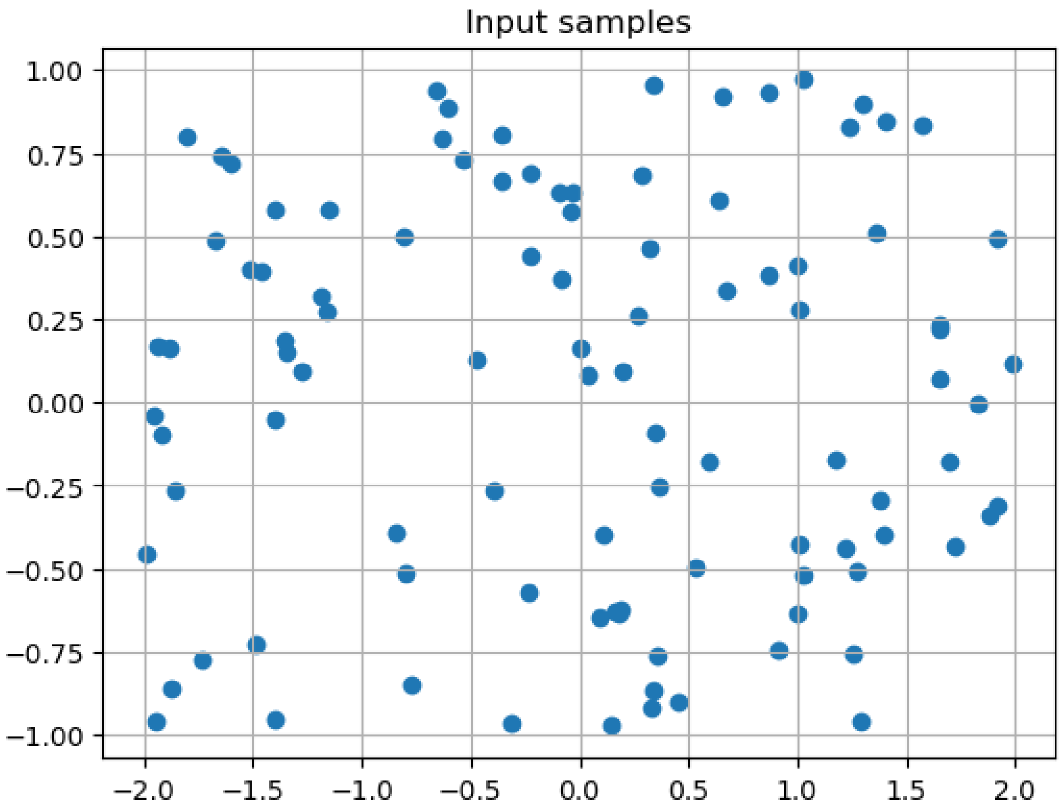
sheet06

December 2, 2024

1 Sheet 6

1.1 1 Autoencoders: theory and practice

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

# create 100 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]:
```python
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
```

2 (a)

We use a ReLU activation on every layer except for the bottleneck as a standard choice. For the bottleneck layer, we wanted to use the sigmoid activation function, so that our latent representations are constrained to [0,1] interval, but that would require a deeper network to invert the function.

[3]:
```python
import torch
from torch import nn
import pytorch_lightning as pl


class Autoencoder(nn.Module):
    def __init__(
        self,
        dims: list[int],
        activation: Optional[type[nn.Module]] = None,
        bottleneck_activation: Optional[type[nn.Module]] = None,
        latent_dim=1,
        input_dim=2,
    ):
        if activation is None:
            activation = nn.ReLU
        if bottleneck_activation is None:
            bottleneck_activation = nn.Identity
        # dims: layer output dims starting from first hidden layer inclusive to
        # bottleneck exclusive
        super().__init__()

        layers = lambda dims: sum(
            [[nn.LazyLinear(i), activation()] for i in dims], start=[]
        )
        self.encoder = nn.Sequential(
            *layers(dims), nn.LazyLinear(latent_dim), bottleneck_activation()
        )
        self.decoder = nn.Sequential(*layers(dims[::-1]), nn.
↪LazyLinear(input_dim))

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


class AutoencoderModule(pl.LightningModule):
    def __init__(
        self,
        lr: Optional[float] = None,
        optim: Optional[type[torch.optim.Optimizer]] = None,
        **model_kwargs,
    ):
        super().__init__()
        self.autoencoder = Autoencoder(**model_kwargs)
        self.loss_curve = []
```

```
        if lr is None:
            lr = 0.001
        self.lr = lr
        if optim is None:
            optim = torch.optim.Adam
        self.optim = optim

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

    def configure_optimizers(self):
        optimizer = self.optim(self.parameters(), lr=self.lr)

        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
```

[4]:
```
def get_module(
    dims,
    act: Optional[type[nn.Module]] = None,
    bact: Optional[type[nn.Module]] = None,
    train=True,
    decoder=None,
    lr=None,
    optim=None,
    batchsize=None,
):
    module = AutoencoderModule(
        dims=dims, activation=act, bottleneck_activation=bact, lr=lr,␣
↪optim=optim
    )
    if decoder is not None:
        for param in decoder.parameters():
            param.requires_grad = False
        module.autoencoder.decoder = decoder
    if not train:
        return module
    trainer = pl.Trainer(max_epochs=1000, enable_checkpointing=False)
```

```
    print("Model overview:", module)
    loader = data_loader
    if batchsize is not None:
        loader = DataLoader(dataset, batch_size=batchsize)
        print("dataloader size:", len(loader))
    trainer.fit(module, loader)
    return module


def plot_loss(module, desc):
    plt.title("loss plot")
    plt.plot(module.loss_curve, label=desc, alpha=0.5)


def plot_data(module, desc):
    # plots latent representation in the original space
    latent = module.autoencoder.encoder(data).detach().numpy()
    plt.figure(figsize=(8, 6))
    plt.scatter(data[:, 0], data[:, 1], c=latent)
    plt.colorbar()
    plt.title(f"Latent representation of the data in the original space, model:␣
 ↪{desc}")
    plt.ylim(-1, 1)
    plt.xlim(-2, 2)
    plt.show()


def plot_space(module, desc, start=-10, end=10):
    latent = torch.linspace(start, end, 1000).reshape(-1, 1)
    reconstructed = module.autoencoder.decoder(latent).detach().numpy()
    plt.figure(figsize=(8, 6))
    plt.scatter(reconstructed[:, 0], reconstructed[:, 1], c=latent)
    plt.colorbar()
    plt.title(f"Latent space embedded in the original space, model: {desc}")
    plt.ylim(-1, 1)
    plt.xlim(-2, 2)
    plt.show()
```

3 (b)

[5]:
```
pca = get_module([], bact=nn.Identity)
small = get_module([20, 10])
big = get_module([50, 50, 50])
```

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

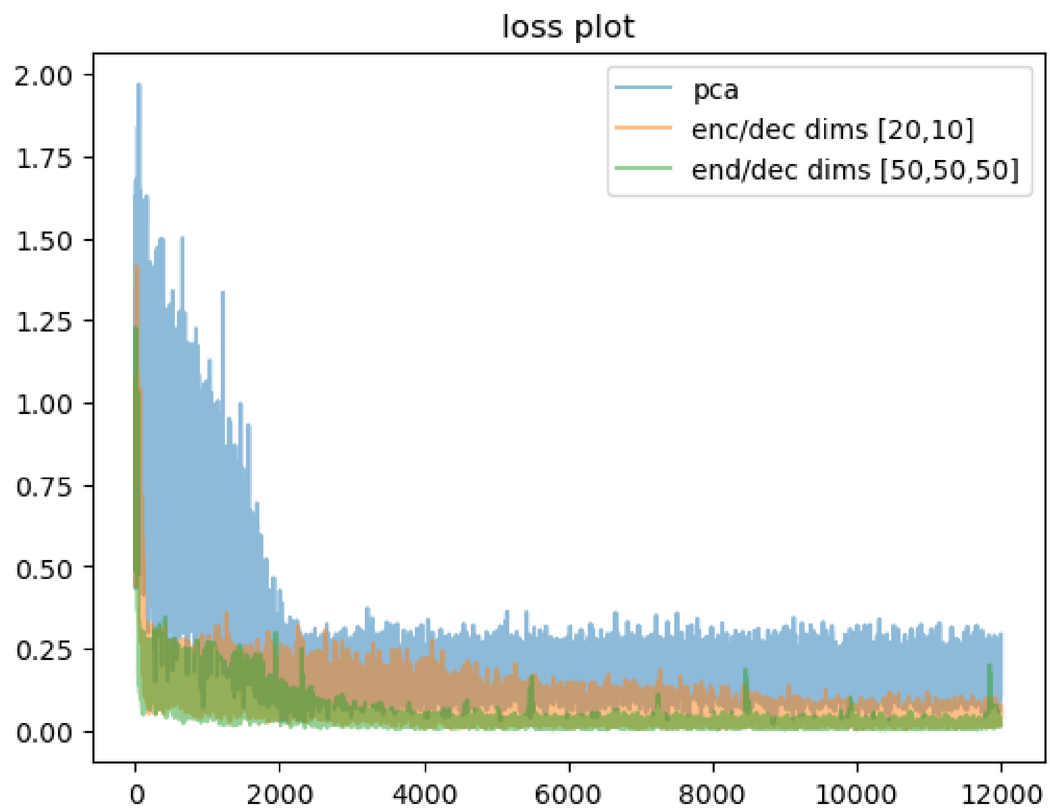
```
/nix/store/68cqjvbnv7xm4ff67zkhm6s1nxyb0z4h-python3-3.12.6-
env/lib/python3.12/site-
packages/pytorch_lightning/utilities/model_summary/model_summary.py:477: The
total number of parameters detected may be inaccurate because the model contains
an instance of `UninitializedParameter`. To get an accurate number, set
`self.example_input_array` in your LightningModule.

  | Name        | Type        | Params | Mode
----------------------------------------------------
0 | autoencoder | Autoencoder | 0      | train
----------------------------------------------------
0         Trainable params
0         Non-trainable params
0         Total params
0.000     Total estimated model params size (MB)
6         Modules in train mode
0         Modules in eval mode

Model overview: AutoencoderModule(
  (autoencoder): Autoencoder(
    (encoder): Sequential(
      (0): LazyLinear(in_features=0, out_features=1, bias=True)
      (1): Identity()
    )
    (decoder): Sequential(
      (0): LazyLinear(in_features=0, out_features=2, bias=True)
    )
  )
)

/nix/store/68cqjvbnv7xm4ff67zkhm6s1nxyb0z4h-python3-3.12.6-
env/lib/python3.12/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=31`
in the `DataLoader` to improve performance.
/nix/store/68cqjvbnv7xm4ff67zkhm6s1nxyb0z4h-python3-3.12.6-
env/lib/python3.12/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: |
                                     …

`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 | 0      | train
----------------------------------------------------
0         Trainable params
0         Non-trainable params
0         Total params
0.000     Total estimated model params size (MB)
14        Modules in train mode
0         Modules in eval mode

Model overview: AutoencoderModule(
  (autoencoder): Autoencoder(
    (encoder): Sequential(
      (0): LazyLinear(in_features=0, out_features=20, bias=True)
      (1): ReLU()
      (2): LazyLinear(in_features=0, out_features=10, bias=True)
      (3): ReLU()
      (4): LazyLinear(in_features=0, out_features=1, bias=True)
      (5): Identity()
    )
    (decoder): Sequential(
      (0): LazyLinear(in_features=0, out_features=10, bias=True)
      (1): ReLU()
      (2): LazyLinear(in_features=0, out_features=20, bias=True)
      (3): ReLU()
      (4): LazyLinear(in_features=0, out_features=2, bias=True)
    )
  )
)

Training: |
 ↪                                  …

`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 | 0      | train
----------------------------------------------------
0         Trainable params
0         Non-trainable params
0         Total params
0.000     Total estimated model params size (MB)
18        Modules in train mode
```

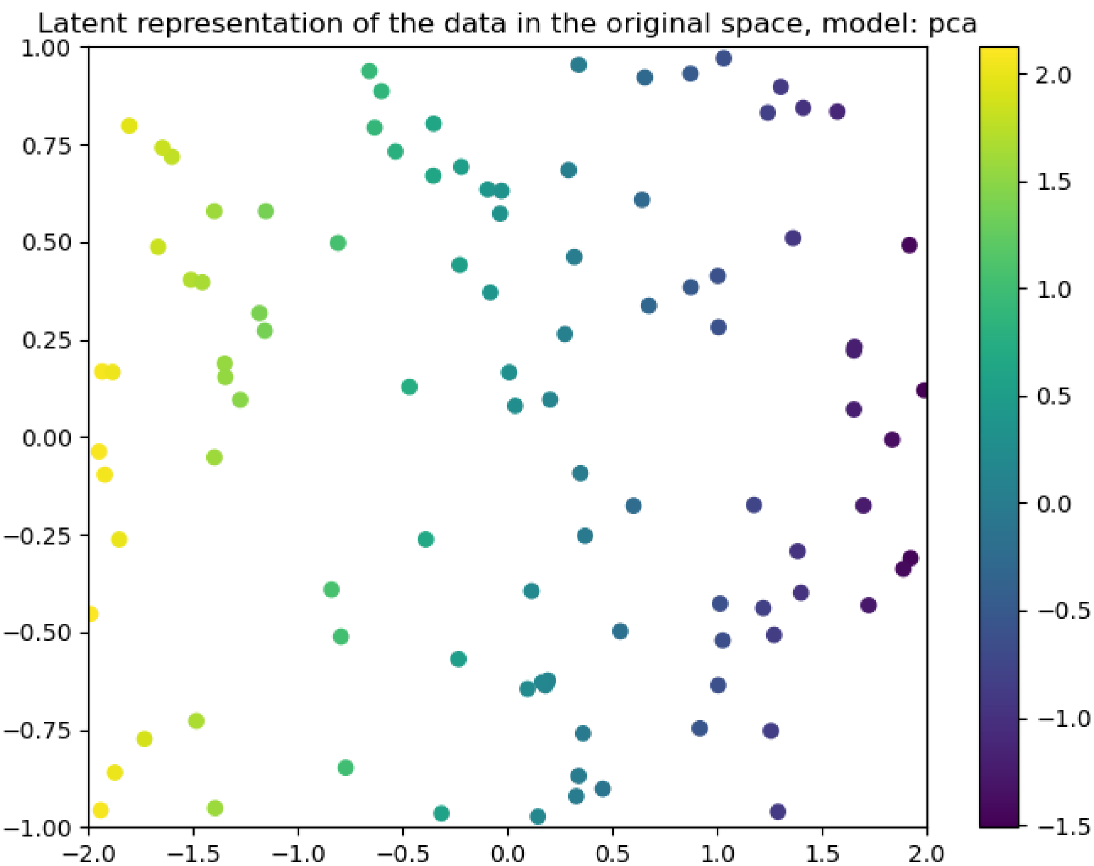
```
0         Modules in eval mode

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

Training: |
 ↪                                …

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

[6]:

```
plot_loss(pca, "pca")
plot_loss(small, "enc/dec dims [20,10]")
plot_loss(big, "end/dec dims [50,50,50]")
plt.legend()
plt.show()
```

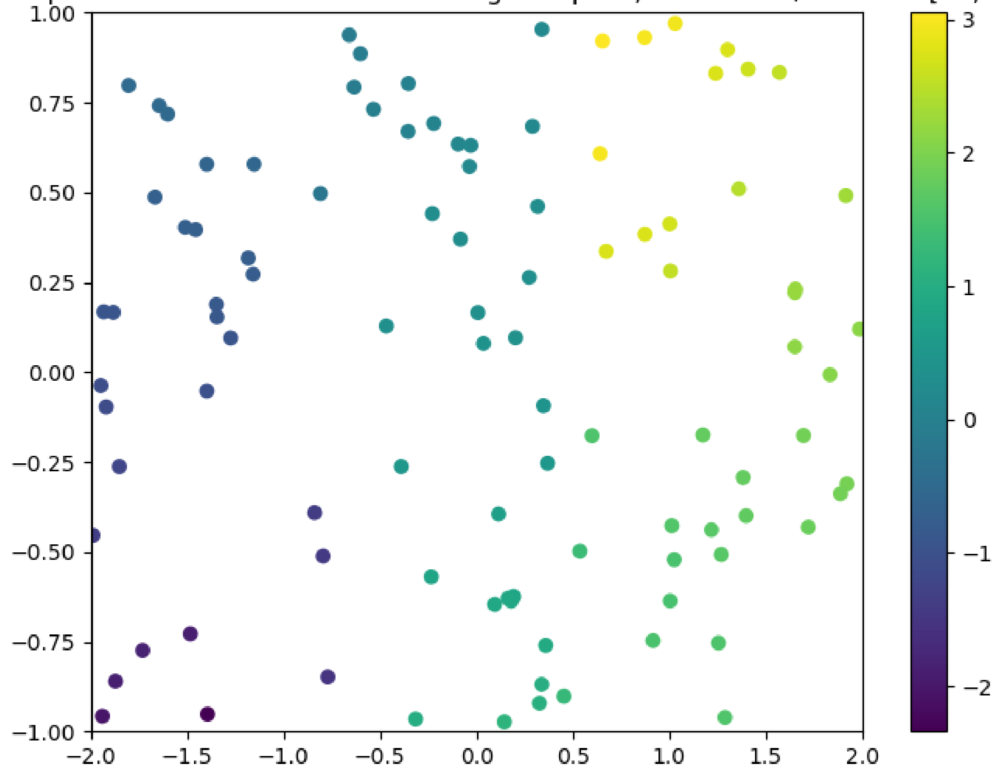


[7]:
```
plot_data(pca, "pca")
plot_data(small, "enc/dec dims [20,10]")
plot_data(big, "end/dec dims [50,50,50]")
```

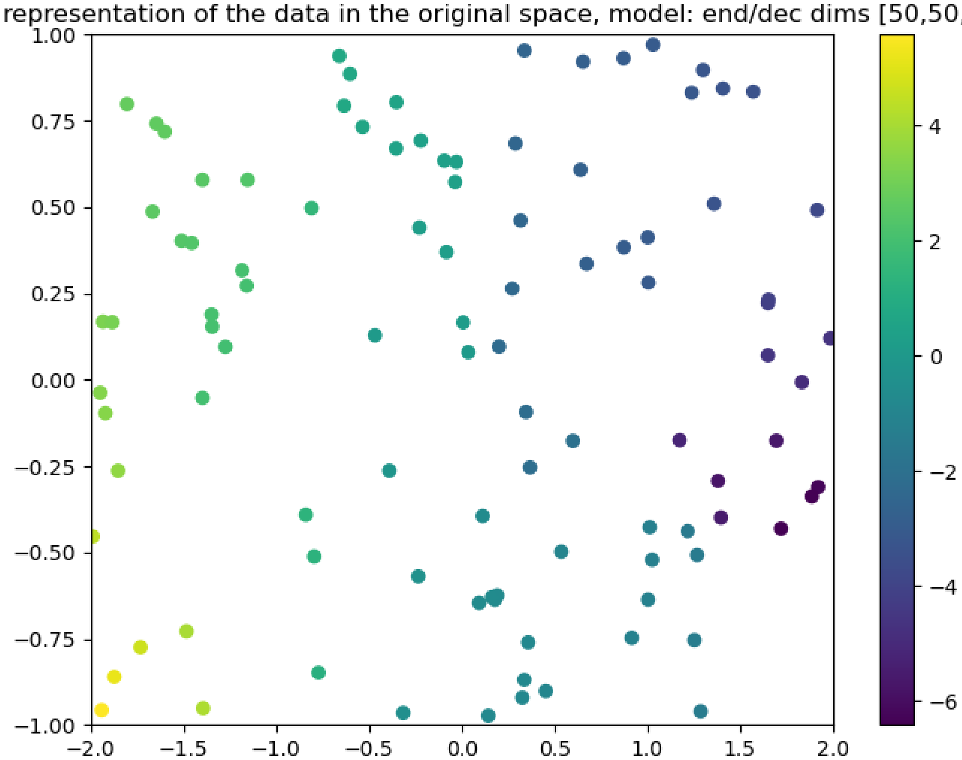


Latent representation of the data in the original space, model: pca
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5

Latent representation of the data in the original space, model: enc/dec dims [20,10]



Latent representation of the data in the original space, model: end/dec dims [50,50,50]

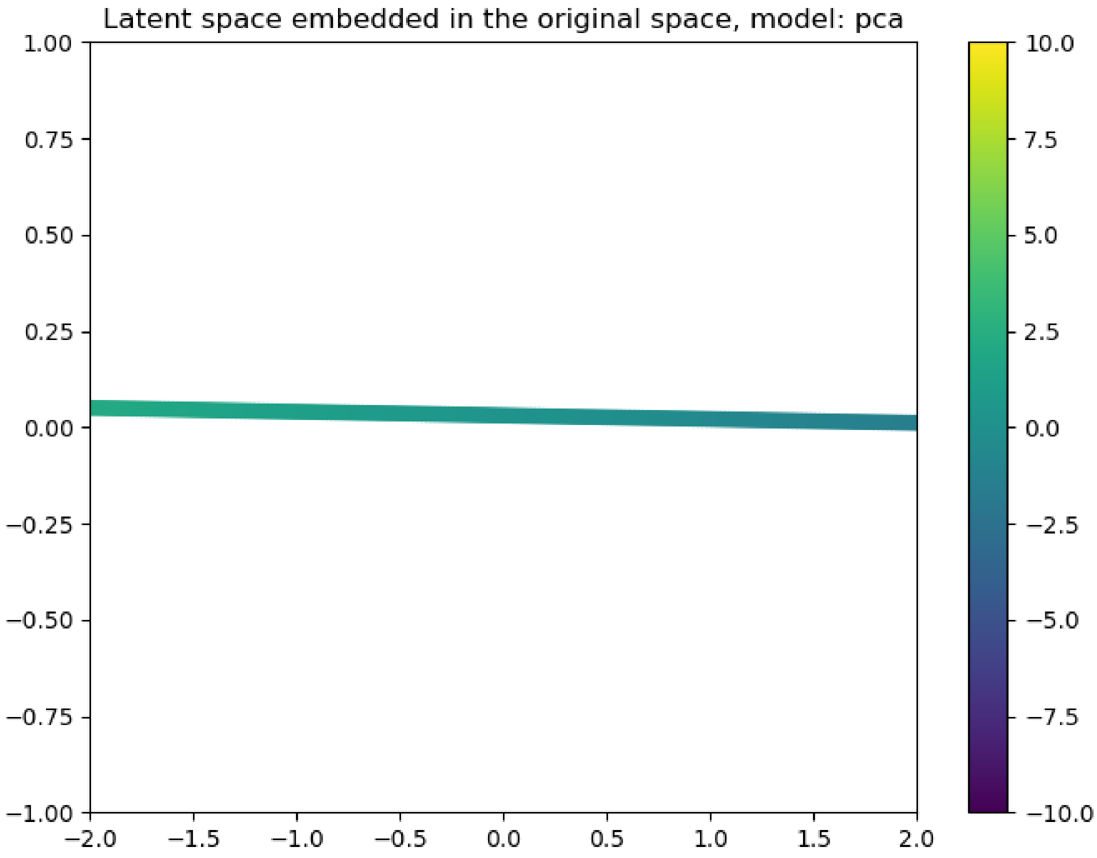


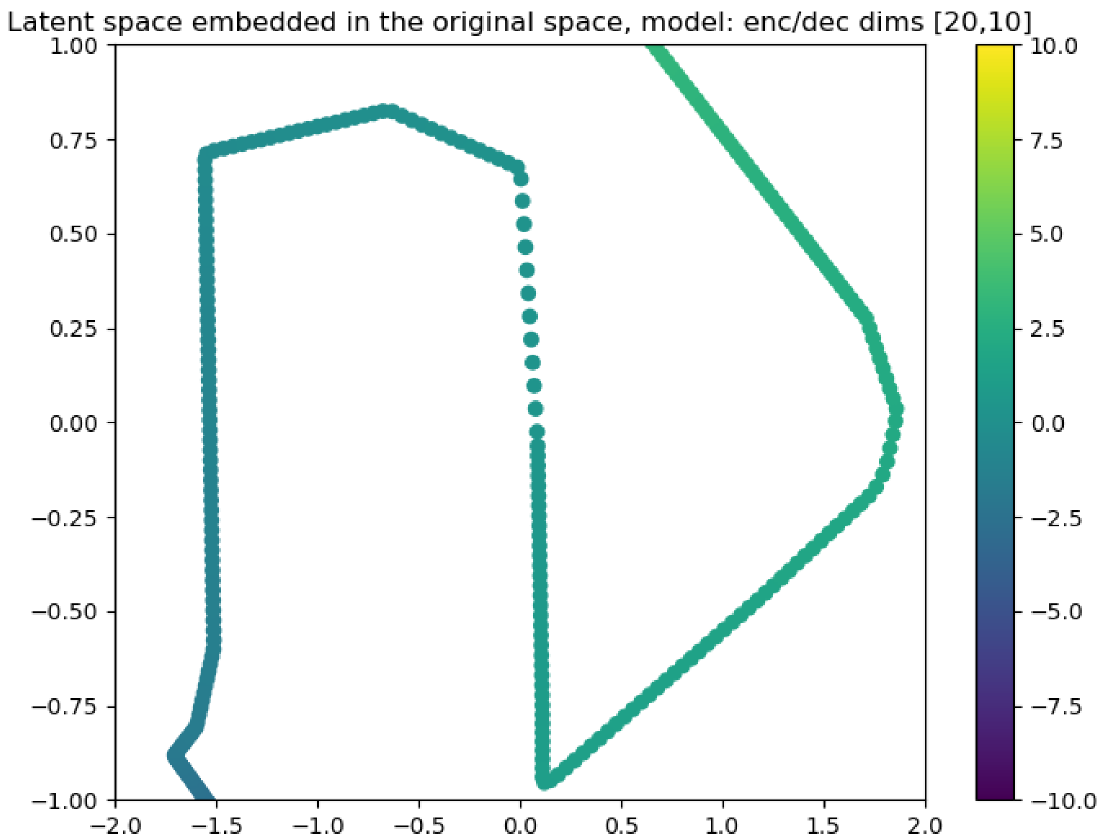
Plots look pretty much the same for all 3 models, except for the much slower convergence for PCA.

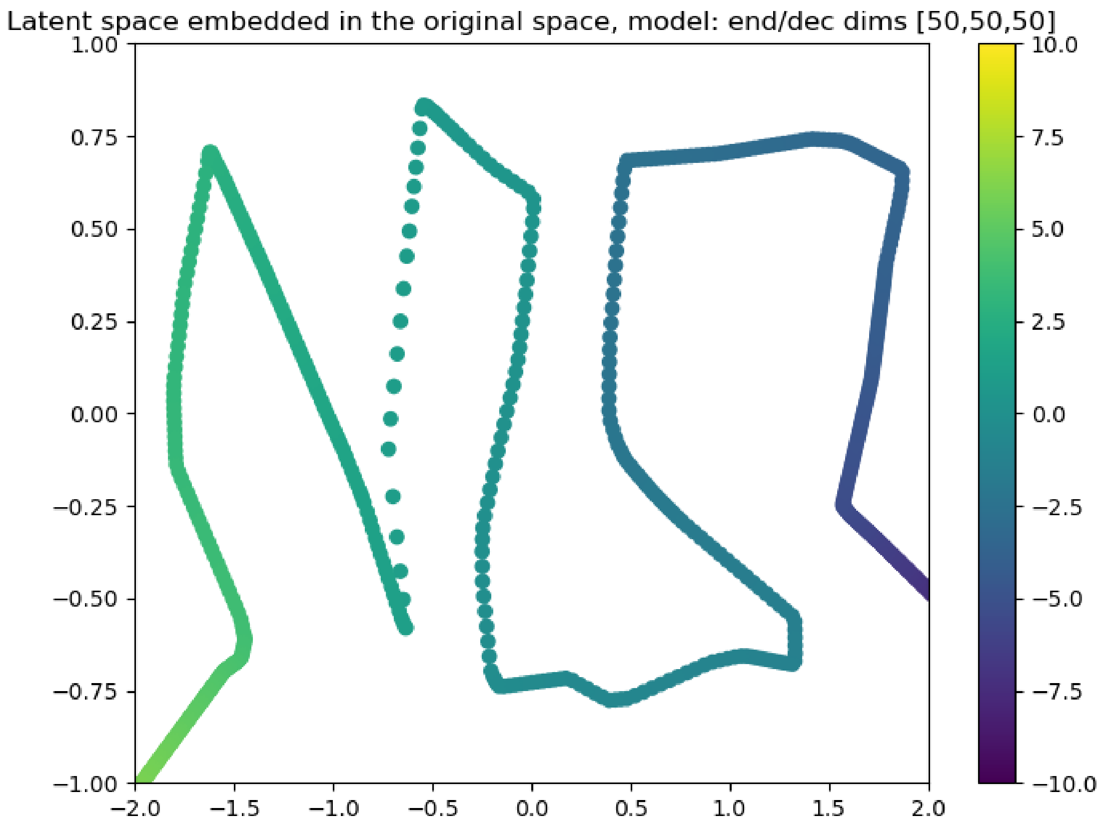
4 (c)

- PCA - a line.
  - Trained: line will be oriented along the x axis, due to the initial distribution
  - Untrained: random orientation
- Small autoencoder - piecewise-linear curve.
  - Trained: the curve will be more or less "dense" in the region that contains data
  - Untrained: most of the breakpoints will be around the origin, due to weight initialization
- Bigger autoencoder - same as the small autoencoder, but with more breakpoints in the curve

[8]:
```
plot_space(pca, "pca", start=-10, end=10)
plot_space(small, "enc/dec dims [20,10]")
plot_space(big, "end/dec dims [50,50,50]")
```

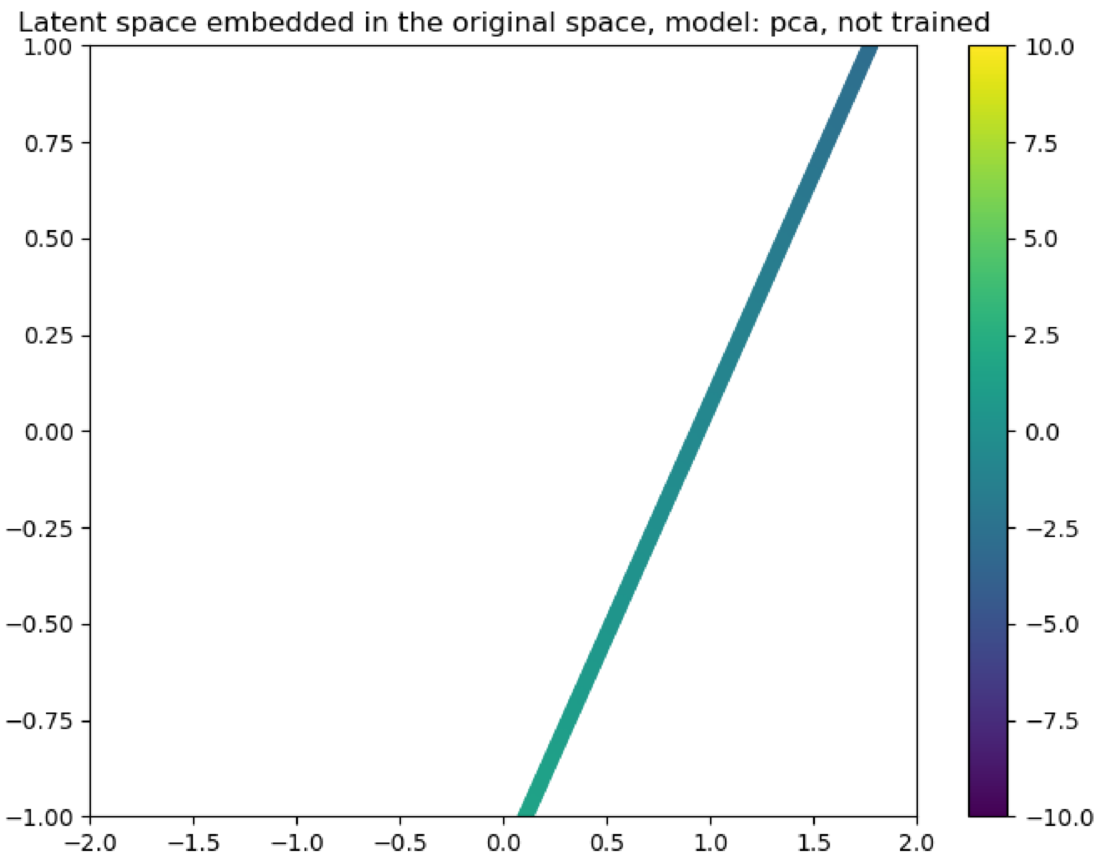



Latent space embedded in the original space, model: enc/dec dims [20,10]
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0

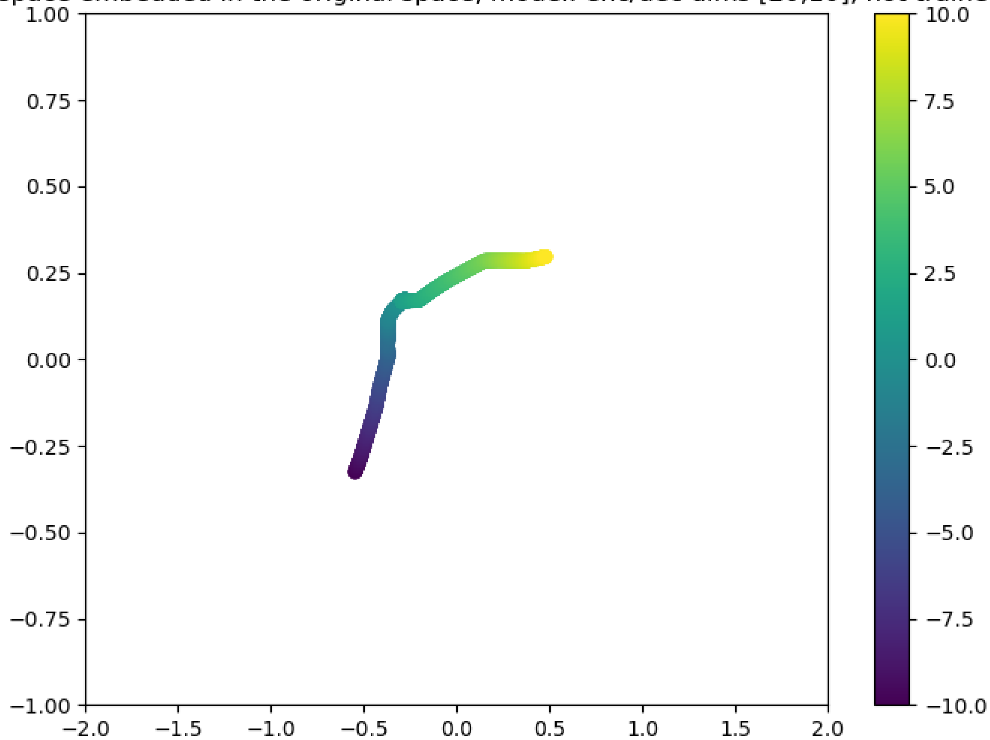


[9]:

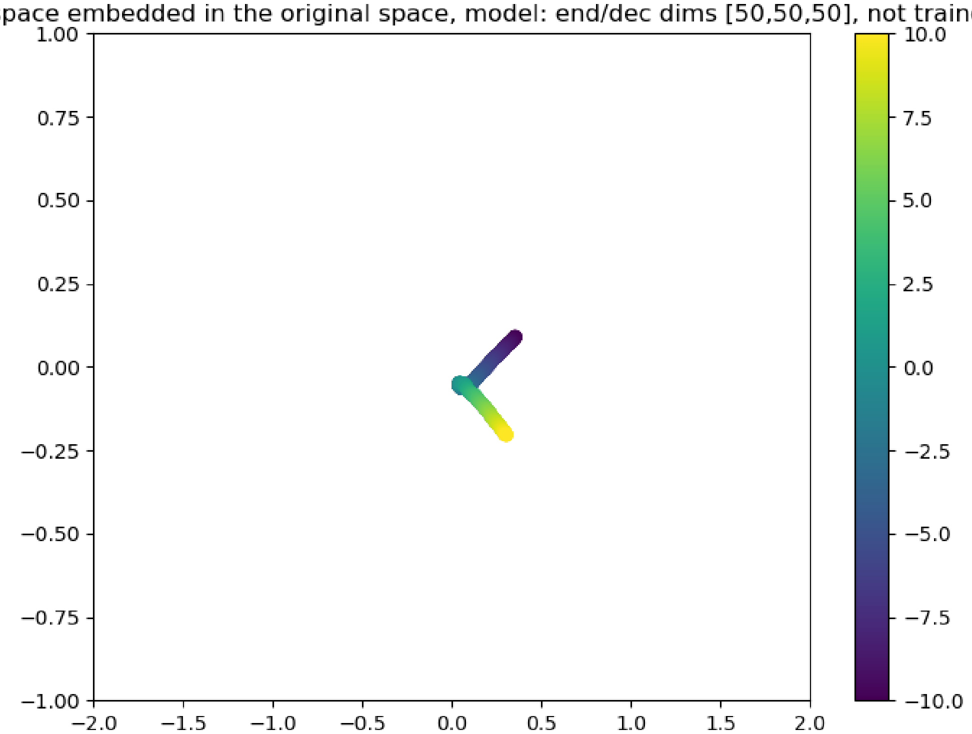
```
plot_space(get_module([], train=False), "pca, not trained", start=-10, end=10)
plot_space(get_module([20, 10], train=False), "enc/dec dims [20,10], not␣
↪trained")
plot_space(
    get_module([50, 50, 50], train=False), "end/dec dims [50,50,50], not␣
↪trained"
)
```


Latent space embedded in the original space, model: pca, not trained
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0

Latent space embedded in the original space, model: enc/dec dims [20,10], not trained



Latent space embedded in the original space, model: end/dec dims [50,50,50], not trained



5 (d)

We can observe the expected behaviour.

6 (e)

Yes. If we pick a simple curve that goes through all n points in the original space, then the latent space can be constructed as a parametrization of this curve. Since we can always find an invertible parametrization, the rest is just a question of finding an architecture that would be able to represent and learn such a parametrization.

7 (f)

The encoder will relearn approximately the same mapping, up to equivalence in the latent space. More concretely, the further the point is from the image of the decoder, the higher the change in latent space under such encoder replacement it is going to experience.

8 (g)

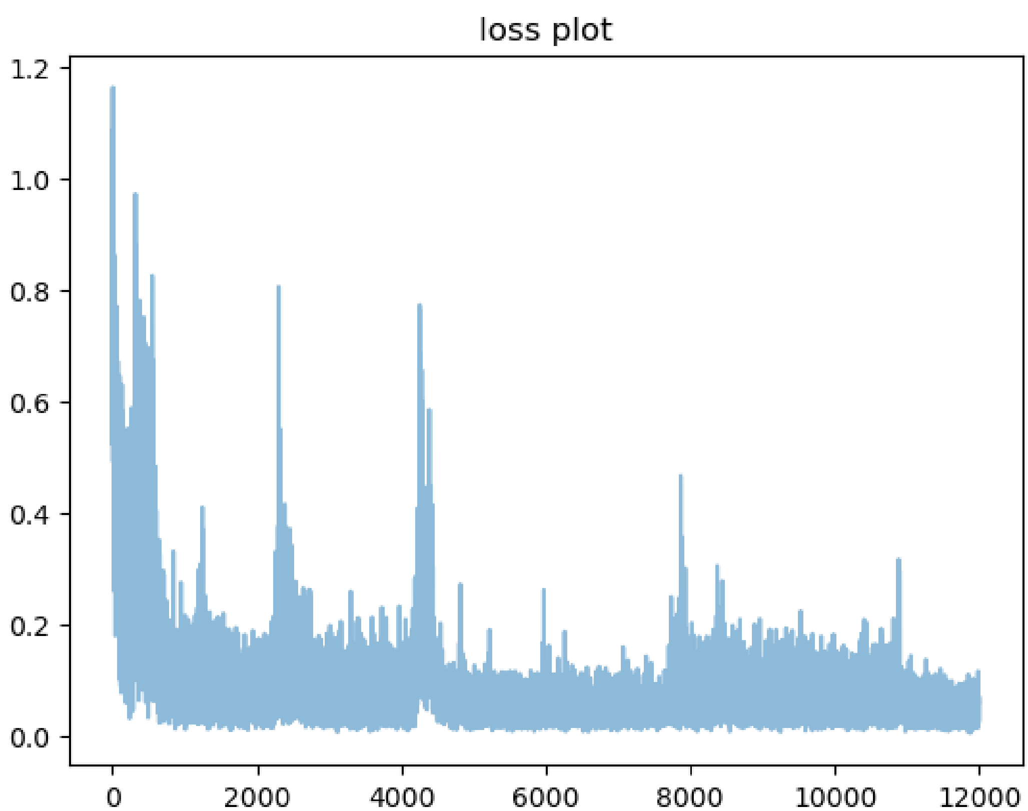
We chose to plot the absolute difference in the latent representation between two encoders

[10]:
```
big2 = get_module([50, 50, 50], train=True, decoder=big.autoencoder.decoder,␣
↪lr=0.01)
plot_loss(big2, desc="")
```

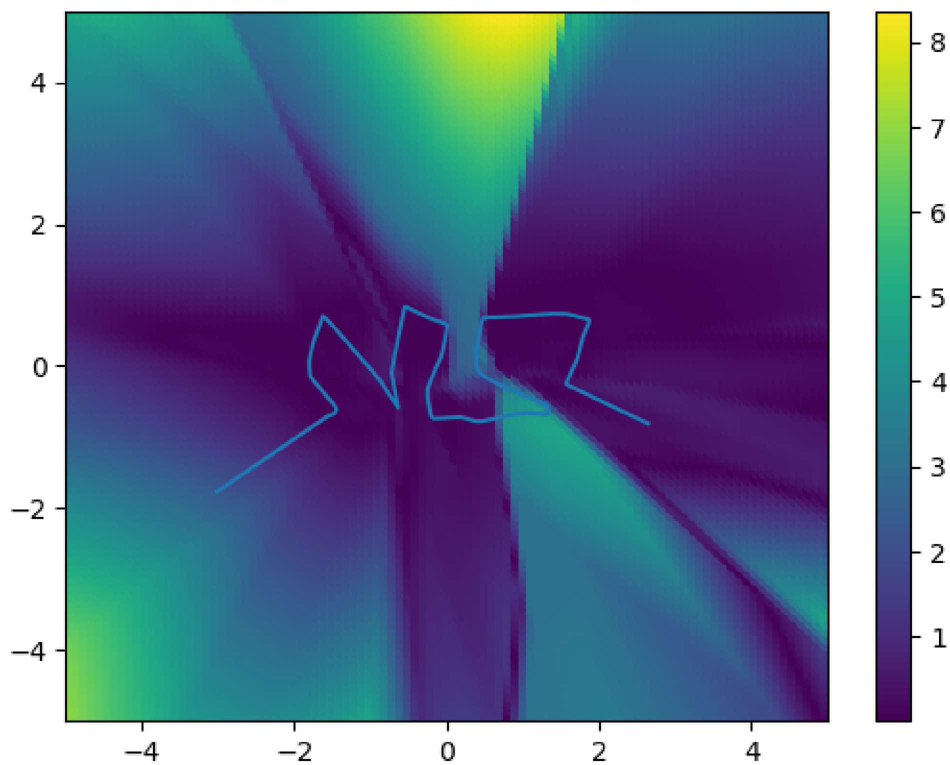
```
GPU available: False, used: False
TPU available: False, using: 0 TPU cores
HPU available: False, using: 0 HPUs

  | Name        | Type        | Params | Mode
----------------------------------------------------
0 | autoencoder | Autoencoder | 5.3 K  | train
----------------------------------------------------
0         Trainable params
5.3 K     Non-trainable params
5.3 K     Total params
0.021     Total estimated model params size (MB)
18        Modules in train mode
0         Modules in eval mode

Model overview: AutoencoderModule(
  (autoencoder): Autoencoder(
    (encoder): Sequential(
      (0): LazyLinear(in_features=0, out_features=50, bias=True)
      (1): ReLU()
```

```
      (2): LazyLinear(in_features=0, out_features=50, bias=True)
      (3): ReLU()
      (4): LazyLinear(in_features=0, out_features=50, bias=True)
      (5): ReLU()
      (6): LazyLinear(in_features=0, out_features=1, bias=True)
      (7): Identity()
    )
    (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=50, bias=True)
      (5): ReLU()
      (6): Linear(in_features=50, out_features=2, bias=True)
    )
  )
)
```

```
Training: |
 ↪                                      …

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



[11]:
```
x, y = torch.meshgrid(
    torch.linspace(-5, 5, 100), torch.linspace(-5, 5, 100), indexing="ij"
)
grid = torch.stack((x, y), dim=-1).reshape(-1, 2)
latent_repr = big.autoencoder.encoder(grid)
latent_repr2 = big2.autoencoder.encoder(grid)
diff = torch.abs(latent_repr2 - latent_repr).detach().numpy()
plt.scatter(grid[:, 0], grid[:, 1], c=diff)

latent_space = torch.linspace(-10, 10, 1000).reshape(-1, 1)
reconstruction = big.autoencoder.decoder(latent_space).detach().numpy()
plt.plot(reconstruction[:, 0], reconstruction[:, 1])

plt.ylim(-5, 5)
plt.xlim(-5, 5)
plt.colorbar()
plt.show()
```



9 (h)

[12]:
```
import numpy as np

big_gd = get_module([50, 50, 50], optim=torch.optim.SGD, batchsize=data.
  ↪shape[0])
gd_loss = big_gd.loss_curve

big_sgd = get_module([50, 50, 50], optim=torch.optim.SGD, batchsize=1, lr=3e-4)
sgd_loss = big_sgd.loss_curve
```

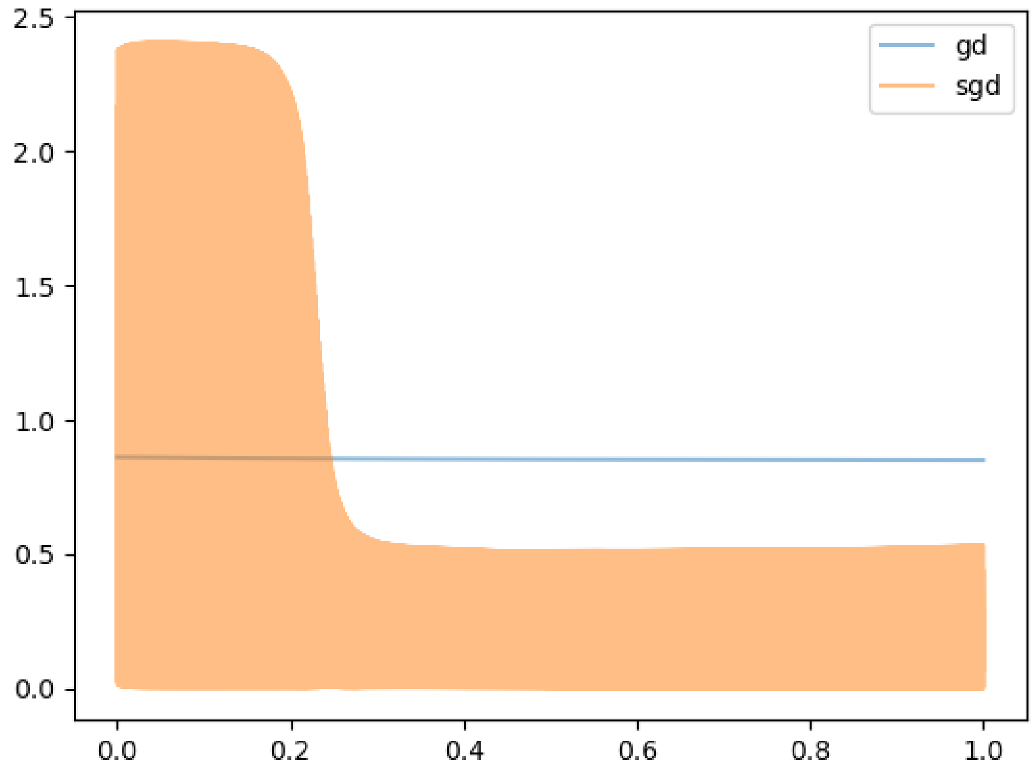
```
GPU available: False, used: False
TPU available: False, using: 0 TPU cores
HPU available: False, using: 0 HPUs

  | Name        | Type        | Params | Mode
----------------------------------------------------
0 | autoencoder | Autoencoder | 0      | train
----------------------------------------------------
0         Trainable params
0         Non-trainable params
0         Total params
0.000     Total estimated model params size (MB)
18        Modules in train mode
0         Modules in eval mode

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

```
)
dataloader size: 1

/nix/store/68cqjvbnv7xm4ff67zkhm6s1nxyb0z4h-python3-3.12.6-
env/lib/python3.12/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: |
 ↪                              …

`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 | 0      | train
----------------------------------------------------
0         Trainable params
0         Non-trainable params
0         Total params
0.000     Total estimated model params size (MB)
18        Modules in train mode
0         Modules in eval mode

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

```
  )
)
dataloader size: 100

Training: |
↪                                        …

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

[13]:

```
plt.plot(np.linspace(0, 1, len(gd_loss)), gd_loss, label="gd", alpha=0.5)
plt.plot(np.linspace(0, 1, len(sgd_loss)), sgd_loss, label="sgd", alpha=0.5)

plt.legend()
plt.show()
```



SGD loss is highly oscillatory