Autoencoder for Dimensionality Reduction

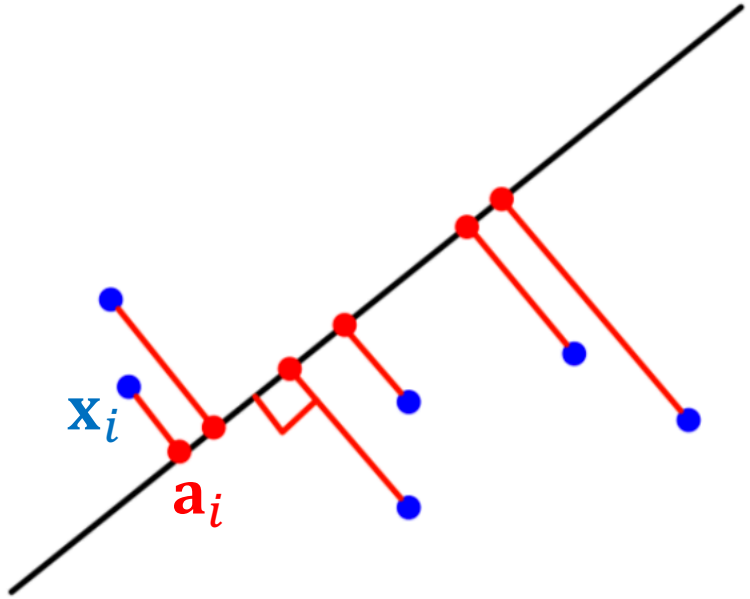
Shusen Wang

Revisit Principal Component Analysis (PCA)

Principal Component Analysis (PCA)

- Input: $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d$ (with zero-mean).

- Output: $\mathbf{a}_1, \cdots, \mathbf{a}_n \in \mathbb{R}^k$ $(k \ll d)$.



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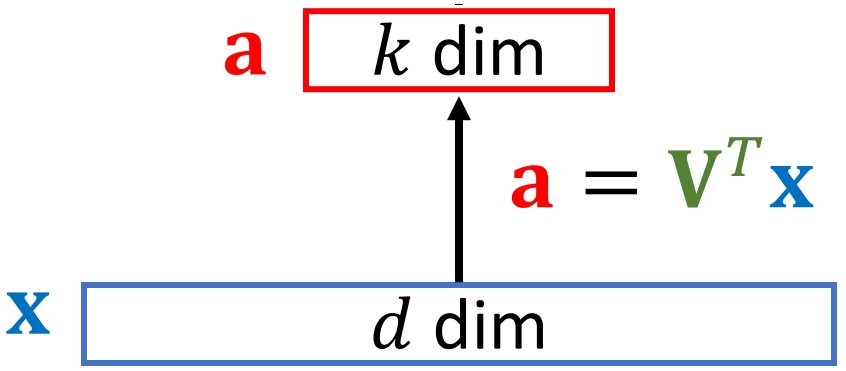
- PCA finds a $d \times k$ column orthogonal matrix $\mathbf{V}$



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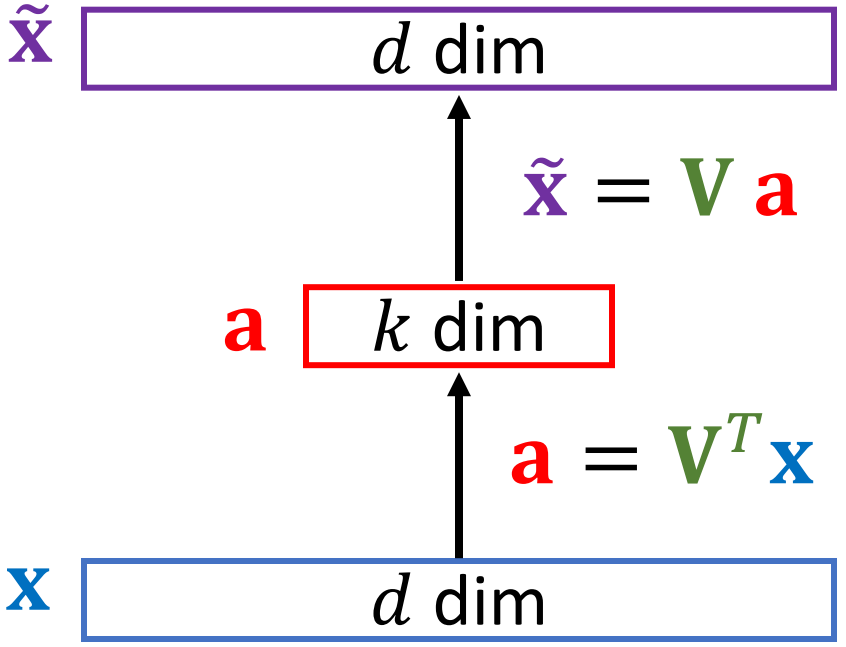
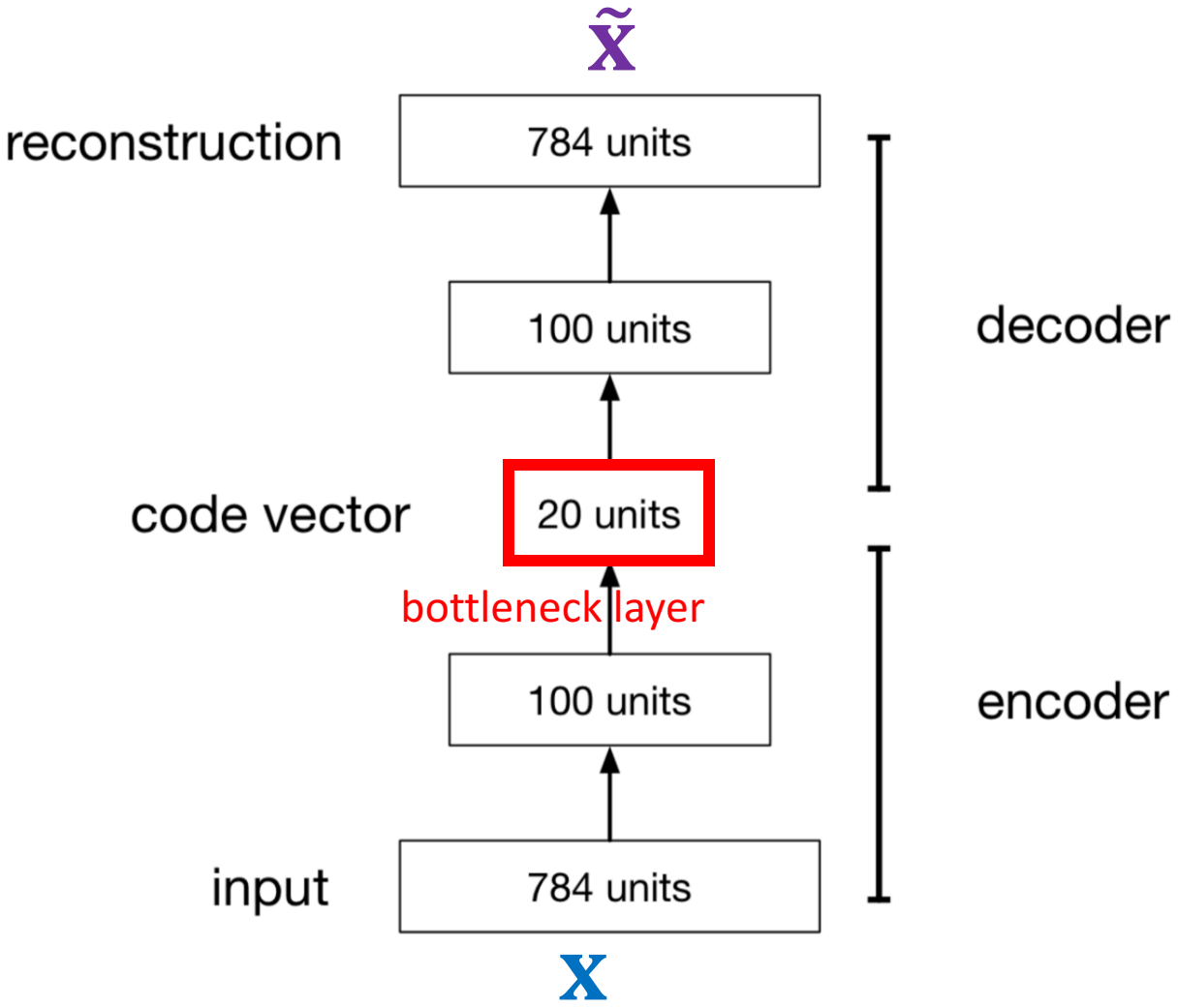
- PCA finds a $d \times k$ column orthogonal matrix $\mathbf{V}$ such that

$$\min_{\mathbf{V}} \sum_{j=1}^{n} \left|\left| \mathbf{x}_j - \tilde{\mathbf{x}}_j \right|\right|_2^2, \quad \text{s.t. } \mathbf{V}^T\mathbf{V} = \mathbf{I}_k.$$



Autoencoder

Autoencoder



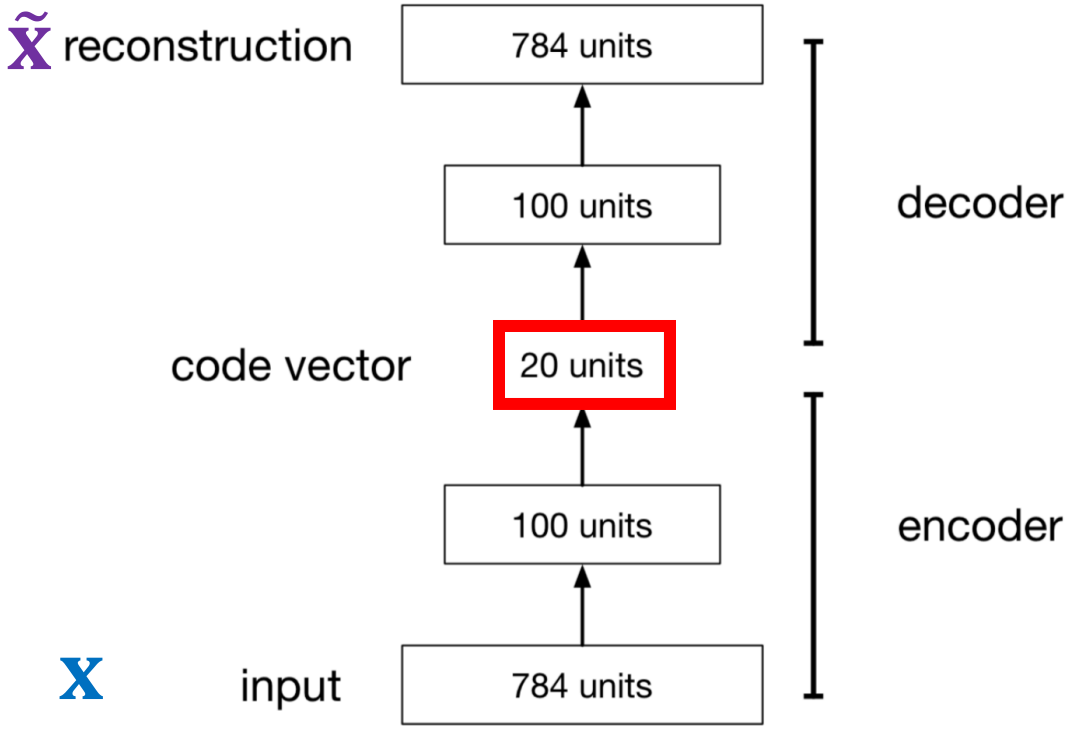
- An autoencoder is a neural net taking an input $\mathbf{x}$ and reconstruct $\mathbf{x}$.
- For dim reduction, we need a bottleneck layer whose dim is much smaller than the input.
- Loss function:

$$\sum_{j=1}^{n} \left|\left|\mathbf{x}_j - \tilde{\mathbf{x}}_j\right|\right|_2^2.$$

Autoencoder v.s. PCA

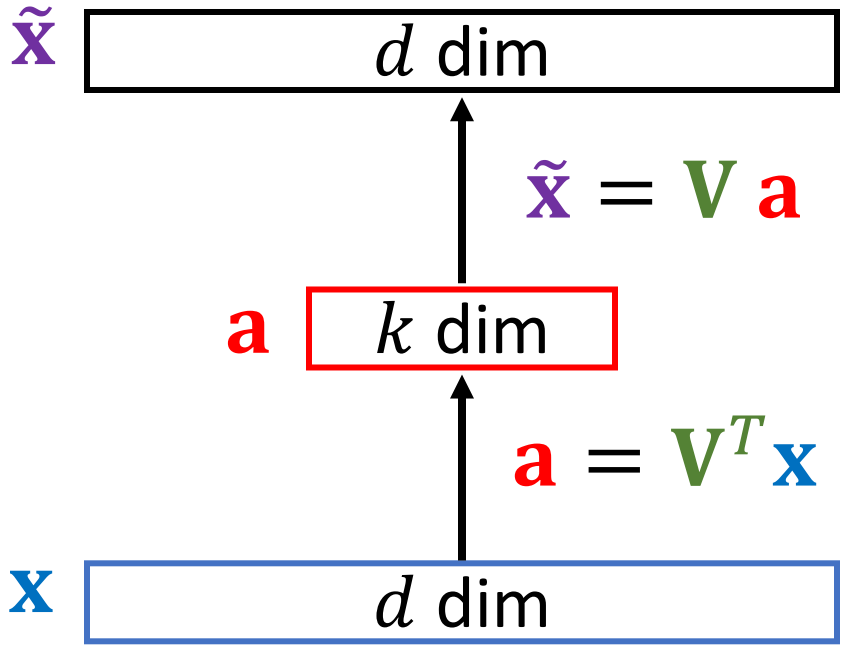
Autoencoder is nonlinear

$$\tilde{\mathbf{x}} = \text{decoder}\big(\text{encoder}(\mathbf{x})\big)$$



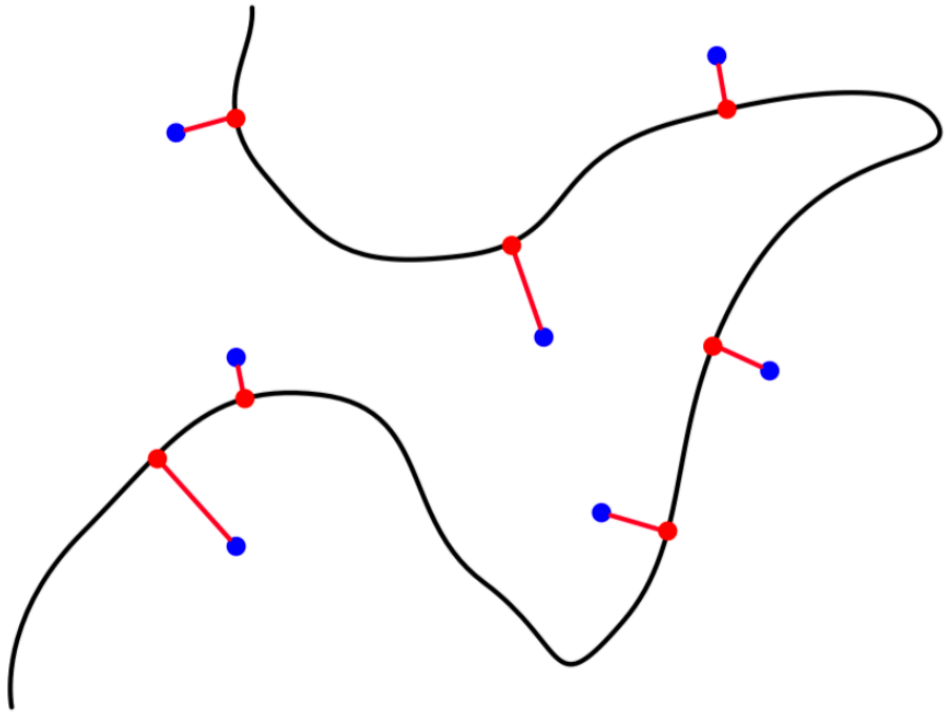
PCA is linear

$$\tilde{\mathbf{x}} = \mathbf{V}\mathbf{V}^T\mathbf{x}$$

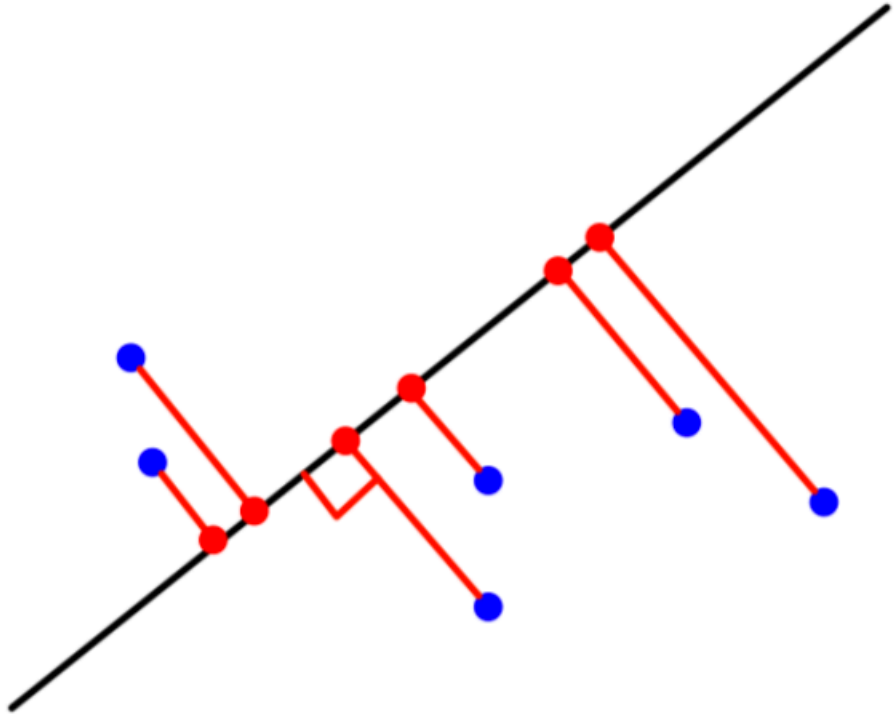


Autoencoder v.s. PCA

Autoencoder projects data onto nonlinear manifold.

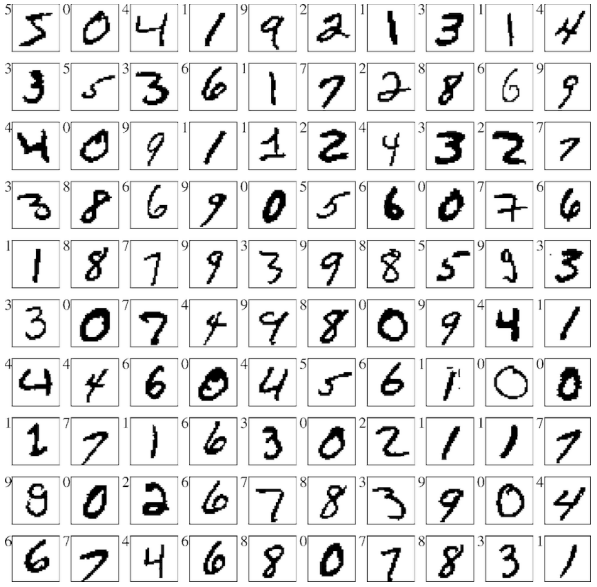


PCA projects data onto a subspace.



Implementation Using Keras

Load Data and Reshape Images to Vectors



The MNIST Dataset

- $n = 60{,}000$ training samples $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_n, y_n)$.
- Each $\mathbf{x}_j$ is a 28×28 image (reshape to 784-dim vector).
- Each y_j is an integer in $\{0, 1, 2, \cdots, 9\}$.

```
print('Shape of x_train_vec: ' + str(x_train_vec.shape))
print('Shape of x_test_vec: ' + str(x_test_vec.shape))
```

```
Shape of x_train_vec: (60000, 784)
Shape of x_test_vec: (10000, 784)
```

2 Ways of Building a Fully-Connected Net

```
from keras.layers import Dense
from keras import models

model = models.Sequential()
model.add(Dense(100, activation='relu',
                input_shape=(784,)))
model.add(Dense(20, activation='relu'))
model.add(Dense(100, activation='relu'))
model.add(Dense(784, activation='relu'))
```

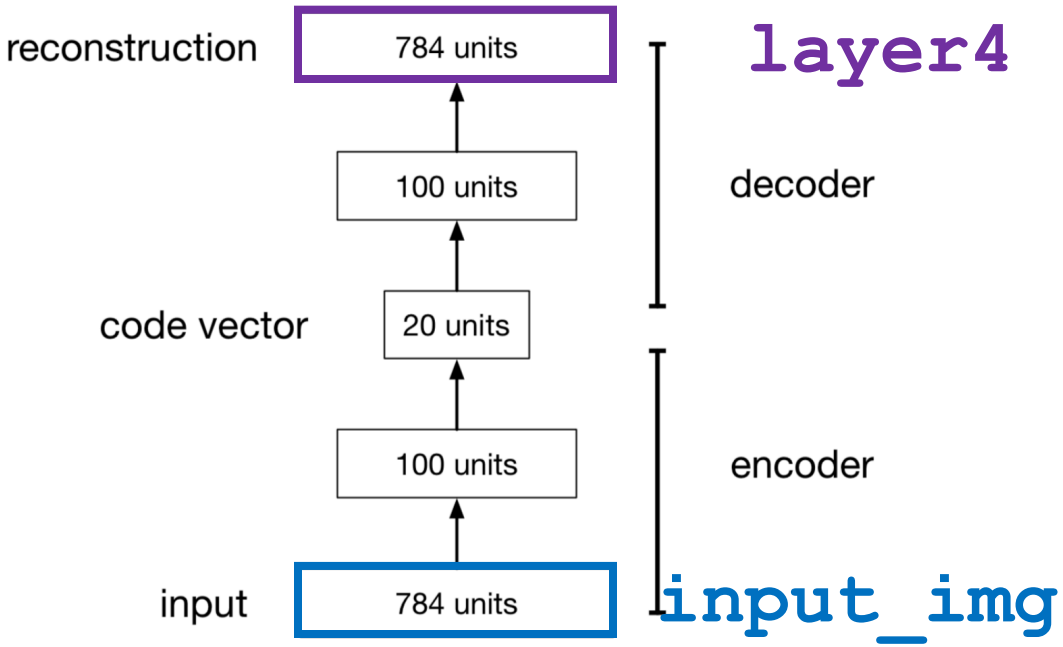
```
from keras.layers import Input, Dense
from keras import models

input_img = Input(shape=(784,))

layer1 = Dense(100, activation='relu')(input_img)
layer2 = Dense(20, activation='relu')(layer1)
layer3 = Dense(100, activation='relu')(layer2)
layer4 = Dense(784, activation='relu')(layer3)

model = models.Model(input_img, layer4)
```

2 Ways of Building a Fully-Connected Net

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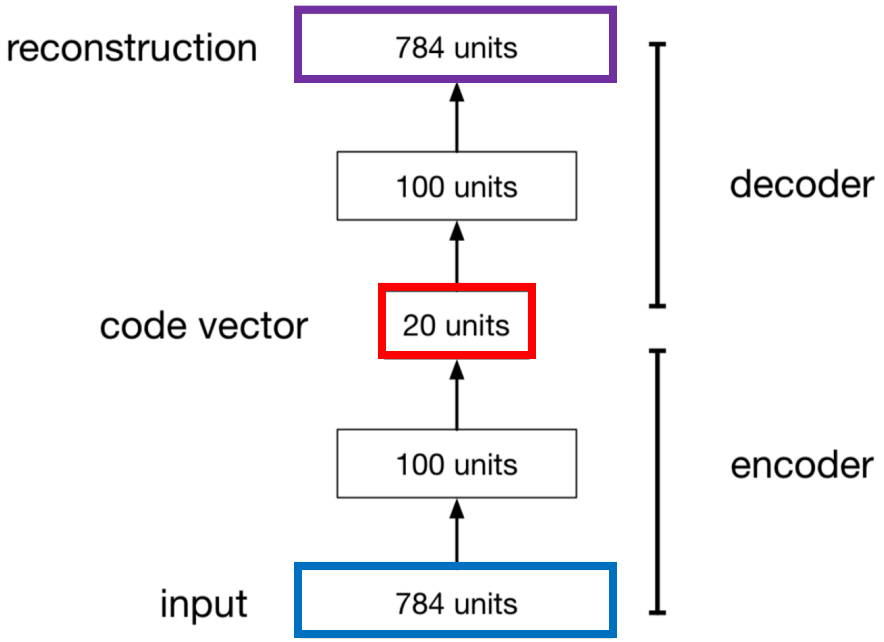


Layer (type)	Output Shape	Param #
input_1 (InputLayer)	(None, 784)	0
dense_5 (Dense)	(None, 100)	78500
dense_6 (Dense)	(None, 20)	2020
dense_7 (Dense)	(None, 100)	2100
dense_8 (Dense)	(None, 784)	79184

Total params: 161,804
Trainable params: 161,804
Non-trainable params: 0

Train the Model

The inputs and targets are the same.

```
model.compile(optimizer='RMSprop', loss='mean_squared_error')
history = model.fit(x_train_vec, x_train_vec, batch_size=128, epochs=50)
```

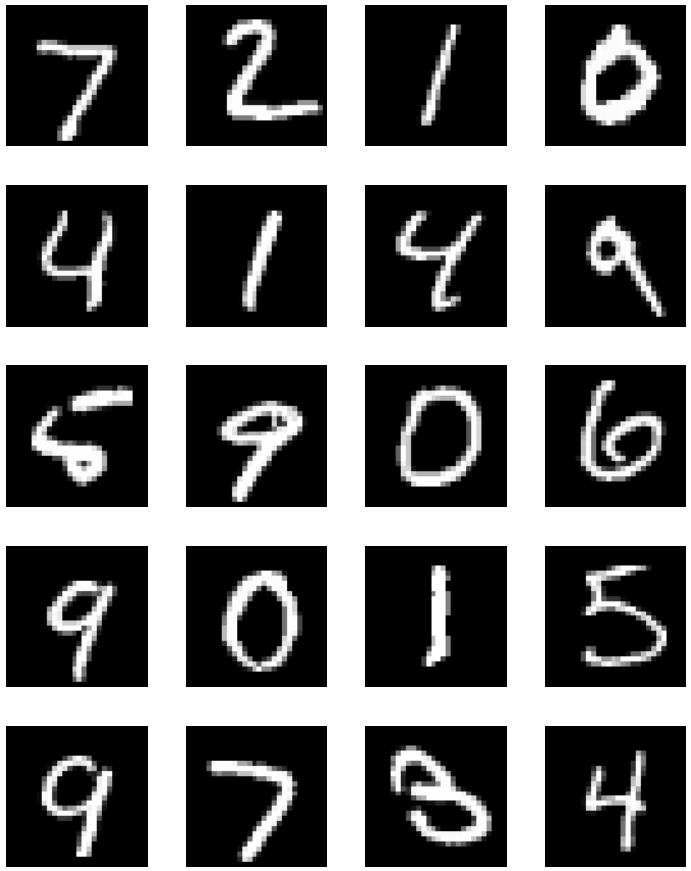
```
Epoch 1/50
60000/60000 [==============================] - 2s 32us/step - loss: 0.0390
Epoch 2/50
60000/60000 [==============================] - 2s 30us/step - loss: 0.0281
```

⋮

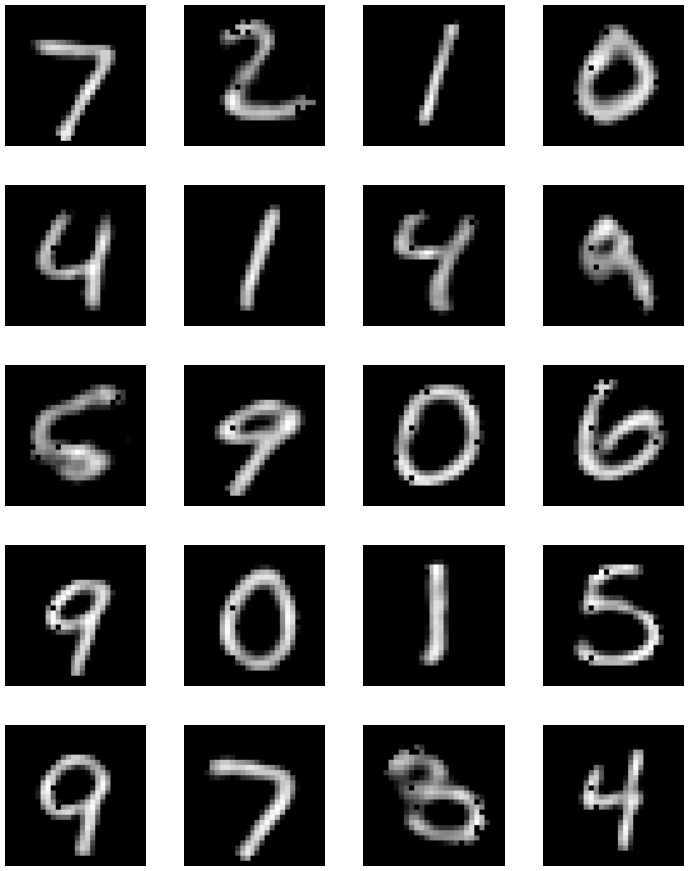
```
Epoch 49/50
60000/60000 [==============================] - 2s 38us/step - loss: 0.0145
Epoch 50/50
60000/60000 [==============================] - 2s 37us/step - loss: 0.0145
```

Results on the Test Set

Input

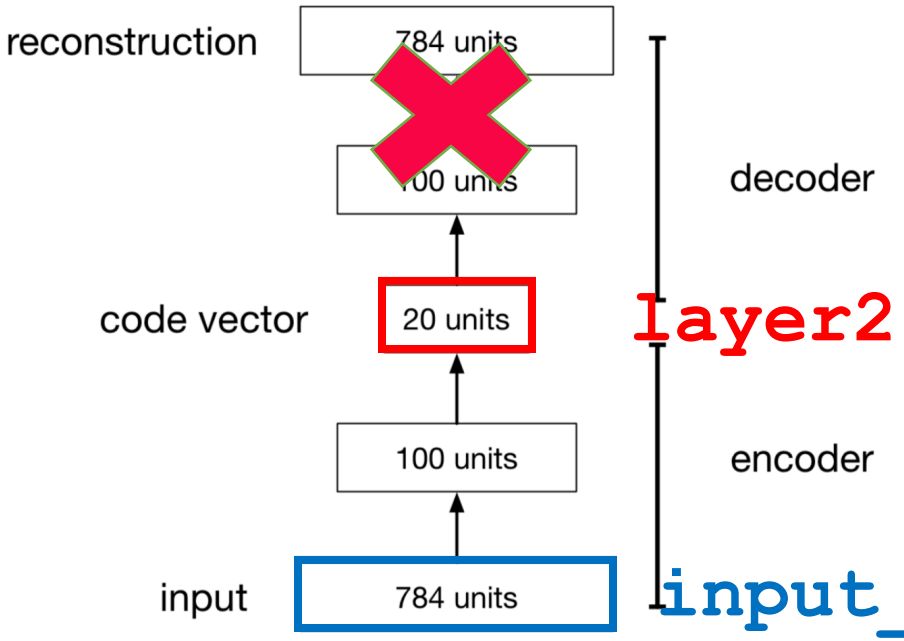


Reconstructed



Dimensionality Reduction

Get the Code Vectors




```
encoder = models.Model(input_img, layer2)
encoder.summary()
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
input_1 (InputLayer)         (None, 784)               0
_________________________________________________________________
dense_5 (Dense)              (None, 100)               78500
_________________________________________________________________
dense_6 (Dense)              (None, 20)                2020
=================================================================
Total params: 80,520
Trainable params: 80,520
Non-trainable params: 0
```

Visualize the Low-Dim Vectors

Get the low-dim code vectors.

20-dim

784-dim

```
encoded_test = encoder.predict(x_test_vec)
print('Shape of encoded_test: ' + str(encoded_test.shape))
```

```
Shape of encoded_test: (10000, 20)
```

Visualize the Low-Dim Vectors

Get the low-dim code vectors.

20-dim

784-dim

```
encoded_test = encoder.predict(x_test_vec)
print('Shape of encoded_test: ' + str(encoded_test.shape))
```

```
Shape of encoded_test: (10000, 20)
```

Project the 20-dim vectors to 2-dim by TSNE

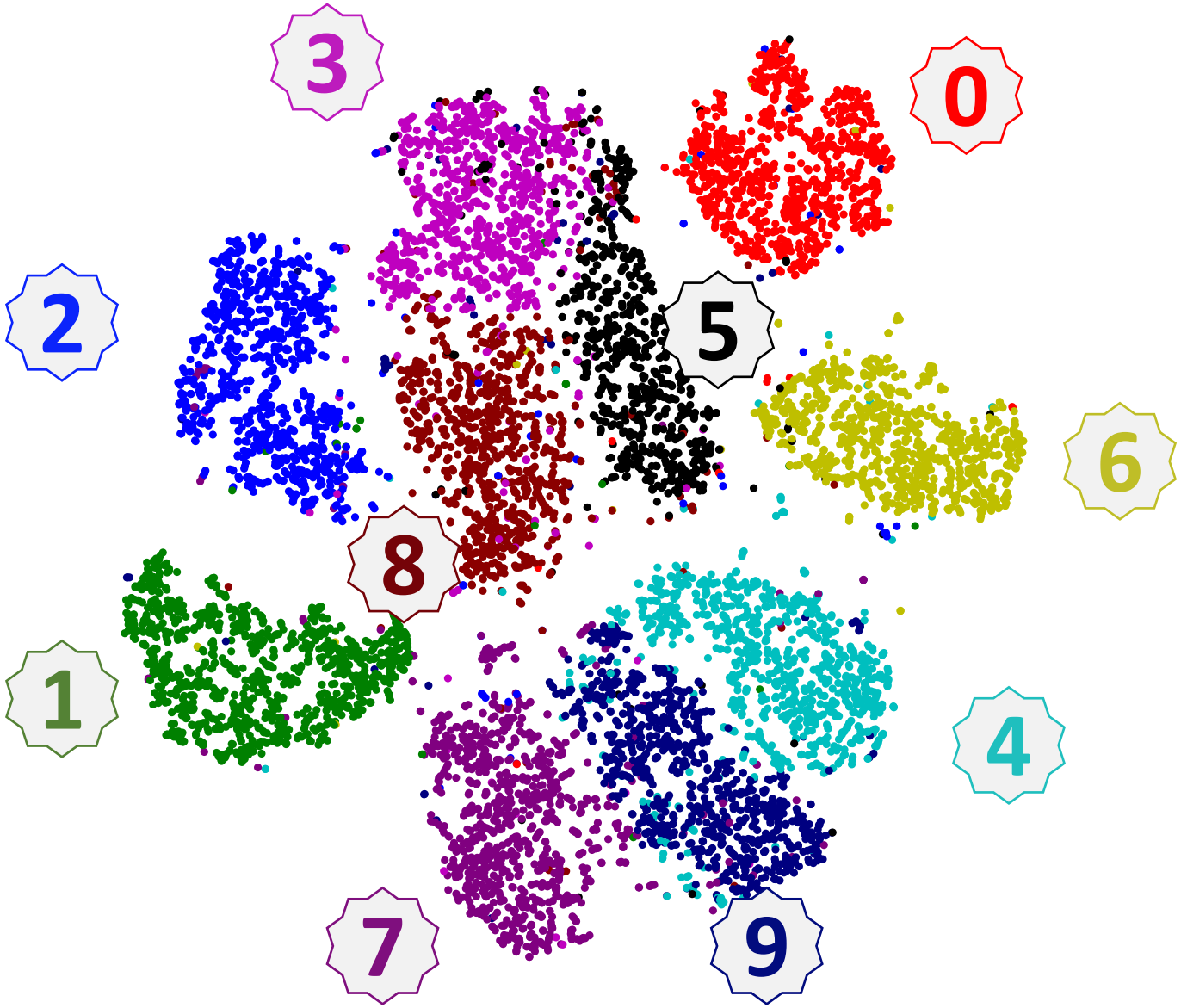
20-dim

2-dim

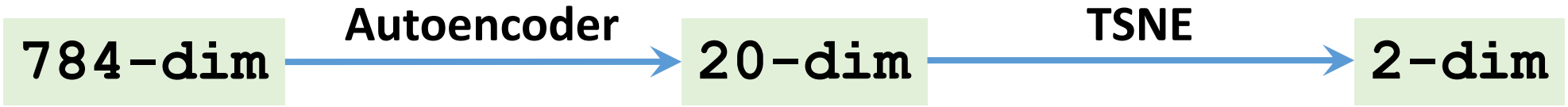
```
from sklearn.manifold import TSNE

embedded_test = TSNE(n_components=2).fit_transform(encoded_test)
print(embedded_test.shape)
```

```
(10000, 2)
```

Scatter Plot of the TSNE Embedding



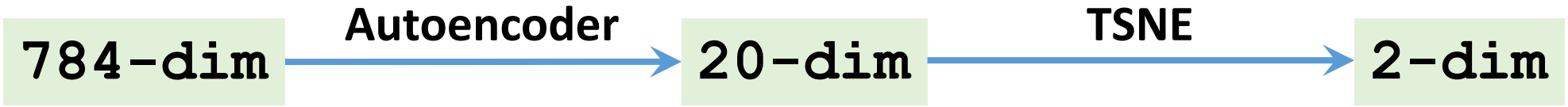
Visualize the Low-Dim Vectors



Question: Why not using Autoencoder to map 784-dim vectors to 2-dim?

Answer: The resulting visualization is not as good as TSNE.

Visualize the Low-Dim Vectors



Question: Why not using Autoencoder to map 784-dim vectors to 2-dim?

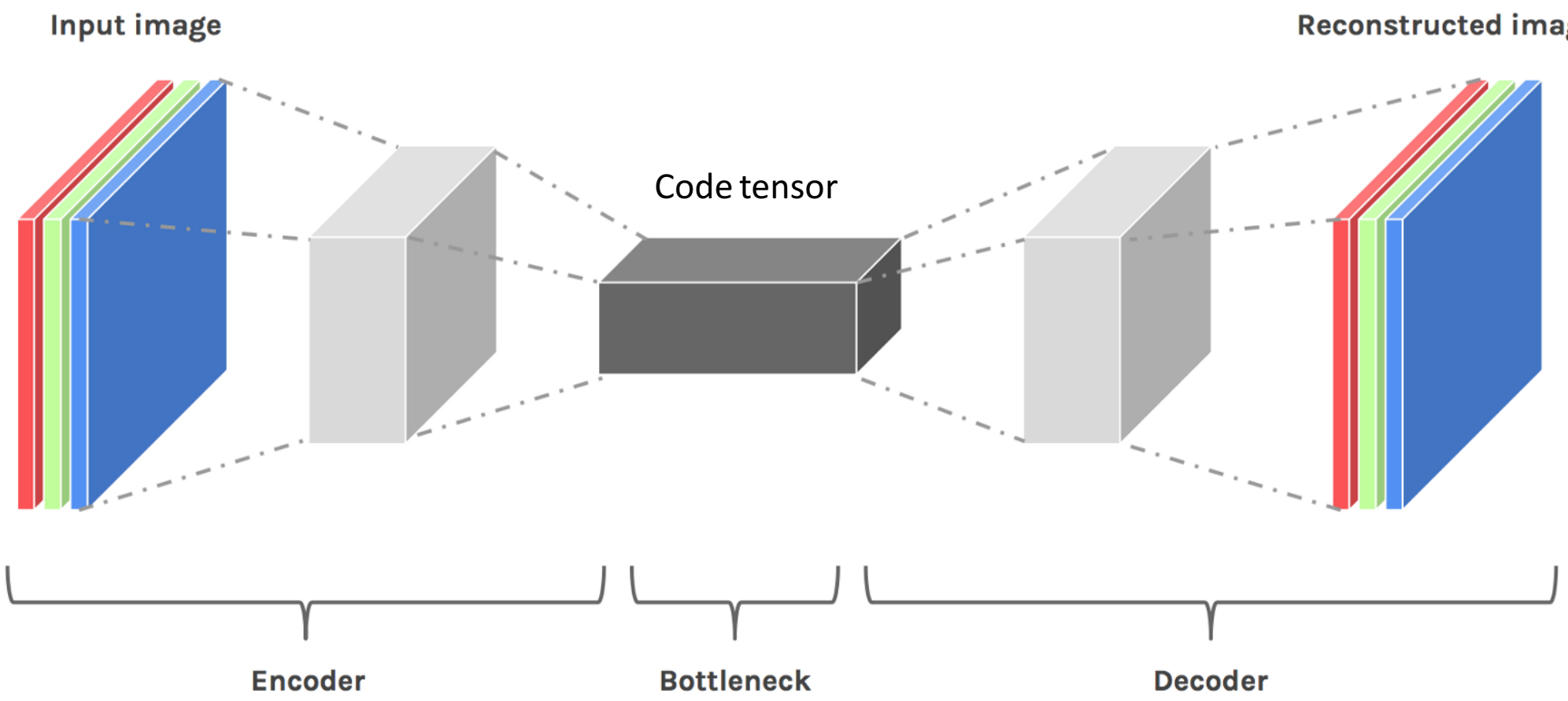
Answer: The resulting visualization is not as good as TSNE.

Question: Why not using TSNE to map 784-dim vectors to 2-dim?

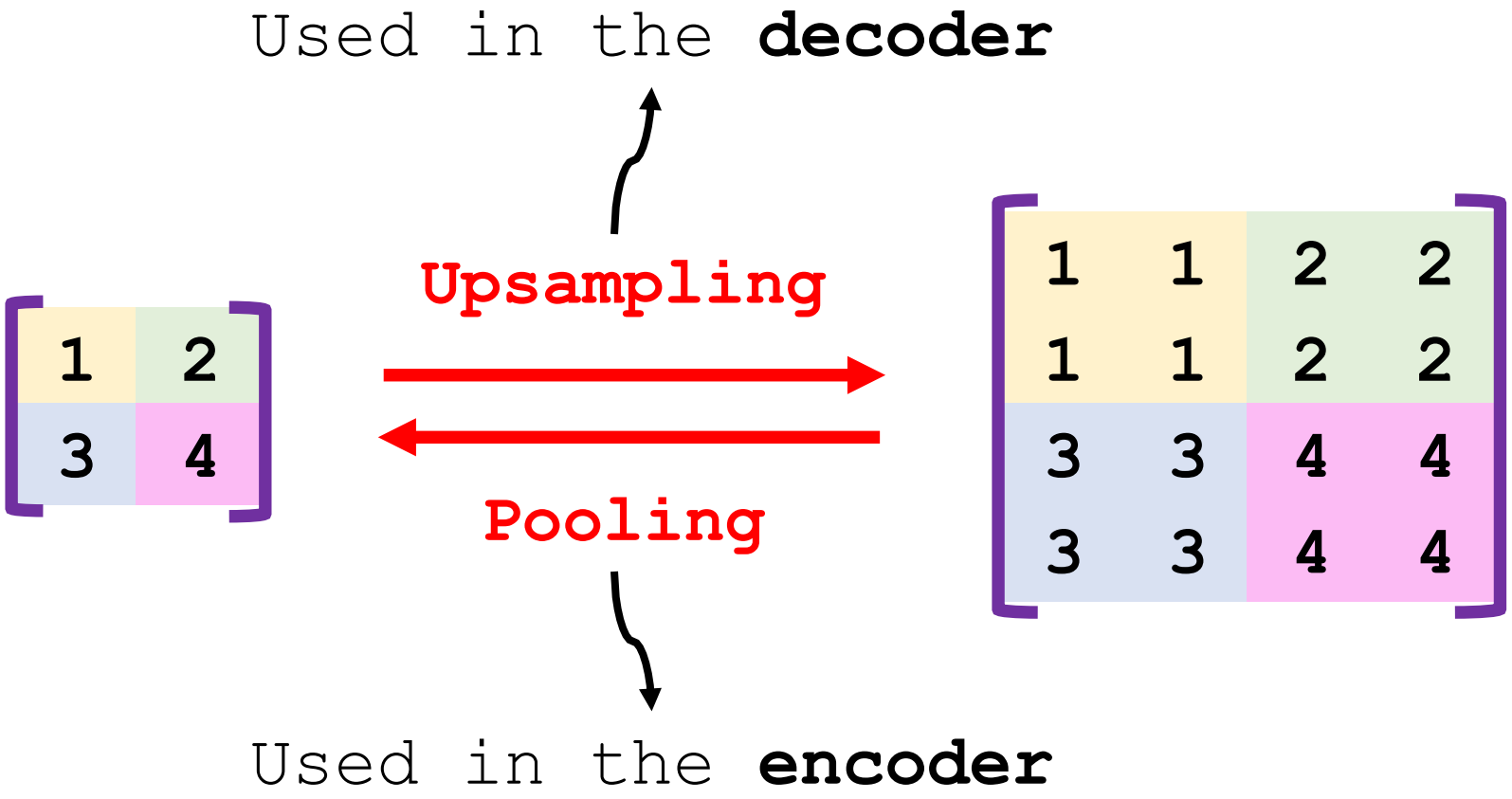
Answer: The results are good, but TSNE is slow for 784-dim vectors.

Convolutional Autoencoder

Convolutional Autoencoder



Pooling v.s. Upsampling



Implementation Using Keras

```
from keras.layers import Input, Dense, Conv2D, MaxPooling2D, UpSampling2D
from keras import models

input_img = Input(shape=(28, 28, 1))

encode1 = Conv2D(8, (3, 3), activation='relu', padding='same')(input_img)
encode2 = MaxPooling2D((2, 2), padding='same')(encode1)
encode3 = Conv2D(4, (3, 3), activation='relu', padding='same')(encode2)
encode4 = MaxPooling2D((2, 2), padding='same')(encode3)
encode5 = Conv2D(4, (3, 3), activation='relu', padding='same')(encode4)
encode6 = MaxPooling2D((2, 2), padding='same')(encode5)

decode1 = Conv2D(4, (3, 3), activation='relu', padding='same')(encode6)
decode2 = UpSampling2D((2, 2))(decode1)
decode3 = Conv2D(4, (3, 3), activation='relu', padding='same')(decode2)
decode4 = UpSampling2D((2, 2))(decode3)
decode5 = Conv2D(8, (3, 3), activation='relu')(decode4)
decode6 = UpSampling2D((2, 2))(decode5)
decode7 = Conv2D(1, (3, 3), activation='relu', padding='same')(decode6)

model = models.Model(input_img, decode7)
```

Implementation Using Keras

Imput image (28×28×1)

Code vector (4×4×4)

Output of decoder(28×28×1)

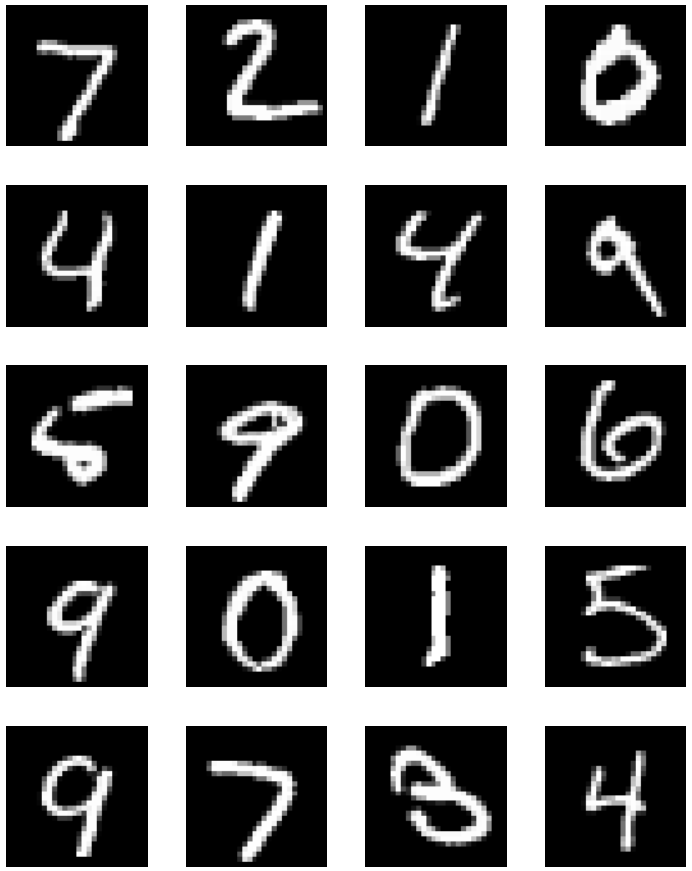
```
model.summary()
```

Layer (type)	Output Shape	Param #
input_1 (InputLayer)	(None, 28, 28, 1)	0
conv2d_1 (Conv2D)	(None, 28, 28, 8)	80
max_pooling2d_1 (MaxPooling2	(None, 14, 14, 8)	0
conv2d_2 (Conv2D)	(None, 14, 14, 4)	292
max_pooling2d_2 (MaxPooling2	(None, 7, 7, 4)	0
conv2d_3 (Conv2D)	(None, 7, 7, 4)	148
max_pooling2d_3 (MaxPooling2	(None, 4, 4, 4)	0
conv2d_4 (Conv2D)	(None, 4, 4, 4)	148
up_sampling2d_1 (UpSampling2	(None, 8, 8, 4)	0
conv2d_5 (Conv2D)	(None, 8, 8, 4)	148
up_sampling2d_2 (UpSampling2	(None, 16, 16, 4)	0
conv2d_6 (Conv2D)	(None, 14, 14, 8)	296
up_sampling2d_3 (UpSampling2	(None, 28, 28, 8)	0
conv2d_7 (Conv2D)	(None, 28, 28, 1)	73

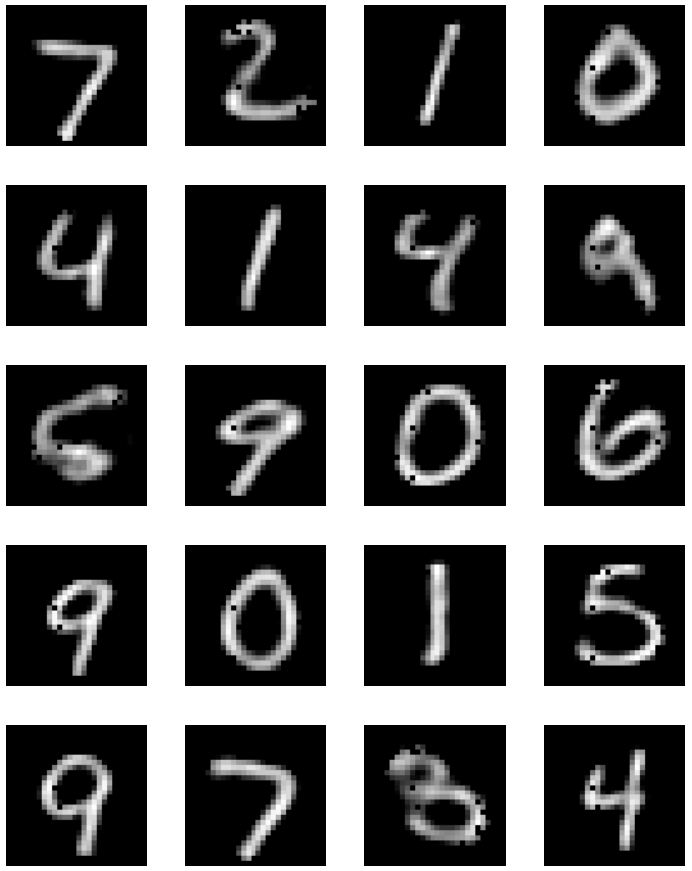
```
Total params: 1,185
Trainable params: 1,185
Non-trainable params: 0
```

Reconstructions (on the Test Set)

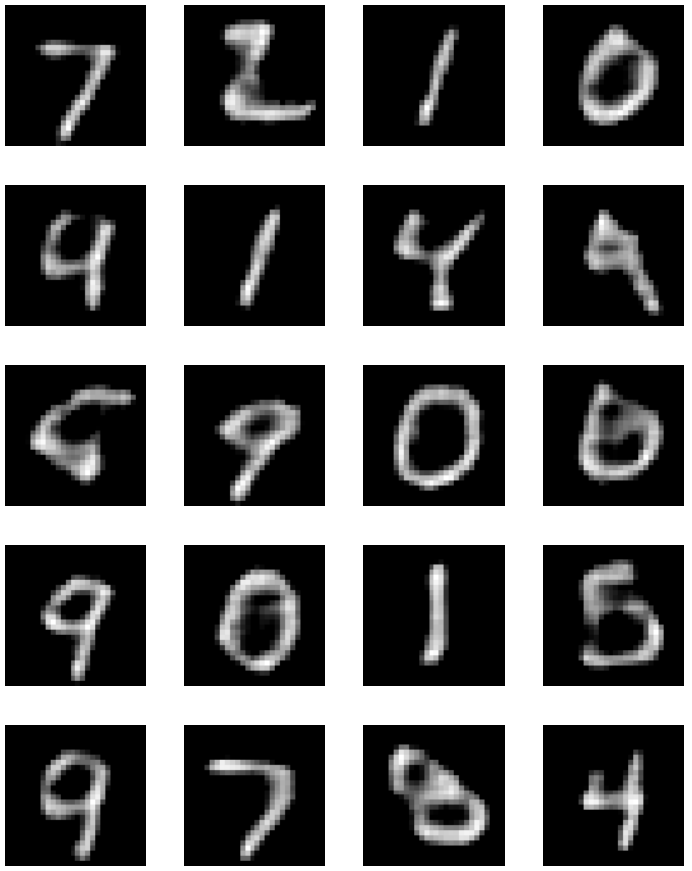
Original Input



Dense Autoencoder



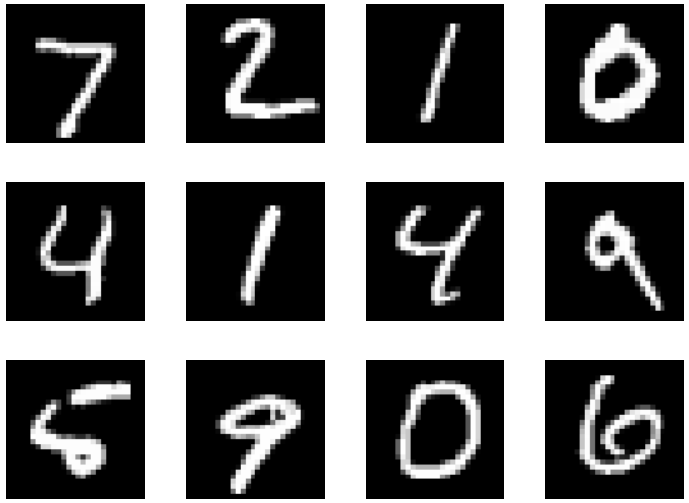
Conv Autoencoder



Denoising Autoencoder

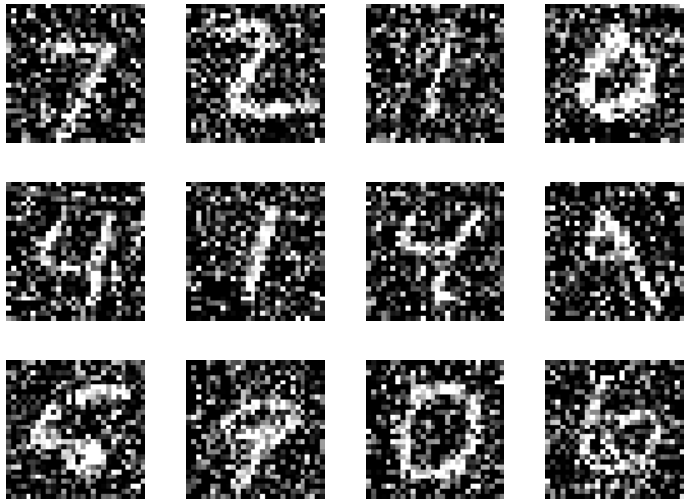
Denoising Autoencoder

Original



add noise

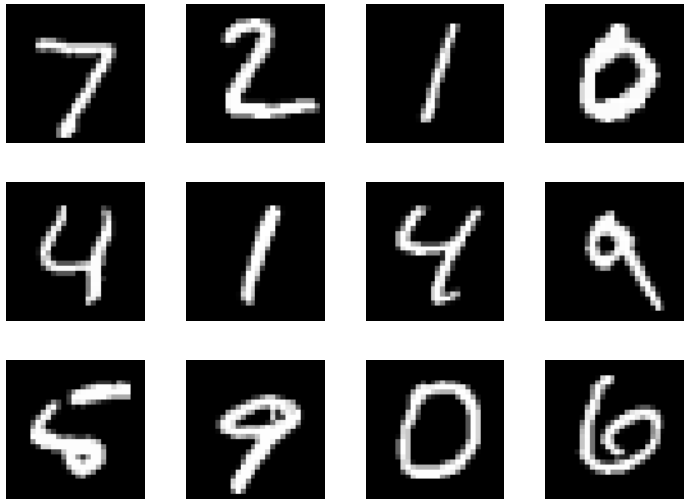
Noisy



```
import numpy as np

noise_factor = 0.5
x_train_noisy = x_train + noise_factor * np.random.normal(loc=0.0, scale=1.0, size=x_train.shape)
x_test_noisy = x_test + noise_factor * np.random.normal(loc=0.0, scale=1.0, size=x_test.shape)

x_train_noisy = np.clip(x_train_noisy, 0., 1.)
x_test_noisy = np.clip(x_test_noisy, 0., 1.)
```

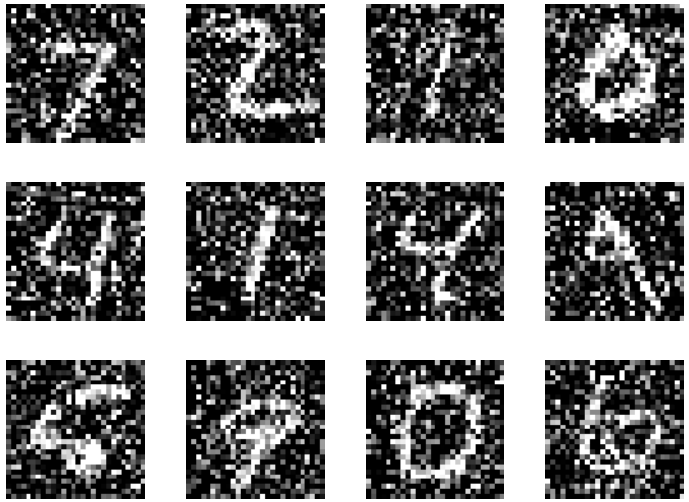
Denoising Autoencoder

Original



add noise

Noisy



Used as targets

Used as inputs

Convolutional Autoencoder

```
from keras.layers import Input, Dense, Conv2D, MaxPooling2D, UpSampling2D
from keras import models

input_img = Input(shape=(28, 28, 1))

encode1 = Conv2D(32, (3, 3), activation='relu', padding='same')(input_img)
encode2 = MaxPooling2D((2, 2), padding='same')(encode1)
encode3 = Conv2D(32, (3, 3), activation='relu', padding='same')(encode2)
encode4 = MaxPooling2D((2, 2), padding='same')(encode3)

decode1 = Conv2D(32, (3, 3), activation='relu', padding='same')(encode4)
decode2 = UpSampling2D((2, 2))(decode1)
decode3 = Conv2D(32, (3, 3), activation='relu', padding='same')(decode2)
decode4 = UpSampling2D((2, 2))(decode3)
decode5 = Conv2D(1, (3, 3), activation='relu', padding='same')(decode4)

model = models.Model(input_img, decode5)
```

Denoising Autoencoder

noisy images as inputs

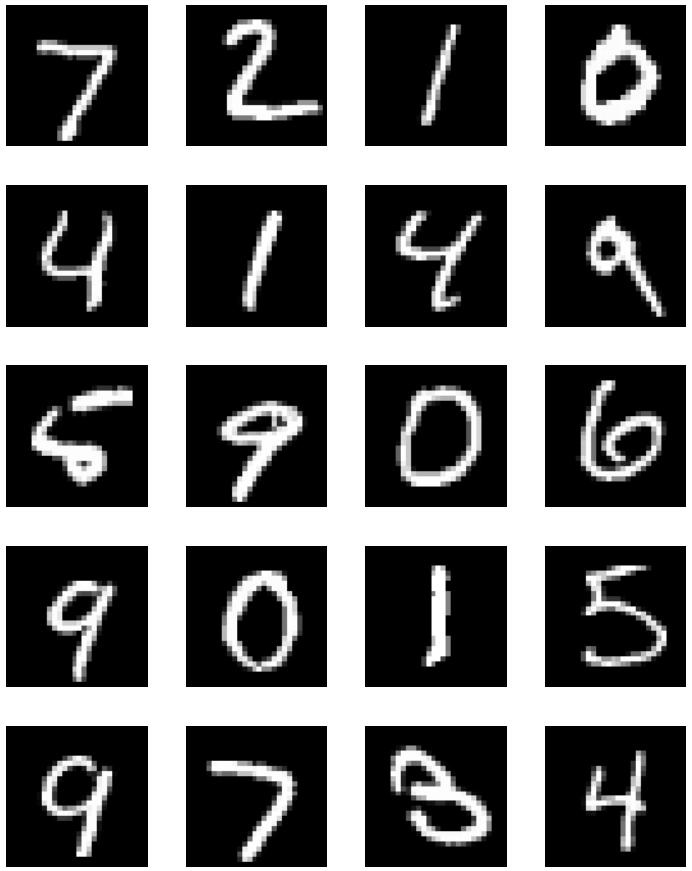
original images as targets

```
model.compile(optimizer='RMSprop', loss='mean_squared_error')
history = model.fit(x_train_noisy, x_train, batch_size=128, epochs=50)
```

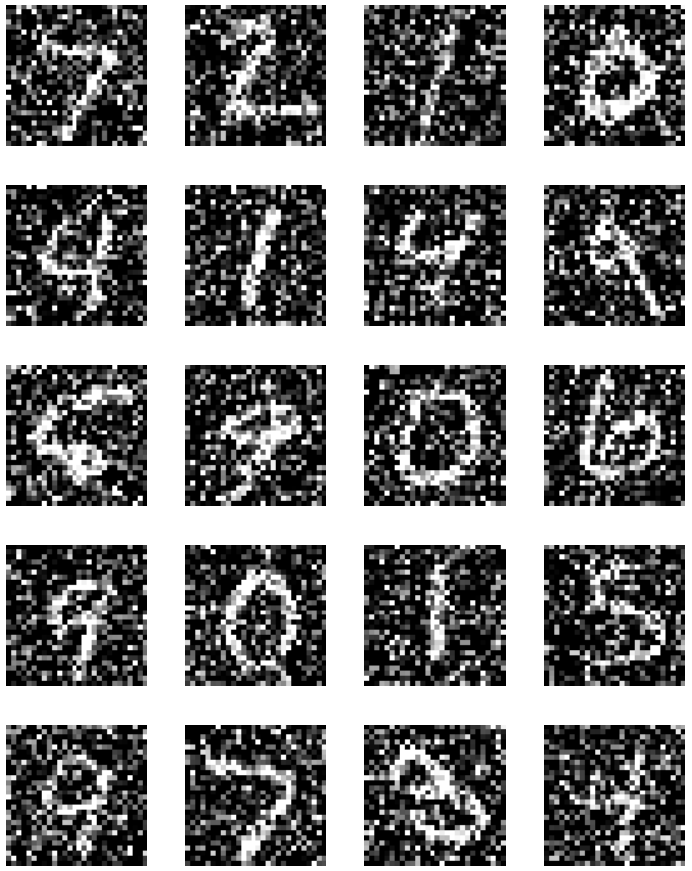
```
Epoch 1/50
60000/60000 [==============================] - 92s 2ms/step - loss: 0.0293
Epoch 2/50
60000/60000 [==============================] - 141s 2ms/step - loss: 0.0162
Epoch 3/50
60000/60000 [==============================] - 130s 2ms/step - loss: 0.0144
    .
    .
    .
Epoch 49/50
60000/60000 [==============================] - 143s 2ms/step - loss: 0.0106
Epoch 50/50
60000/60000 [==============================] - 122s 2ms/step - loss: 0.0106
```

Results on the Test Set

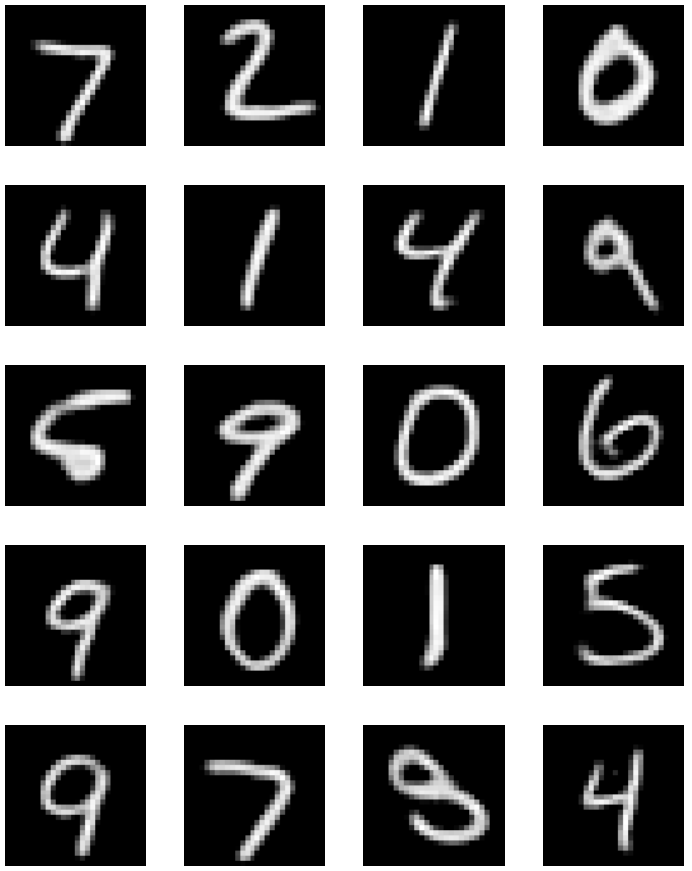
Original



Noisy



Reconstructed



Summary

- Autoencoder: generalizations of (linear) PCA.
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- Autoencoder = Encoder + Decoder.
- Training:
  - Inputs: original or noisy images.
  - targets: original images.
- Application 1: Dimensionality reduction (using the code vector).
- Application 2: Denoising.