

sheet06

December 2, 2024

1 Sheet 6

1.1 1 Autoencoders: theory and practice

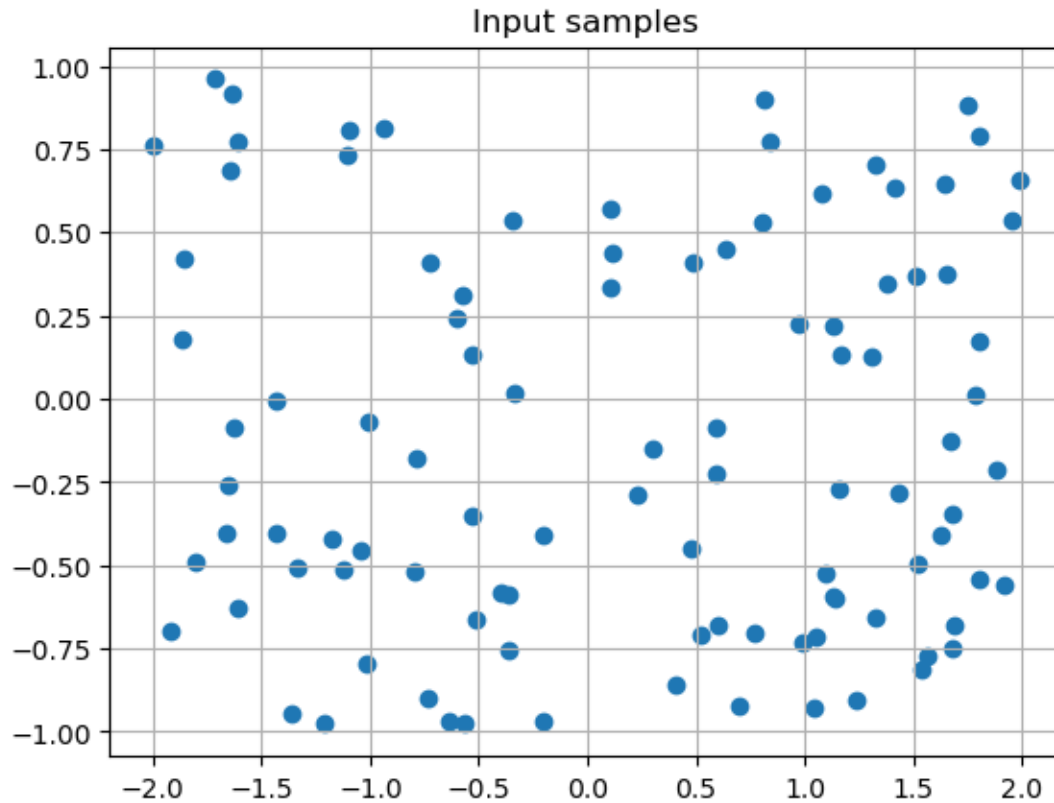
by Oliver Sange, Sam Rouppe van der Voort and Elias Huber

```
[7]: import torch
import matplotlib.pyplot as plt
import numpy as np

# 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()

max_epochs_run = 1000
```



```
[8]: 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
```

1.2 (a)

```
[9]: # 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, activation=nn.
    ↪ReLU, PCA=False):
        super().__init__()

        if not PCA:
            # TODO: implement the encoder and decoder
            layers_encoder = []
            layers_decoder = []
            n_layers = len(hidded_channels)

            layers_encoder.append(nn.Linear(input_dim, hidded_channels[0])) # ↪
            ↪adding input layer
            #layers_encoder.append(input_dim)
            layers_encoder.append(activation())
            pass_latent = False
            for i, (l_in, l_out) in enumerate(zip(hidded_channels[:
            ↪-1], hidded_channels[1:])):
                if pass_latent:
                    layers_decoder.append(nn.Linear(l_in, l_out))
                    if i != n_layers-2: # no relu activation of output?
                        layers_decoder.append(activation())
                else:
                    if l_out == latent_dim:
                        pass_latent = True
                    layers_encoder.append(nn.Linear(l_in, l_out))
                    if not pass_latent: # no activation applied on the latent ↪
            ↪space
                    layers_encoder.append(activation())

            self.encoder = nn.Sequential(*layers_encoder)
            self.decoder = nn.Sequential(*layers_decoder)
        else:
            # Linear encoder
            self.encoder = nn.Linear(input_dim, latent_dim)
            # Linear decoder
            self.decoder = nn.Linear(latent_dim, input_dim)

    def forward(self, x):
```

```

        x = self.encoder(x)
        x = self.decoder(x)
        return x

    def encode(self, x):
        x_encoded = self.encoder(x)
        return x_encoded

    def decode(self, x):
        x_decoded = self.decoder(x)
        return x_decoded

    """
        #self.encoder = nn.ModuleList(layers_encoder)
        #self.decoder = nn.ModuleList(layers_decoder)
    # when using the nn.ModuleList one must define the forward pass explicitly as_
    ↪in understood, example with loop like:
        # def forward(self, x):
        #     for layer in self.encoder:
        #         x = layer(x)
        #     for layer in self.decoder:
        #         x = layer(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())#, weight_decay=1e-5)

        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

```

For the Network architecture we used the ReLU activation function since we want to handle a regression problem and the ReLU is the state of the art for these classes of problems. We also decided to not put an activation function on the latent space since it would only half the space and project the negative encoder output to zero.

```

[10]: hidded_channels_small = [20, 10, 1, 10, 20, 2]
autoencoder_module_small = □
    ↳AutoencoderModule(hidded_channels=hidded_channels_small,latent_dim=1,□
    ↳input_dim=2, activation=nn.ReLU) #Autoencoder(hidded_channels_small)# #□
    ↳TODO: specify the model here
print("small Model overview:", autoencoder_module_small)

hidded_channels_big = [50, 50, 50, 1, 50, 50, 50, 2]
autoencoder_module_big = □
    ↳AutoencoderModule(hidded_channels=hidded_channels_big,latent_dim=1,□
    ↳input_dim=2, activation=nn.ReLU )
print("big Model overview:", autoencoder_module_big)

PCA_autoencoder = AutoencoderModule(hidded_channels=None,PCA=True,latent_dim=1,□
    ↳input_dim=2)
print("pca like Model overview:", PCA_autoencoder)

```

```

small 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)
    )
  )
)

```

```

)
big 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=50, bias=True)
      (5): ReLU()
      (6): 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=50, bias=True)
      (5): ReLU()
      (6): Linear(in_features=50, out_features=2, bias=True)
    )
  )
)
)
pca like Model overview: AutoencoderModule(
  (autoencoder): Autoencoder(
    (encoder): Linear(in_features=2, out_features=1, bias=True)
    (decoder): Linear(in_features=1, out_features=2, bias=True)
  )
)

```

1.3 (b)

```

[11]: # start the training using a PyTorch Lightning Trainer
trainer_small = pl.Trainer(max_epochs=max_epochs_run,
    ↪enable_checkpointing=False) # was max_epochs=max_epochs_run (1000 for test)

trainer_small.fit(autoencoder_module_small, data_loader)

```

```

GPU available: False, used: False
TPU available: False, using: 0 TPU cores
HPU available: False, using: 0 HPUs
/home/elias/miniconda3/envs/mlph3/lib/python3.9/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

```
| 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)
/home/elias/miniconda3/envs/mlph3/lib/python3.9/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.
/home/elias/miniconda3/envs/mlph3/lib/python3.9/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]
```

IOPub message rate exceeded.

The Jupyter server will temporarily stop sending output
to the client in order to avoid crashing it.

To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.

Current values:

ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)

ServerApp.rate_limit_window=3.0 (secs)

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

```
[12]: # start the training using a PyTorch Lightning Trainer
trainer_big = pl.Trainer(max_epochs=max_epochs_run, enable_checkpointing=False)

trainer_big.fit(autoencoder_module_big, 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 | 10.6 K | train
-----
10.6 K      Trainable params
```

```

0          Non-trainable params
10.6 K     Total params
0.042      Total estimated model params size (MB)

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

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

```

```

[13]: # start the training using a PyTorch Lightning Trainer
PCA_trainer = pl.Trainer(max_epochs=max_epochs_run, enable_checkpointing=False)

PCA_trainer.fit(PCA_autoencoder, 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	7	train

```

7          Trainable params
0          Non-trainable params
7          Total params
0.000      Total estimated model params size (MB)

```

```

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

```

```

IOPub message rate exceeded.
The Jupyter server will temporarily stop sending output
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To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.

```

```

Current values:
ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
ServerApp.rate_limit_window=3.0 (secs)

```

```

IOPub message rate exceeded.
The Jupyter server will temporarily stop sending output
to the client in order to avoid crashing it.
To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.

```

```

Current values:
ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
ServerApp.rate_limit_window=3.0 (secs)

```

```

IOPub message rate exceeded.
The Jupyter server will temporarily stop sending output

```


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ServerApp.rate_limit_window=3.0 (secs)

IOPub message rate exceeded.
The Jupyter server will temporarily stop sending output
to the client in order to avoid crashing it.
To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.

Current values:
ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
ServerApp.rate_limit_window=3.0 (secs)

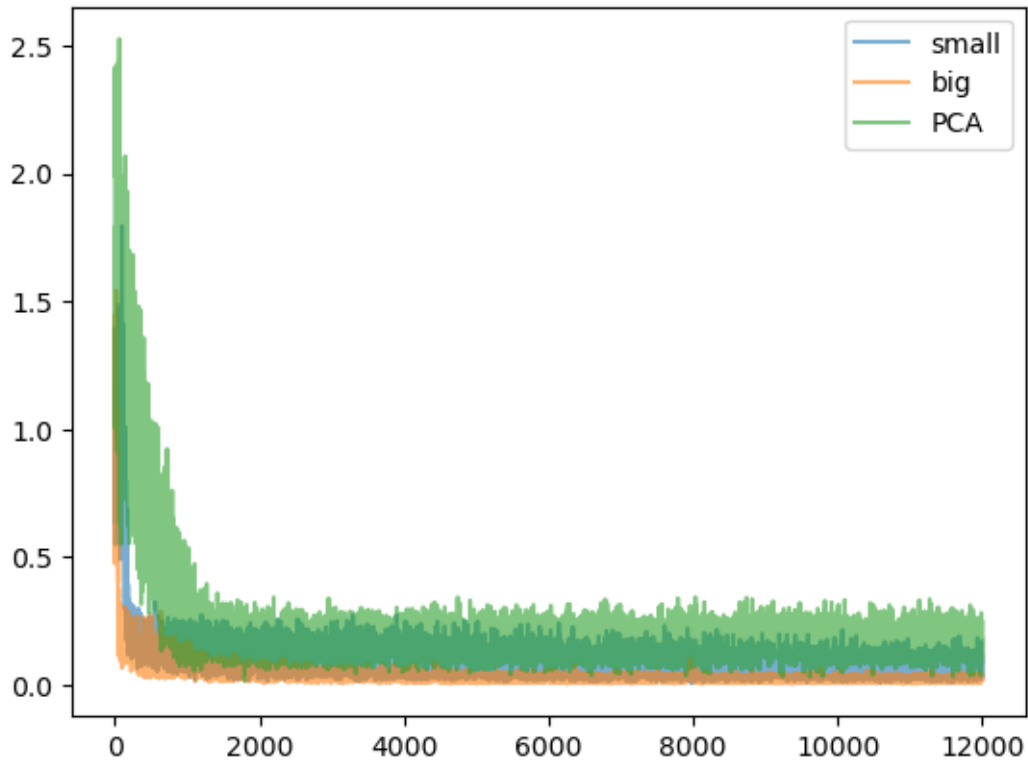
IOPub message rate exceeded.
The Jupyter server will temporarily stop sending output
to the client in order to avoid crashing it.
To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.

Current values:
ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
ServerApp.rate_limit_window=3.0 (secs)

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

```
[14]: # len(autoencoder_module_big.loss_curve)
      ## here im not completely sure what i should actually plot, probably average_
      ↪over each epoch makes more sense,
      # i dont understand why the loss_curve length is so long.
      plt.plot(range(len(autoencoder_module_small.
      ↪loss_curve)),autoencoder_module_small.loss_curve,label="small",alpha = 0.6)
      plt.plot(range(len(autoencoder_module_big.loss_curve)),autoencoder_module_big.
      ↪loss_curve,label="big",alpha = 0.6)
      plt.plot(range(len(PCA_autoencoder.loss_curve)),PCA_autoencoder.
      ↪loss_curve,label="PCA",alpha = 0.6)
      plt.legend()
```

[14]: <matplotlib.legend.Legend at 0x7fda4c5076a0>



```
[40]: latent_embedding_small = autoencoder_module_small.autoencoder.encode(data)
latent_embedding_big = autoencoder_module_big.autoencoder.encode(data)
latent_embedding_PCA = PCA_autoencoder.autoencoder.encode(data)

# Flatten the grid for encoding
x_grid, y_grid = np.meshgrid(np.linspace(-2, 2, 100), np.linspace(-1, 1, 100))
# Convert grid to PyTorch tensors
x_tensor = torch.from_numpy(x_grid).float() # Shape: (100, 100)
y_tensor = torch.from_numpy(y_grid).float() # Shape: (100, 100)

# Step 2: Combine x and y into a grid tensor for encoding
grid = torch.stack((x_tensor, y_tensor), dim=-1)

grid_flat = grid.view(-1, 2) # Flatten to shape (10000, 2)

# Encode the grid points using the autoencoders
contour_values1 = autoencoder_module_small.autoencoder.encode(grid_flat)
contour_values2 = autoencoder_module_big.autoencoder.encode(grid_flat)
contour_values3 = PCA_autoencoder.autoencoder.encode(grid_flat)

# Reshape the encoded values back to a 2D grid for contourf
contour_values1 = contour_values1.view(100, 100).detach().numpy()
```

```

contour_values2 = contour_values2.view(100, 100).detach().numpy()
contour_values3 = contour_values3.view(100, 100).detach().numpy()

# Plot
fig, axes = plt.subplots(2, 2, figsize=(14, 10)) # Adjust figsize for better
↳ layout

# Plot latent embeddings for each model
contour1 = axes[0, 0].contourf(x_grid, y_grid, contour_values1, levels=50,
↳ cmap='coolwarm', alpha=0.7)
contour2 = axes[0, 1].contourf(x_grid, y_grid, contour_values2, levels=50,
↳ cmap='coolwarm', alpha=0.7)
contour3 = axes[1, 0].contourf(x_grid, y_grid, contour_values3, levels=50,
↳ cmap='coolwarm', alpha=0.7)

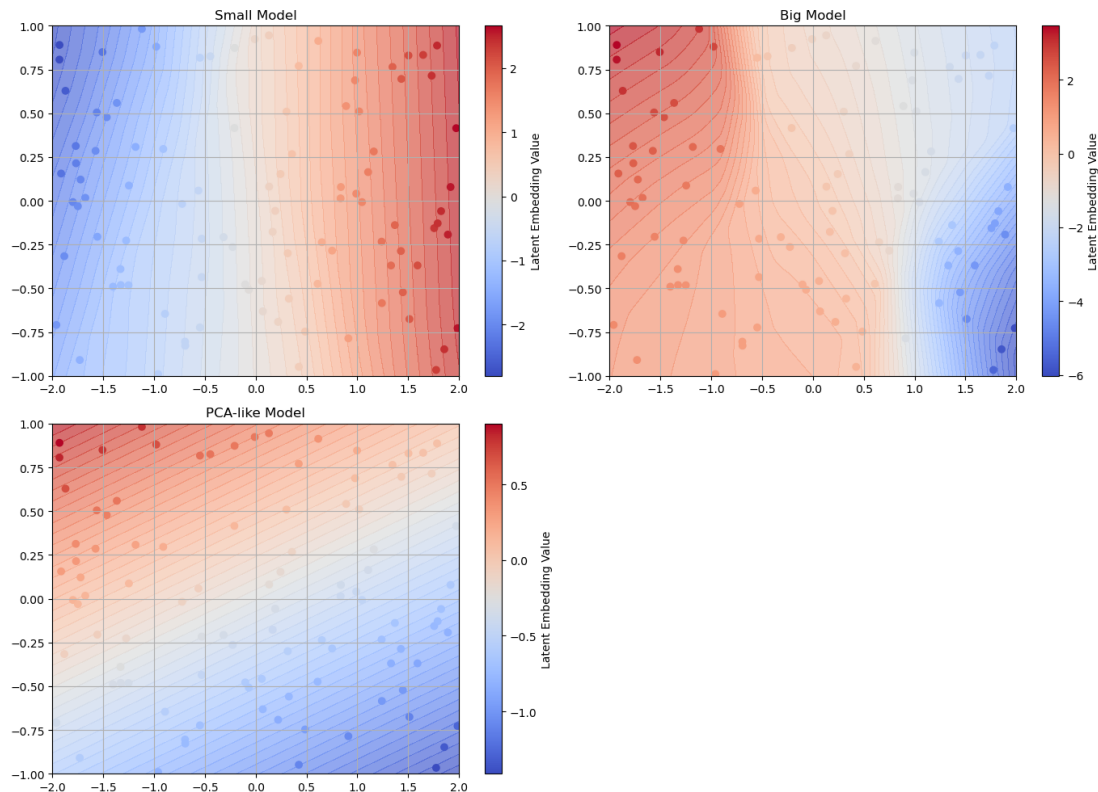
scatter1 = axes[0, 0].scatter(data[:, 0], data[:, 1], c=latent_embedding_small.
↳ detach().numpy(), cmap='coolwarm')
scatter2 = axes[0, 1].scatter(data[:, 0], data[:, 1], c=latent_embedding_big.
↳ detach().numpy(), cmap='coolwarm')
scatter3 = axes[1, 0].scatter(data[:, 0], data[:, 1], c=latent_embedding_PCA.
↳ detach().numpy(), cmap='coolwarm')

fig.colorbar(scatter1, ax=axes[0, 0], label="Latent Embedding Value")
fig.colorbar(scatter2, ax=axes[0, 1], label="Latent Embedding Value")
fig.colorbar(scatter3, ax=axes[1, 0], label="Latent Embedding Value")

axes[0, 0].set_title("Small Model")
axes[0, 1].set_title("Big Model")
axes[1, 0].set_title("PCA-like Model")
axes[0, 0].grid(True)
axes[0, 1].grid(True)
axes[1, 0].grid(True)

# Hide the empty subplot (bottom-right) as we only need 3 plots
axes[1, 1].axis('off')
plt.tight_layout()
plt.show()

```



The PCA model prefers a color gradient around the X2 axis, the X1 axis seems to influence the embedding less. This can be due to getting the X2 axis wrong leads to a higher loss than for the X1 axis, due to the stretch in the sample space.

1.4 (c)

1.5 also make a prediction before looking at plots below

If we sample points from an interval in the latent space, the decoder can attempt to map them to a curve in the ambient/input space. Guess what these curves may look like: i) After random initialization of the MLP parameters, and ii) After training the respective architecture.

1.5.1 i)

A random walk like line.

1.5.2 ii)

We think its a line following the color change seen above.

1.6 (d)

```
[15]: import numpy as np

latent_space_samples = np.linspace(-2, 2, 100) # somewhat arbitrary choice for
↳ ReLu maybe, should just include origin
# if we change the non linearity to sigmoid, then from -1 to 1 i would say,
# but also we need to think if we should have a non linearity in latent space
# for this random num task i dont see why not but idk
latent_space_samples = torch.tensor(latent_space_samples, dtype=torch.float32).
↳ view(100, 1)

samples_decoded_trained_small = autoencoder_module_small.autoencoder.
↳ decode(latent_space_samples)
samples_decoded_trained_big = autoencoder_module_big.autoencoder.
↳ decode(latent_space_samples)
samples_decoded_trained_PCA = PCA_autoencoder.autoencoder.
↳ decode(latent_space_samples)

fig, axes = plt.subplots(2, 2, figsize=(14, 10)) # Adjust figsize for better
↳ layout

# Plot latent embeddings for each model

scatter1 = axes[0,0].scatter(samples_decoded_trained_small[:, 0].detach().
↳ numpy(), samples_decoded_trained_small[:, 1].detach().
↳ numpy(), c=latent_space_samples.detach().numpy(), cmap='viridis')
scatter2 = axes[0,1].scatter(samples_decoded_trained_big[:, 0].detach().
↳ numpy(), samples_decoded_trained_big[:, 1].detach().
↳ numpy(), c=latent_space_samples.detach().numpy(), cmap='viridis')
scatter3 = axes[1,0].scatter(samples_decoded_trained_PCA[:, 0].detach().
↳ numpy(), samples_decoded_trained_PCA[:, 1].detach().
↳ numpy(), c=latent_space_samples.detach().numpy(), cmap='viridis')

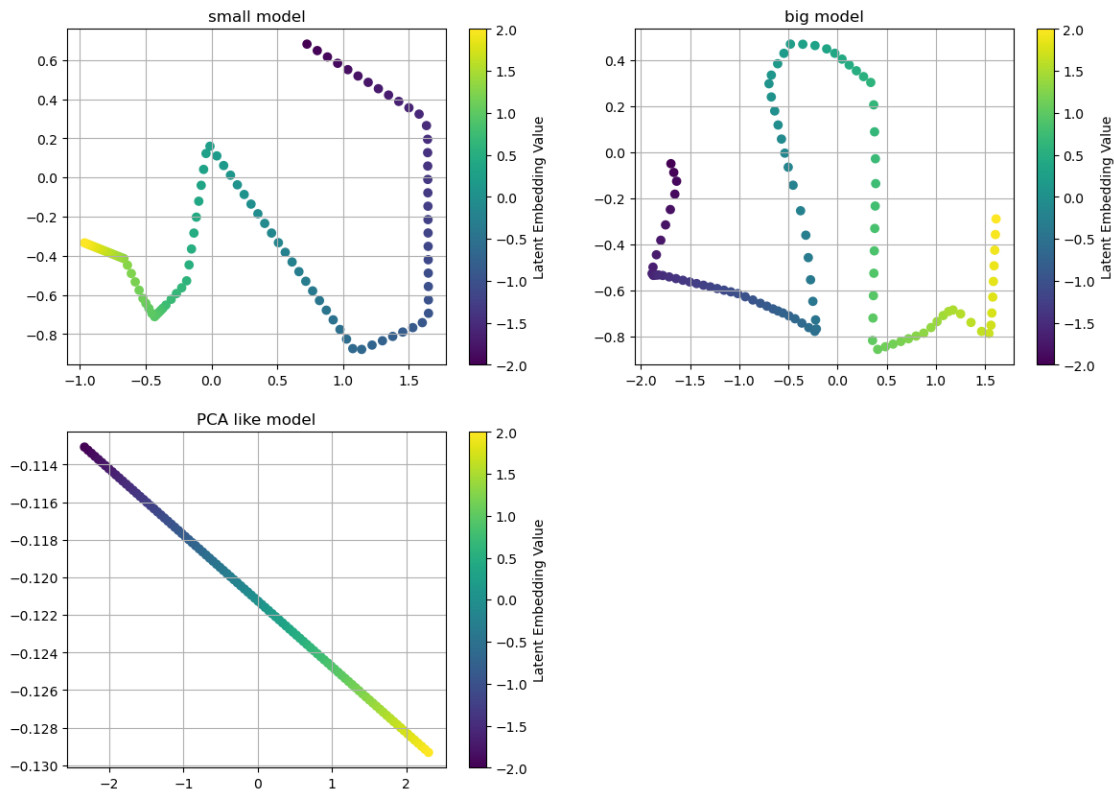
fig.colorbar(scatter1, ax=axes[0, 0], label="Latent Embedding Value")
fig.colorbar(scatter2, ax=axes[0, 1], label="Latent Embedding Value")
fig.colorbar(scatter3, ax=axes[1, 0], label="Latent Embedding Value")

axes[0,0].set_title("small model")
axes[0,1].set_title("big model")
axes[1,0].set_title("PCA like model")

axes[0,0].grid(True)
axes[0,1].grid(True)
axes[1,0].grid(True)
```

```
fig.suptitle('Trained',fontsize=20)
# Hide the empty subplot (bottom-right) as we only need 3 plots
axes[1, 1].axis('off')
plt.show()
```

Trained



```
[16]: # init untrained models
untrained_autoencoder_small = ␣
    ␣AutoencoderModule(hidded_channels=hidded_channels_small,latent_dim=1,␣
    ␣input_dim=2, activation=nn.ReLU)
untrained_autoencoder_big = ␣
    ␣AutoencoderModule(hidded_channels=hidded_channels_big,latent_dim=1,␣
    ␣input_dim=2, activation=nn.ReLU )
untrained_PCA_autoencoder = ␣
    ␣AutoencoderModule(hidded_channels=None,PCA=True,latent_dim=1, input_dim=2)

samples_decoded_untrained_small = untrained_autoencoder_small.autoencoder.
    ␣decode(latent_space_samples)
samples_decoded_untrained_big = untrained_autoencoder_big.autoencoder.
    ␣decode(latent_space_samples)
```

```

samples_decoded_untrained_PCA = untrained_PCA_autoencoder.autoencoder.
    ↳ decode(latent_space_samples)

fig, axes = plt.subplots(2, 2, figsize=(14, 10)) # Adjust figsize for better
    ↳ layout

scatter1 = axes[0,0].scatter(samples_decoded_untrained_small[:, 0].detach().
    ↳ numpy(), samples_decoded_untrained_small[:, 1].detach().
    ↳ numpy(), c=latent_space_samples.detach().numpy(), cmap='viridis')
scatter2 = axes[0,1].scatter(samples_decoded_untrained_big[:, 0].detach().
    ↳ numpy(), samples_decoded_untrained_big[:, 1].detach().
    ↳ numpy(), c=latent_space_samples.detach().numpy(), cmap='viridis')
scatter3 = axes[1,0].scatter(samples_decoded_untrained_PCA[:, 0].detach().
    ↳ numpy(), samples_decoded_untrained_PCA[:, 1].detach().
    ↳ numpy(), c=latent_space_samples.detach().numpy(), cmap='viridis')

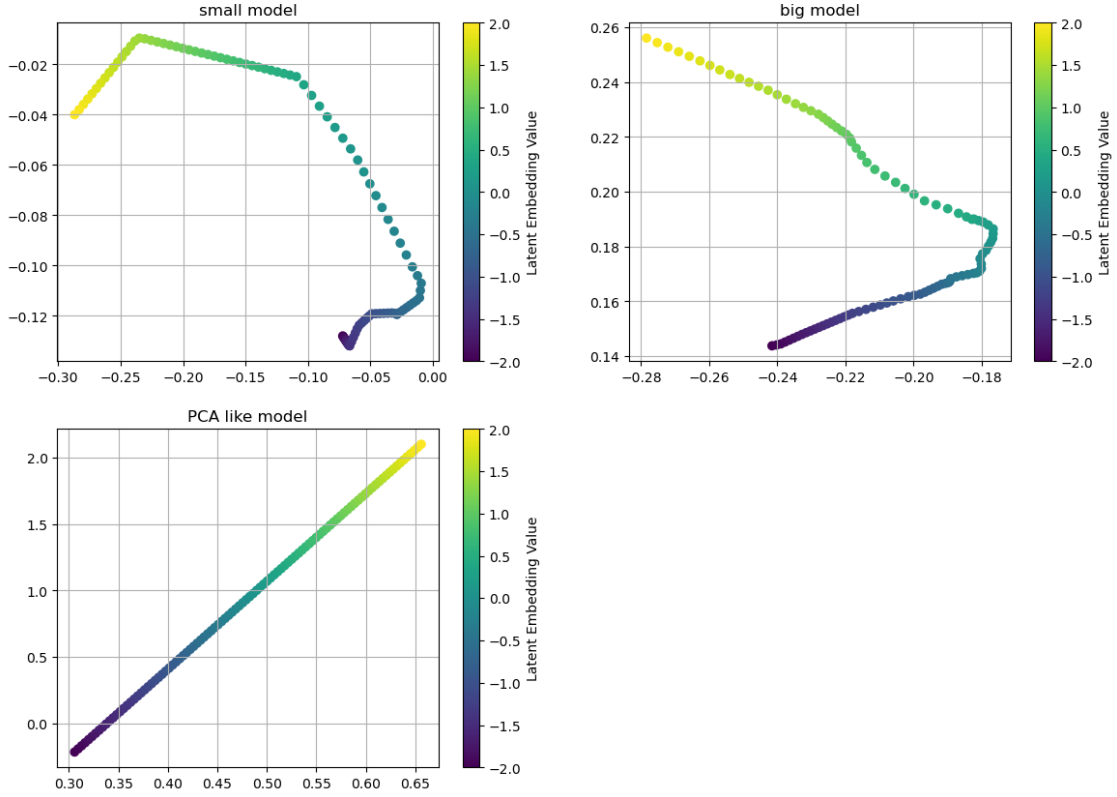
fig.colorbar(scatter1, ax=axes[0, 0], label="Latent Embedding Value")
fig.colorbar(scatter2, ax=axes[0, 1], label="Latent Embedding Value")
fig.colorbar(scatter3, ax=axes[1, 0], label="Latent Embedding Value")

axes[0,0].set_title("small model")
axes[0,1].set_title("big model")
axes[1,0].set_title("PCA like model")

axes[0,0].grid(True)
axes[0,1].grid(True)
axes[1,0].grid(True)
fig.suptitle('Untrained', fontsize=20)
# Hide the empty subplot (bottom-right) as we only need 3 plots
axes[1, 1].axis('off')
plt.show()

```


Untrained



We observe that the trained model curve tries to cover most of the space where the data points are placed. This is contrary to the untrained model where the region where the path goes is stretched on a smaller region.

1.7 (e) and (f) discussion

1.7.1 (e)

Given enough parameters, the encoder can reconstruct the finite number of points by fitting the interpolation polynomial that fits all the points. This representation however is not very useful due to extreme overfitting.

An MLP autoencoder with a bottleneck dimension of 1 can theoretically reconstruct all data points given a sufficiently complex architecture and effective training. Since MLPs are universal approximators, they can approximate the necessary mappings if they have enough width and depth. However, practical challenges, such as optimization difficulties or finite numerical precision, can affect the model's performance. While perfect reconstruction theoretically possible, achieving it in practice is often very difficult.

1.7.2 (f)

The encoder will with high likelihood converge to a embedding close to the original encoder. But due to inefficiencies during training and the now less possible output values (since the decoder is fixed) the result will be less accurate then the original encoder.

```
[17]: hidded_channels_big = [50, 50, 50, 1, 50, 50, 50, 2]
autoencoder_module_big_retrain = _
    ↪ AutoencoderModule(hidded_channels=hidded_channels_big, latent_dim=1, _
    ↪ input_dim=2, activation=nn.ReLU )

# start the training using a PyTorch Lightning Trainer
retrain_trainer = pl.Trainer(max_epochs=max_epochs_run, _
    ↪ enable_checkpointing=False)

retrain_trainer.fit(autoencoder_module_big_retrain, data_loader)
plt.plot(autoencoder_module_big_retrain.loss_curve, label="first training")

latent_space_data_trained = autoencoder_module_big_retrain.autoencoder.
    ↪ encoder(data).detach().numpy()

#now fix decoder parameters
for parameter in autoencoder_module_big_retrain.autoencoder.decoder.
    ↪ parameters():
    parameter.requires_grad = False

# reinitialize parameters for the encoder
for parameter in autoencoder_module_big_retrain.autoencoder.encoder.
    ↪ parameters():
    if isinstance(parameter, nn.Linear):
        nn.init.normal_(parameter.weight, mean=0.0, std=1)
        nn.init.zeros_(parameter.bias)

retrain_trainer = pl.Trainer(max_epochs=max_epochs_run, _
    ↪ enable_checkpointing=False)
retrain_trainer.fit(autoencoder_module_big_retrain, data_loader)
plt.plot(autoencoder_module_big_retrain.loss_curve, label="retraining")
plt.legend()
plt.grid()
plt.show()

latent_space_data_retrained = autoencoder_module_big_retrain.autoencoder.
    ↪ encoder(data).detach().numpy()
```

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	10.6 K	train

10.6 K	Trainable params
0	Non-trainable params
10.6 K	Total params
0.042	Total estimated model params size (MB)

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	10.6 K	train

5.3 K	Trainable params
5.3 K	Non-trainable params
10.6 K	Total params
0.042	Total estimated model params size (MB)

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

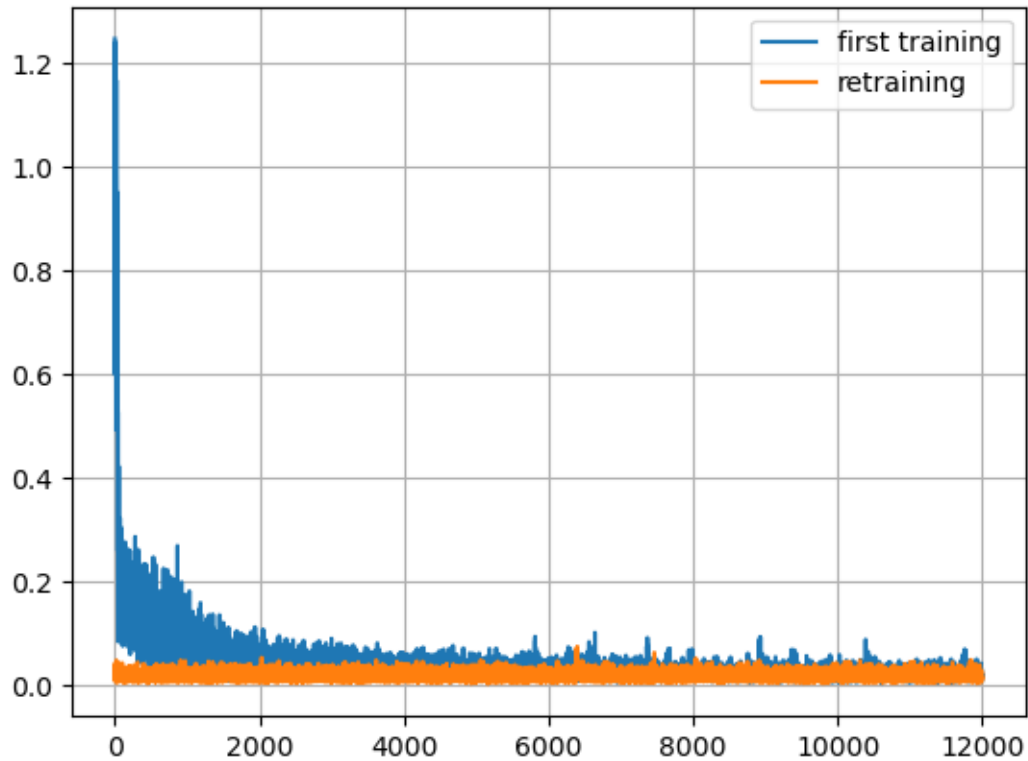
IOPub message rate exceeded.
The Jupyter server will temporarily stop sending output
to the client in order to avoid crashing it.
To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.

Current values:
ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
ServerApp.rate_limit_window=3.0 (secs)

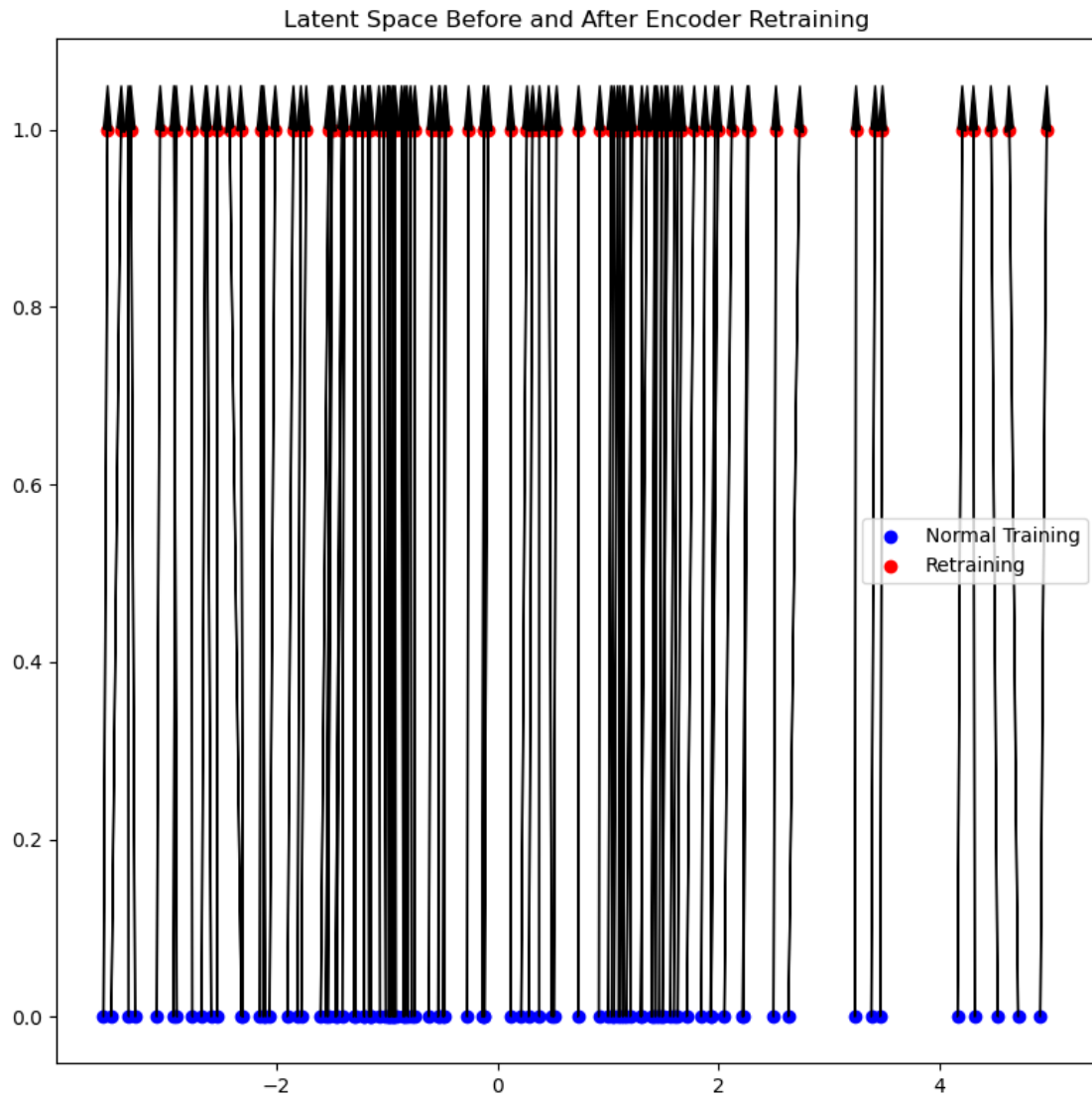
IOPub message rate exceeded.
The Jupyter server will temporarily stop sending output
to the client in order to avoid crashing it.
To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.

Current values:
ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
ServerApp.rate_limit_window=3.0 (secs)

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



```
[21]: fig, ax = plt.subplots(figsize=(8, 8))
ax.scatter(latent_space_data_trained[:, 0], np.
    ↪zeros_like(latent_space_data_trained[:, 0]), color='blue',
        label='Normal Training')
ax.scatter(latent_space_data_retrained[:, 0], np.
    ↪zeros_like(latent_space_data_retrained[:, 0])+1,
        color='red', label='Retraining')
# Add arrows showing how the encoder's output changed after retraining
for i in range(len(latent_space_data_trained)):
    ax.arrow(latent_space_data_trained[i, 0], 0, latent_space_data_retrained[i, 0],
    ↪0] -
        latent_space_data_trained[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()
```



1.8 (h)

```
[22]: # define model that uses SGD
class AutoencoderModuleSGD(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.SGD(self.parameters(), weight_decay=1e-5)

    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

```

```

[26]: hidded_channels_big = [50, 50, 50, 1, 50, 50, 50, 2]
autoencoder_module_big_retrain = _
    ↪ AutoencoderModule(hidded_channels=hidded_channels_big, latent_dim=1, _
    ↪ input_dim=2, activation=nn.ReLU)
dataset = TensorDataset(data, data)
data_loader = DataLoader(dataset, batch_size=100, shuffle=True, drop_last=True)

num_training_examples = [list(range(8, 8*12*max_epochs_run+1, 8)), _
    ↪ list(range(100, 100*1*max_epochs_run+1, 100))]
# num training samples given by step=num batch size, and total _
    ↪ train_data_seen=batch_size*num_batches*epochs

# start the training using a PyTorch Lightning Trainer
retrain_trainer = pl.Trainer(max_epochs=max_epochs_run, _
    ↪ enable_checkpointing=False)

retrain_trainer.fit(autoencoder_module_big_retrain, data_loader)
plt.plot(num_training_examples[1], autoencoder_module_big_retrain.
    ↪ loss_curve, label="first training GD", alpha = 0.6)

# now fix decoder parameters
for parameter in autoencoder_module_big_retrain.autoencoder.decoder.
    ↪ parameters():
    parameter.requires_grad = False

# reinitialize parameters for the encoder
for parameter in autoencoder_module_big_retrain.autoencoder.encoder.
    ↪ parameters():
    if isinstance(parameter, nn.Linear):

```

```

        nn.init.normal_(parameter.weight,mean=0.0,std=1)
        nn.init.zeros_(parameter.bias)

retrain_trainer = pl.Trainer(max_epochs=max_epochs_run,
    ↪enable_checkpointing=False)
retrain_trainer.fit(autoencoder_module_big_retrain, data_loader)
plt.plot(num_training_examples[1],autoencoder_module_big_retrain.
    ↪loss_curve,label="retraining GD",alpha=0.6)

## now the same task for SGD
    ↪#####

dataset = TensorDataset(data, data)
data_loader = DataLoader(dataset, batch_size=8, shuffle=True, drop_last=True)

autoencoder_module_big_retrain =
    ↪AutoencoderModuleSGD(hidded_channels=hidded_channels_big,latent_dim=1,
    ↪input_dim=2, activation=nn.ReLU)

# start the training using a PyTorch Lightning Trainer
retrain_trainer = pl.Trainer(max_epochs=max_epochs_run,
    ↪enable_checkpointing=False)

retrain_trainer.fit(autoencoder_module_big_retrain, data_loader)
plt.plot(num_training_examples[0],autoencoder_module_big_retrain.
    ↪loss_curve,label="first training SGD",alpha = 0.6)

#now fix decoder parameters
for parameter in autoencoder_module_big_retrain.autoencoder.decoder.
    ↪parameters():
    parameter.requires_grad = False

# reinitialize parameters for the encoder
for parameter in autoencoder_module_big_retrain.autoencoder.encoder.
    ↪parameters():
    if isinstance(parameter,nn.Linear):
        nn.init.normal_(parameter.weight,mean=0.0,std=1)
        nn.init.zeros_(parameter.bias)

retrain_trainer = pl.Trainer(max_epochs=max_epochs_run,
    ↪enable_checkpointing=False)
retrain_trainer.fit(autoencoder_module_big_retrain, data_loader)
plt.plot(num_training_examples[0],autoencoder_module_big_retrain.
    ↪loss_curve,label="retraining SGD", alpha = 0.6)

```

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

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	10.6 K	train
10.6 K	Trainable params			
0	Non-trainable params			
10.6 K	Total params			
0.042	Total estimated model params size (MB)			

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	10.6 K	train
5.3 K	Trainable params			
5.3 K	Non-trainable params			
10.6 K	Total params			
0.042	Total estimated model params size (MB)			

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

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0	Non-trainable params			
10.6 K	Total params			
0.042	Total estimated model params size (MB)			

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

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5.3 K	Trainable params			
5.3 K	Non-trainable params			
10.6 K	Total params			
0.042	Total estimated model params size (MB)			

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

IOPub message rate exceeded.
The Jupyter server will temporarily stop sending output
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To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.

Current values:
ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
ServerApp.rate_limit_window=3.0 (secs)

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Current values:
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ServerApp.rate_limit_window=3.0 (secs)

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To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.`

Current values:

ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
ServerApp.rate_limit_window=3.0 (secs)

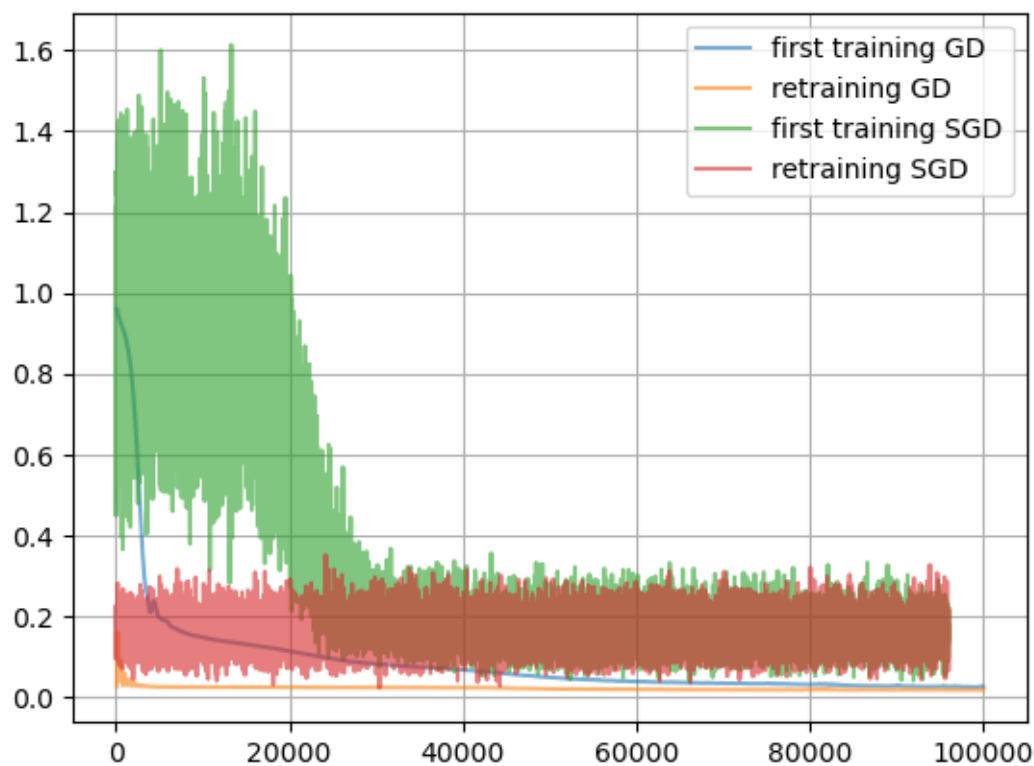
IOPub message rate exceeded.

The Jupyter server will temporarily stop sending output to the client in order to avoid crashing it.
To change this limit, set the config variable
`--ServerApp.iopub_msg_rate_limit`.`

Current values:

ServerApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
ServerApp.rate_limit_window=3.0 (secs)

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



We see the gradient descent algorithm trains the network faster, when comparing to the examples seen, while in return taking more computing time.

[]:

DATA

Which dataset do you want to use?



Ratio of training to test data: 50%



Noise: 0



Batch size: 14



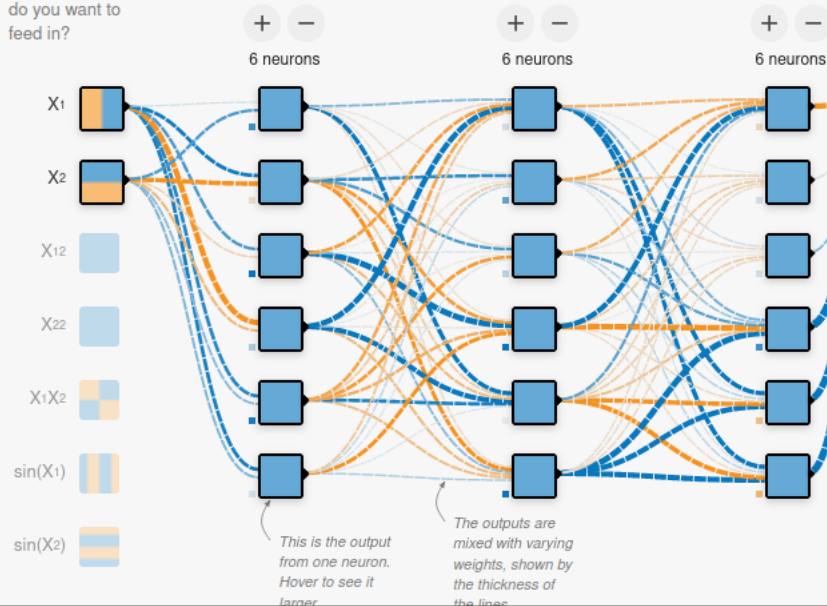
REGENERATE

FEATURES

Which properties do you want to feed in?

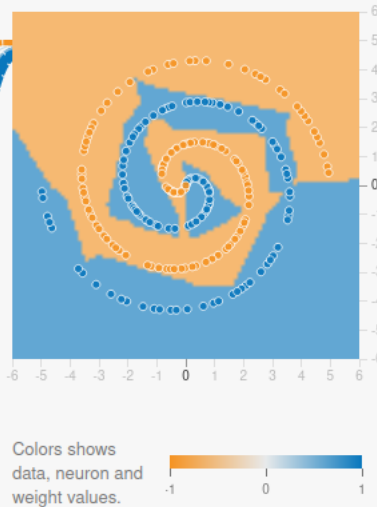
- X1
- X2
- X12
- X22
- X1X2
- sin(X1)
- sin(X2)

3 HIDDEN LAYERS



OUTPUT

Test loss 0.041
Training loss 0.016



Text

DATA

Which dataset do you want to use?



Ratio of training to test data: 50%



Noise: 0



Batch size: 14



REGENERATE

FEATURES

Which properties do you want to feed in?

- X1
- X2
- X12
- X22
- X1X2
- sin(X1)
- sin(X2)

6 HIDDEN LAYERS

+

-

8 neurons

+

-

8 neurons

+

-

8 neurons

+

-

8 neurons

+

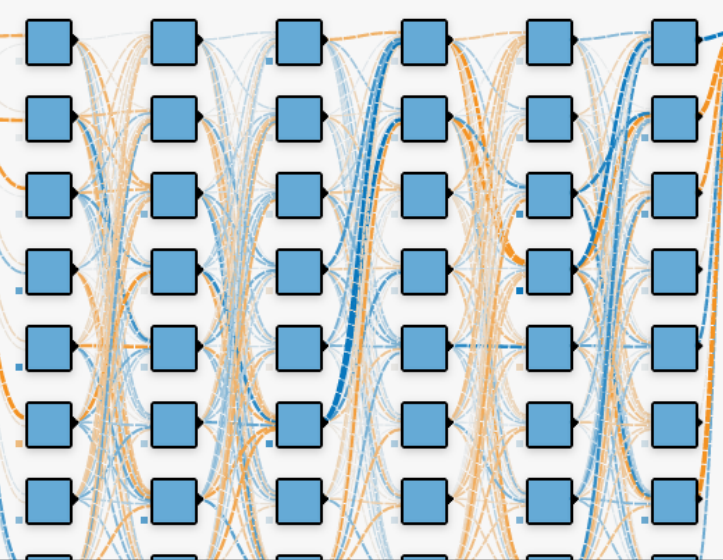
-

8 neurons

+

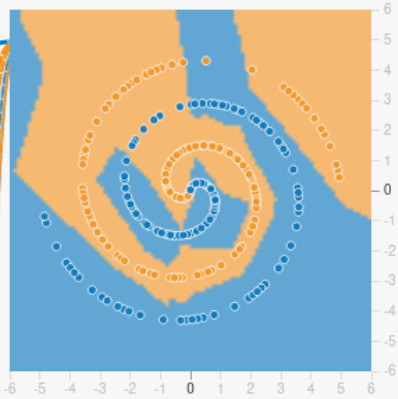
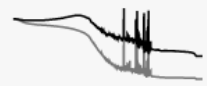
-

8 neurons

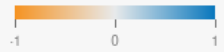


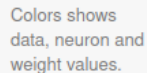
OUTPUT

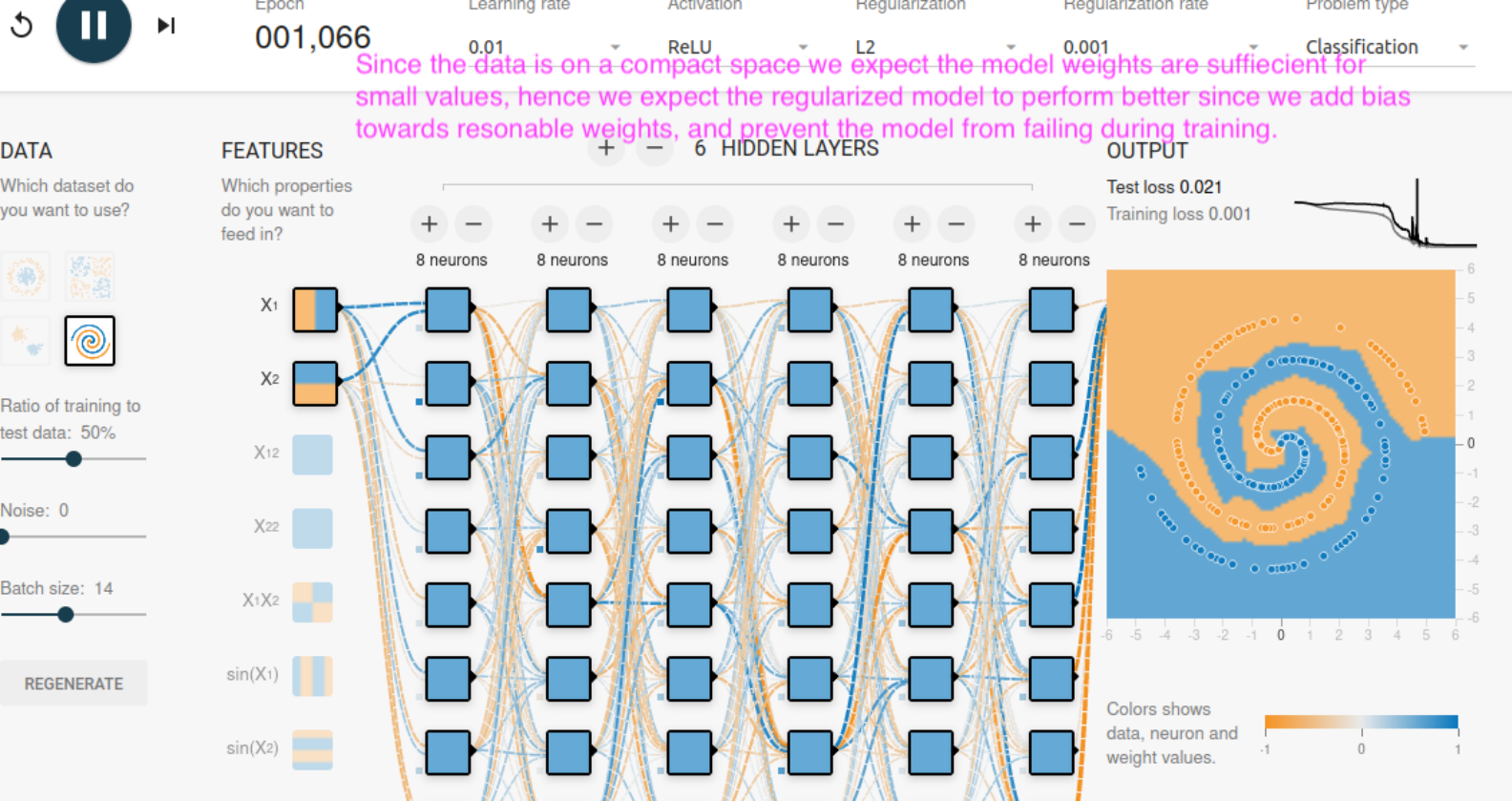
Test loss 0.231
Training loss 0.066



Colors shows data, neuron and weight values.







Epoch 000,885 Learning rate 0.1 Activation ReLU Regularization None Regularization rate 0 Problem type Classification

we observe that the model is able to almost perfectly fit the training data while not being able to perform well on the validation data at all. Classic overfitting.

DATA

Which dataset do you want to use?



Ratio of training to test data: 10%

Noise: 50

Batch size: 14

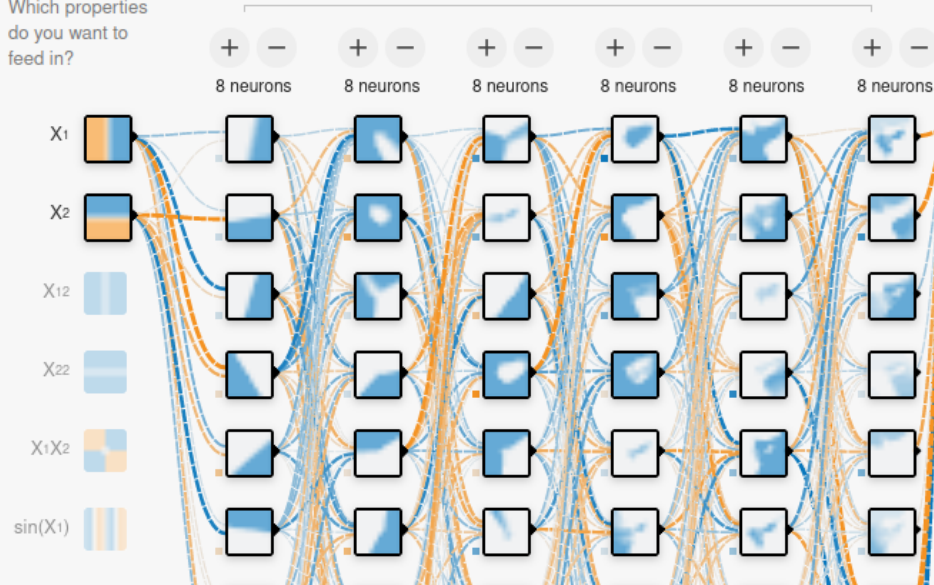
REGENERATE

FEATURES

Which properties do you want to feed in?

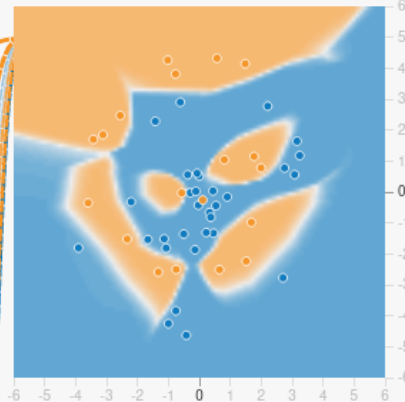
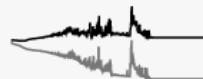
- X1
- X2
- X12
- X22
- X1X2
- sin(X1)

6 HIDDEN LAYERS



OUTPUT

Test loss 0.545
Training loss 0.040



Colors shows data, neuron and