torch.isnan(torch.exp(logvar)).sum(), torch.isinf(torch.exp(logvar)).
      ⇒sum())
     var = torch.exp(logvar)
     indices = np.load(indices file)
     colors = np.load(colors_file)
     latent dim = mu.shape[1]
     print(f"Latent dim: {latent_dim}")
    tensor(0) tensor(0)
    tensor(0) tensor(0)
    tensor(0) tensor(0)
    Latent dim: 512
[]: print(mu.min(), mu.mean(), mu.max())
     print(mu.min(), mu.median(), mu.max())
     print(torch.pow(mu.var(), 0.5))
    tensor(-23.5699) tensor(0.0091) tensor(24.2539)
    tensor(-23.5699) tensor(0.0129) tensor(24.2539)
    tensor(1.7325)
[]: print(torch.sqrt(var).min(), torch.sqrt(var).mean(), torch.sqrt(var).max())
     print(torch.sqrt(var).min(), torch.sqrt(var).median(), torch.sqrt(var).max())
    tensor(0.1050) tensor(0.6477) tensor(3.2188)
    tensor(0.1050) tensor(0.6550) tensor(3.2188)
[]:|dataset = ReferenceChannelDatasetInMemory(data_path, imsize=256) if channel ==__
      →"reference" else FUCCIChannelDatasetInMemory(data_path, imsize=256)
```

2 Exploration

```
[]: # plot the mean and standard deviation of each channel in the latent space
d = 4
# q = torch.Tensor([1 / d * i for i in range(d + 1)])
q = torch.Tensor([0.2, 0.4, 0.5, 0.6, 0.8])
q = torch.Tensor([0.25, 0.5, 0.75])
```

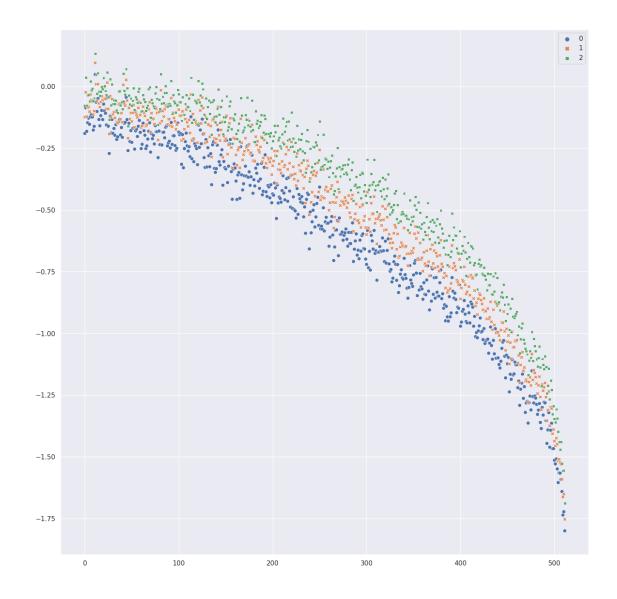
```
mu_q = torch.quantile(mu, q, dim=0)
     print(mu_q.shape)
     print(mu_q[:10, :10])
     # diff = mu_q[O] - mu_q[-1]
     # print(diff.shape)
     # metric = diff
     emp_std = torch.std(mu, dim=0)
     print(emp std.shape)
     metric = emp_std
     sorted_indices = np.argsort(metric.numpy())
     # print(sorted_indices)
     std_q = torch.quantile(torch.sqrt(var), q, dim=0)
     print(std_q.shape)
     print(std_q[:10, :10])
    torch.Size([3, 512])
    tensor([[-1.2359e-03, -1.0187e+00, -4.3665e-01, -1.7756e-01, -2.5400e+00,
             -1.3507e+00, -2.0323e+00, -1.9944e+00, -1.1807e+00, 5.7138e-02],
            [7.7602e-01, -2.0527e-01, -2.0637e-01, 1.0002e-01, -5.5196e-01,
              1.4063e-01, 4.4951e-01, -5.5006e-01, -2.8806e-01, 7.6298e-01],
            [ 1.4028e+00, 7.1308e-01, 6.4150e-02, 3.2896e-01, 1.6964e+00,
              1.5954e+00, 2.8392e+00, 1.0428e+00, 7.3232e-01, 1.3649e+00]])
    torch.Size([512])
    torch.Size([3, 512])
    tensor([[0.5579, 0.4984, 0.7269, 0.7574, 0.2768, 0.3585, 0.2320, 0.3698, 0.4345,
             0.5535],
            [0.6514, 0.5635, 0.8029, 0.8382, 0.3087, 0.3902, 0.2531, 0.4117, 0.5026,
             0.6341],
            [0.7435, 0.6478, 0.8633, 0.9194, 0.3491, 0.4380, 0.2815, 0.4606, 0.5843,
             0.7126]])
[]: mu_q_sorted = mu_q[:, sorted_indices]
     sns.set(rc={'figure.figsize':(16,16)})
     sns.scatterplot(data=mu_q_sorted.T.numpy())
```

[]: <Axes: >



```
[]: std_q_sorted = std_q[:, sorted_indices]
sns.scatterplot(data=torch.log(std_q_sorted).T.numpy())
```

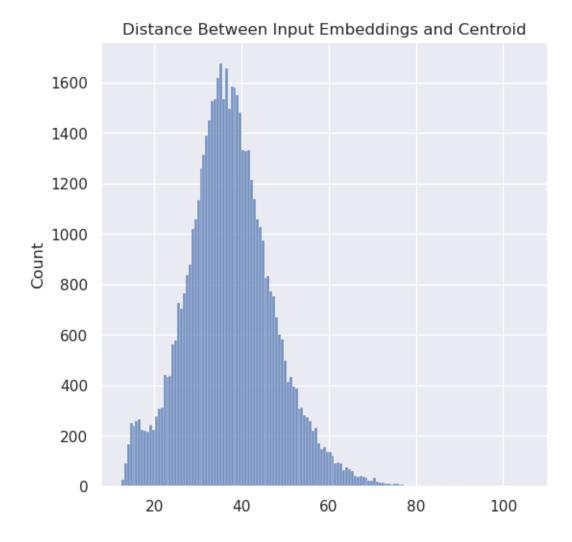
[]: <Axes: >



```
[]: sns.set(rc={'figure.figsize':(6,6)})
    centroid = torch.mean(mu, dim=0)
    print(centroid.shape)
    distances = torch.linalg.vector_norm(mu[:, :] - centroid[None, :], dim=1)
    sns.histplot(distances)
    plt.title("Distance Between Input Embeddings and Centroid")
```

torch.Size([512])

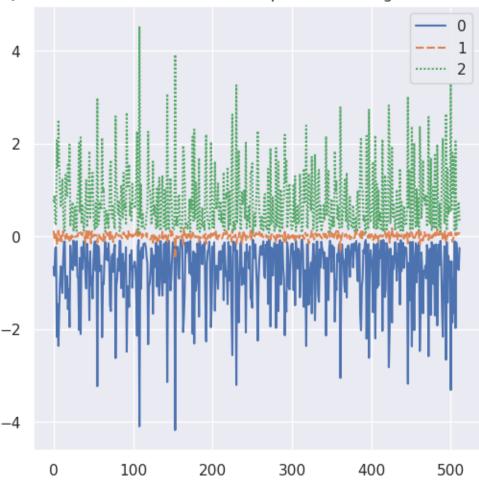
[]: Text(0.5, 1.0, 'Distance Between Input Embeddings and Centroid')



```
[]: centroid = torch.mean(mu, dim=0)
    distances = mu[:, :] - centroid[None, :]
    dimension_quantiles = torch.quantile(distances, q, dim=0)
    sns.lineplot(data=dimension_quantiles.T.numpy())
    plt.title("Quantiles of Distance Between Input Embeddings and Centroid")
```

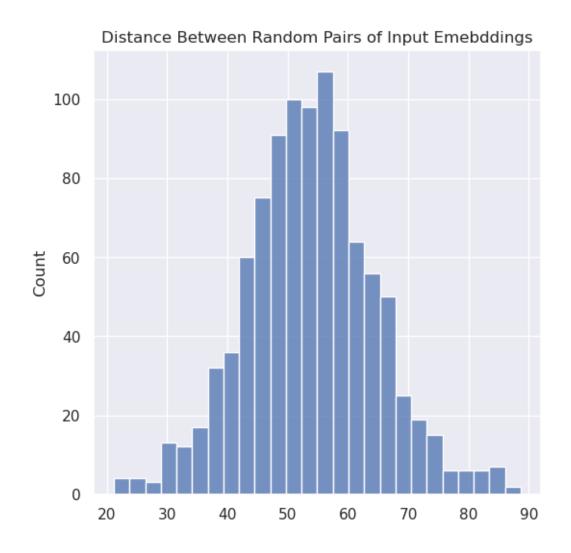
[]: Text(0.5, 1.0, 'Quantiles of Distance Between Input Embeddings and Centroid')

Quantiles of Distance Between Input Embeddings and Centroid



```
[]: sample_indices = np.random.choice(len(dataset), 1000, replace=False)
    sample_mu = mu[sample_indices]
    partner_indices = np.random.choice(len(dataset), 1000, replace=False)
    partner_mu = mu[partner_indices]
    distance = torch.linalg.vector_norm(sample_mu[:, :] - partner_mu[:, :], dim=1)
    print(distance.mean(), distance.std())
    sns.set(rc={'figure.figsize':(6,6)})
    sns.histplot(distance)
    plt.title("Distance Between Random Pairs of Input Emebddings")
    plt.show()
```

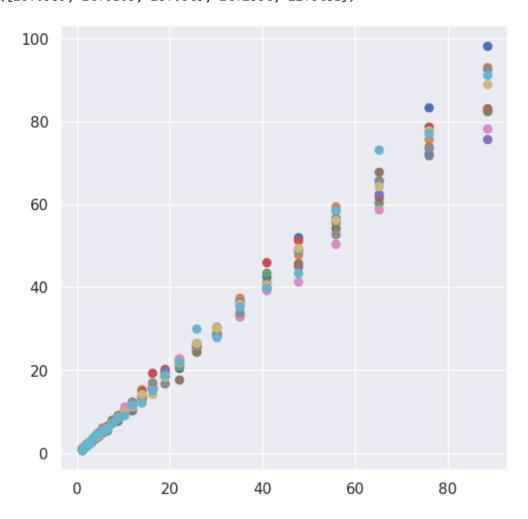
tensor(53.8331) tensor(10.7382)



3 Error-Distance Dependency

```
print(scale)
    tensor(21.2073) tensor(88.6392)
    tensor(1.) tensor(88.6392)
    tensor([ 1.0000, 1.1672, 1.3624, 1.5903, 1.8563, 2.1667, 2.5290, 2.9520,
             3.4457, 4.0219, 4.6946, 5.4797, 6.3961, 7.4658, 8.7143, 10.1717,
            11.8728, 13.8584, 16.1760, 18.8812, 22.0389, 25.7247, 30.0268, 35.0484,
            40.9099, 47.7516, 55.7375, 65.0589, 75.9392, 88.6392])
    tensor([6.6970e-04, 9.1243e-04, 1.2431e-03, 1.6937e-03, 2.3076e-03, 3.1440e-03,
            4.2835e-03, 5.8360e-03, 7.9512e-03, 1.0833e-02, 1.4759e-02, 2.0109e-02,
            2.7397e-02, 3.7327e-02, 5.0857e-02, 6.9289e-02, 9.4403e-02, 1.2862e-01,
            1.7524e-01, 2.3875e-01, 3.2528e-01, 4.4318e-01, 6.0381e-01, 8.2266e-01,
            1.1208e+00, 1.5271e+00, 2.0805e+00, 2.8346e+00, 3.8620e+00, 5.2618e+00])
[]: sample_indices = np.random.choice(len(dataset), samples_ct, replace=False)
     sample mu = mu[sample indices]
     emp_std = torch.sqrt(scale[:, None] * mu.var(dim=0)[None, :])
     print(sample_mu.shape)
     eps_shape = [samples_ct, replicates, latent_dim] # 5 samples per example data_
      \rightarrow point
     # for d in sample mu.shape:
           eps_shape.append(d)
     eps = torch.randn(eps_shape)
     print(eps.shape, emp_std.shape, sample_mu.shape)
     samples = eps[:, :, :] * emp std[None, :, :] + sample mu[:, None, :]
     print(samples.shape, emp_std.shape, sample_mu.shape)
     print(samples.min(), samples.mean(), samples.max())
    torch.Size([10, 512])
    torch.Size([10, 30, 512]) torch.Size([30, 512]) torch.Size([10, 512])
    torch.Size([10, 30, 512]) torch.Size([30, 512]) torch.Size([10, 512])
    tensor(-46.0173) tensor(0.0159) tensor(28.4996)
[]: sample_dist = (samples[:, :, :] - sample_mu[:, None, :]).squeeze()
     sample_diff = torch.linalg.vector_norm(sample_dist, dim=2)
     print(sample diff.shape)
     print(torch.mean(sample_diff, dim=1)[:5])
     print(torch.std(sample_diff, dim=1)[:5])
     for i in range(samples_ct):
         plt.scatter(target_distances, sample_diff[i, :])
     plt.show()
     print(sample_dist.min(), sample_dist.mean(), sample_dist.max())
    torch.Size([10, 30])
```

```
tensor([21.2127, 20.6668, 19.7837, 20.7525, 19.7129])
tensor([26.0939, 24.6168, 23.0545, 24.2384, 22.5451])
```



tensor(-44.3663) tensor(0.0034) tensor(22.4845)

```
[]: samples = samples.reshape(-1, samples.shape[-1])

# samples = torch.stack([samples, samples], dim=1)

# samples[:, 1, :] = 0
```

```
class CustomWriter(BasePredictionWriter):

    def __init__(self, output_dir, write_interval):
        super().__init__(write_interval)
        self.output_dir = output_dir

    def write_on_epoch_end(self, trainer, pl_module, predictions,ubatch_indices):
```

```
# this will create N (num processes) files in `output_dir` each
      ⇔containing
            # the predictions of it's respective rank
            torch.save(predictions, os.path.join(self.output_dir,_

¬f"predictions_{trainer.global_rank}.pt"))

            # optionally, you can also save `batch_indices` to get the information_
      ⇒about the data index
            # from your prediction data
            torch.save(batch_indices, os.path.join(self.output_dir,_
      []: from torch.utils.data import Dataset
    class SimpleDataset(Dataset):
        def init (self, tensor) -> None:
            self.tensor = tensor
        def __getitem__(self, index):
            return self.tensor[index]
        def __len__(self):
            return self.tensor.size(0)
[]: predictions_dir = save_path / "sample_predictions"
    if not predictions_dir.exists():
        os.mkdir(predictions_dir)
    for f in predictions_dir.glob("*"):
        f.unlink()
    pred_writer = CustomWriter(output_dir=predictions_dir, write_interval="epoch")
    sample_dm = pl.LightningDataModule.
     ⇔from datasets(predict dataset=SimpleDataset(samples), batch_size=replicates, ⊔
     →num_workers=1)
    print(samples.shape)
    print(len(SimpleDataset(samples)))
    print(len(sample_dm.predict_dataloader()))
    model.set_predict_mode("sampling")
    trainer = pl.Trainer(accelerator="gpu", devices=1, callbacks=[pred_writer])
    trainer.predict(model, datamodule=sample_dm, return_predictions=False)
    GPU available: True (cuda), used: True
```

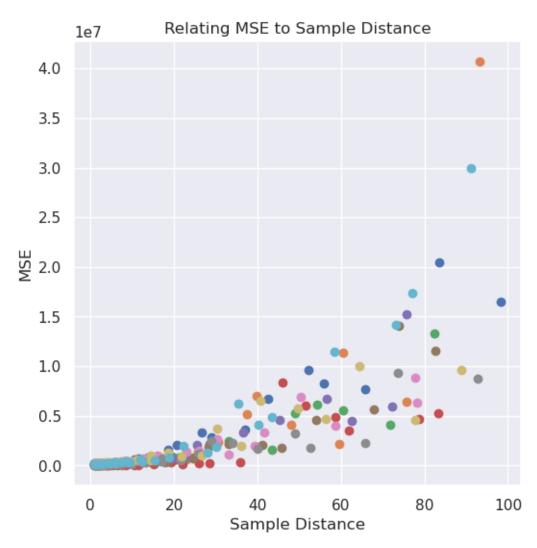
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs

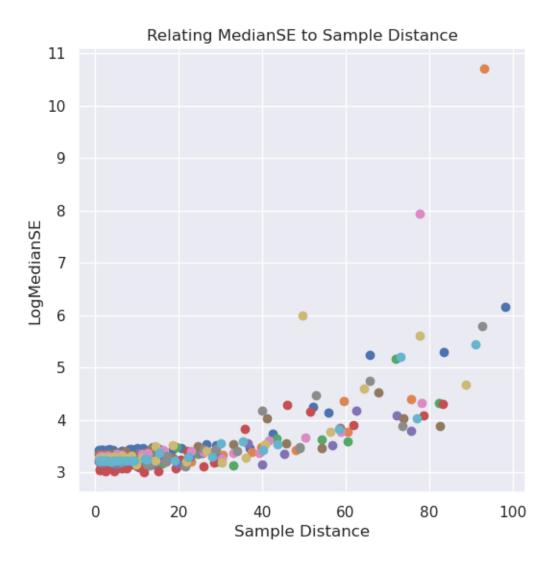
```
torch.Size([300, 512])
    300
    10
    You are using a CUDA device ('NVIDIA A100-SXM4-40GB') that has Tensor Cores. To
    properly utilize them, you should set
    `torch.set_float32_matmul_precision('medium' | 'high')` which will trade-off
    precision for performance. For more details, read https://pytorch.org/docs/stabl
    e/generated/torch.set_float32_matmul_precision.html#torch.set_float32_matmul_pre
    cision
    LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1,2,3,4,5,6,7]
    /home/ishang/miniconda3/envs/implicit/lib/python3.10/site-
    packages/lightning/pytorch/trainer/connectors/data_connector.py:430:
    PossibleUserWarning: The dataloader, predict dataloader, does not have many
    workers which may be a bottleneck. Consider increasing the value of the
    `num workers` argument` (try 256 which is the number of cpus on this machine) in
    the `DataLoader` init to improve performance.
      rank_zero_warn(
    Predicting: 0it [00:00, ?it/s]
[]: !ls /data/ishang/nb_data/sample_predictions/
    batch_indices_0.pt predictions_0.pt
[]: batch indices = torch.load(predictions dir / "batch indices 0.pt")[0]
     predictions = torch.load(predictions_dir / "predictions_0.pt")
     print(len(batch_indices), len(predictions))
     print(len(batch_indices), predictions[0].shape)
     predictions = torch.stack(predictions, dim=0)
    10 10
    10 torch.Size([30, 2, 256, 256])
[]: indices = [i for batch in batch_indices for i in batch]
     for i in range(len(indices)):
         assert indices[i] == i
[]: targets = dataset[sample_indices]
     print(predictions.shape, targets.shape)
     se = torch.pow(predictions[:, :, :, :] - targets[:, None, :, :], 2)
     mse = se.mean(dim=(2, 3, 4))
     med = se.reshape(samples_ct, replicates, -1).median(dim=(2)).values
     for i in range(10):
         plt.scatter(sample_diff[i], mse[i])
     plt.xlabel("Sample Distance")
     plt.ylabel("MSE")
```

```
plt.title(f"Relating MSE to Sample Distance")
plt.show()

plt.clf()
for i in range(10):
    plt.scatter(sample_diff[i], torch.log(med[i]))
plt.xlabel("Sample Distance")
plt.ylabel("LogMedianSE")
plt.title(f"Relating MedianSE to Sample Distance")
plt.show()
```

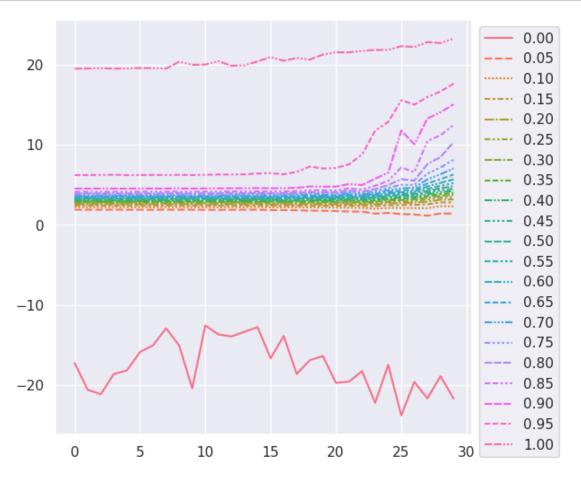
torch.Size([10, 30, 2, 256, 256]) torch.Size([10, 2, 256, 256])





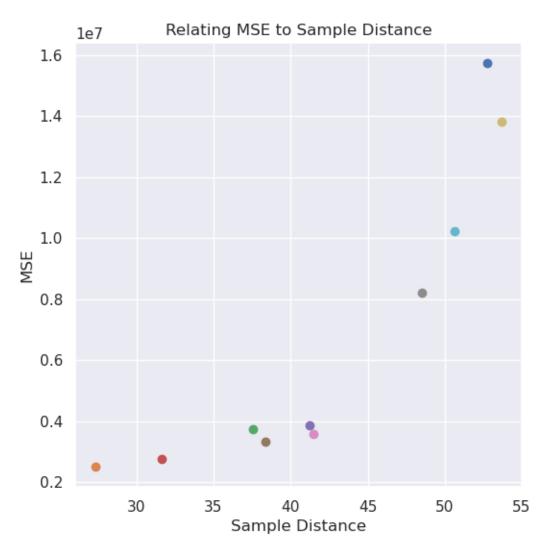
torch.Size([10, 30]) torch.Size([10, 30]) torch.Size([10, 30])

```
(21, 30)
```



```
plt.scatter(distance[i], mse[i])
plt.xlabel("Sample Distance")
plt.ylabel("MSE")
plt.title(f"Relating MSE to Sample Distance")
plt.show()
```

```
torch.Size([10, 512]) torch.Size([10, 512])
torch.Size([10, 2, 256, 256]) torch.Size([10, 2, 256, 256])
torch.Size([10]) torch.Size([10])
```



4 Attractor Detection

```
[]: # quick and dirty check for fixed-point
     sample indices = np.random.choice(len(dataset), 10, replace=False)
     samples = dataset[sample_indices]
     print(sample_indices)
     predictions_dir = save_path / "sample_embeddings"
     if not predictions_dir.exists():
        os.mkdir(predictions_dir)
     for f in predictions_dir.glob("*"):
        f.unlink()
     pred_writer = CustomWriter(output_dir=predictions_dir, write_interval="epoch")
     sample_dm = pl.LightningDataModule.
      afrom_datasets(predict_dataset=SimpleDataset(samples), batch_size=2,_
      print(samples.shape)
     print(len(SimpleDataset(samples)))
     print(len(sample_dm.predict_dataloader()))
     model.set_predict_mode("embedding")
     trainer = pl.Trainer(accelerator="gpu", devices=1, callbacks=[pred writer])
     trainer.predict(model, datamodule=sample_dm, return_predictions=False)
    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
    You are using a CUDA device ('NVIDIA A100-SXM4-40GB') that has Tensor Cores. To
    properly utilize them, you should set
    `torch.set_float32_matmul_precision('medium' | 'high')` which will trade-off
    precision for performance. For more details, read https://pytorch.org/docs/stabl
    e/generated/torch.set_float32_matmul_precision.html#torch.set_float32_matmul_pre
    cision
    [19885 35760 49121 50637 17209 28716 46642 16838 29640 1898]
    torch.Size([10, 2, 256, 256])
    10
    LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1,2,3,4,5,6,7]
    /home/ishang/miniconda3/envs/implicit/lib/python3.10/site-
    packages/lightning/pytorch/trainer/connectors/data_connector.py:430:
    PossibleUserWarning: The dataloader, predict_dataloader, does not have many
    workers which may be a bottleneck. Consider increasing the value of the
    `num_workers` argument` (try 256 which is the number of cpus on this machine) in
```

```
rank_zero_warn(
    Predicting: 0it [00:00, ?it/s]
[]: predictions = torch.load(predictions_dir / "predictions_0.pt")
     print(len(predictions))
     batch_indices = torch.load(predictions_dir / "batch_indices_0.pt")[0]
     print(len(batch indices))
     print(predictions[0][0].mean(), predictions[0][1].mean())
     print(predictions[0][0].var(), predictions[0][1].var())
     print(predictions[0][0].min(), predictions[0][1].min())
     print(predictions[0][0].max(), predictions[0][1].max())
     predicted_mu = torch.cat([p[0] for p in predictions])
     print(predicted_mu.shape)
     batch_indices = [i for batch in batch_indices for i in batch]
     print(len(batch_indices), len(sample_indices))
     print(batch_indices)
    5
    tensor(0.0097) tensor(-1.2204)
    tensor(3.4139) tensor(0.6144)
    tensor(-9.7099) tensor(-3.6796)
    tensor(11.0675) tensor(0.1135)
    torch.Size([10, 512])
    10 10
    [0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
[]: mu_sample = mu[[sample_indices[i] for i in batch_indices]]
     assert torch.all(dataset[[sample_indices[i] for i in batch_indices]] == samples)
     print(mu_sample.shape, predicted_mu.shape)
     distance = torch.linalg.vector_norm(mu_sample[:, :] - predicted_mu[:, :], dim=1)
     print(distance.shape)
     print(distance.min(), distance.mean(), distance.max())
     print(distance)
    torch.Size([10, 512]) torch.Size([10, 512])
    torch.Size([10])
    tensor(0.0112) tensor(0.0148) tensor(0.0170)
    tensor([0.0121, 0.0138, 0.0164, 0.0148, 0.0162, 0.0168, 0.0170, 0.0153, 0.0112,
            0.01447)
[]: # sample images then calculate the jacobian of the combined encoder and decoder
     device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")
     num_samples = 10
     sample_indices = np.random.choice(len(dataset), num_samples, replace=False)
     predictions_dir = save_path / "sample_predictions"
```

the `DataLoader` init to improve performance.

```
samples = torch.Tensor(dataset[sample_indices]).to(device)
E = model.encoder
D = model.decoder
class SimpleAE(nn.Module):
   def __init__(self, encoder, decoder):
        super(). init ()
        self.encoder = encoder
        self.decoder = decoder
   def forward(self, x):
       mu, var = self.encoder(x)
       x_hat = self.decoder(mu)
        return x_hat
simple_model = SimpleAE(E, D).cuda()
samples.requires_grad = True
reconstruction = simple_model(samples).reshape(num_samples, -1)
samples = samples.reshape(num_samples, -1)
jacob = torch.autograd.grad(reconstruction, samples, grad_outputs=torch.
 ⇔ones like(reconstruction))[0]
print(type(jacob), type(samples), type(reconstruction))
print(jacob.shape, samples.shape, reconstruction.shape)
(eigenvalues, eigenvectors) = torch.linalg.eig(jacob)
# from torch.autograd.functional import jacobian
# j = jacobian(simple_model, samples[None, 0])
# print(j.shape)
```

```
RuntimeError Traceback (most recent call last)

Cell In[52], line 28

26 reconstruction = simple_model(samples).reshape(num_samples, -1)

27 samples = samples.reshape(num_samples, -1)

---> 28 jacob = torch.autograd.grad(reconstruction, samples, grad_outputs=torch

ones_like(reconstruction))[0]

29 print(type(jacob), type(samples), type(reconstruction))

30 print(jacob.shape, samples.shape, reconstruction.shape)

File ~/miniconda3/envs/implicit/lib/python3.10/site-packages/torch/autograd/

-_init__.py:303, in grad(outputs, inputs, grad_outputs, retain_graph, create_graph, only_inputs, allow_unused, is_grads_batched)

301 return _vmap_internals._vmap(vjp, 0, 0, u)

-allow_none_pass_through=True)(grad_outputs_)
```