Exercise06_Kusch_Reckermann_Weinreich

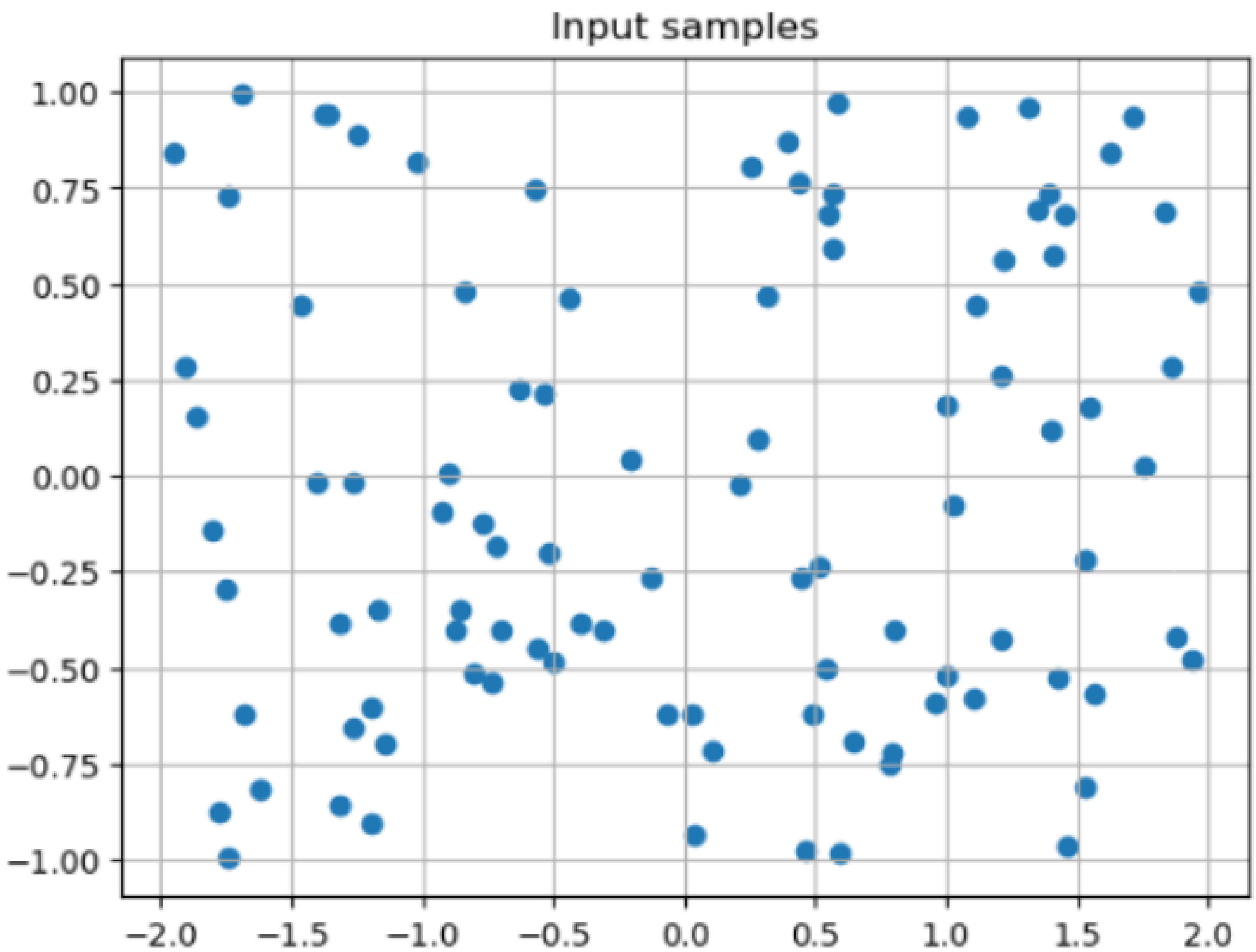
December 2, 2024

1 Sheet 6

1.1 1 Autoencoders: theory and practice

[1]:
```
import numpy as np
```

[2]:
```
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()
```



[3]:
```
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,y)
print("x.shape:", x.shape)
print("y.shape:", y.shape)
print("all x == y:", torch.all(x == y).item())
```

```
tensor([[-0.5185, -0.1993],
        [ 1.0801,  0.9392],
        [ 1.3905,  0.7348],
        [ 1.5648, -0.5684],
        [ 1.4512,  0.6837],
        [-1.7427,  0.7308],
        [-1.3621,  0.9411],
        [-1.9089,  0.2855]]) tensor([[-0.5185, -0.1993],
```

```
        [ 1.0801,  0.9392],
        [ 1.3905,  0.7348],
        [ 1.5648, -0.5684],
        [ 1.4512,  0.6837],
        [-1.7427,  0.7308],
        [-1.3621,  0.9411],
        [-1.9089,  0.2855]])
x.shape: torch.Size([8, 2])
y.shape: torch.Size([8, 2])
all x == y: True
```

[36]:

```
# TODO: define the Autoencoder architecture

import torch
from torch import nn
import pytorch_lightning as pl

class Autoencoder(nn.Module):
    def __init__(self, hidded_channels, latent_dim=1, input_dim=2):
        super().__init__()
        encoder_layers = []
        layer_sizes = np.concatenate((np.array([input_dim]), np.
 ↪array(hidded_channels), np.array([latent_dim])))
        for i in range(len(layer_sizes) - 1):
            encoder_layers.append(nn.Linear(layer_sizes[i], layer_sizes[i + 1]))
            if i < len(layer_sizes) - 2:  # Don't add activation to the last␣
 ↪layer
                encoder_layers.append(nn.ReLU())
        self.encoder = nn.Sequential(*encoder_layers)

        decoder_layers = []
        for i in range(len(layer_sizes) - 1, 0, -1):
            decoder_layers.append(nn.Linear(layer_sizes[i], layer_sizes[i - 1]))
            if i > 1:  # Don't add activation to the last layer
                decoder_layers.append(nn.ReLU())
        self.decoder = nn.Sequential(*decoder_layers)

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

class AutoencoderModule(pl.LightningModule):
    def __init__(self, **model_kwargs):
```

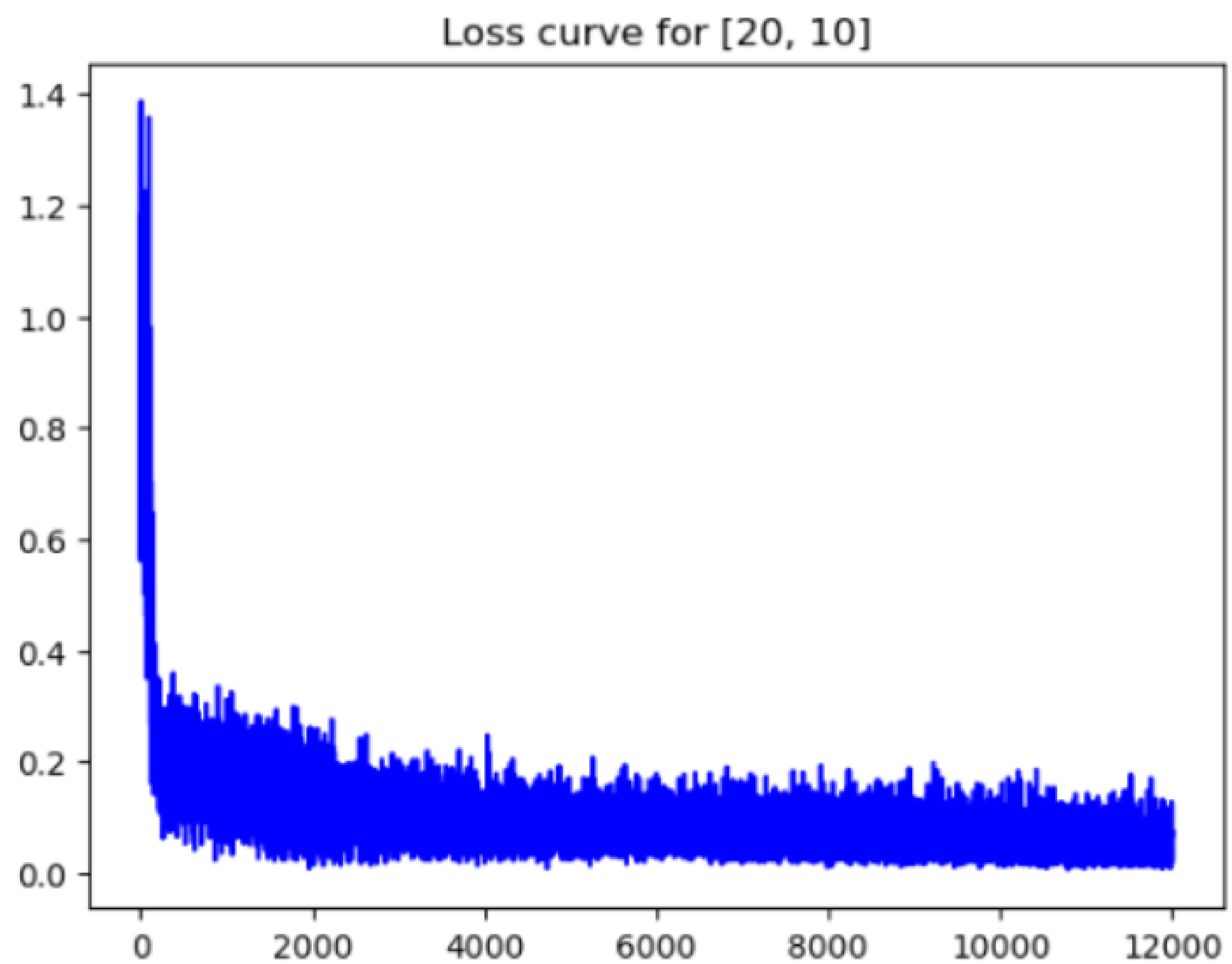
```python
        super().__init__()
        self.autoencoder = Autoencoder(**model_kwargs)
        self.loss_curve = []

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

    def embedder(self, x):
        x = self.autoencoder.embedder(x)
        return 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
        #print(batch)
        x_hat = self.autoencoder(x)
        #print(x_hat)
        loss = nn.MSELoss()(x_hat, x)
        #print(loss.item())
        self.loss_curve.append(loss.item())
        return loss
```

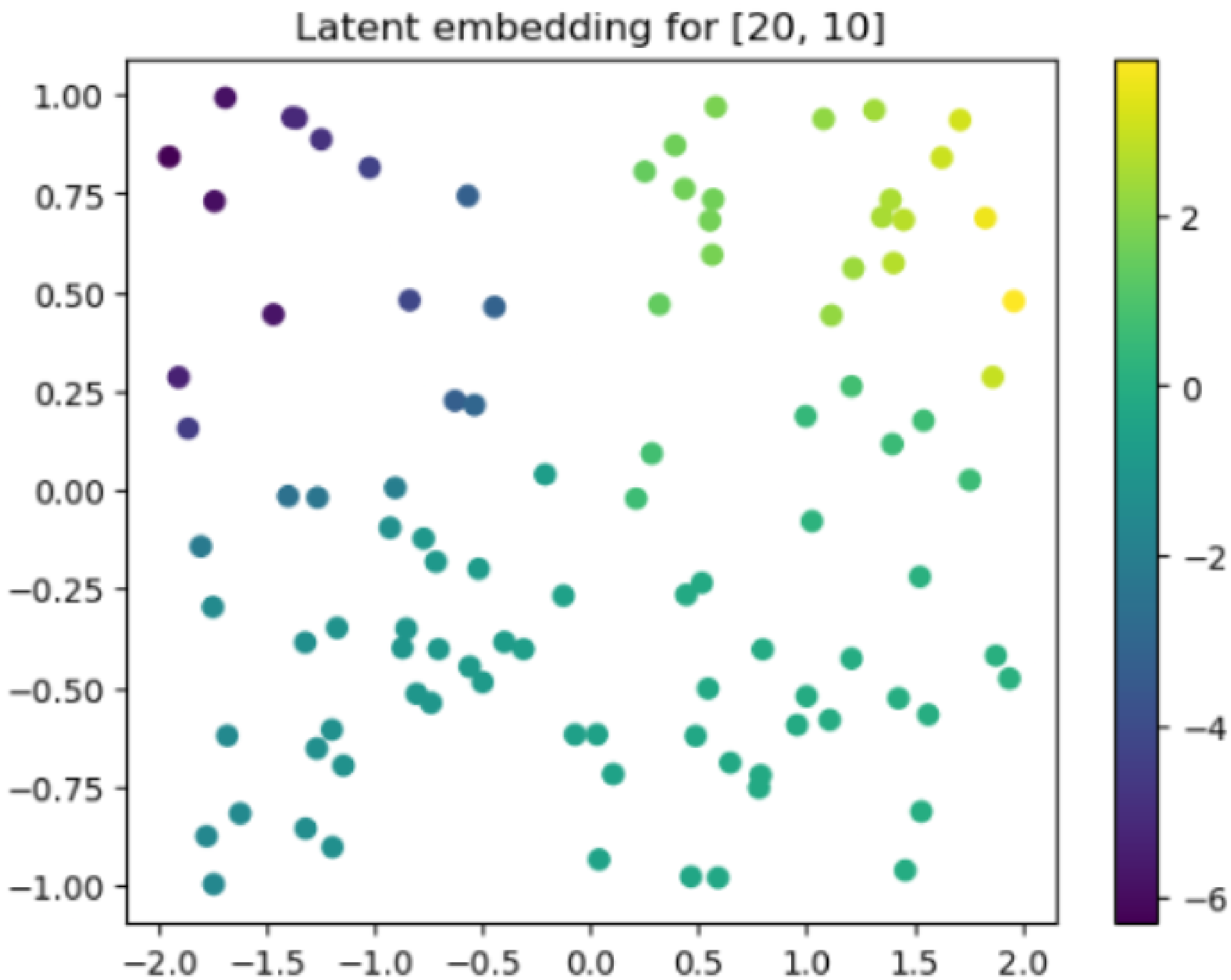
[58]:
```python
# start the training using a PyTorch Lightning Trainer
def plot_all(hidded_channels, epochs = 1000):
    trainer = pl.Trainer(max_epochs=epochs)
    autoencoder_module = AutoencoderModule( hidded_channels = hidded_channels)
    autoencoder_module.forward
    trainer.fit(autoencoder_module, data_loader)

    loss = autoencoder_module.loss_curve
    latent = autoencoder_module.embedder(data)
    x = data[:,0].detach().numpy()
    y = data[:,1].detach().numpy()
    latent = latent.detach().numpy()

    plt.plot(loss, color = "b")
```

```python
    plt.title(f"Loss curve for {hidded_channels}")
    plt.show()
    plt.scatter(x, y, c=latent)
    plt.title(f"Latent embedding for {hidded_channels}")
    plt.colorbar()
    plt.show()
```

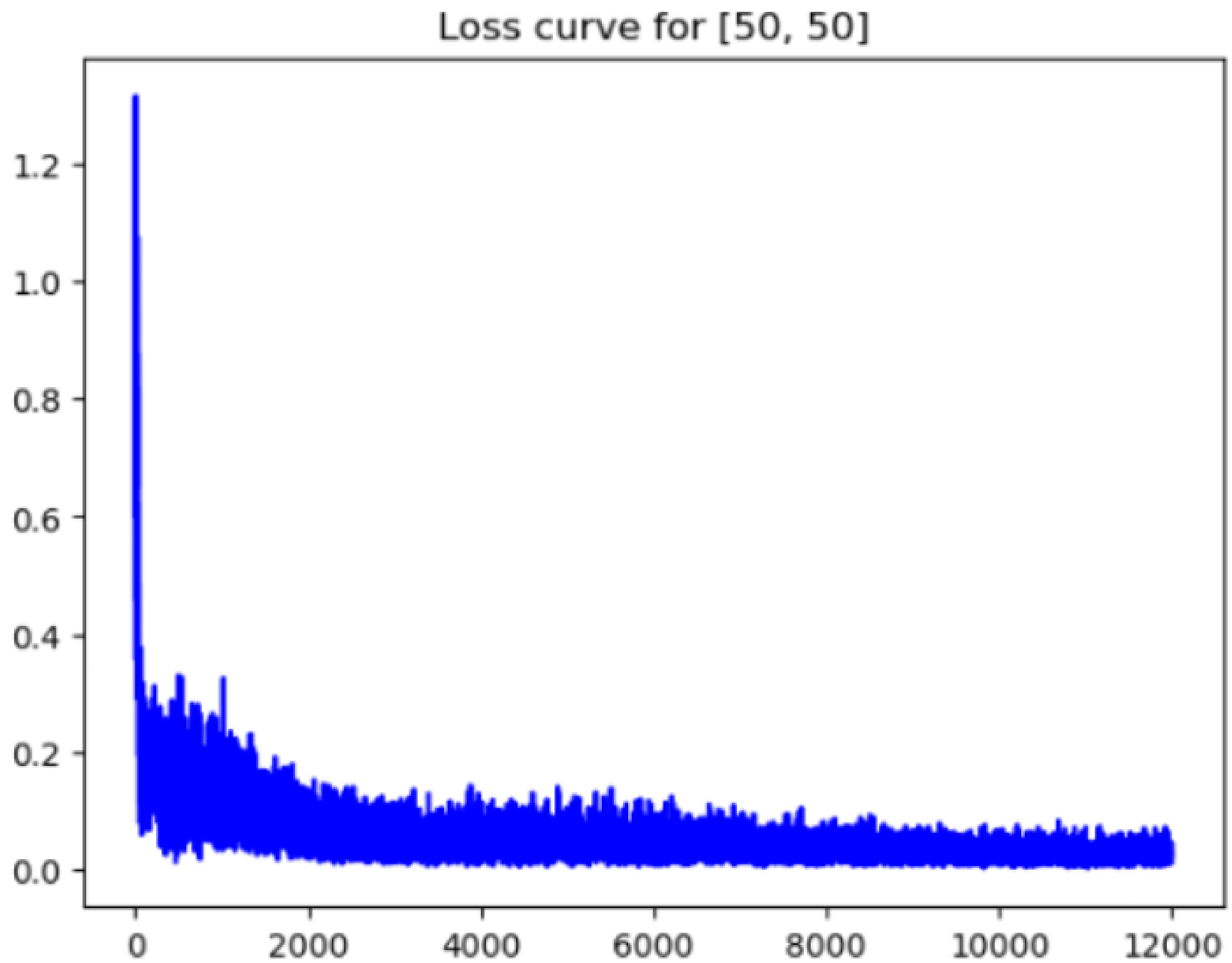
[60]:
```python
dims = [[20, 10], [50, 50]]
for dim in dims:
    plot_all(dim)
```

```
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 | 563    | train
----------------------------------------------------
563       Trainable params
0         Non-trainable params
563       Total params
0.002     Total estimated model params size (MB)
13        Modules in train mode
0         Modules in eval mode
c:\Users\janre\OneDrive\Studium\MachineLearning\sheet01\.conda\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=7`
in the `DataLoader` to improve performance.
c:\Users\janre\OneDrive\Studium\MachineLearning\sheet01\.conda\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.
```

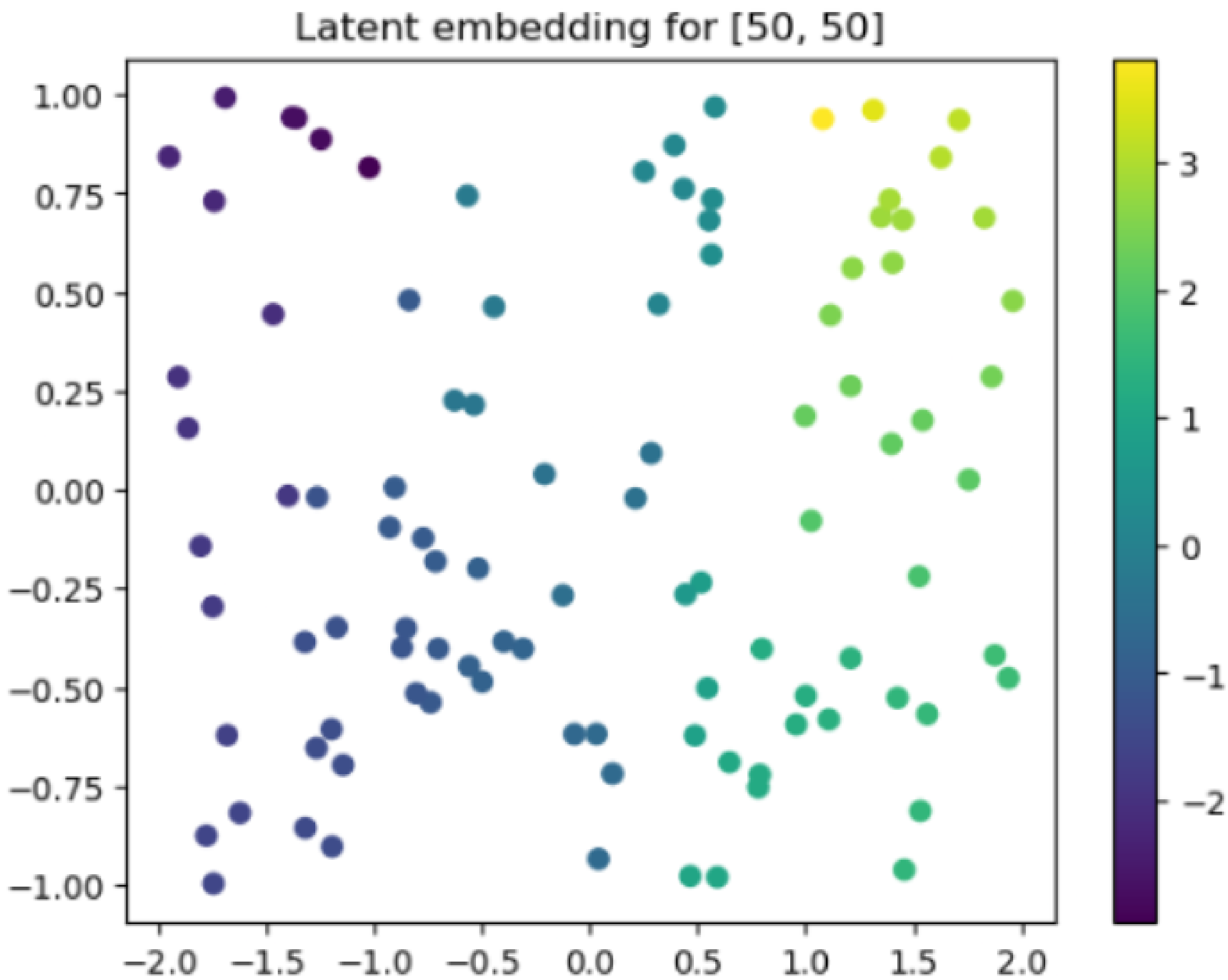

Loss curve for [20, 10]
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
2000
4000
6000
8000
10000
12000




```
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)
13        Modules in train mode
0         Modules in eval mode

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

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



Loss curve for [50, 50]
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
2000
4000
6000
8000
10000
12000



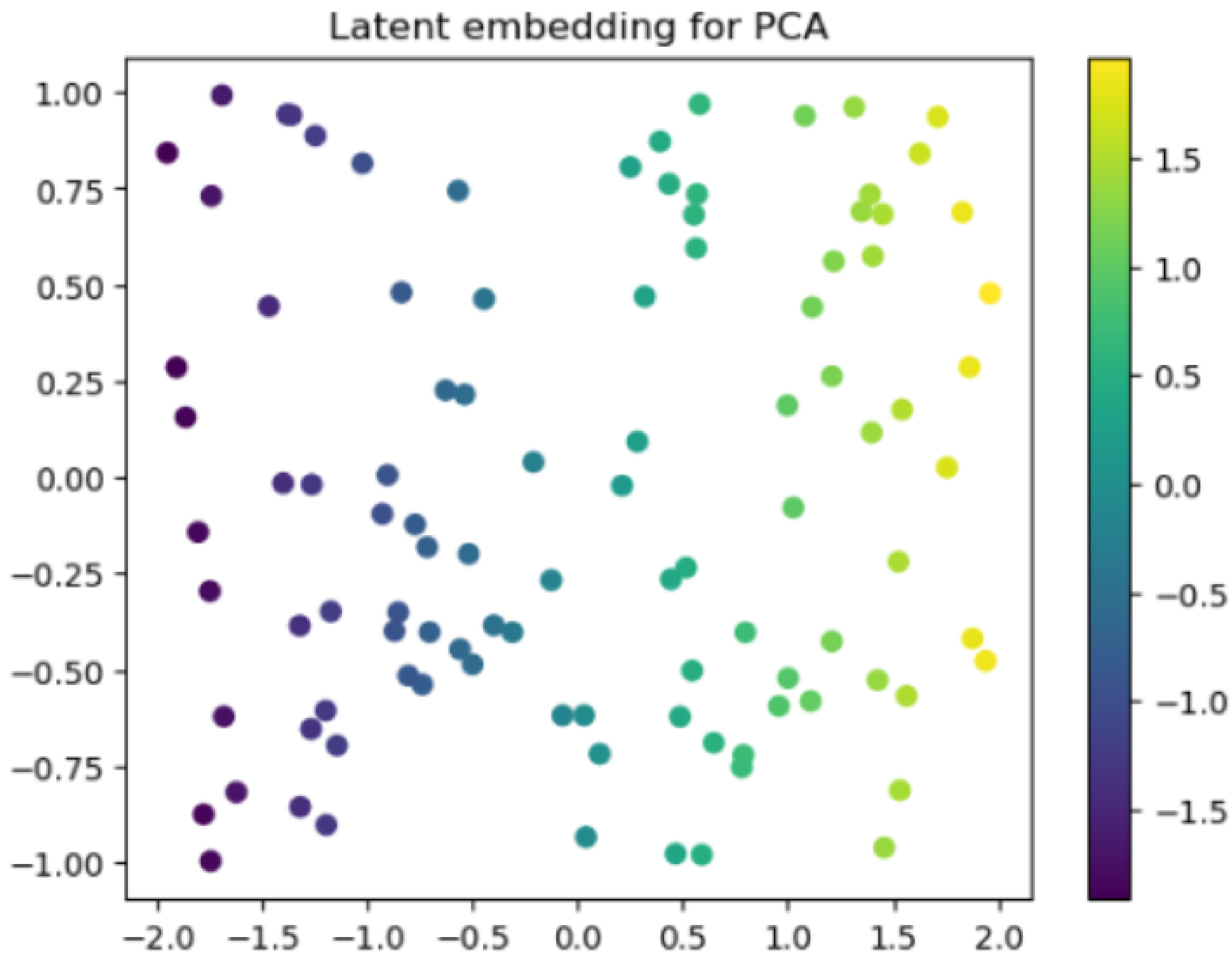
PCA

[20]:
```python
import torch

def pca(data, num_components):

    # Center the data
    mean = torch.mean(data, dim=0)
    centered_data = data - mean

    # Compute the covariance matrix
    covariance_matrix = torch.mm(centered_data.T, centered_data) / (data.
 ↪shape[0] - 1)

    # Calculate eigenvalues and eigenvectors using torch.linalg.eig()
    eigenvalues, eigenvectors = torch.linalg.eig(covariance_matrix)

    # Convert complex eigenvalues to real (if negligible imaginary parts exist)
    eigenvalues = eigenvalues.real
    eigenvectors = eigenvectors.real
```

```python
    # Sort by descending eigenvalues
    sorted_indices = torch.argsort(eigenvalues, descending=True)
    eigenvalues = eigenvalues[sorted_indices]
    eigenvectors = eigenvectors[:, sorted_indices]

    # Select the top principal components
    components = eigenvectors[:, :num_components]
    projected_data = torch.mm(centered_data, components)

    # Explained variance
    explained_variance = eigenvalues[:num_components]

    return projected_data, explained_variance, components

# Example: Applying PCA to generated data
num_components = 1
projected_data, explained_variance, components = pca(data, num_components)

print("Projected Data (first 5 samples):", projected_data[:5])
```

```
Projected Data (first 5 samples): tensor([[-1.8399],
        [-0.6167],
        [-1.8759],
        [ 0.4803],
        [ 1.3702]])
```

[57]:
```python
x = data[:,0].detach().numpy()
y = data[:,1].detach().numpy()
latent = projected_data[:, 0].detach().numpy()

plt.scatter(x, y, c=latent)
plt.title("Latent embedding for PCA")
plt.colorbar()
plt.show()
```



1.1.1 c)

Autoencoder 1: {20, 10, 1, 10, 20, 2}

i)

- With random initialization of weights, the decoder's mapping will essentially behave like a random function. Sampling points from the latent space will map to arbitrary, irregular curves in the input space. These curves will not follow any discernible structure as no meaningful relationship between the latent and input spaces has been learned.

ii)

- After training, the decoder learns to map latent space points back to the input space in a structured way. Since the bottleneck dimension is 1, the decoder will map the latent interval to a 1D manifold in the 2D input space.
- The manifold will resemble the underlying shape of the input data distribution (e.g., a straight or curved line, depending on the data geometry). The exact shape will depend on the data distribution and how well the autoencoder has learned it.

Autoencoder 2: {50, 50, 1, 50, 50, 2}

i)

- Due to the higher number of parameters, the decoder at random initialization will likely produce more complex, erratic, and jagged curves compared to `AE1`. The larger network introduces more random interactions between latent space points and their input space mapping.

ii)

- After training, the mapping from the latent space to the input space will be more flexible and capable of representing complex structures in the data.
- Sampling points from the latent space will map to a 1D manifold, but it may capture finer nuances and non-linearities in the input data compared to `AE1`.

PCA Autoencoder

i)

- At random initialization, the PCA-based architecture will behave like a linear projection with untrained weights. Sampling points from the latent space will map to straight lines or simple affine transformations in the input space. The lack of non-linearities restricts the curve's complexity.

ii)

- After training, the decoder will map the latent space to a linear subspace in the input space. Sampling an interval from the latent space will produce a straight line segment in the input space.
- This is because PCA inherently learns a linear relationship between the latent and input spaces, so the curve will not bend or follow any non-linear structure.

1.1.2 e)

Yes, an MLP autoencoder with a bottleneck dimension of 1 **can perfectly reconstruct all n points in $\mathbb{R}^p$**, given a sufficiently large architecture and proper training.

Explanation:

Mapping n Points to a Bottleneck Dimension of 1: - A bottleneck dimension of 1 implies that the encoder maps each input $x_i \in \mathbb{R}^p$ to a single scalar $z_i \in \mathbb{R}$. - The encoder can learn to assign unique scalars z_i to each point x_i, creating a one-to-one mapping from the input points to the bottleneck representation. This is achievable because the number of unique values z_i required is finite (n).

Decoder Reconstruction: - The decoder maps the scalar z_i back to the corresponding point $x_i \in \mathbb{R}^p$. If the decoder has sufficient capacity (enough layers and neurons), it can learn the mapping from z_i to x_i for all n points. - In essence, the network learns a look-up table encoded in its weights, allowing for perfect reconstruction of the n points.

1.1.3 f)

When the decoder is fixed and the encoder is retrained:

1. **New Latent Representations:** The encoder learns new latent representations for the inputs, which may differ from the original ones but aim to minimize reconstruction error.

2. **Decoder Constraints:** The fixed decoder acts as a constraint. The encoder must adapt its outputs to match what the decoder can map back to the inputs, potentially limiting performance.
3. **Possible Outcomes:**
   - **Ideal Case:** Perfect reconstruction if the decoder is flexible and well-aligned with the dataset.
   - **Suboptimal Reconstruction:** Increased reconstruction error if the decoder cannot adequately map the encoder's new outputs to the inputs.
   - **Degenerate Representations:** The encoder may collapse to suboptimal mappings if the decoder is overly constrained.

In summary, retraining the encoder adapts the latent space to the fixed decoder, but reconstruction quality depends on the decoder's capacity and alignment with the data.

g) / h) ?