ICE535 Machine Leaning – Homework♯9

Quize

Given a set of observations $\{x^{(1)}, x^{(2)}, \dots, x^{(n)}\}$, where each observation is a d-dimensional real vector, K-means clustering aims to partition the n observations into $K(\leq n)$ sets $S = \{1, 2, \dots, K\}$ so as to minimize the within-cluster sum of squares (WCSS) (sum of distance functions of each point in the cluster to the K center). Specifically, its objective is to find:

$$\min_{\{r_{ij}\},\{\mu_j\}} J(r_{11}, \dots, r_{mK}, \mu_1, \dots, \mu_K) = \frac{1}{m} \sum_{i=1}^{m} \sum_{j=1}^{K} r_{ij} \left\| \mathbf{x}^{(i)} - \mu_j \right\|^2$$

where $r_{ij} \in \{0, 1\}$ for $1 \leq i \leq m$, $1 \leq j \leq K$, and $\sum_{j=1}^{K} r_{ij} = 1$ for $1 \leq i \leq m$.

Show that the K-means algorithm is developed by alternating between the two steps:

- Find $\{r_{ij}\}$ to minimize $J(r_{11}, \dots, r_{mK}, \mu_1, \dots, \mu_K)$ with fixed $\{\mu_j\}$;
- Find $\{\mu_j\}$ to minimize $J(r_{11}, \dots, r_{mK}, \mu_1, \dots, \mu_K)$ with fixed $\{r_{ij}\}$.

Please provide the derivations for the above two steps.

1 Let's build an autoencoder by Keras

We'll start simple, with a single fully-connected neural layer as encoder and as decoder:

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

# this is the size of our encoded representations
encoding_dim = 32  # 32 floats -> compression of factor 24.5, assuming the input is 784
    floats

# this is our input placeholder
input_img = Input(shape=(784,))
# "encoded" is the encoded representation of the input
encoded = Dense(encoding_dim, activation='relu')(input_img)
# "decoded" is the lossy reconstruction of the input
decoded = Dense(784, activation='sigmoid')(encoded)

# this model maps an input to its reconstruction
autoencoder = Model(input_img, decoded)
```

Let's also create a separate encoder model:

```python
# this model maps an input to its encoded representation
encoder = Model(input_img, encoded)
```

As well as the decoder model:

```python
# create a placeholder for an encoded (32-dimensional) input
encoded_input = Input(shape=(encoding_dim,))
# retrieve the last layer of the autoencoder model
decoder_layer = autoencoder.layers[-1]
# create the decoder model
decoder = Model(encoded_input, decoder_layer(encoded_input))
```

Now let's train our autoencoder to reconstruct MNIST digits.

First, we'll configure our model to use a per-pixel binary crossentropy loss, and the Adadelta optimizer:

```python
autoencoder.compile(optimizer='adadelta', loss='binary_crossentropy')
```

Let's prepare our input data. We're using MNIST digits, and we're discarding the labels (since we're only interested in encoding/decoding the input images).

```python
from keras.datasets import mnist
import numpy as np
(x_train, _), (x_test, _) = mnist.load_data()
```

We will normalize all values between 0 and 1 and we will flatten the 28x28 images into vectors of size 784.

```python
x_train = x_train.astype('float32') / 255.
x_test = x_test.astype('float32') / 255.
x_train = x_train.reshape((len(x_train), np.prod(x_train.shape[1:])))
x_test = x_test.reshape((len(x_test), np.prod(x_test.shape[1:])))
print(x_train.shape[0], 'train samples')
print(x_test.shape[0], 'test samples')
```

Now let's train our autoencoder for 50 epochs:

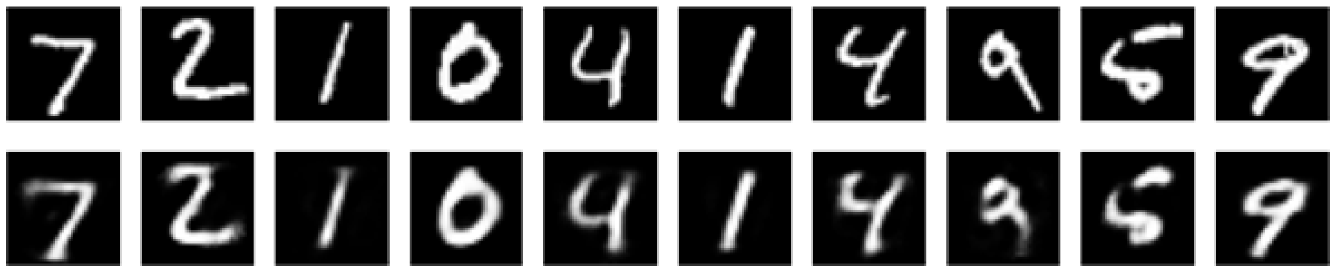
```python
autoencoder.fit(x_train, x_train,
                epochs=50,
                batch_size=256,
                shuffle=True,
                validation_data=(x_test, x_test))
```

After 50 epochs, the autoencoder seems to reach a stable train/test loss value of about 0.11. We can try to visualize the reconstructed inputs and the encoded representations. We will use Matplotlib.

```python
# encode and decode some digits
# note that we take them from the *test* set
encoded_imgs = encoder.predict(x_test)
decoded_imgs = decoder.predict(encoded_imgs)
```

```python
# use Matplotlib (don't ask)
import matplotlib.pyplot as plt

n = 10  # how many digits we will display
plt.figure(figsize=(20, 4))
for i in range(n):
    # display original
    ax = plt.subplot(2, n, i + 1)
    plt.imshow(x_test[i].reshape(28, 28))
    plt.gray()
    ax.get_xaxis().set_visible(False)
    ax.get_yaxis().set_visible(False)

    # display reconstruction
    ax = plt.subplot(2, n, i + 1 + n)
    plt.imshow(decoded_imgs[i].reshape(28, 28))
    plt.gray()
    ax.get_xaxis().set_visible(False)
    ax.get_yaxis().set_visible(False)
plt.show()
```

Here's what we get. The top row is the original digits, and the bottom row is the reconstructed digits. We are losing quite a bit of detail with this basic approach.



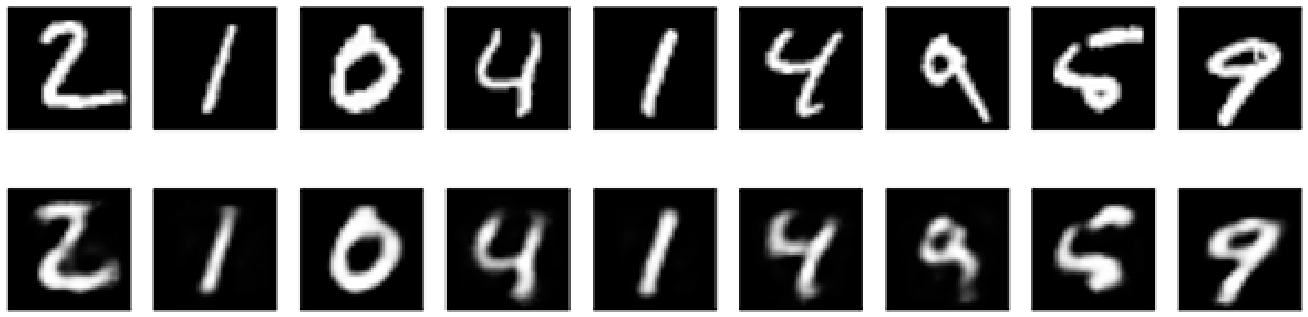
2 Adding a sparsity constraint on the encoded representations

In the previous example, the representations were only constrained by the size of the hidden layer (32). In such a situation, what typically happens is that the hidden layer is learning an approximation of PCA (principal component analysis). But another way to constrain the representations to be compact is to add a sparsity contraint on the activity of the hidden representations, so fewer units would "fire" at a given time. In Keras, this can be done by adding an activity_regularizer to our Dense layer:

```python
from keras import regularizers

encoding_dim = 32

input_img = Input(shape=(784,))
# add a Dense layer with a L1 activity regularizer
encoded = Dense(encoding_dim, activation='relu',
                activity_regularizer=regularizers.l1(10e-5))(input_img)
decoded = Dense(784, activation='sigmoid')(encoded)

autoencoder = Model(input_img, decoded)
```

Let's train this model for 100 epochs (with the added regularization the model is less likely to overfit and can be trained longer). The models ends with a train loss of 0.11 and test loss of 0.10. The difference between the two is mostly due to the regularization term being added to the loss during training (worth about 0.01).

Here's a visualization of our new results:



They look pretty similar to the previous model, the only significant difference being the sparsity of the encoded representations. encoded_imgs.mean() yields a value 3.33 (over our 10,000 test images), whereas with the previous model the same quantity was 7.30. So our new model yields encoded representations that are twice sparser.

3 Deep autoencoder

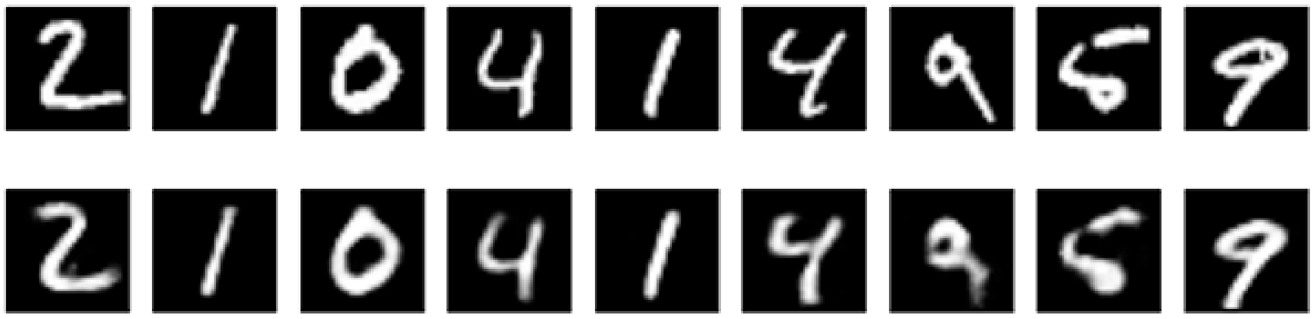
We do not have to limit ourselves to a single layer as encoder or decoder, we could instead use a stack of layers, such as:

```
input_img = Input(shape=(784,))
encoded = Dense(128, activation='relu')(input_img)
encoded = Dense(64, activation='relu')(encoded)
encoded = Dense(32, activation='relu')(encoded)

decoded = Dense(64, activation='relu')(encoded)
decoded = Dense(128, activation='relu')(decoded)
decoded = Dense(784, activation='sigmoid')(decoded)
```

Let's try this:

```
autoencoder = Model(input_img, decoded)
autoencoder.compile(optimizer='adadelta', loss='binary_crossentropy')

autoencoder.fit(x_train, x_train,
                epochs=100,
                batch_size=256,
                shuffle=True,
                validation_data=(x_test, x_test))
```

After 100 epochs, it reaches a train and test loss of 0.097, a bit better than our previous models. Our reconstructed digits look a bit better too:



4 Convolutional autoencoder

Since our inputs are images, it makes sense to use convolutional neural networks (convnets) as encoders and decoders. In practical settings, autoencoders applied to images are always convolutional autoencoders –they simply perform much better.

Let's implement one. The encoder will consist in a stack of Conv2D and MaxPooling2D layers (max pooling being used for spatial down-sampling), while the decoder will consist in a stack of Conv2D and UpSampling2D layers.

```python
from keras.layers import Input, Dense, Conv2D, MaxPooling2D, UpSampling2D
from keras.models import Model
from keras import backend as K

input_img = Input(shape=(28, 28, 1))  # adapt this if using `channels_first` image data format

x = Conv2D(16, (3, 3), activation='relu', padding='same')(input_img)
x = MaxPooling2D((2, 2), padding='same')(x)
x = Conv2D(8, (3, 3), activation='relu', padding='same')(x)
x = MaxPooling2D((2, 2), padding='same')(x)
x = Conv2D(8, (3, 3), activation='relu', padding='same')(x)
encoded = MaxPooling2D((2, 2), padding='same')(x)

# at this point the representation is (4, 4, 8) i.e. 128-dimensional

x = Conv2D(8, (3, 3), activation='relu', padding='same')(encoded)
x = UpSampling2D((2, 2))(x)
x = Conv2D(8, (3, 3), activation='relu', padding='same')(x)
x = UpSampling2D((2, 2))(x)
x = Conv2D(16, (3, 3), activation='relu')(x)
x = UpSampling2D((2, 2))(x)
decoded = Conv2D(1, (3, 3), activation='sigmoid', padding='same')(x)

autoencoder = Model(input_img, decoded)
autoencoder.compile(optimizer='adadelta', loss='binary_crossentropy')
```

To train it, we will use the original MNIST digits with shape (samples, 3, 28, 28), and we will just normalize pixel values between 0 and 1.

```python
from keras.datasets import mnist
import numpy as np

(x_train, _), (x_test, _) = mnist.load_data()

x_train = x_train.astype('float32') / 255.
x_test = x_test.astype('float32') / 255.
x_train = np.reshape(x_train, (len(x_train), 28, 28, 1))  # adapt this if using `channels_first` image data format
x_test = np.reshape(x_test, (len(x_test), 28, 28, 1))  # adapt this if using `channels_first`
```

```
    image data format
```

Then let's train our model with 50 epochs, which might spend you more than two hours for this train. If you only what to test your code without getting low loss, you can try 10 epochs.

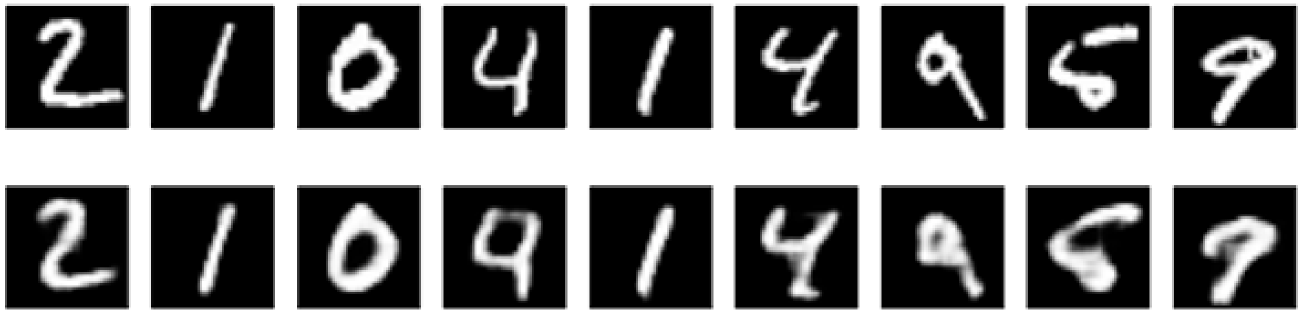
```
autoencoder.fit(x_train, x_train,
                epochs=50,
                batch_size=128,
                shuffle=True,
                validation_data=(x_test, x_test))
```

The model converges to a loss of 0.094, significantly better than our previous models (this is in large part due to the higher entropic capacity of the encoded representation, 128 dimensions vs. 32 previously). Let's take a look at the reconstructed digits:

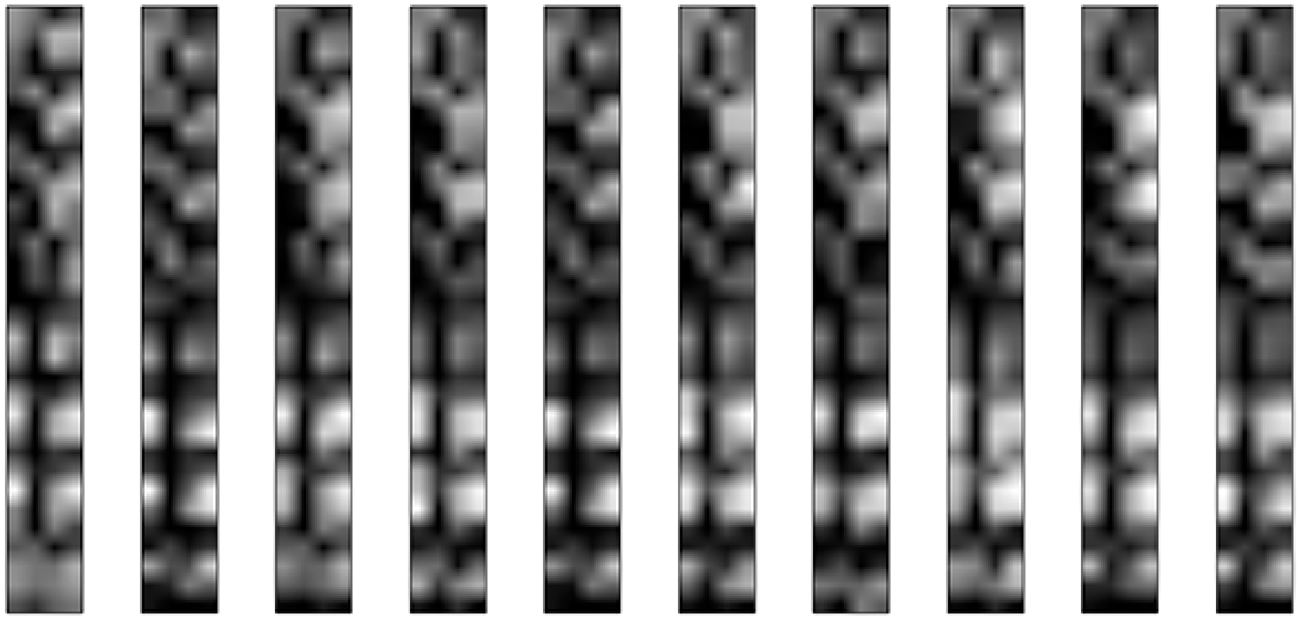
```
# use Matplotlib
import matplotlib.pyplot as plt

decoded_imgs = autoencoder.predict(x_test)

n = 10
plt.figure(figsize=(20, 4))
for i in range(n):
    # display original
    ax = plt.subplot(2, n, i)
    plt.imshow(x_test[i].reshape(28, 28))
    plt.gray()
    ax.get_xaxis().set_visible(False)
    ax.get_yaxis().set_visible(False)

    # display reconstruction
    ax = plt.subplot(2, n, i + n)
    plt.imshow(decoded_imgs[i].reshape(28, 28))
    plt.gray()
    ax.get_xaxis().set_visible(False)
    ax.get_yaxis().set_visible(False)
plt.show()
```

We can also have a look at the 128-dimensional encoded representations. These representations are 8x4x4, so we reshape them to 4x32 in order to be able to display them as grayscale images.

```
# this model maps an input to its encoded representation
encoder = Model(input=input_img, output=encoded)
encoded_imgs = encoder.predict(x_test)

n = 10
plt.figure(figsize=(20, 8))
for i in range(n):
    ax = plt.subplot(1, n, i + 1)
```



```
    plt.imshow(encoded_imgs[i].reshape(4, 4 * 8).T)
    plt.gray()
    ax.get_xaxis().set_visible(False)
    ax.get_yaxis().set_visible(False)
plt.show()
```



5 Application to image denoising

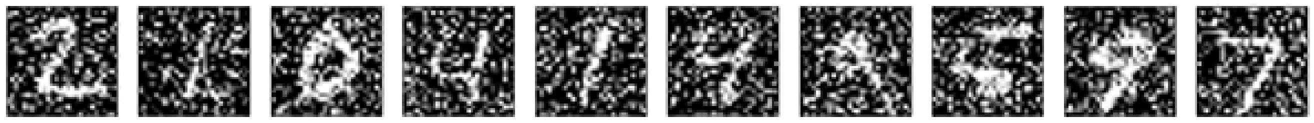
Let's put our convolutional autoencoder to work on an image denoising problem. It's simple: we will train the autoencoder to map noisy digits images to clean digits images.

Here's how we will generate synthetic noisy digits: we just apply a gaussian noise matrix and clip the images between 0 and 1.

```python
from keras.datasets import mnist
import numpy as np

(x_train, _), (x_test, _) = mnist.load_data()

x_train = x_train.astype('float32') / 255.
x_test = x_test.astype('float32') / 255.
x_train = np.reshape(x_train, (len(x_train), 28, 28, 1))  # adapt this if using `channels_first` image data format
x_test = np.reshape(x_test, (len(x_test), 28, 28, 1))  # adapt this if using `channels_first` image data format

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.)
```

Here's what the noisy digits look like:

```python
n = 10
plt.figure(figsize=(20, 2))
for i in range(n):
    ax = plt.subplot(1, n, i)
    plt.imshow(x_test_noisy[i].reshape(28, 28))
    plt.gray()
    ax.get_xaxis().set_visible(False)
    ax.get_yaxis().set_visible(False)
plt.show()
```



If you squint you can still recognize them, but barely. Can our autoencoder learn to recover the original digits? Let's find out.

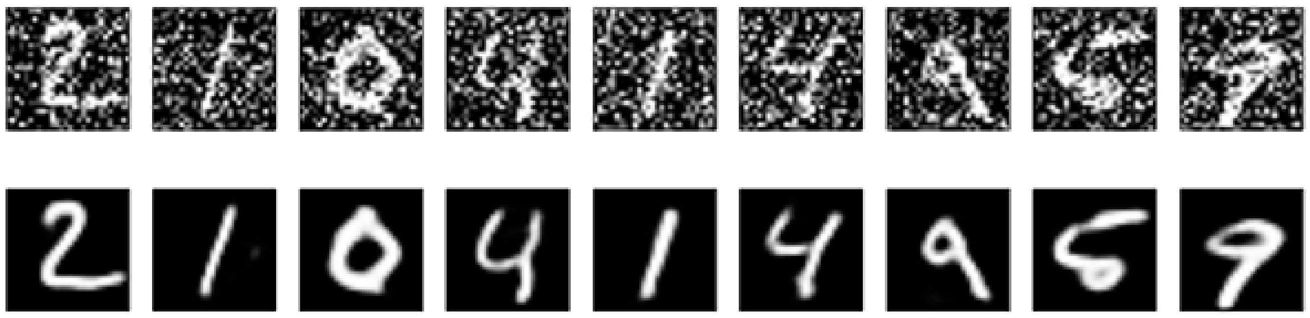
Compared to the previous convolutional autoencoder, in order to improve the quality of the reconstructed, we'll use a slightly different model with more filters per layer:

```
input_img = Input(shape=(28, 28, 1))  # adapt this if using `channels_first` image data
    format

x = Conv2D(32, (3, 3), activation='relu', padding='same')(input_img)
x = MaxPooling2D((2, 2), padding='same')(x)
x = Conv2D(32, (3, 3), activation='relu', padding='same')(x)
encoded = MaxPooling2D((2, 2), padding='same')(x)

# at this point the representation is (7, 7, 32)

x = Conv2D(32, (3, 3), activation='relu', padding='same')(encoded)
x = UpSampling2D((2, 2))(x)
x = Conv2D(32, (3, 3), activation='relu', padding='same')(x)
x = UpSampling2D((2, 2))(x)
decoded = Conv2D(1, (3, 3), activation='sigmoid', padding='same')(x)

autoencoder = Model(input_img, decoded)
autoencoder.compile(optimizer='adadelta', loss='binary_crossentropy')
```

Let's train it for 100 epochs:

```
autoencoder.fit(x_train_noisy, x_train,
                epochs=100,
                batch_size=128,
                shuffle=True,
                validation_data=(x_test_noisy, x_test),
                callbacks=[TensorBoard(log_dir='/tmp/tb', histogram_freq=0, write_graph=False
                    )])
```

Now let's take a look at the results. Top, the noisy digits fed to the network, and bottom, the digits are reconstructed by the network.



It seems to work pretty well. If you scale this process to a bigger convnet, you can start building document denoising or audio denoising models.