

sheet06

November 27, 2024

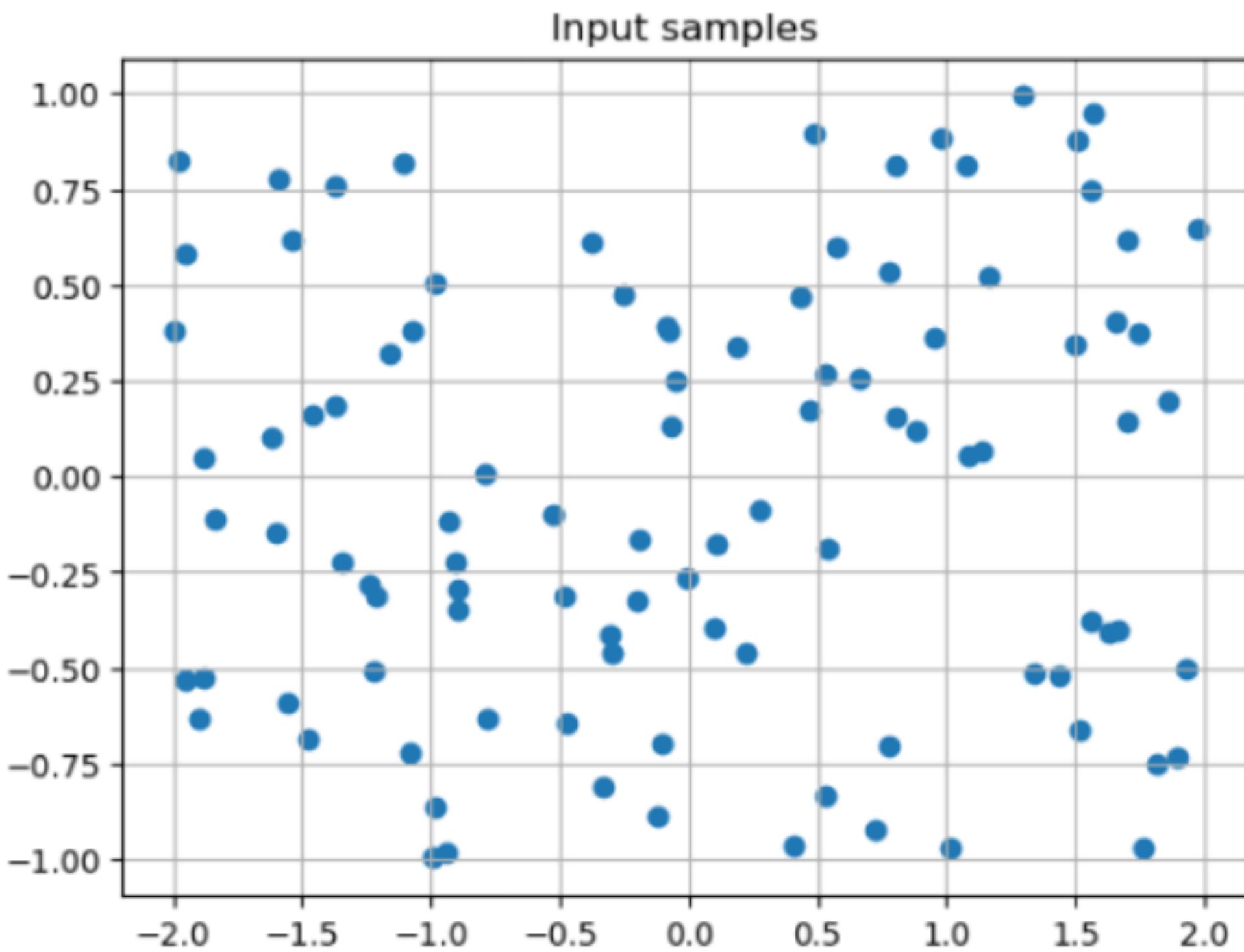
1 Sheet 6

1.1 1 Autoencoders: theory and practice

```
[1]: import torch
import matplotlib.pyplot as plt

# create 1000 uniform samples from a rectangle [-2, 2] x [-1, 1]
num_samples = 100
data = torch.zeros(num_samples, 2)
data[:, 0] = torch.rand(num_samples) * 4 - 2
data[:, 1] = torch.rand(num_samples) * 2 - 1

# plot the samples
plt.scatter(data[:, 0], data[:, 1])
plt.title("Input samples")
plt.grid(True)
plt.show()
```



```
[2]: from torch.utils.data import DataLoader, TensorDataset
```

```
# Prepare data loader
dataset = TensorDataset(data, data)
data_loader = DataLoader(dataset, batch_size=8, shuffle=True, drop_last=True)
```

```
# get batched data from the data loader
```

```
x, y = next(iter(data_loader))
print("x.shape:", x.shape)
print("y.shape:", y.shape)
print("all x == y:", torch.all(x == y).item())
```

```
x.shape: torch.Size([8, 2])
y.shape: torch.Size([8, 2])
all x == y: True
```

1.1.1 (a)

```
[3]: # TODO: define the Autoencoder architecture

import torch
from torch import nn
import pytorch_lightning as pl

class Autoencoder(nn.Module):
    def __init__(self, hidden_channels, latent_dim=1, input_dim=2): #hidden_
    ↵channels as list
        super().__init__()

        # TODO: implement the encoder and decoder
        if hidden_channels == 0:
            self.encoder = nn.Linear(input_dim, latent_dim, bias=False) #_
    ↵Linear layer with no bias
            self.decoder = nn.Linear(latent_dim, input_dim, bias=False)
        else:
            encoder_layers = []
            current_dim = input_dim
            for h in hidden_channels:
                encoder_layers.append(nn.Linear(current_dim, h))
                encoder_layers.append(nn.ReLU())
                current_dim = h
            encoder_layers.append(nn.Linear(current_dim, latent_dim)) #_
    ↵Bottleneck layer
            self.encoder = nn.Sequential(*encoder_layers)

            #decoder as mirrored encoder
            decoder_layers = []
            current_dim = latent_dim
            for h in reversed(hidden_channels):
                decoder_layers.append(nn.Linear(current_dim, h))
                decoder_layers.append(nn.ReLU())
                current_dim = h
            decoder_layers.append(nn.Linear(current_dim, input_dim)) # Output_
    ↵layer
            self.decoder = nn.Sequential(*decoder_layers)

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

```

class AutoencoderModule(pl.LightningModule):
    def __init__(self, **model_kwargs):
        super().__init__()
        self.autoencoder = Autoencoder(**model_kwargs)
        self.loss_curve = []

    def forward(self, x):
        return self.autoencoder(x)

    def configure_optimizers(self):
        # as default use Adam optimizer:
        optimizer = torch.optim.Adam(self.parameters())

        return optimizer

    def on_train_start(self):
        self.loss_curve = []
        return super().on_train_start()

    def training_step(self, batch):
        x, _ = batch
        x_hat = self.autoencoder(x)
        loss = nn.MSELoss()(x_hat, x)
        self.loss_curve.append(loss.item())
        return loss

```

ReLU is a simple and effective non-linearity, therefore it was chosen. The activation was left out for the bottleneck and the output as those should be unconstrained. In the case of PCA no nonlinearities are added in the network.

1.1.2 (b)

```

[4]: # start the training using a PyTorch Lightning Trainer
autoencoder_module_1 = AutoencoderModule(hidden_channels=[20, 10]) # TODO: ↴
    ↴ specify the model here
autoencoder_module_2 = AutoencoderModule(hidden_channels=[50, 50]) # TODO: ↴
    ↴ specify the model here
autoencoder_module_pca = AutoencoderModule(hidden_channels=0) # TODO: specify ↴
    ↴ the model here

models = [autoencoder_module_1, autoencoder_module_2, autoencoder_module_pca]

[5]: for model in models:
    trainer = pl.Trainer(max_epochs=1000)
    print("Model overview:", model)
    trainer.fit(model, data_loader)

```

```
GPU available: False, used: False
TPU available: False, using: 0 TPU cores
HPU available: False, using: 0 HPUs
c:\Users\sasch\miniconda3\envs\mlph3\lib\site-packages\pytorch_lightning\trainer
\connectors\logger_connector\logger_connector.py:75: Starting from v1.9.0,
`tensorboardX` has been removed as a dependency of the `pytorch_lightning`
package, due to potential conflicts with other packages in the ML ecosystem. For
this reason, `logger=True` will use `CSVLogger` as the default logger, unless
the `tensorboard` or `tensorboardX` packages are found. Please `pip install
lightning[extra]` or one of them to enable TensorBoard support by default
Missing logger folder:
c:\Users\sasch\iCloudDrive\Uni\mlph_w24\sheet06\lightning_logs

| Name           | Type      | Params | Mode
-----
0 | autoencoder | Autoencoder | 563    | train
-----
563       Trainable params
0         Non-trainable params
563       Total params
0.002     Total estimated model params size (MB)

Model overview: AutoencoderModule(
    (autoencoder): Autoencoder(
        (encoder): Sequential(
            (0): Linear(in_features=2, out_features=20, bias=True)
            (1): ReLU()
            (2): Linear(in_features=20, out_features=10, bias=True)
            (3): ReLU()
            (4): Linear(in_features=10, out_features=1, bias=True)
        )
        (decoder): Sequential(
            (0): Linear(in_features=1, out_features=10, bias=True)
            (1): ReLU()
            (2): Linear(in_features=10, out_features=20, bias=True)
            (3): ReLU()
            (4): Linear(in_features=20, out_features=2, bias=True)
        )
    )
)
c:\Users\sasch\miniconda3\envs\mlph3\lib\site-
packages\pytorch_lightning\trainer\connectors\data_connector.py:424: The
'train_dataloader' does not have many workers which may be a bottleneck.
Consider increasing the value of the `num_workers` argument` to `num_workers=3`-
in the `DataLoader` to improve performance.
c:\Users\sasch\miniconda3\envs\mlph3\lib\site-
packages\pytorch_lightning\loops\fit_loop.py:298: The number of training batches
(12) is smaller than the logging interval Trainer(log_every_n_steps=50). Set a
```

```
lower value for log_every_n_steps if you want to see logs for the training epoch.
```

```
Training: | 0/? [00:00<?, ?it/s]
```

```
`Trainer.fit` stopped: `max_epochs=1000` reached.
```

```
GPU available: False, used: False
```

```
TPU available: False, using: 0 TPU cores
```

```
HPU available: False, using: 0 HPUs
```

	Name	Type	Params	Mode
0	autoencoder	Autoencoder	5.5 K	train
5.5 K	Trainable params			
0	Non-trainable params			
5.5 K	Total params			
0.022	Total estimated model params size (MB)			

```
Model overview: AutoencoderModule(  
    (autoencoder): Autoencoder(  
        (encoder): Sequential(  
            (0): Linear(in_features=2, out_features=50, bias=True)  
            (1): ReLU()  
            (2): Linear(in_features=50, out_features=50, bias=True)  
            (3): ReLU()  
            (4): Linear(in_features=50, out_features=1, bias=True)  
        )  
        (decoder): Sequential(  
            (0): Linear(in_features=1, out_features=50, bias=True)  
            (1): ReLU()  
            (2): Linear(in_features=50, out_features=50, bias=True)  
            (3): ReLU()  
            (4): Linear(in_features=50, out_features=2, bias=True)  
        )  
    )  
)
```

```
Training: | 0/? [00:00<?, ?it/s]
```

```
`Trainer.fit` stopped: `max_epochs=1000` reached.
```

```
GPU available: False, used: False
```

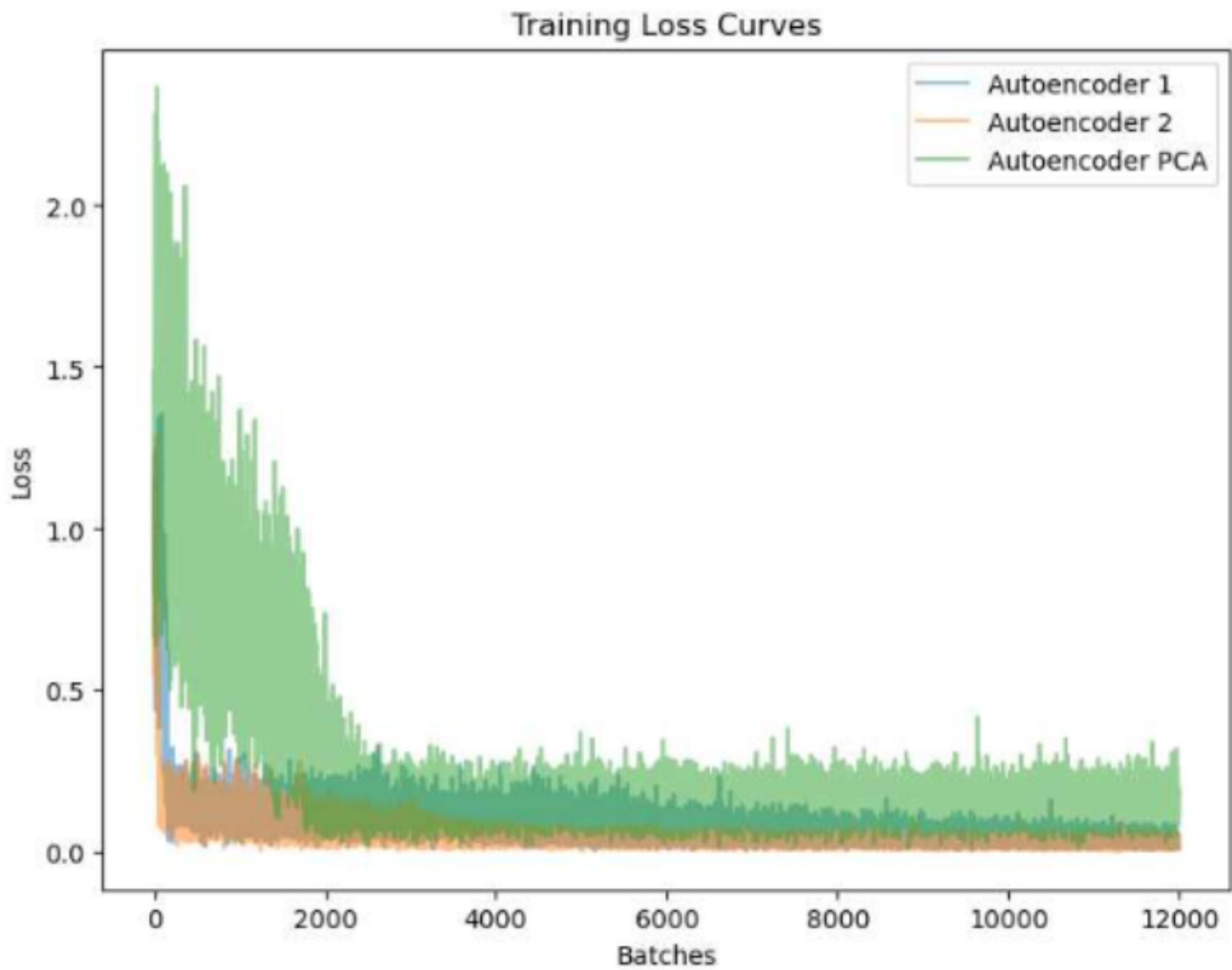
```
TPU available: False, using: 0 TPU cores
```

```
HPU available: False, using: 0 HPUs
```

	Name	Type	Params	Mode
0	autoencoder	Autoencoder	4	train

```
-----  
4      Trainable params  
0      Non-trainable params  
4      Total params  
0.000   Total estimated model params size (MB)  
  
Model overview: AutoencoderModule(  
    (autoencoder): Autoencoder(  
        (encoder): Linear(in_features=2, out_features=1, bias=False)  
        (decoder): Linear(in_features=1, out_features=2, bias=False)  
    )  
)  
  
Training: |          | 0/? [00:00<?, ?it/s]  
  
`Trainer.fit` stopped: `max_epochs=1000` reached.
```

```
[6]: autoencoder_names = ["1", "2", "PCA"]  
plt.figure(figsize=(8, 6))  
for i, model in enumerate(models):  
    plt.plot(model.loss_curve, label=f"Autoencoder {autoencoder_names[i]}",  
             alpha=0.5)  
plt.xlabel("Batches")  
plt.ylabel("Loss")  
plt.title("Training Loss Curves")  
plt.legend()  
plt.show()
```



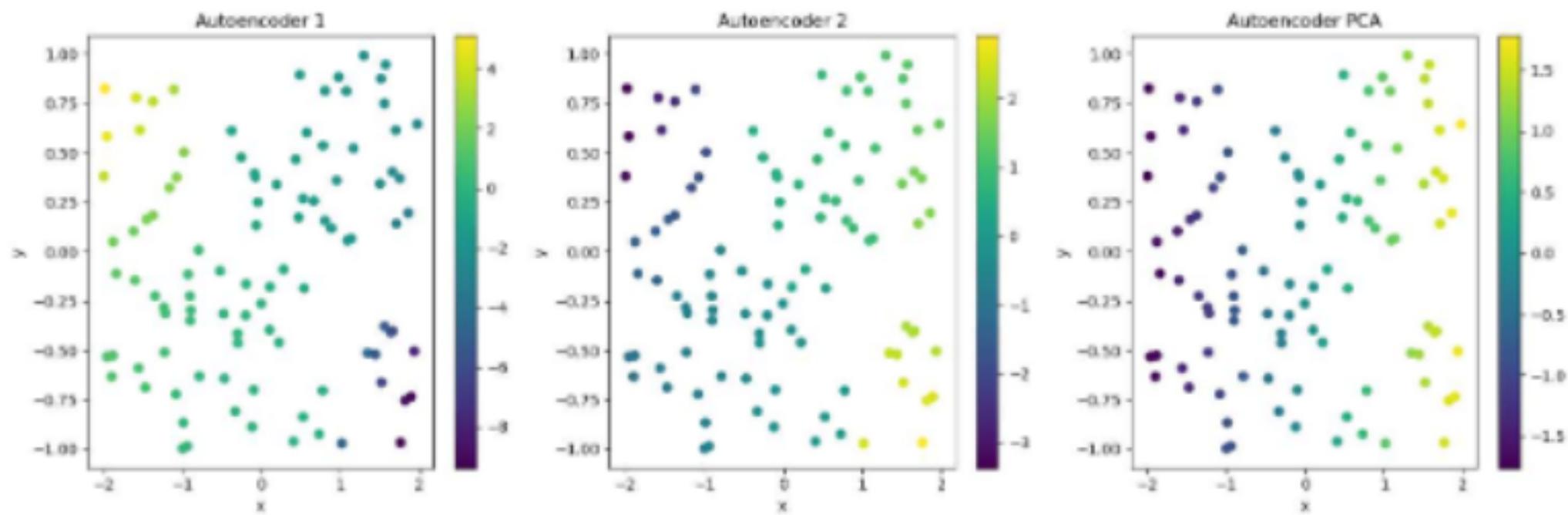
Autoencoder 2 gives the best convergence and the lowest loss on the training data. This Autoencoder is the preferred one. PCA has the worst convergence and the highest loss. It is least suitable for dimensionality reduction.

```
[7]: # Visualize latent embeddings
fig, axes = plt.subplots(1, 3, figsize=(15, 5))

for i, model in enumerate(models):
    with torch.no_grad():
        embeddings = model.autoencoder.encoder(data).squeeze().numpy()

        scatter = axes[i].scatter(data[:, 0], data[:, 1], c=embeddings, cmap='viridis')
        axes[i].set_title(f"Autoencoder {autoencoder_names[i]}")
        axes[i].set_xlabel("x")
        axes[i].set_ylabel("y")
        fig.colorbar(scatter, ax=axes[i])

plt.tight_layout()
plt.show()
```



Autoencoder 1 increases with higher x and higher y. Autoencoder 2 increases with higher x and lower y. Autoencoder PCA increases with x.

1.1.3 (c)

- i) The random initialization gives random distributions for all encoders. The more parameters the AE has the more random the distribution will be.
- ii) In the case of AE 1 after training a linear dependency of x and y is expected. In the case of AE 2 after training a parabolic dependency is expected. In the case of AE PCA a constant relation is expected.

Both AE's are universal function approximators

1.1.4 (d)

```
[ ]: random_autoencoder_module_1 = AutoencoderModule(hidden_channels=[20, 10]) # ↵
    ↵TODO: specify the model here
random_autoencoder_module_2 = AutoencoderModule(hidden_channels=[50, 50]) # ↵
    ↵TODO: specify the model here
random_autoencoder_module_pca = AutoencoderModule(hidden_channels=0) # TODO: ↵
    ↵specify the model here

random_models = [random_autoencoder_module_1, random_autoencoder_module_2, ↵
    ↵random_autoencoder_module_pca]

latent_samples = torch.linspace(-1.5, 1.5, 500).unsqueeze(1)

fig, axs = plt.subplots(3, 2, figsize=(12, 12))

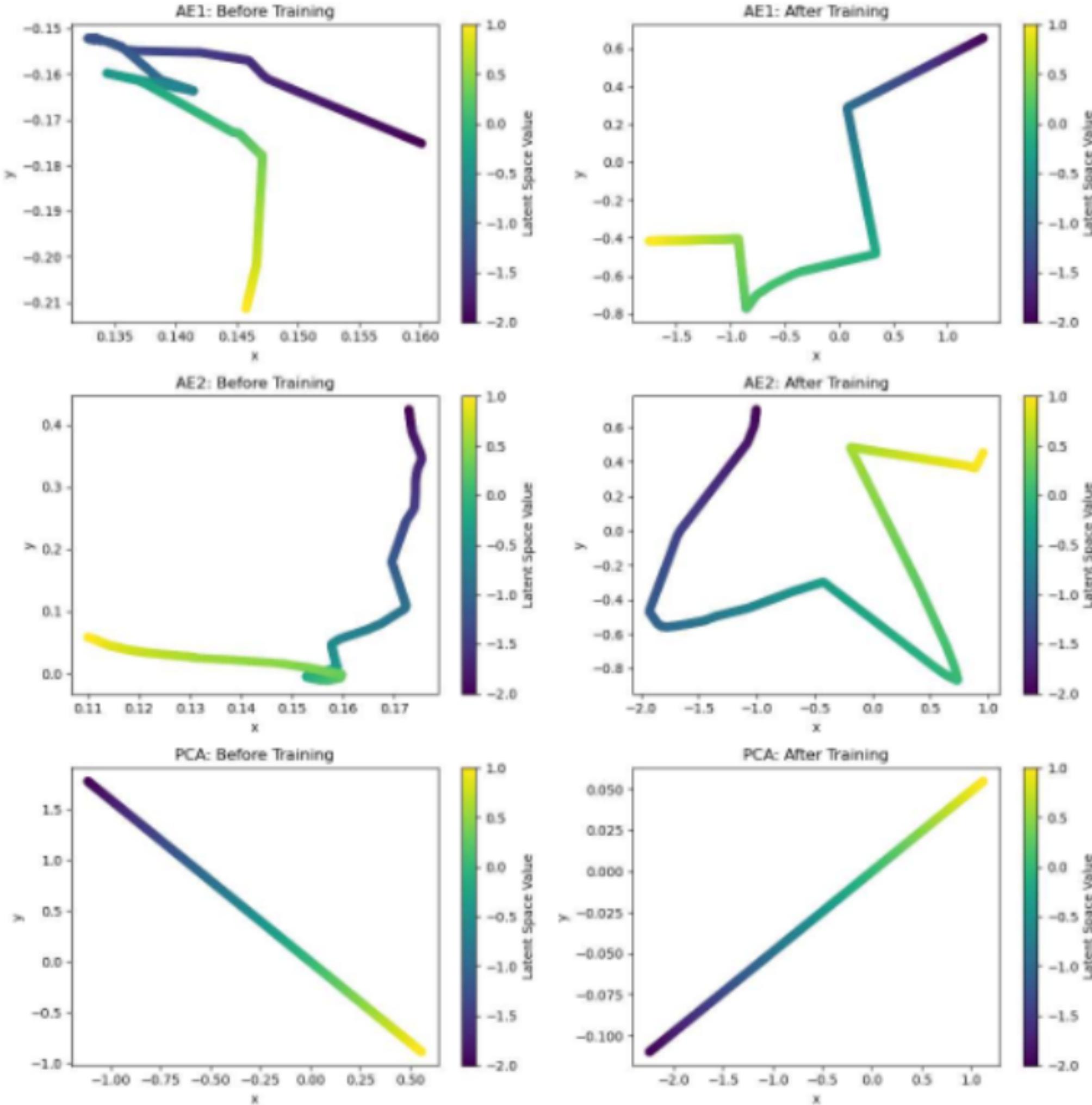
for i, (model, name) in enumerate(zip(models, ["AE1", "AE2", "PCA"])):
    random_decoder = random_models[i].autoencoder.decoder
    decoder = model.autoencoder.decoder

    with torch.no_grad():
        random_outputs = random_decoder(latent_samples)
        sc1 = axs[i, 0].scatter(random_outputs[:, 0], random_outputs[:, 1], ↵
            ↵c=latent_samples.squeeze(), cmap="viridis")
```

```
axs[i, 0].set_title(f"{name}: Before Training")
axs[i, 0].set_xlabel("x")
axs[i, 0].set_ylabel("y")
plt.colorbar(sc1, ax=axs[i, 0], orientation='vertical', label='Latent Space Value')

# After training
with torch.no_grad():
    trained_outputs = decoder(latent_samples)
    sc2 = axs[i, 1].scatter(trained_outputs[:, 0], trained_outputs[:, 1], c=latent_samples.squeeze(), cmap="viridis")
    axs[i, 1].set_title(f"{name}: After Training")
    axs[i, 1].set_xlabel("x")
    axs[i, 1].set_ylabel("y")
    plt.colorbar(sc2, ax=axs[i, 1], orientation='vertical', label='Latent Space Value')

plt.tight_layout()
plt.show()
```



The expectations for the random weights were fulfilled. For the trained case the AE 1 fulfilled the increase with lower x and less dependency on y despite not observing higher values with decreasing y. AE2 does not correspond to the expected outcome as the highest values were expected in the lower right corner. AE PCA behaves as expected. It increases in the x direction and the y direction has only minor influence.

1.1.5 (e)

Given a sufficient amount of parameters and non-linearities the model will be able to reconstruct the data due to the universal approximation theorem and the ability to map n datapoints to distinct values in \mathbb{R}^1 which can then be reconstructed. The drawback is that the model overfits and loses generalizability in this case as it memorizes the dataset.

1.1.6 (f)

The training of the encoder will be constrained by the fixed values of the decoder. This results into less efficient, structured and interpretable latent representations, loss of generalizability due to the focus of the encoder on the discriminator and lower reconstruction quality. Those are the causes of an imbalanced training.

1.1.7 (g)

```
[9]: autoencoder_module_2_for_retraining = AutoencoderModule(hidden_channels=[50, ↴50])
      trainer = pl.Trainer(max_epochs=1000)
      print("Model overview:", autoencoder_module_2_for_retraining)
      trainer.fit(autoencoder_module_2_for_retraining, data_loader)
```

GPU available: False, used: False
TPU available: False, using: 0 TPU cores
HPU available: False, using: 0 HPUs

	Name	Type	Params	Mode
0	autoencoder	Autoencoder	5.5 K	train

5.5 K Trainable params
0 Non-trainable params
5.5 K Total params
0.022 Total estimated model params size (MB)

Model overview: AutoencoderModule(
 (autoencoder): Autoencoder(
 (encoder): Sequential(
 (0): Linear(in_features=2, out_features=50, bias=True)
 (1): ReLU()
 (2): Linear(in_features=50, out_features=50, bias=True)
 (3): ReLU()
 (4): Linear(in_features=50, out_features=1, bias=True)
)
 (decoder): Sequential(
 (0): Linear(in_features=1, out_features=50, bias=True)
 (1): ReLU()
 (2): Linear(in_features=50, out_features=50, bias=True)
 (3): ReLU()
 (4): Linear(in_features=50, out_features=2, bias=True)
)
)
)

Training: | 0/? [00:00<?, ?it/s]

```

`Trainer.fit` stopped: `max_epochs=1000` reached.

[10]: import numpy as np
encoded_data = autoencoder_module_2_for_retraining.autoencoder.encoder(data).
        .detach().numpy()

for param in autoencoder_module_2_for_retraining.autoencoder.decoder.
    .parameters():
    param.requires_grad = False

# Initialize encoder weights using a normal distribution (example)
for m in autoencoder_module_2_for_retraining.autoencoder.encoder:
    if isinstance(m, nn.Linear):
        nn.init.normal_(m.weight, mean=0.0, std=1) # initialization (normal
        distribution)
        nn.init.zeros_(m.bias) # Zero initialization for biases

trainer = pl.Trainer(max_epochs=1000)
print("Model overview:", autoencoder_module_2_for_retraining)
trainer.fit(autoencoder_module_2_for_retraining, data_loader)

```

GPU available: False, used: False
 TPU available: False, using: 0 TPU cores
 HPU available: False, using: 0 HPUs

	Name	Type	Params	Mode
0	autoencoder	Autoencoder	5.5 K	train
2.8 K		Trainable params		
2.8 K		Non-trainable params		
5.5 K		Total params		
0.022		Total estimated model params size (MB)		

Model overview: AutoencoderModule(
 (autoencoder): Autoencoder(
 (encoder): Sequential(
 (0): Linear(in_features=2, out_features=50, bias=True)
 (1): ReLU()
 (2): Linear(in_features=50, out_features=50, bias=True)
 (3): ReLU()
 (4): Linear(in_features=50, out_features=1, bias=True)
)
 (decoder): Sequential(
 (0): Linear(in_features=1, out_features=50, bias=True)
 (1): ReLU()
 (2): Linear(in_features=50, out_features=50, bias=True)
 (3): ReLU()

```
(4): Linear(in_features=50, out_features=2, bias=True)
)
)
)

Training: |          0/? [00:00<?, ?it/s]

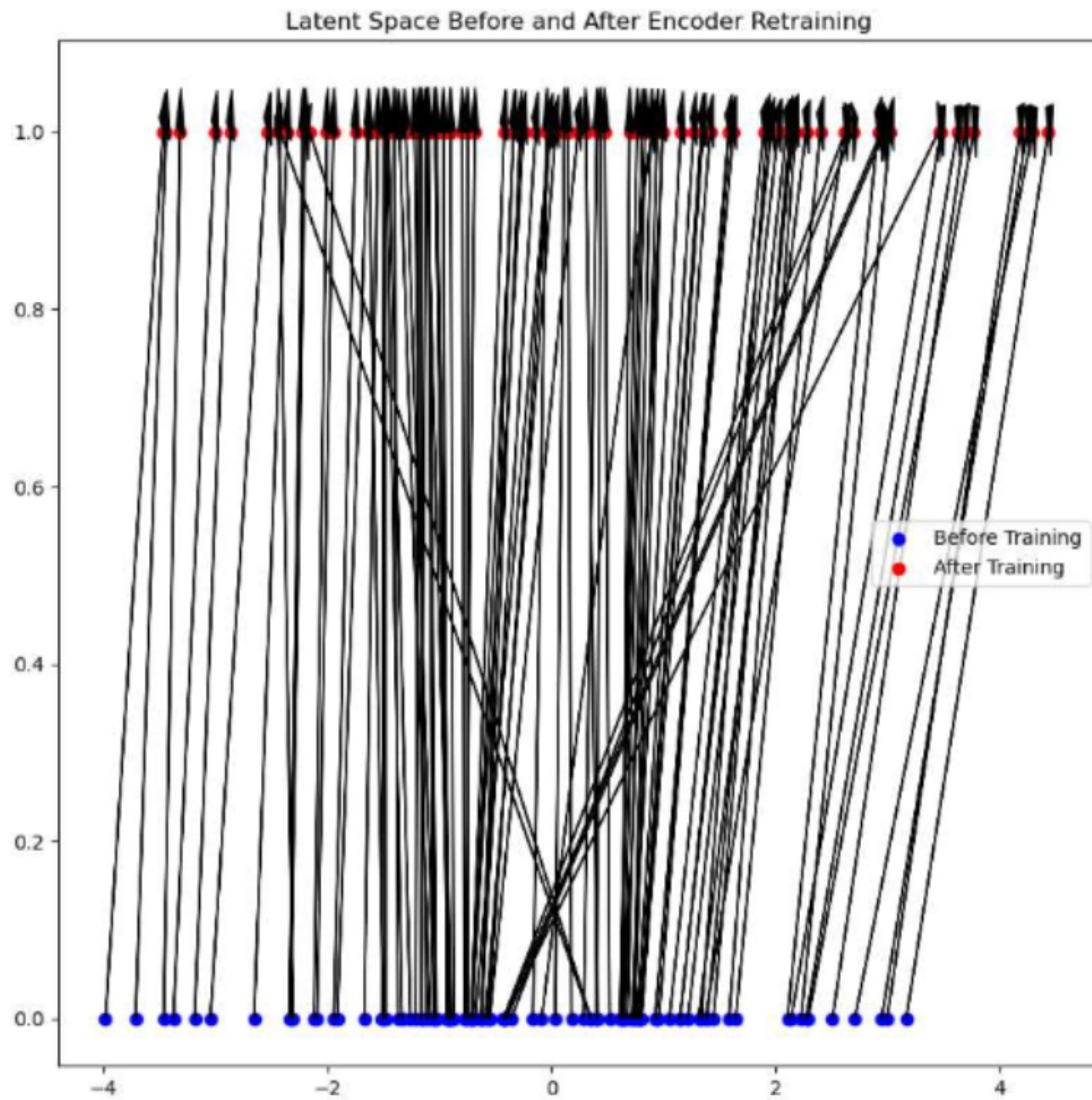
`Trainer.fit` stopped: `max_epochs=1000` reached.

[11]: encoded_data_after = autoencoder_module_2_for_retraining.autoencoder.
       encoder(data).detach().numpy()

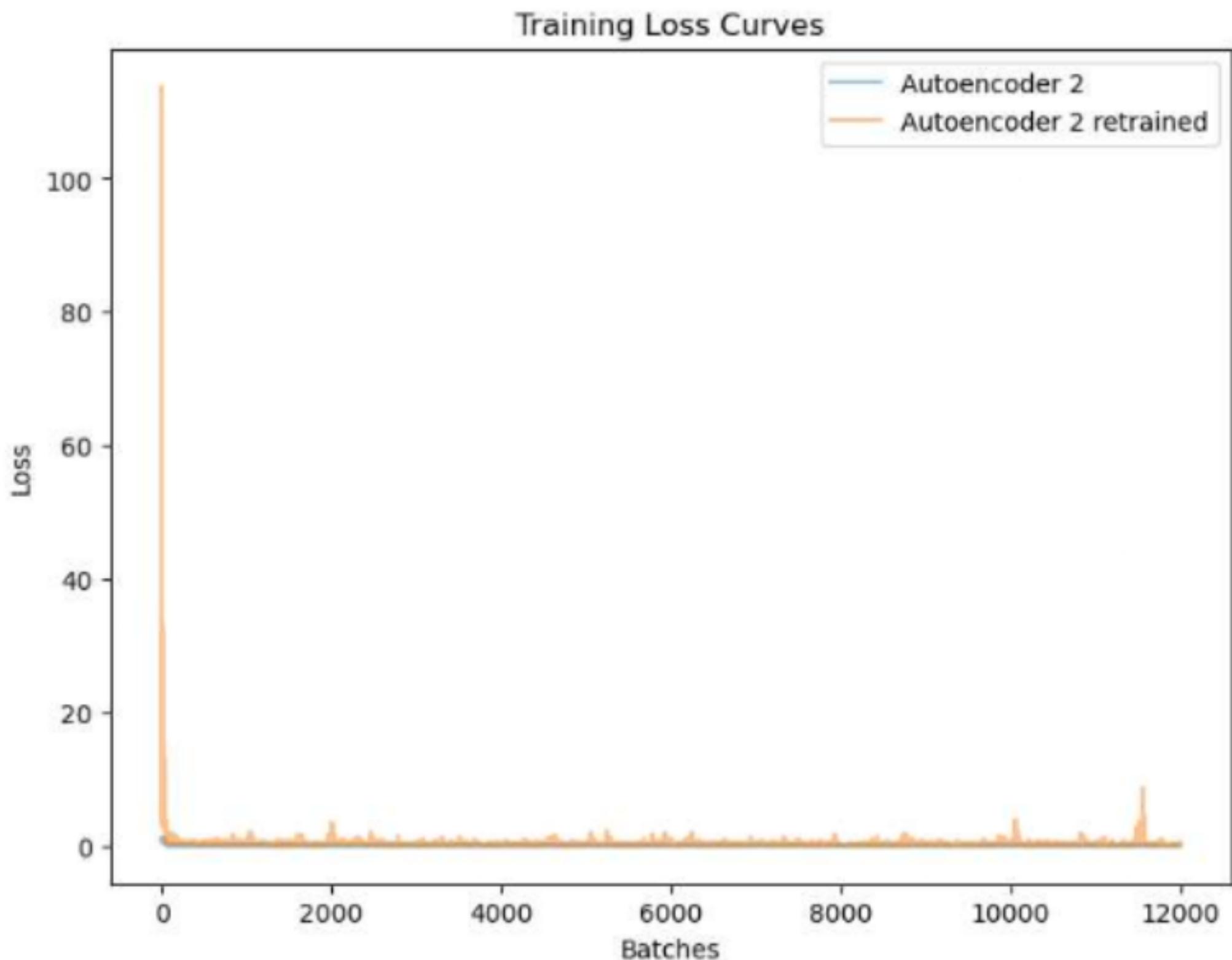
fig, ax = plt.subplots(figsize=(8, 8))
ax.scatter(encoded_data[:, 0], np.zeros_like(encoded_data[:, 0]), color='blue', label='Before Training')
ax.scatter(encoded_data_after[:, 0], np.zeros_like(encoded_data_after[:, 0])+1, color='red', label='After Training')

# Add arrows showing how the encoder's output changed after retraining
for i in range(len(data)):
    ax.arrow(encoded_data[i, 0], 0, encoded_data_after[i, 0] - encoded_data[i, 0], 1, head_width=0.07, head_length=0.05, fc='black', ec='black')

ax.set_title('Latent Space Before and After Encoder Retraining')
ax.legend()
plt.tight_layout()
plt.show()
```



```
[12]: autoencoder_names = ["2", "2 retrained"]
models = [autoencoder_module_2, autoencoder_module_2_for_retraining]
plt.figure(figsize=(8, 6))
for i, model in enumerate(models):
    plt.plot(model.loss_curve, label=f"Autoencoder {autoencoder_names[i]}",
             alpha=0.5)
plt.xlabel("Batches")
plt.ylabel("Loss")
plt.title("Training Loss Curves")
plt.legend()
plt.show()
```



The new latent space is different from the original one. The spread is determined by the width of the gaussian that is used for the reinitialization. The new latent space is not a scaled version as arrows from the embeddings cross each other. The loss of the retrained network is more variable and higher. This approves the hypothesis.

1.1.8 (h)

```
[13]: # Autoencoder module with SGD instead of Adam optimizer
```

```
class AutoencoderModule(pl.LightningModule):
    def __init__(self, **model_kwargs):
        super().__init__()
        self.autoencoder = Autoencoder(**model_kwargs)
        self.loss_curve = []

    def forward(self, x):
        return self.autoencoder(x)

    def configure_optimizers(self):
        optimizer = torch.optim.SGD(self.parameters())
```

```

    return optimizer

    def on_train_start(self):
        self.loss_curve = []
        return super().on_train_start()

    def training_step(self, batch):
        x, _ = batch
        x_hat = self.autoencoder(x)
        loss = nn.MSELoss()(x_hat, x)
        self.loss_curve.append(loss.item())
        return loss

```

```
[14]: autoencoder_module_2_sgd = AutoencoderModule(hidden_channels=[50, 50])
trainer = pl.Trainer(max_epochs=1000)
print("Model overview:", autoencoder_module_2_sgd)
trainer.fit(autoencoder_module_2_sgd, data_loader)
```

GPU available: False, used: False
TPU available: False, using: 0 TPU cores
HPU available: False, using: 0 HPUs

	Name	Type	Params	Mode
0	autoencoder	Autoencoder	5.5 K	train
5.5 K		Trainable params		
0		Non-trainable params		
5.5 K		Total params		
0.022		Total estimated model params size (MB)		

Model overview: AutoencoderModule(
(autoencoder): Autoencoder(
(encoder): Sequential(
(0): Linear(in_features=2, out_features=50, bias=True)
(1): ReLU()
(2): Linear(in_features=50, out_features=50, bias=True)
(3): ReLU()
(4): Linear(in_features=50, out_features=1, bias=True)
)
(decoder): Sequential(
(0): Linear(in_features=1, out_features=50, bias=True)
(1): ReLU()
(2): Linear(in_features=50, out_features=50, bias=True)
(3): ReLU()
(4): Linear(in_features=50, out_features=2, bias=True)
)

```
)  
)  
Training: | 0/? [00:00<?, ?it/s]
```

`Trainer.fit` stopped: `max_epochs=1000` reached.

```
[18]: # dataloader with only one batch to make GD instead of SGD  
data_loader = DataLoader(dataset, batch_size=100, shuffle=True, drop_last=True)  
autoencoder_module_2_gd = AutoencoderModule(hidden_channels=[50, 50])  
trainer = pl.Trainer(max_epochs=1000)  
print("Model overview:", autoencoder_module_2_gd)  
trainer.fit(autoencoder_module_2_gd, data_loader)
```

GPU available: False, used: False
TPU available: False, using: 0 TPU cores
HPU available: False, using: 0 HPUs

	Name	Type	Params	Mode
0	autoencoder	Autoencoder	5.5 K	train
			5.5 K	Trainable params
			0	Non-trainable params
			5.5 K	Total params
			0.022	Total estimated model params size (MB)

Model overview: AutoencoderModule(
 (autoencoder): Autoencoder(
 (encoder): Sequential(
 (0): Linear(in_features=2, out_features=50, bias=True)
 (1): ReLU()
 (2): Linear(in_features=50, out_features=50, bias=True)
 (3): ReLU()
 (4): Linear(in_features=50, out_features=1, bias=True)
)
 (decoder): Sequential(
 (0): Linear(in_features=1, out_features=50, bias=True)
 (1): ReLU()
 (2): Linear(in_features=50, out_features=50, bias=True)
 (3): ReLU()
 (4): Linear(in_features=50, out_features=2, bias=True)
)
)
)

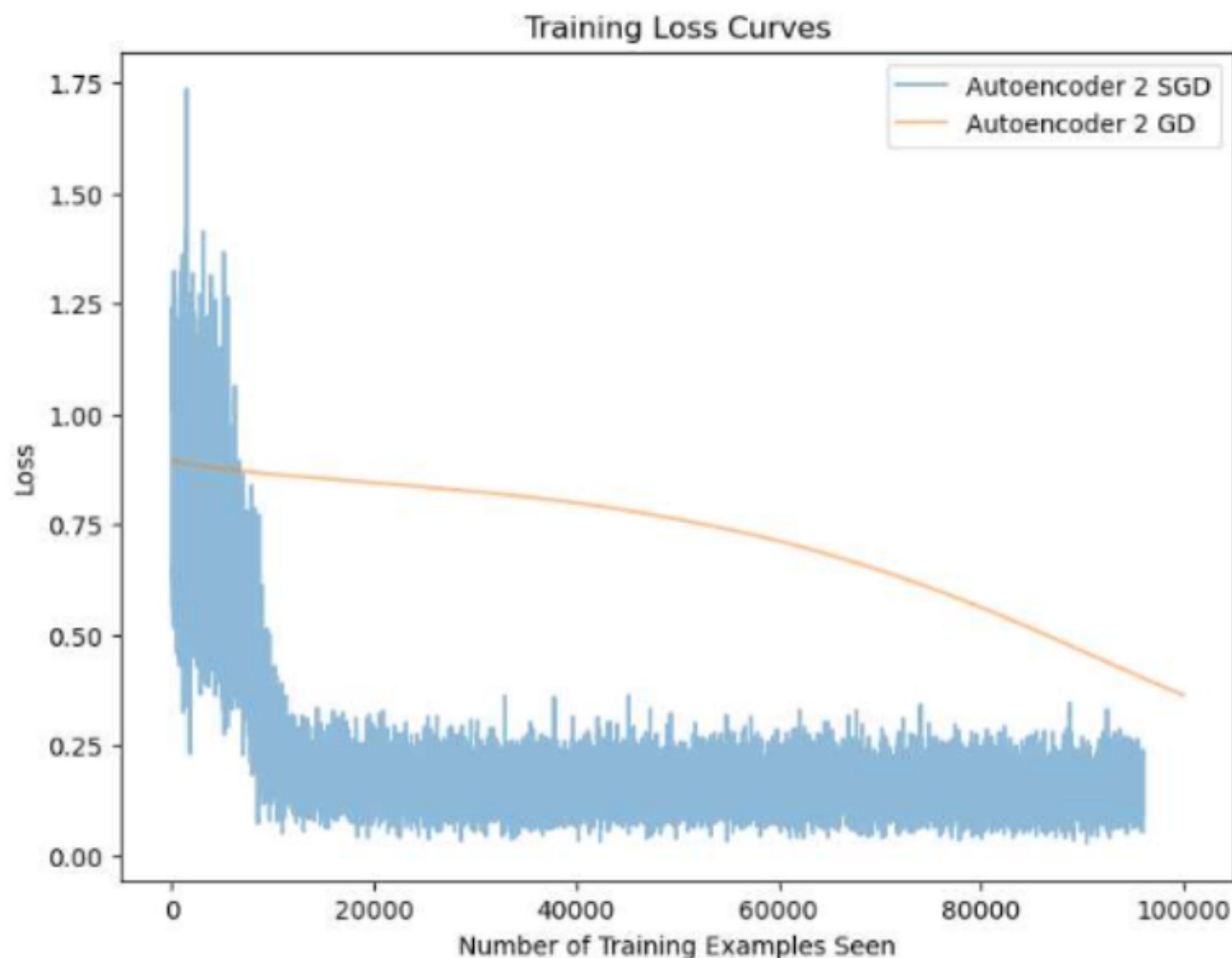
c:\Users\sasch\miniconda3\envs\mlph3\lib\site-packages\pytorch_lightning\loops\fit_loop.py:298: The number of training batches (1) is smaller than the logging interval Trainer(log_every_n_steps=50). Set a

lower value for log_every_n_steps if you want to see logs for the training epoch.

Training: | 0/? [00:00<?, ?it/s]

`Trainer.fit` stopped: `max_epochs=1000` reached.

```
[38]: autoencoder_names = ["2 SGD", "2 GD"]
models = [autoencoder_module_2_sgd, autoencoder_module_2_gd]
num_training_examples = [list(range(8, 8*12*1000+1, 8)), list(range(100, 100*1*1000+1, 100))] #num training samples given by step=num batch size, and total train_data_seen=batch_size*num_batches*epochs+
plt.figure(figsize=(8, 6))
for i, model in enumerate(models):
    plt.plot(num_training_examples[i], model.loss_curve, label=f"Autoencoder {autoencoder_names[i]}", alpha=0.5)
plt.xlabel("Number of Training Examples Seen")
plt.ylabel("Loss")
plt.title("Training Loss Curves")
plt.legend()
plt.show()
```



As expected gradient descent has less variation of the loss but decreases slower.

[]:

2 Bonus: Training of an MLP

a)



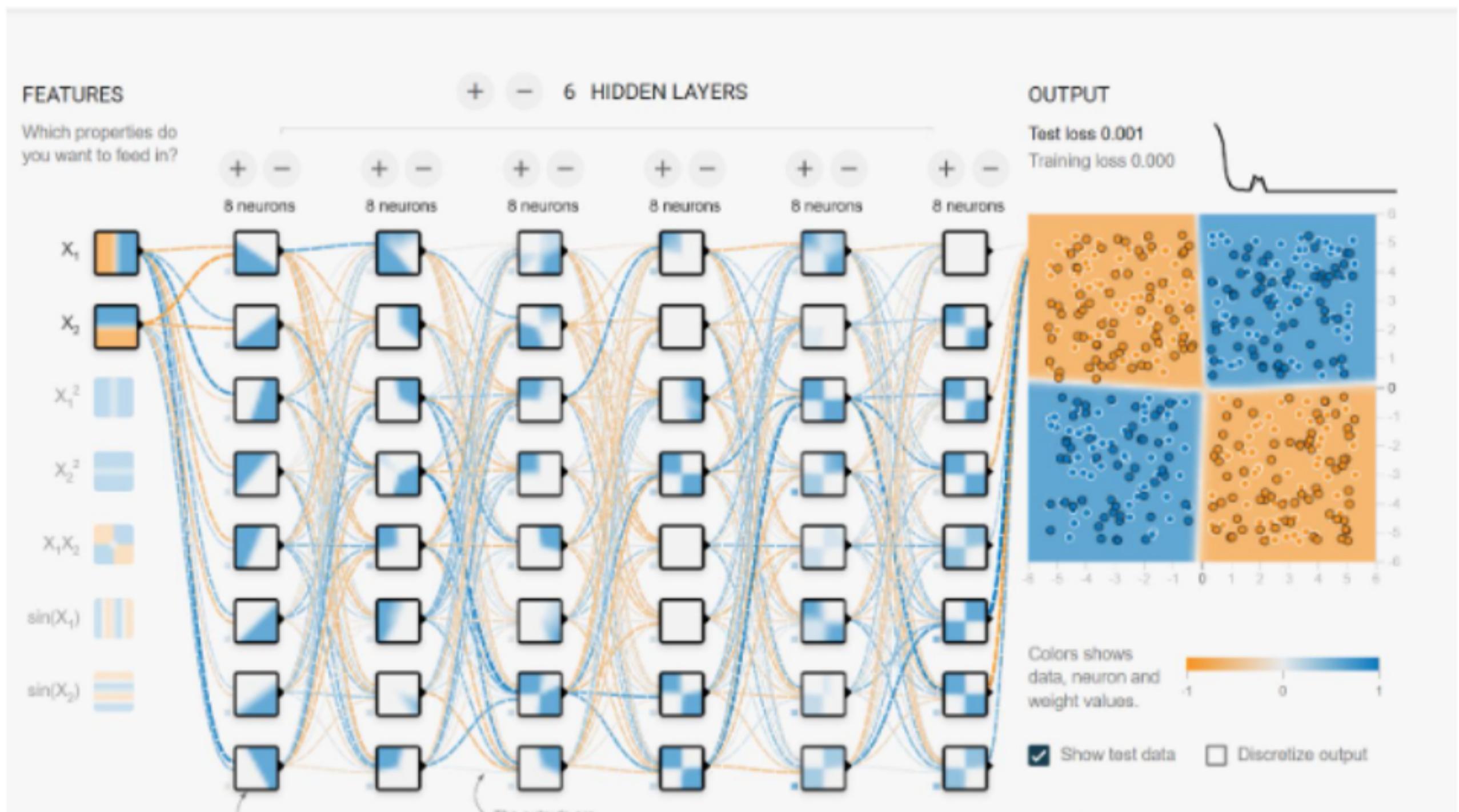
The best NN configuration we could find in terms of fast loss convergence, a low loss and little model complexity can be seen in the screenshot above. The loss converged at around 250. General observations are listed below:

- Ratio of training to test data: In all cases, increasing the ratio of training to test data, significantly increased the ability of the network to fit the data. However, for our configuration this is kept standard at 50% as we wanted to avoid low variance.
- Number of Neurons per layer: It was observed, that a high number of neurons per layer is preferable. Adding just one layer with less neurons increases the loss. This is likely due to the complexity of the data, which makes the loss of information due to less neurons in a layer quite significant. This could be observed in the picture of the neurons and the final fit, which become more chunky and less round.
- Number of layers: Adding more than two layers yielded no advantage. The training took longer and was less stable.
- Learning rate: 0.1 seemed the largest possible learning rate. Larger ones created a less stable loss curve with large jumps in the error. Smaller ones are possible but the training takes longer.
- Activation function: Tanh and sigmoid took a significant amount of training time, especially at the beginning. This is likely due to the vanishing gradients of these loss functions, which ReLU does not have

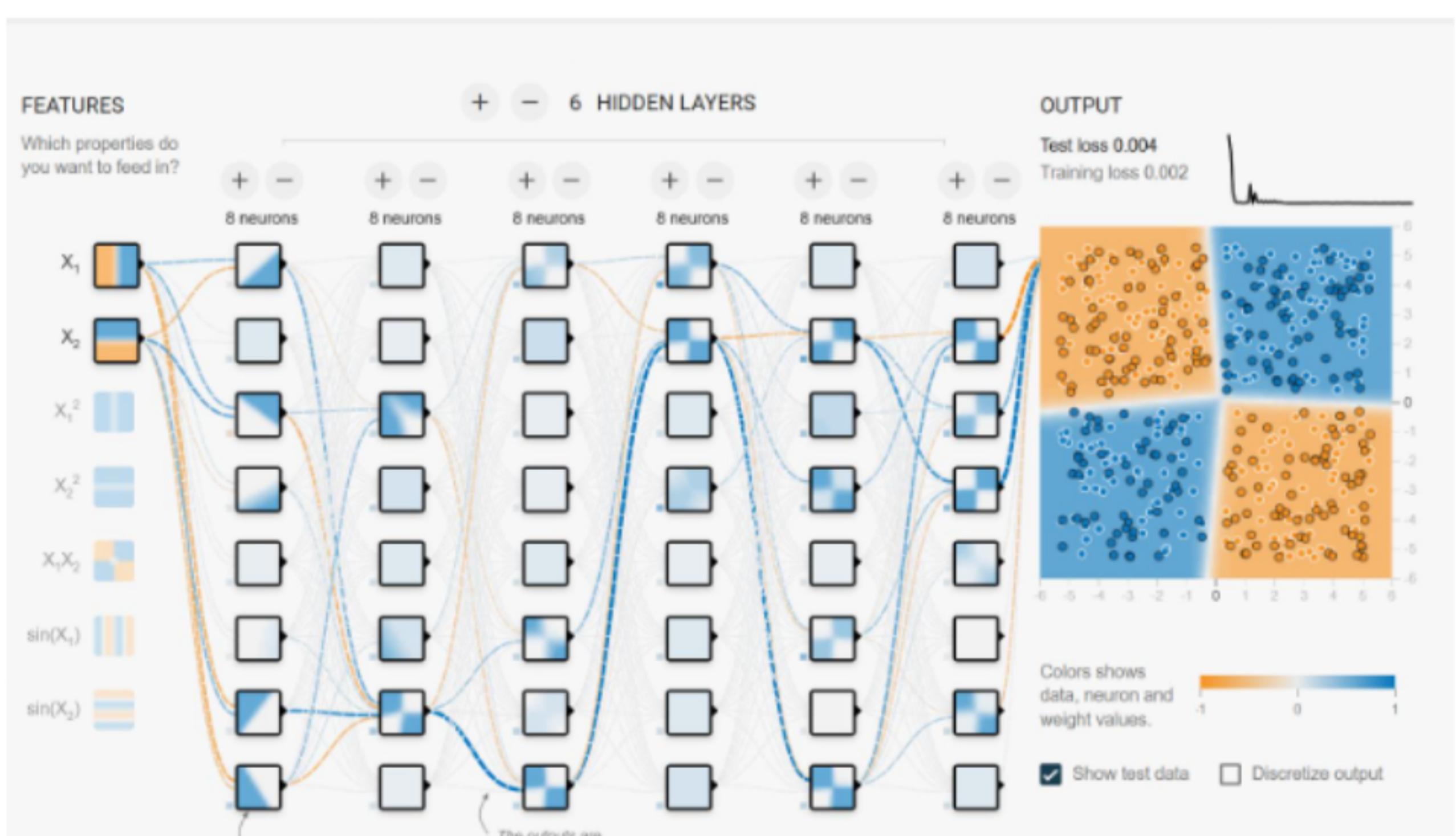
b)

Without regularization, we expect many neurons to be similar, meaning “they have learned the same”. Making many of them redundant. With L_2 we expect that the weight of those redundant neurons becomes less, with L_1 even zero. This expected behaviour could very well be seen in the following three screenshots.

Epoch	Learning rate	Activation	Regularization	Regularization rate	Problem type
000,046	0.1	ReLU	None	0	Classification

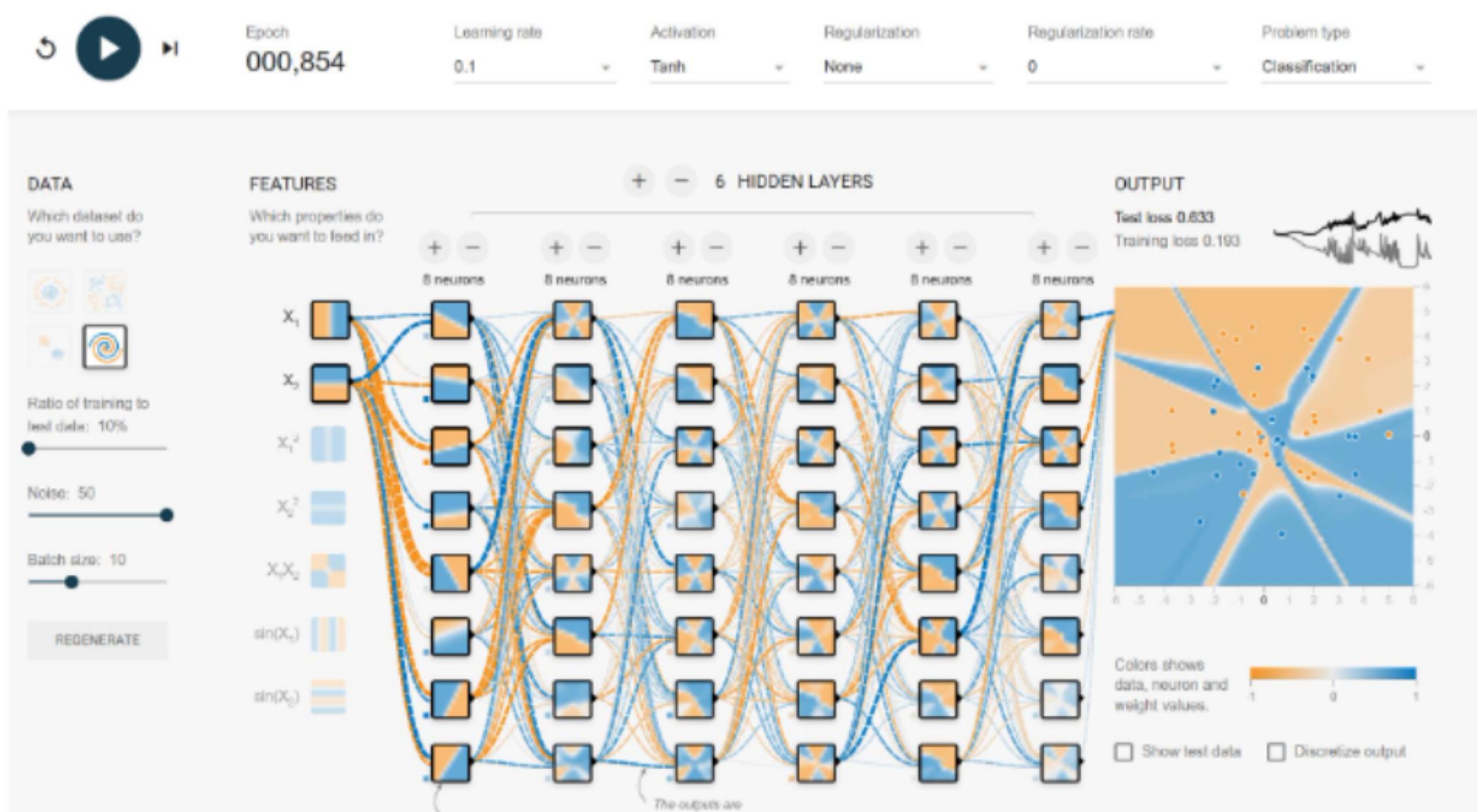


Epoch	Learning rate	Activation	Regularization	Regularization rate	Problem type
000,084	0.1	ReLU	L1	0.003	Classification





c)



We can see, that the training loss is relatively low in comparison to the test loss. The test data is a spiral, whereas the training data looks rather random. I was not possible however to train the net perfectly.