Autoencoder

Industrial AI Lab.

Prof. Seungchul Lee

Unsupervised Learning

- Many applications such as image synthesis, denoising, super-resolution, speech synthesis, compression, etc. require to go beyond classification and regression, and model explicitly a high dimension signal.

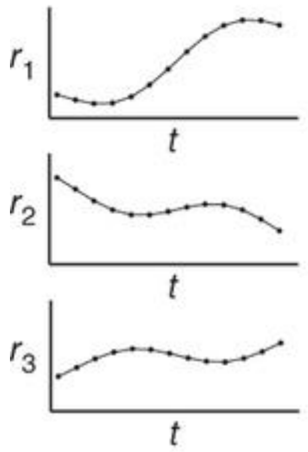
- This modeling consists of finding "meaningful degrees of freedom" that describe the signal, and are of lesser dimension.

Unsupervised Learning

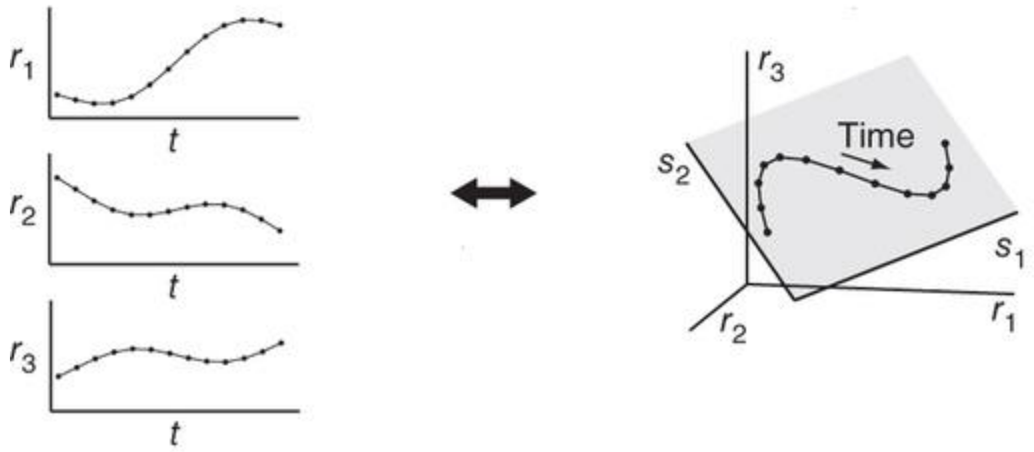
- Definition
  - Unsupervised learning refers to most attempts to extract information from a distribution that do not require human labor to annotate example
  - Main task is to find the ‘best’ representation of the data

- Dimension Reduction
  - Attempt to compress as much information as possible in a smaller representation
  - Preserve as much information as possible while obeying some constraint aimed at keeping the representation simpler

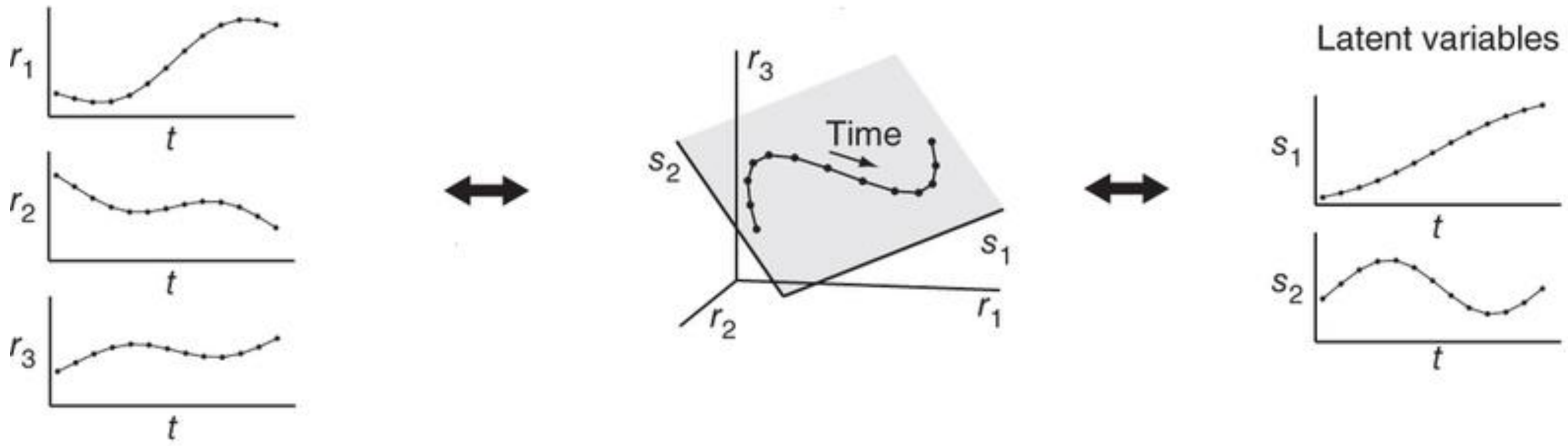
Unsupervised Learning



Unsupervised Learning

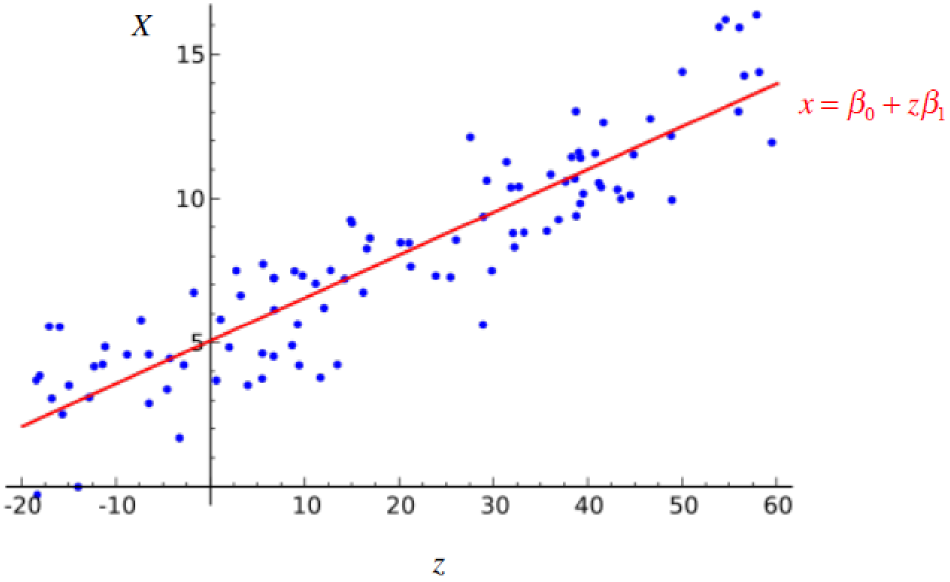


Unsupervised Learning



Recap: Linear Regression

- Most people think of linear regression as points and a straight line:

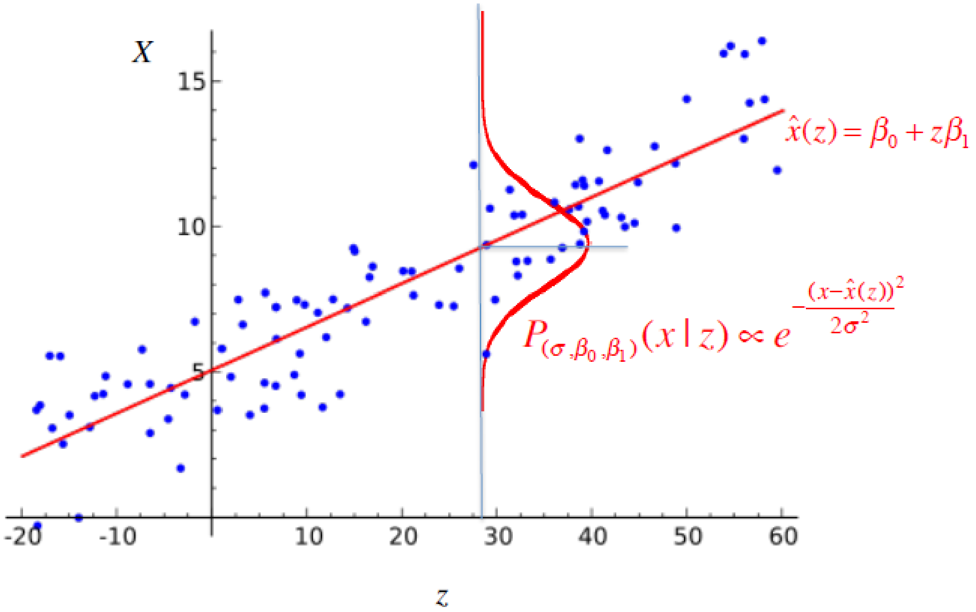


Recap: Linear Regression

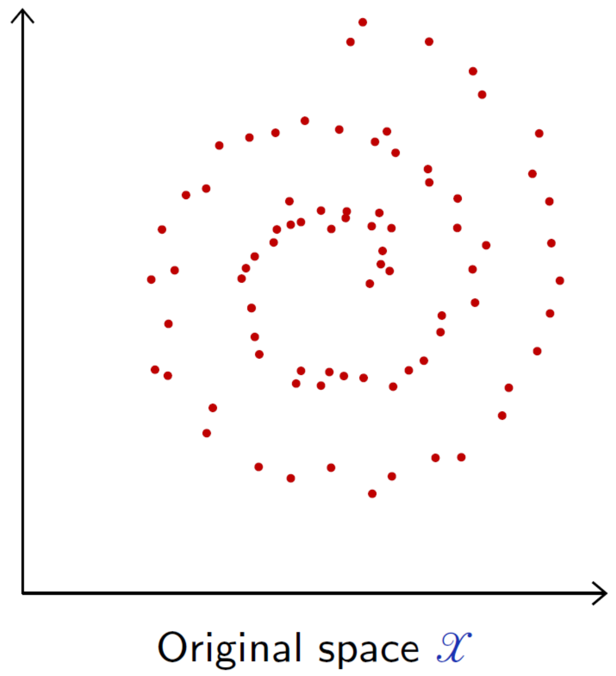
- Statisticians additionally have $P_\theta(X|Z)$
- True model
  - May not be too complicated as opposed to original data
- Observed data = true model + error
- Benefits of having an error model:
  - How likely is a data point
  - Confidence bounds
  - Compare models

- Q: how to find an unseen true model

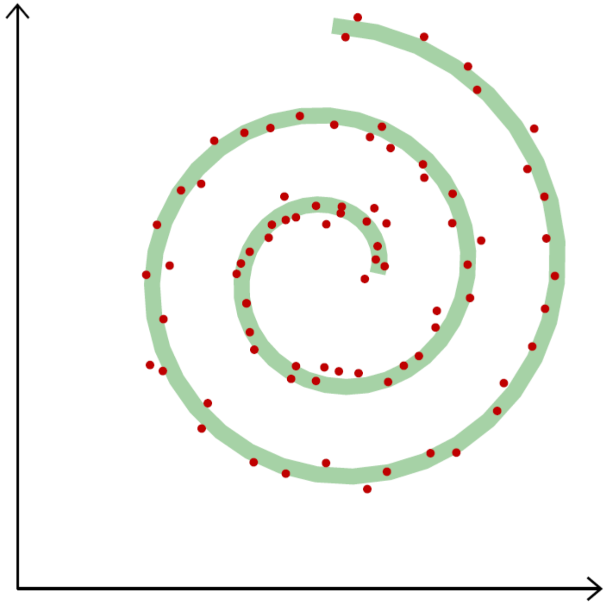
  (we never know the true model)



Original Space and Latent Space



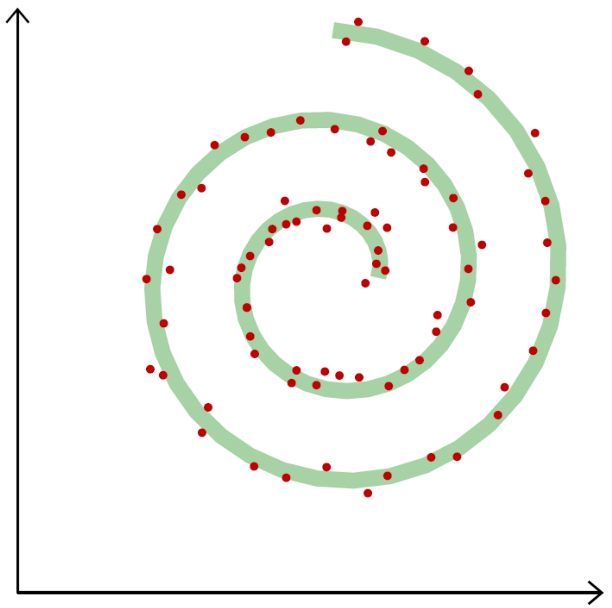
Original Space and Latent Space

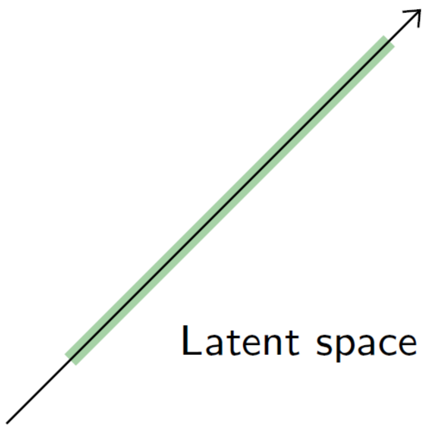


Original space $\mathscr{X}$

Source: Dr. Francois Fleuret at EPEL

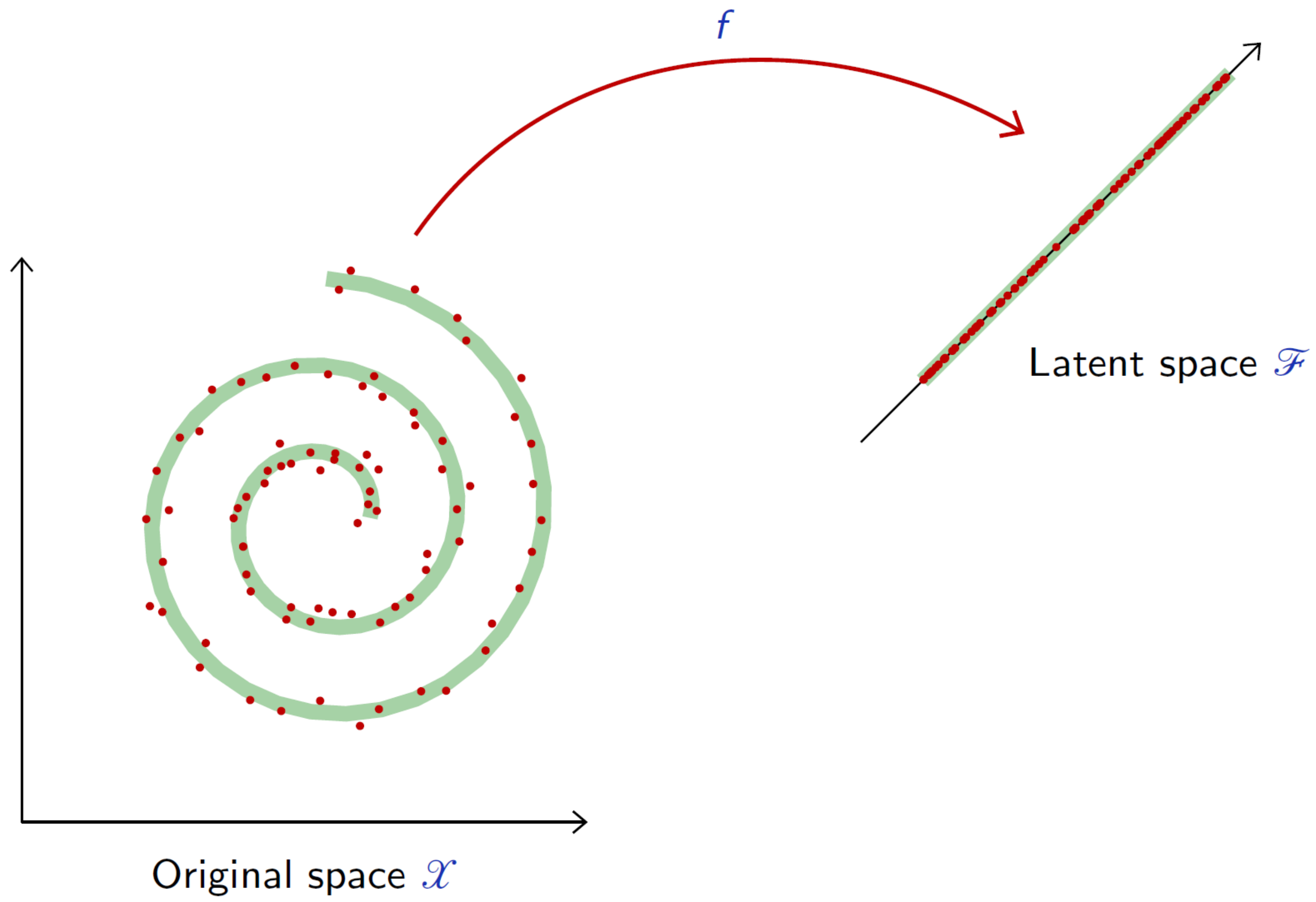
Original Space and Latent Space





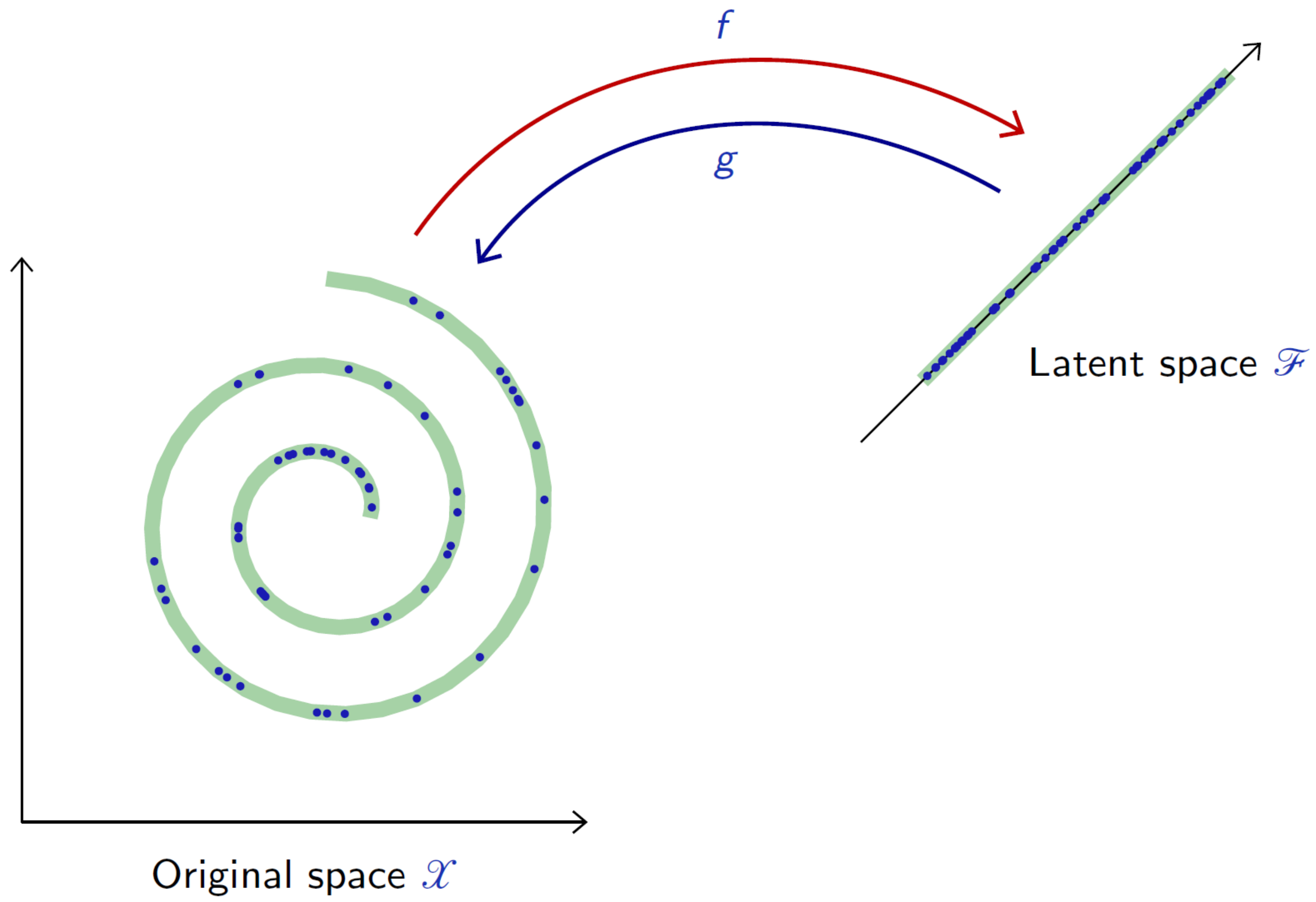
Source: Dr. Francois Fleuret at EPEL

Original Space and Latent Space



Source: Dr. Francois Fleuret at EPEL

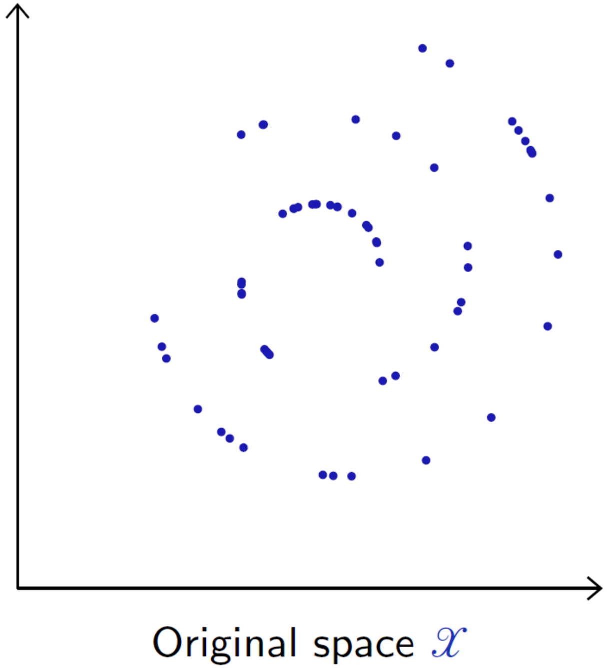
Original Space and Latent Space



Source: Dr. Francois Fleuret at EPEL

Original Space and Latent Space

- We can generate data



Autoencoders

- It is like 'deep learning version' of unsupervised learning

- Definition
  - An autoencoder is a neural network that is trained to attempt to copy its input to its output
  - The network consists of two parts: an encoder and a decoder that produce a reconstruction

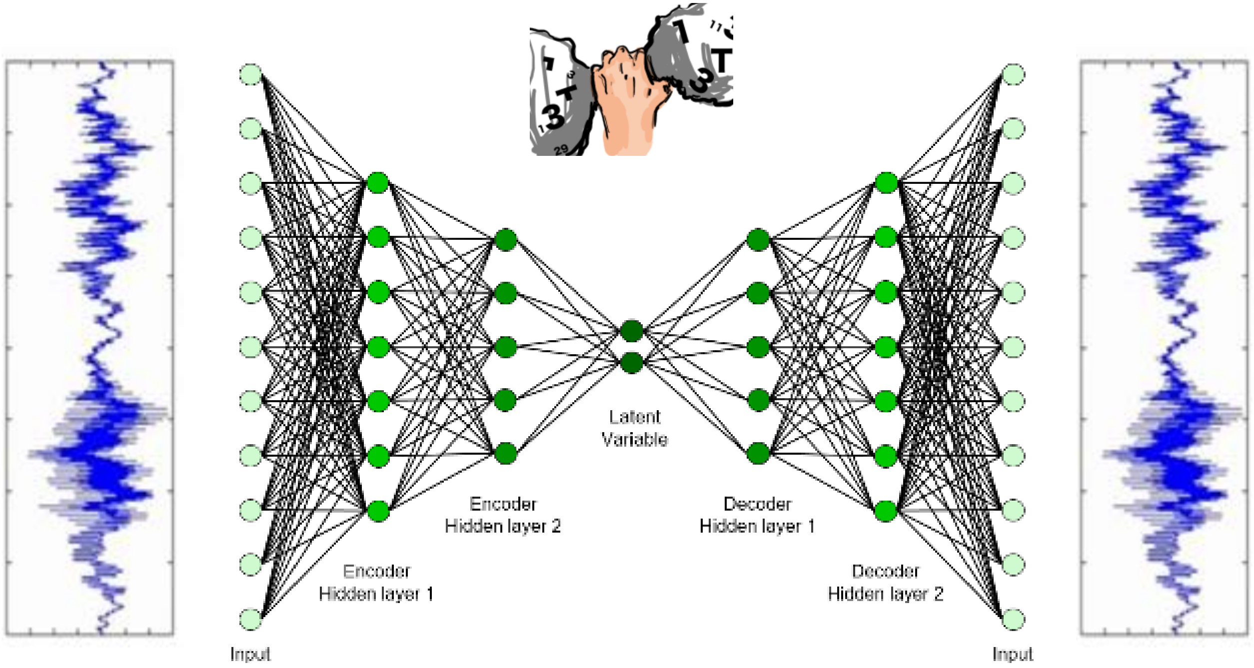
- Encoder and Decoder
  - Encoder function : $z = f(x)$
  - Decoder function : $x = g(z)$
  - We learn to set $g\big(f(x)\big) = x$

Autoencoder

- Dimension reduction
- Recover the input data

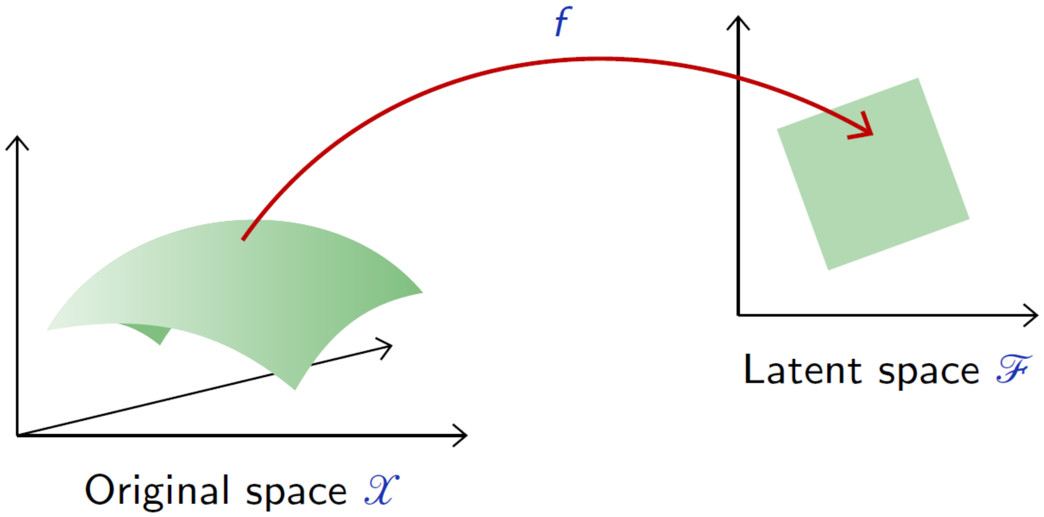
Autoencoder

- Dimension reduction
- Recover the input data
  - Learns an encoding of the inputs so as to recover the original input from the encodings as well as possible



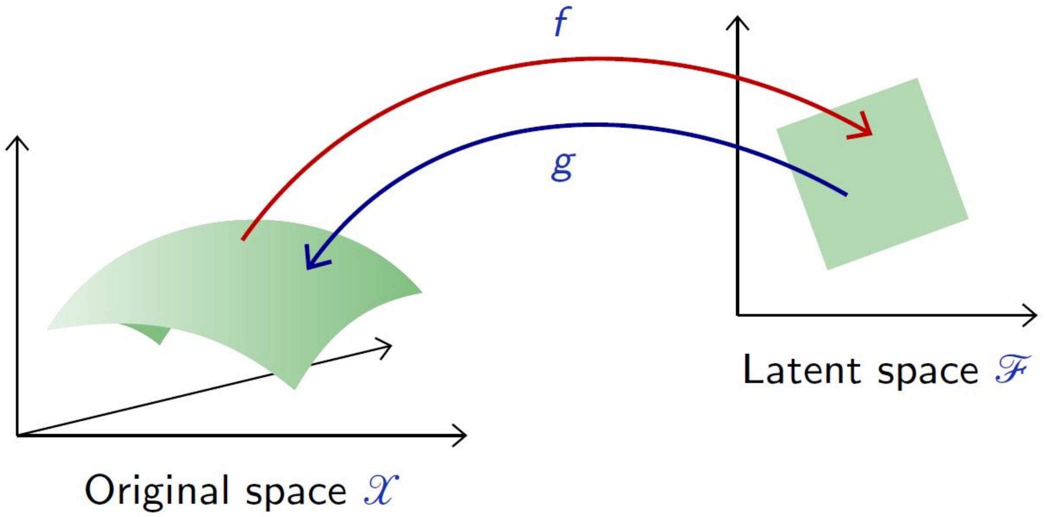
Autoencoder

- Autoencoder combines an encoder f from the original space $\mathcal{X}$ to a latent space $\mathcal{F}$, and a decoder g to map back to $\mathcal{X}$, such that $g \circ f$ is [close to] the identity on the data



Autoencoder

- Autoencoder combines an encoder f from the original space $\mathcal{X}$ to a latent space $\mathcal{F}$, and a decoder g to map back to $\mathcal{X}$, such that $g \circ f$ is [close to] the identity on the data



- A proper autoencoder has to capture a "good" parametrization of the signal, and in particular the statistical dependencies between the signal components.

Source: Dr. Francois Fleuret at EPEL

Autoencoder

Let q be the data distribution over $\mathscr{X}$. A good autoencoder could be characterized with the quadratic loss

$$\mathbb{E}_{X \sim q}\left[\|X - g \circ f(X)\|^2\right] \simeq 0.$$

Given two parametrized mappings $f(\cdot\,;w)$ and $g(\cdot\,;w)$, training consists of minimizing an empirical estimate of that loss

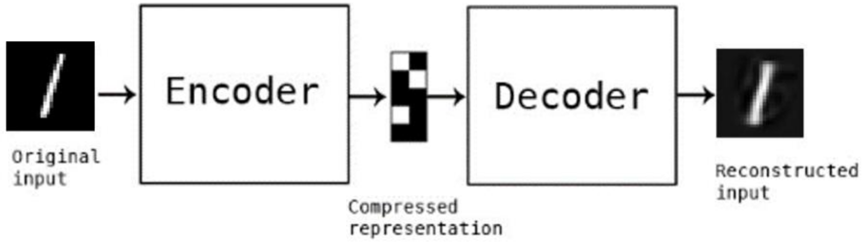
$$\hat{w}_f, \hat{w}_g = \underset{w_f, w_g}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} \|x_n - g(f(x_n; w_f); w_g)\|^2 .$$

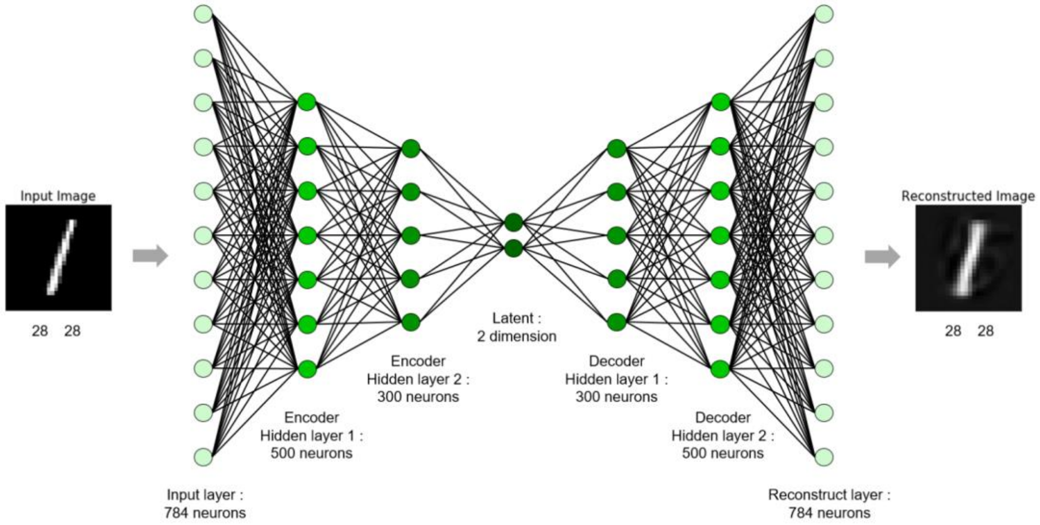
A simple example of such an autoencoder would be with both f and g linear, in which case the optimal solution is given by PCA. Better results can be achieved with more sophisticated classes of mappings, in particular deep architectures.

Autoencoder with MNIST

Autoencoder with TensorFlow

- MNIST example
- Use only (1, 5, 6) digits to visualize in 2-D





Import Libraries and Load MNIST Data

```
import numpy as np
import matplotlib.pyplot as plt
import tensorflow as tf
%matplotlib inline
```

```
from tensorflow.examples.tutorials.mnist import input_data
mnist = input_data.read_data_sets("MNIST_data/", one_hot=True)
```

- Only use (1, 5, 6) digits to visualize latent space in 2-D

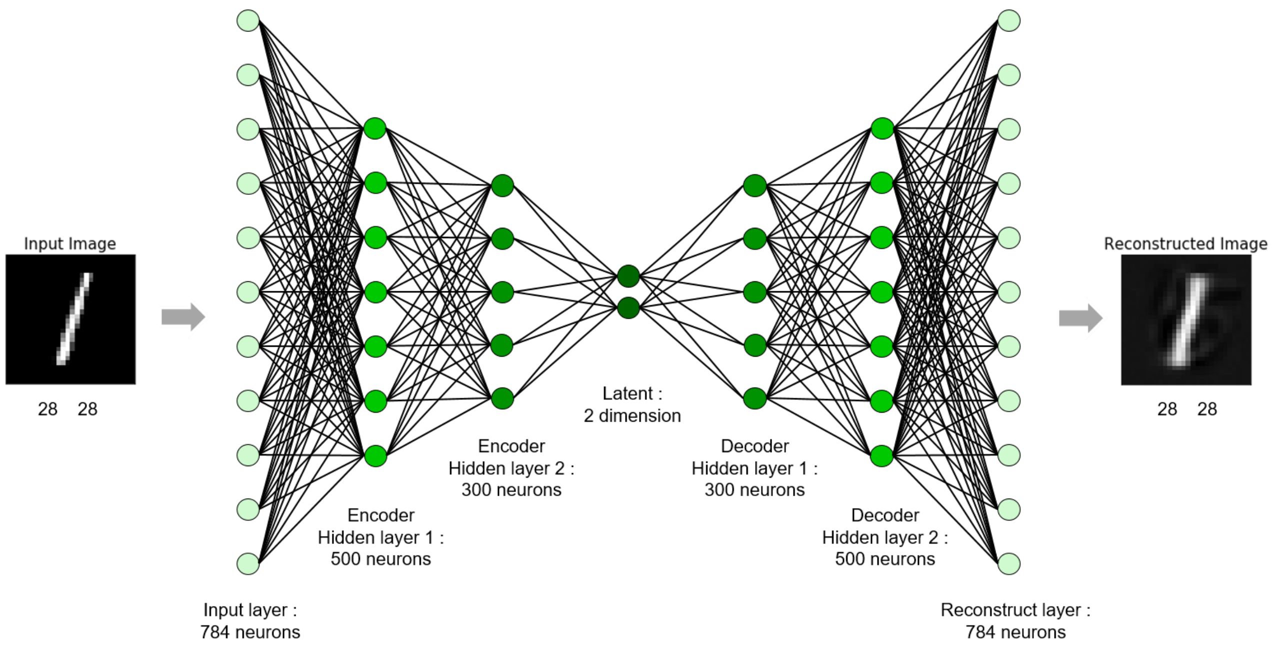
```
train_idx = ((np.argmax(mnist.train.labels, 1) == 1) | \
             (np.argmax(mnist.train.labels, 1) == 5) | \
             (np.argmax(mnist.train.labels, 1) == 6))
test_idx = ((np.argmax(mnist.test.labels, 1) == 1) | \
            (np.argmax(mnist.test.labels, 1) == 5) | \
            (np.argmax(mnist.test.labels, 1) == 6))

train_imgs   = mnist.train.images[train_idx]
train_labels = mnist.train.labels[train_idx]
test_imgs    = mnist.test.images[test_idx]
test_labels  = mnist.test.labels[test_idx]
n_train      = train_imgs.shape[0]
n_test       = test_imgs.shape[0]

print ("The number of training images : {}, shape : {}".format(n_train, train_imgs.shape))
print ("The number of testing images : {}, shape : {}".format(n_test, test_imgs.shape))
```

```
The number of training images : 16583, shape : (16583, 784)
The number of testing images : 2985, shape : (2985, 784)
```

Structure of Autoencoder

- Input shape and latent variable shape
- Encoder shape
- Decoder shape

```
# Shape of input and latent variable

n_input = 28*28

# Encoder structure
n_encoder1 = 500
n_encoder2 = 300

n_latent = 2

# Decoder structure
n_decoder2 = 300
n_decoder1 = 500
```



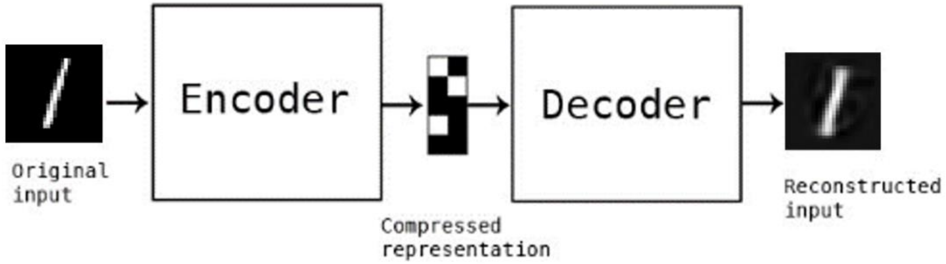
Weights & Biases, and Placeholder

- Define weights and biases for encoder and decoder, separately
- Based on the pre-defined layer size
- Initialize with normal distribution of $\mu = 0$ and $\sigma = 0.1$

```
weights = {
    'encoder1' : tf.Variable(tf.random_normal([n_input, n_encoder1], stddev = 0.1)),
    'encoder2' : tf.Variable(tf.random_normal([n_encoder1, n_encoder2], stddev = 0.1)),
    'latent' : tf.Variable(tf.random_normal([n_encoder2, n_latent], stddev = 0.1)),
    'decoder2' : tf.Variable(tf.random_normal([n_latent, n_decoder2], stddev = 0.1)),
    'decoder1' : tf.Variable(tf.random_normal([n_decoder2, n_decoder1], stddev = 0.1)),
    'reconst' : tf.Variable(tf.random_normal([n_decoder1, n_input], stddev = 0.1))
}

biases = {
    'encoder1' : tf.Variable(tf.random_normal([n_encoder1], stddev = 0.1)),
    'encoder2' : tf.Variable(tf.random_normal([n_encoder2], stddev = 0.1)),
    'latent' : tf.Variable(tf.random_normal([n_latent], stddev = 0.1)),
    'decoder2' : tf.Variable(tf.random_normal([n_decoder2], stddev = 0.1)),
    'decoder1' : tf.Variable(tf.random_normal([n_decoder1], stddev = 0.1)),
    'reconst' : tf.Variable(tf.random_normal([n_input], stddev = 0.1))
}
```

```
x = tf.placeholder(tf.float32, [None, n_input])
```

Build a Model




```python
def encoder(x, weights, biases):
    encoder1 = tf.add(tf.matmul(x, weights['encoder1']), biases['encoder1'])
    encoder1 = tf.nn.tanh(encoder1)

    encoder2 = tf.add(tf.matmul(encoder1, weights['encoder2']), biases['encoder2'])
    encoder2 = tf.nn.tanh(encoder2)

    latent = tf.add(tf.matmul(encoder2, weights['latent']), biases['latent'])

    return latent
```

```python
def decoder(latent, weights, biases):
    decoder2 = tf.add(tf.matmul(latent, weights['decoder2']), biases['decoder2'])
    decoder2 = tf.nn.tanh(decoder2)

    decoder1 = tf.add(tf.matmul(decoder2, weights['decoder1']), biases['decoder1'])
    decoder1 = tf.nn.tanh(decoder1)

    reconst = tf.add(tf.matmul(decoder1, weights['reconst']), biases['reconst'])

    return reconst
```

Loss and Optimizer

- Loss
  – Squared loss

$$\frac{1}{m}\sum_{i=1}^{m}(t_i - y_i)^2$$

- Optimizer
  – AdamOptimizer: the most popular optimizer

```
LR = 0.0001

latent = encoder(x, weights, biases)
reconst = decoder(latent, weights, biases)
loss = tf.square(tf.subtract(x, reconst))
loss = tf.reduce_mean(loss)

optm = tf.train.AdamOptimizer(LR).minimize(loss)
```

Define Optimization Configuration and Batch Maker

- Define parameters for training autoencoder
  - n_batch: batch size for mini-batch gradient descent
  - n_iter: the number of iterations steps
  - n_prt: check loss for every n_prt iteration

```
n_batch = 50
n_iter = 2500
n_prt = 250
```

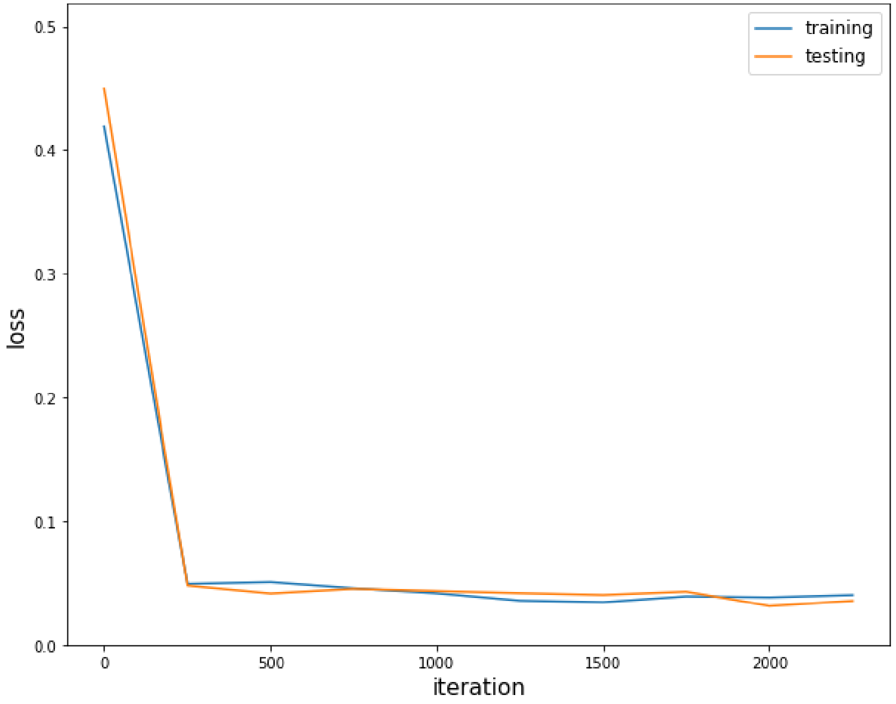
- Batch maker

```
def train_batch_maker(batch_size):
    random_idx = np.random.randint(n_train, size = batch_size)
    return train_imgs[random_idx], train_labels[random_idx]
```

```
def test_batch_maker(batch_size):
    random_idx = np.random.randint(n_test, size = batch_size)
    return test_imgs[random_idx], test_labels[random_idx]
```

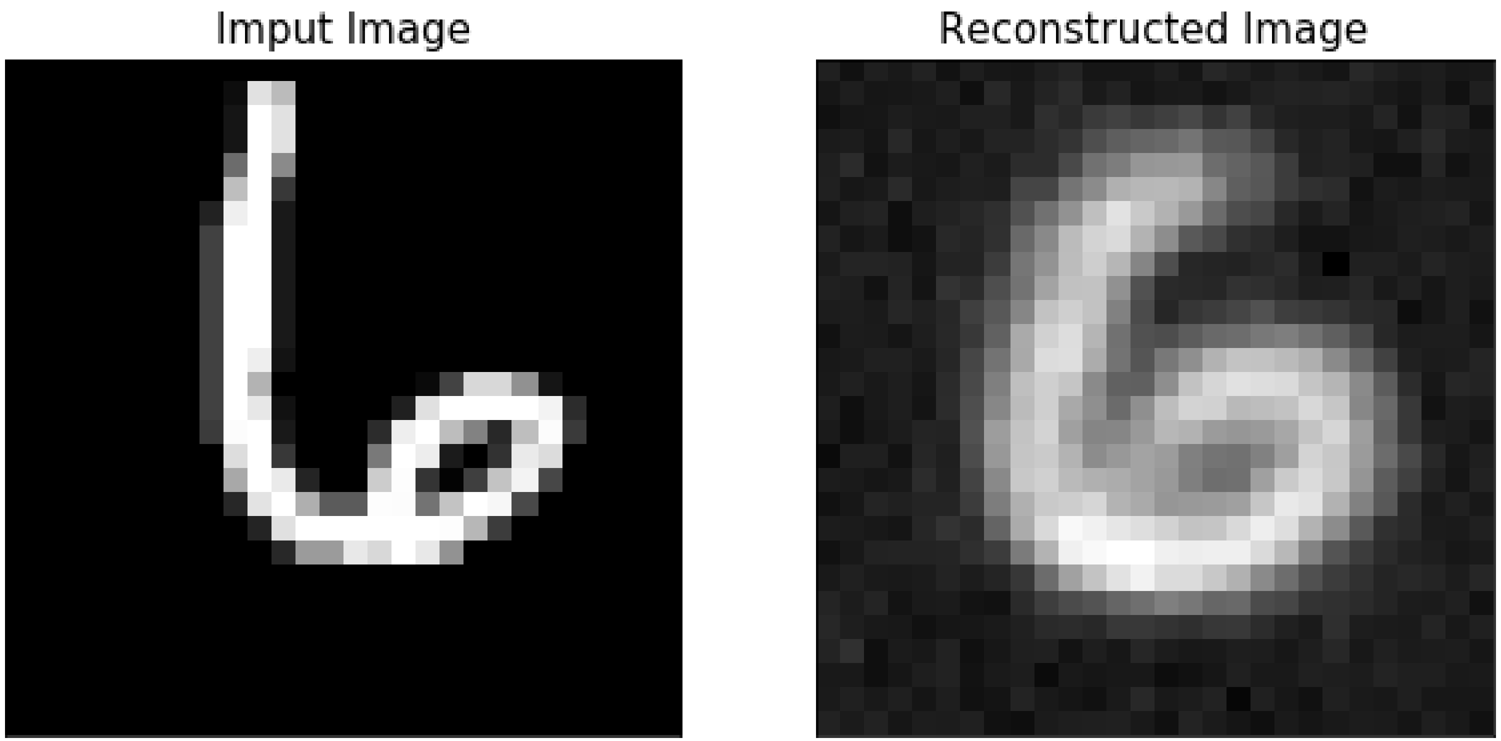
Optimization

```python
sess = tf.Session()
init = tf.global_variables_initializer()
sess.run(init)

loss_record_train = []
loss_record_test = []
for epoch in range(n_iter):
    train_x, _ = train_batch_maker(n_batch)
    sess.run(optm, feed_dict = {x : train_x})

    if epoch % n_prt == 0:
        test_x, _ = test_batch_maker(n_batch)
        c1 = sess.run(loss, feed_dict = {x: train_x})
        c2 = sess.run(loss, feed_dict = {x: test_x})
        loss_record_train.append(c1)
        loss_record_test.append(c2)
        print ("Iter : {}".format(epoch))
        print ("Cost : {}".format(c1))
```



Test or Evaluation

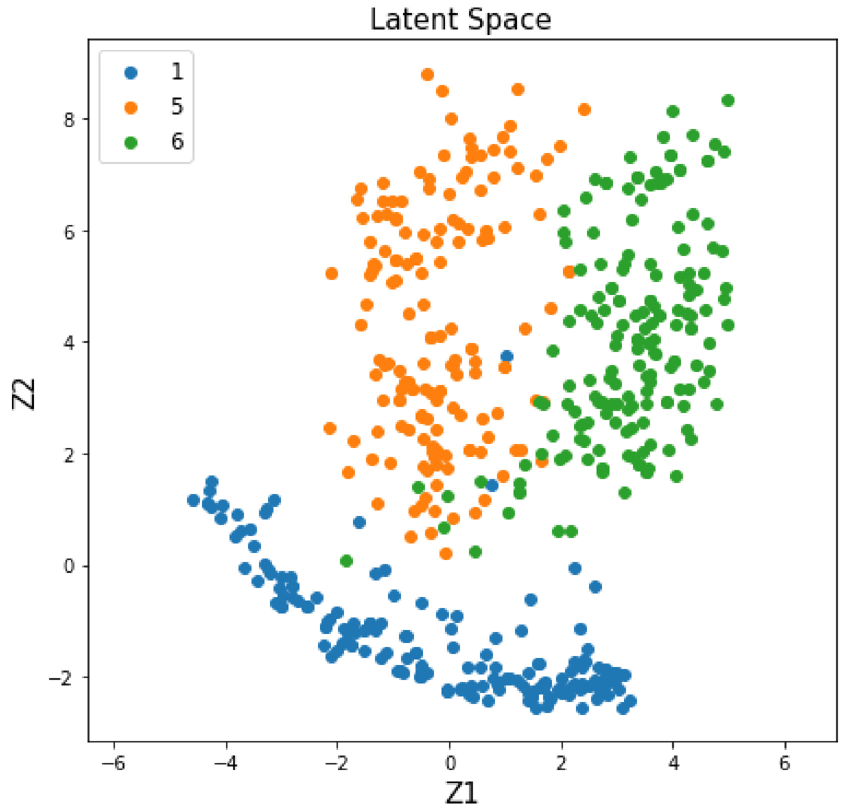
```
test_x, _ = test_batch_maker(1)
x_reconst = sess.run(reconst, feed_dict = {x: test_x})
```



Distribution in Latent Space

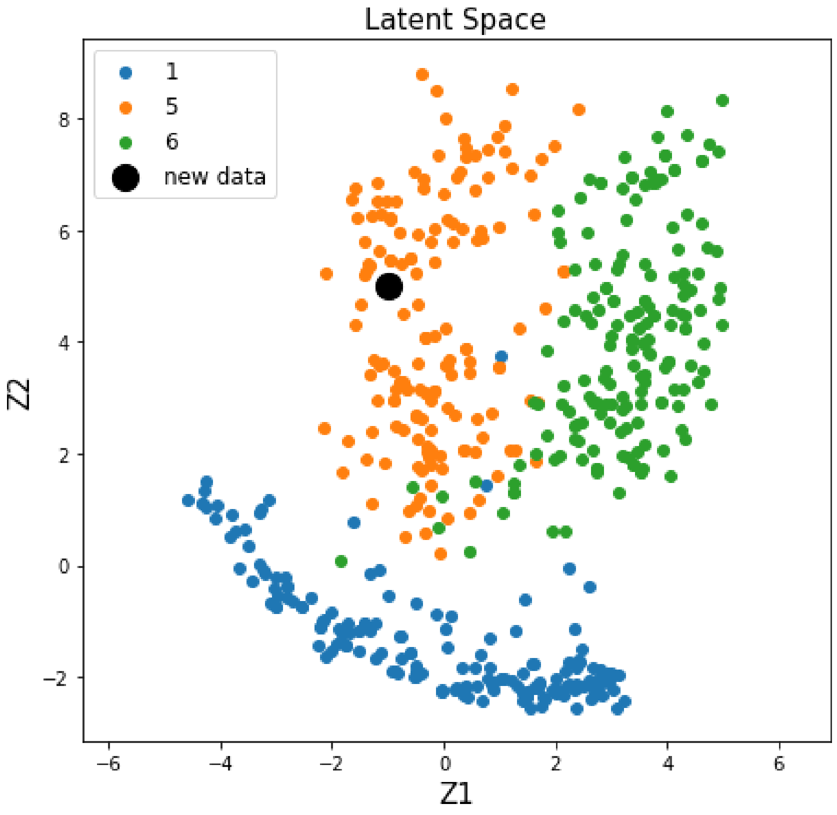
- Make a projection of 784-dim image onto 2-dim latent space

```
test_x, test_y = test_batch_maker(500)
test_y = np.argmax(test_y, axis = 1)
test_latent = sess.run(latent, feed_dict = {x: test_x})
```

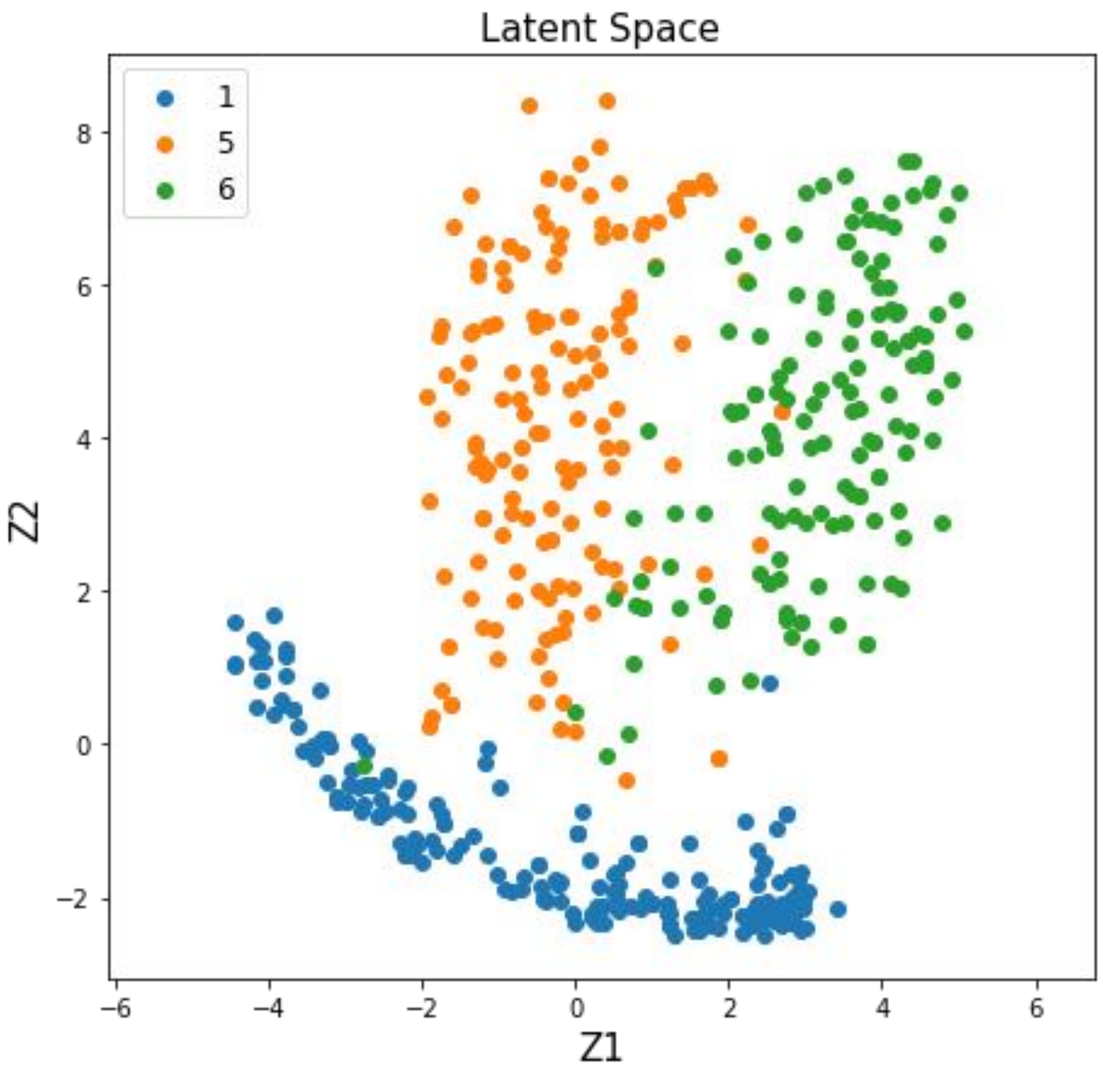


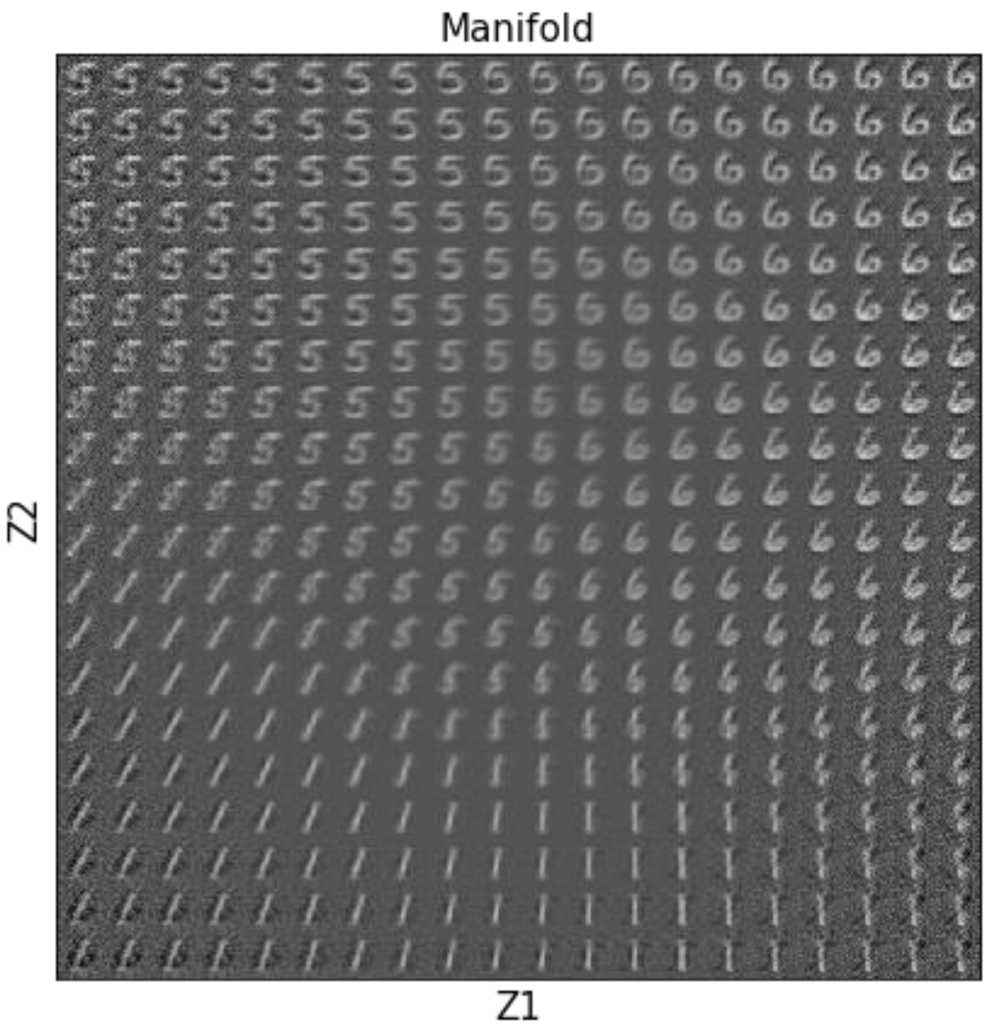
Data Generation

```
new_data = np.array([[-1, 5]])

latent_input = tf.placeholder(tf.float32, [None, n_latent])
reconst = decoder(latent_input, weights, biases)
fake_image = sess.run(reconst, feed_dict = {latent_input: new_data})
```



Visualization

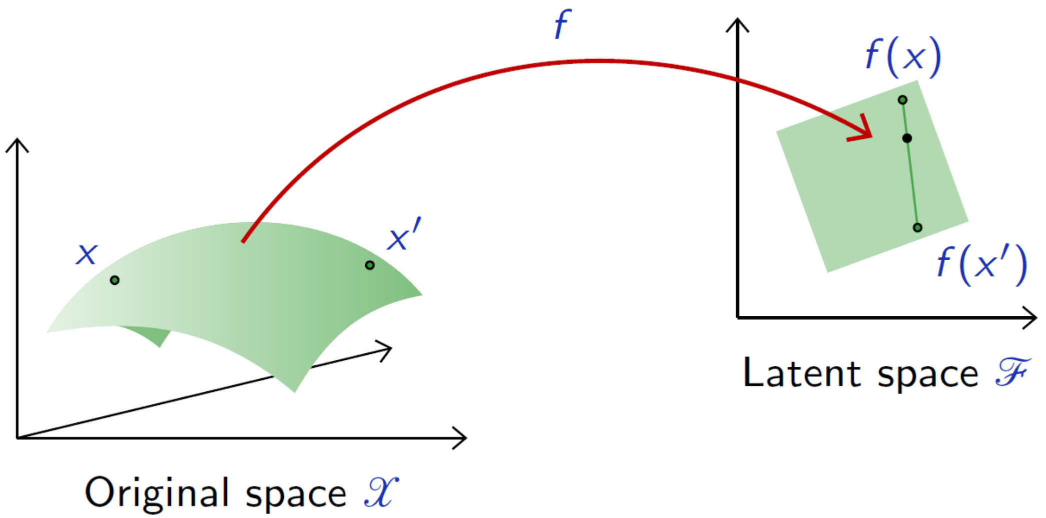




Autoencoder as Generative Model

Latent Representation

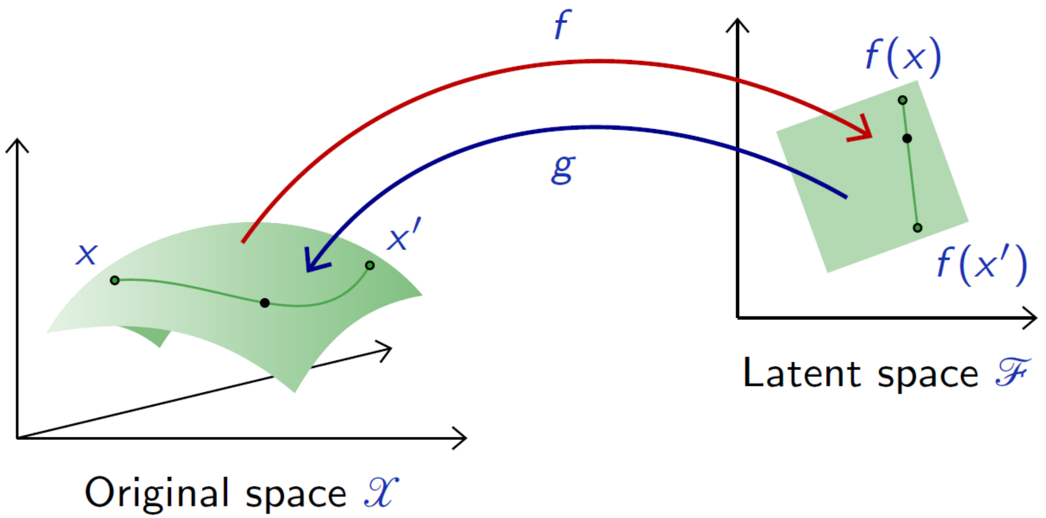
- To get an intuition of the latent representation, we can pick two samples x and x' at random and interpolate samples along the line in the latent space



Latent Representation

- To get an intuition of the latent representation, we can pick two samples x and x' at random and interpolate samples along the line in the latent space

$$\forall x, x' \in \mathscr{X}^2, \ \alpha \in [0,1], \quad \xi(x, x', \alpha) = g((1-\alpha)f(x) + \alpha f(x')).$$

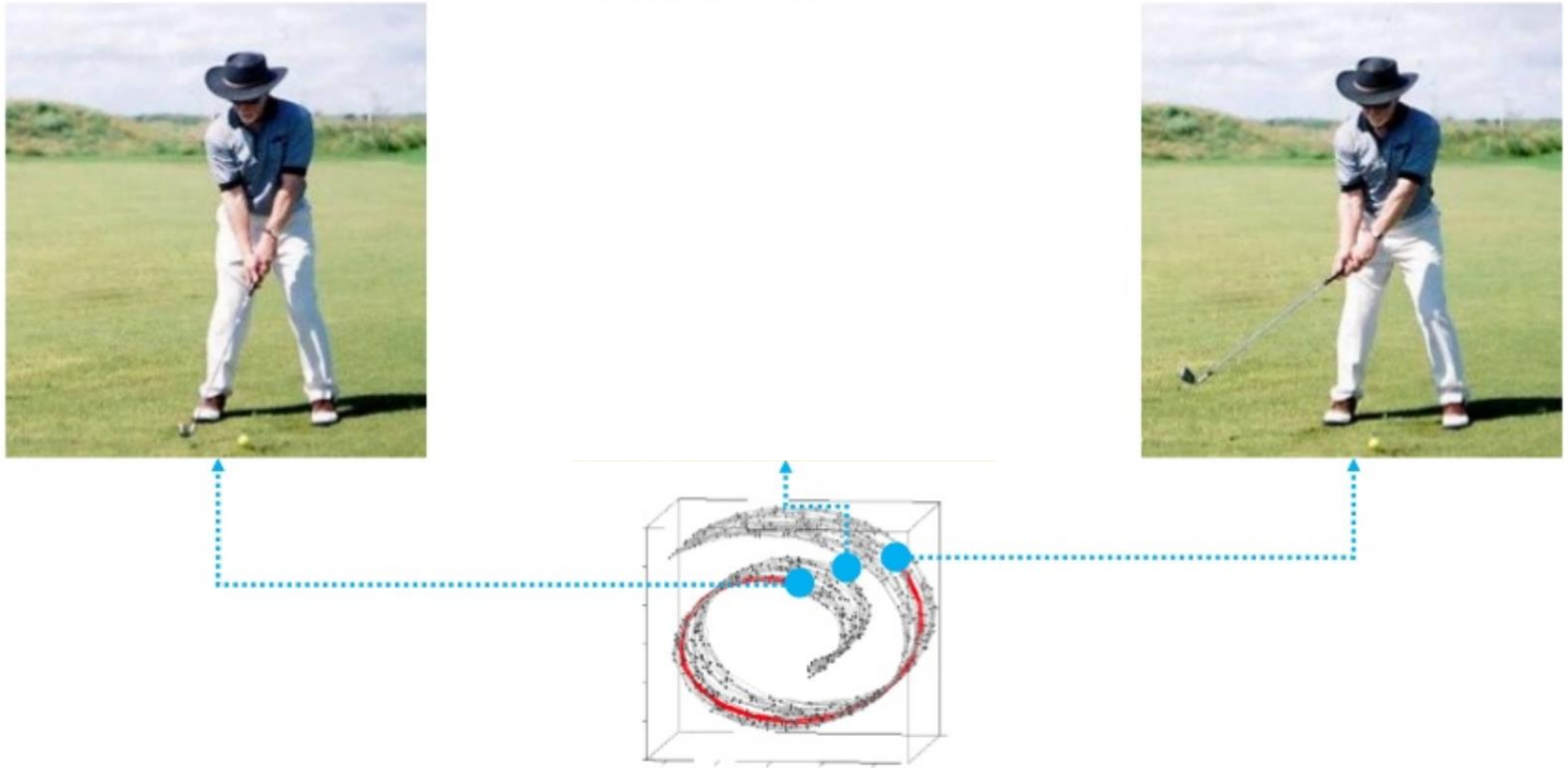


Source: Dr. Francois Fleuret at EPEL

Interpolation in High Dimension

Reasonable distance metric

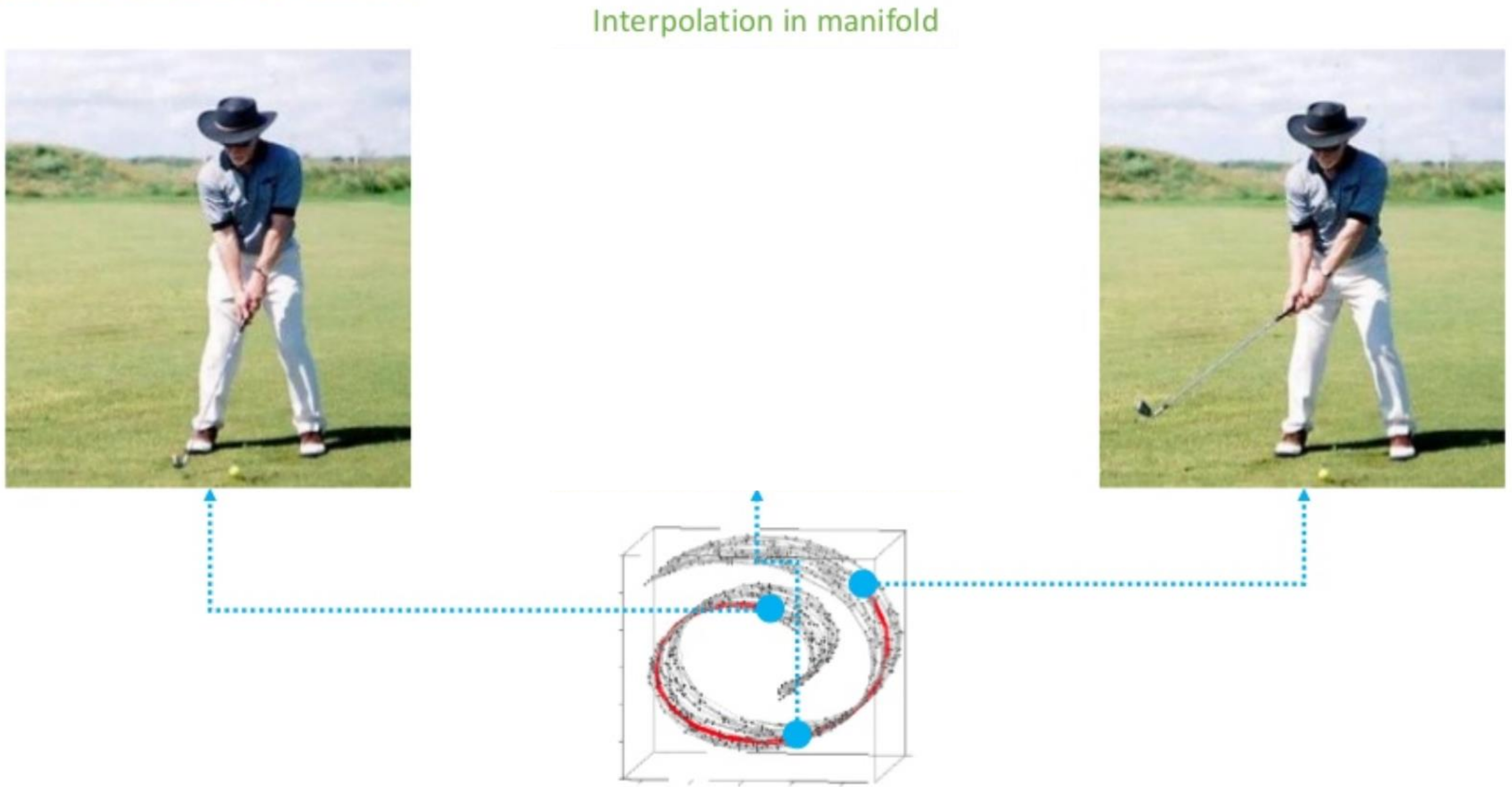
Interpolation in high dimension



https://www.cs.cmu.edu/~efros/courses/AP06/presentations/ThompsonDimensionalityReduction.pdf

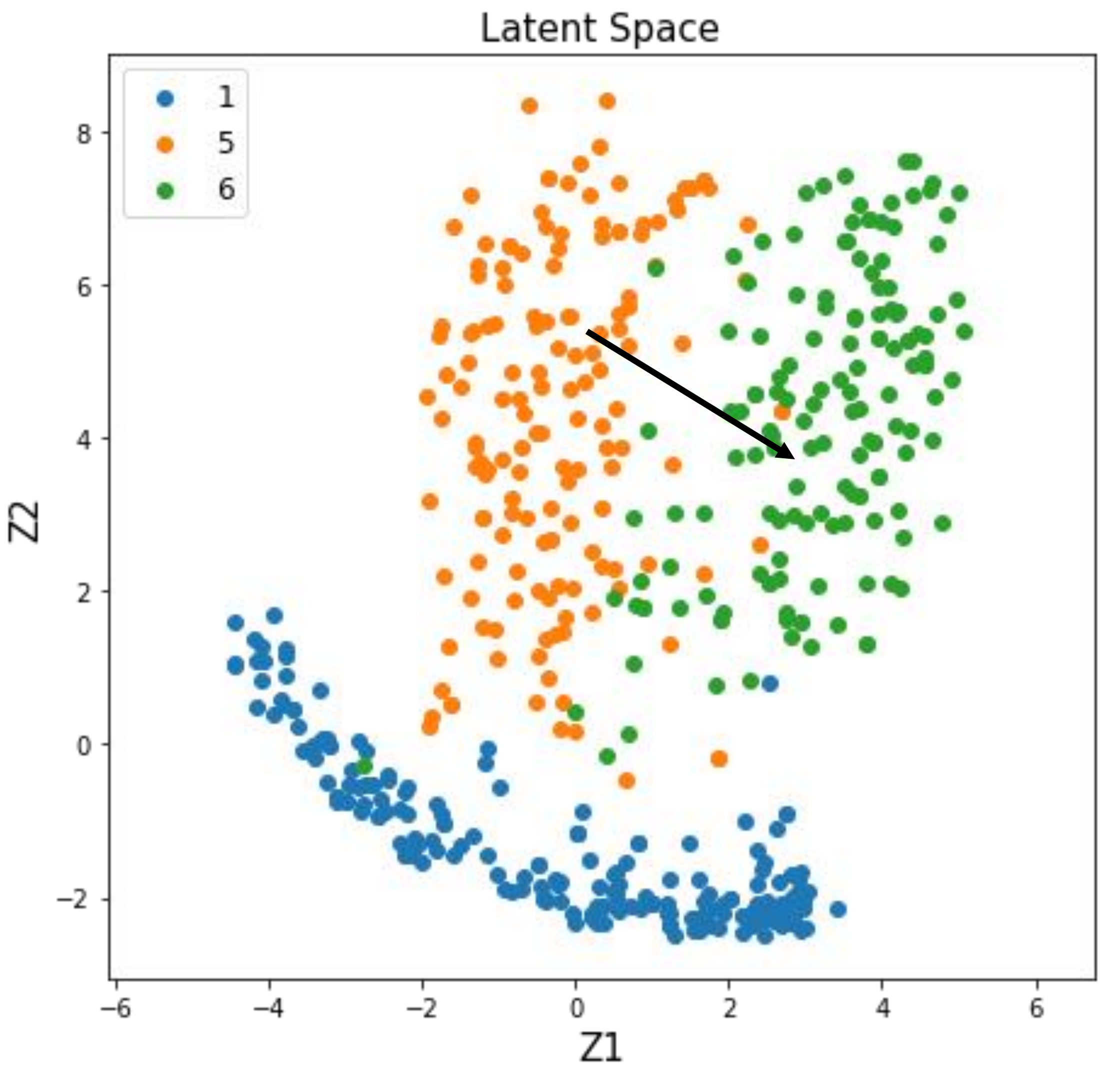
Interpolation in Manifold

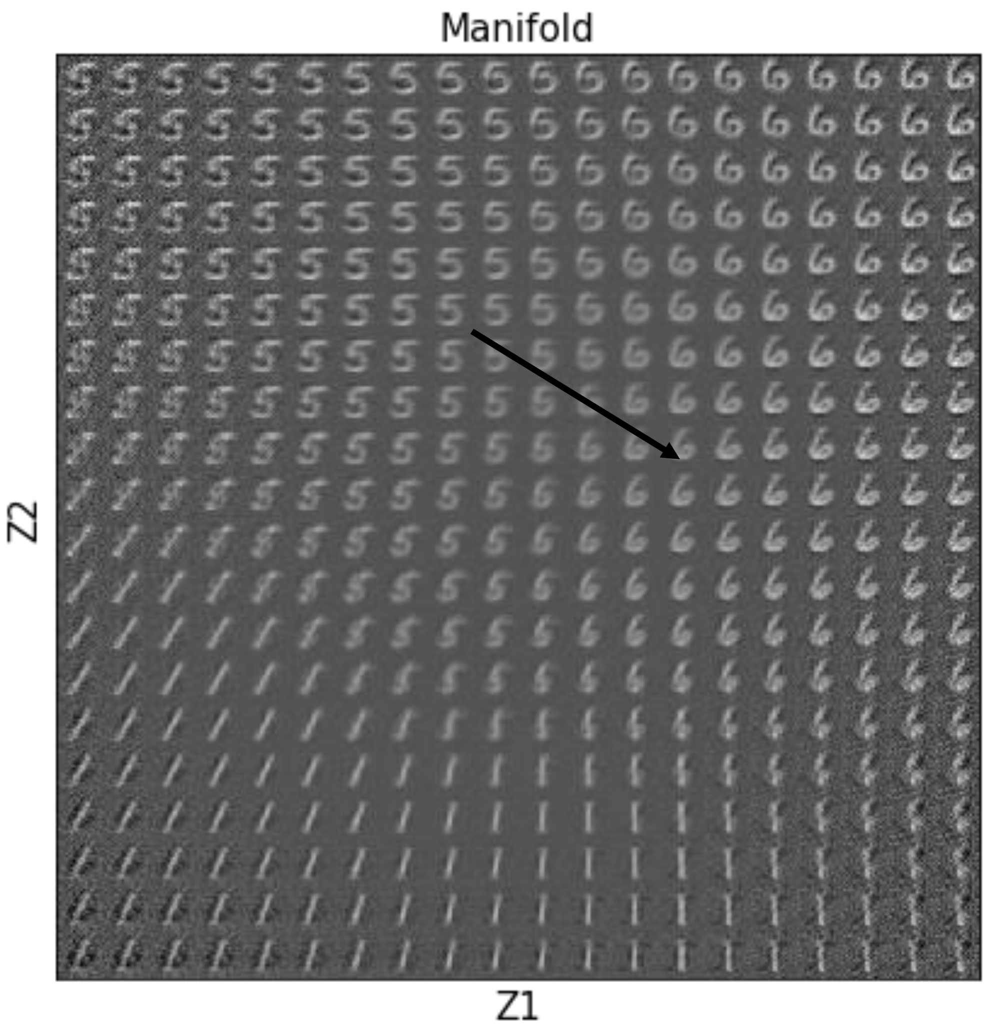
Reasonable distance metric



https://www.cs.cmu.edu/~efros/courses/AP06/presentations/ThompsonDimensionalityReduction.pdf

MNIST Example: Walk in the Latent Space





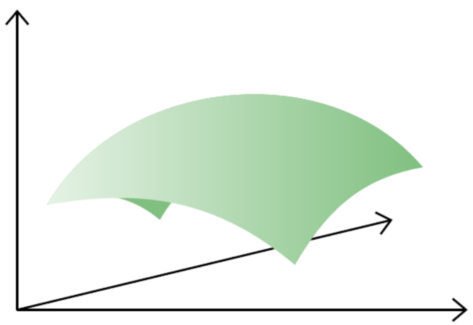
Generative Capabilities

- We can assess the generative capabilities of the decoder g by introducing a [simple] density model q^Z over the latent space $\mathcal{F}$, sample there, and map the samples into the image space $\mathcal{X}$ with g.

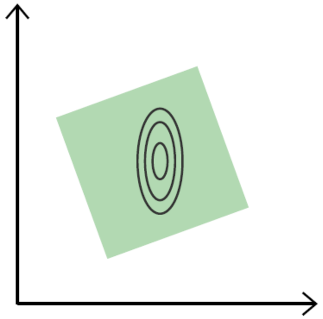
We can for instance use a Gaussian model with diagonal covariance matrix.

$$f(X) \sim \mathcal{N}(\hat{m}, \hat{\Delta})$$

where $\hat{m}$ is a vector and $\hat{\Delta}$ a diagonal matrix, both estimated on training data.



Original space $\mathscr{X}$



Latent space $\mathscr{F}$

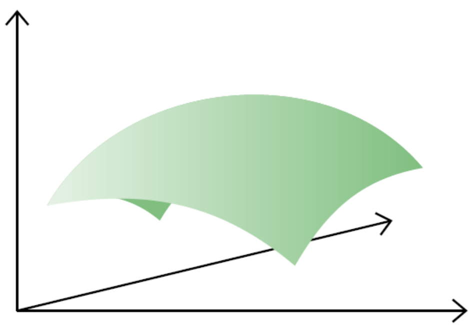
Generative Capabilities

- We can assess the generative capabilities of the decoder g by introducing a [simple] density model q^Z over the latent space $\mathcal{F}$, sample there, and map the samples into the image space $\mathcal{X}$ with g.

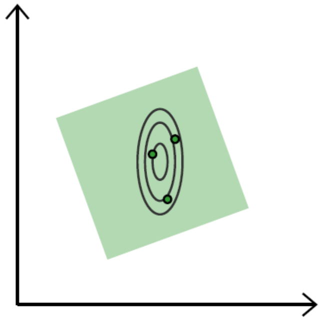
We can for instance use a Gaussian model with diagonal covariance matrix.

$$f(X) \sim \mathcal{N}(\hat{m}, \hat{\Delta})$$

where $\hat{m}$ is a vector and $\hat{\Delta}$ a diagonal matrix, both estimated on training data.



Original space $\mathscr{X}$



Latent space $\mathscr{F}$

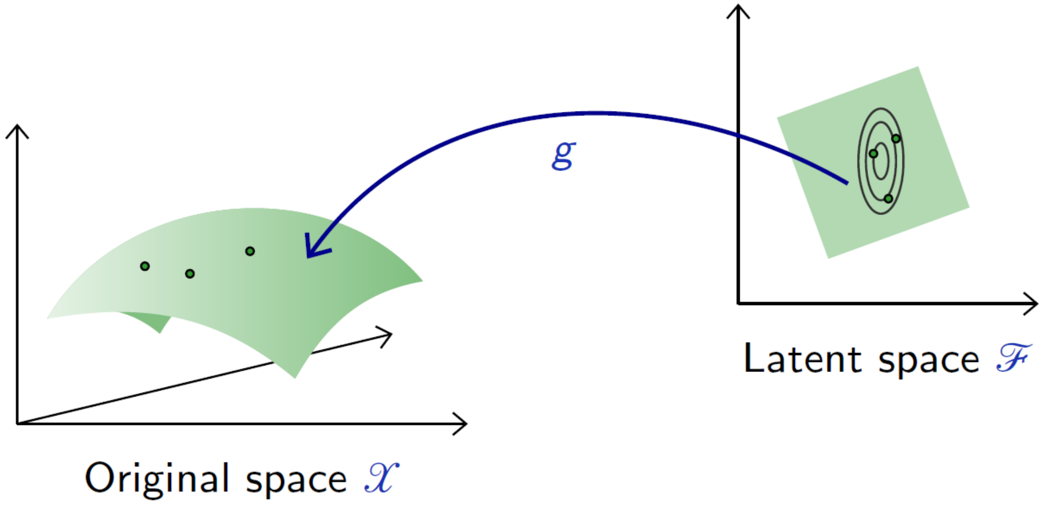
Generative Capabilities

- We can assess the generative capabilities of the decoder g by introducing a [simple] density model q^Z over the latent space $\mathcal{F}$, sample there, and map the samples into the image space $\mathcal{X}$ with g.

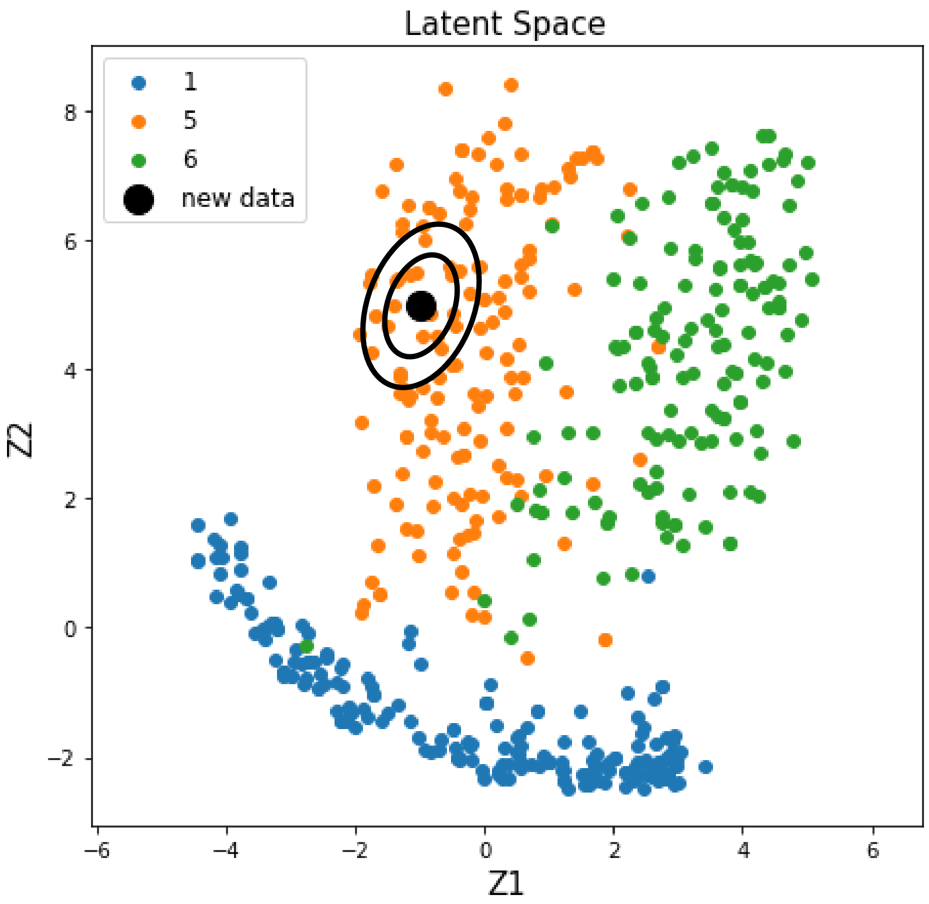
We can for instance use a Gaussian model with diagonal covariance matrix.

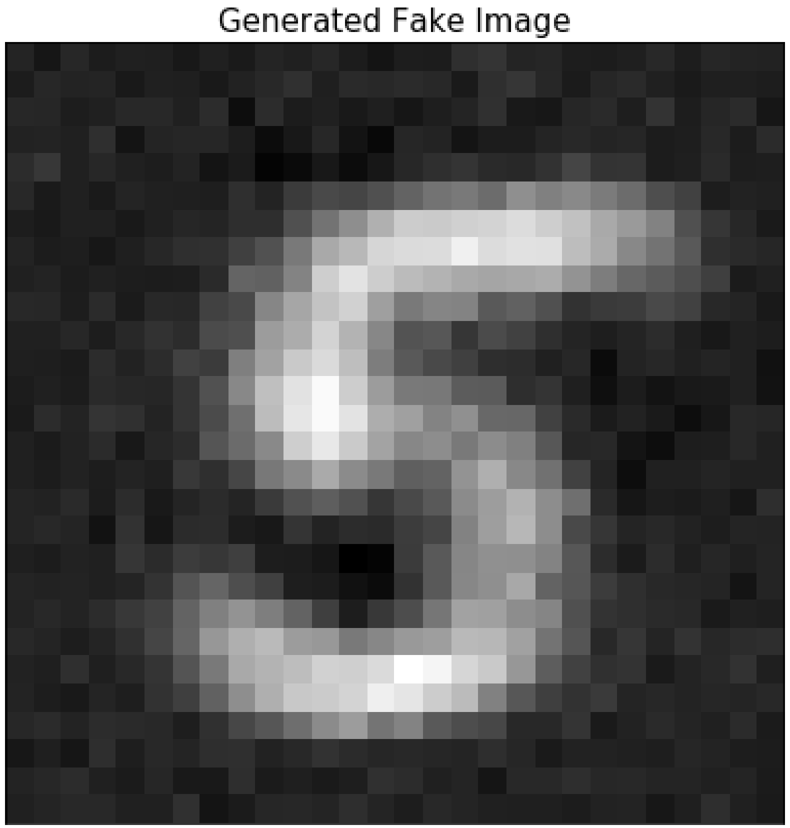
$$f(X) \sim \mathcal{N}(\hat{m}, \hat{\Delta})$$

where $\hat{m}$ is a vector and $\hat{\Delta}$ a diagonal matrix, both estimated on training data.



MNIST Example





Generative Models

- It generates something that makes sense.

- These results are unsatisfying, because the density model used on the latent space $\mathcal{F}$ is too simple and inadequate.

- Building a “good” model amounts to our original problem of modeling an empirical distribution, although it may now be in a lower dimension space.

- This is a motivation to VAE or GAN.