Principal Component Analysis (PCA)

We will implement the PCA algorithm. We will first implement PCA, then apply it (once again) to the MNIST digit dataset.

Learning objective

- 1. Write code that implements PCA.
- 2. Write code that implements PCA for high-dimensional datasets

Let's first import the packages we need for this week.

```
In [47]:
```

```
# PACKAGE: DO NOT EDIT
import numpy as np
import scipy
import scipy.stats
```

```
In [48]:
```

```
import matplotlib.pyplot as plt
from ipywidgets import interact

plt.style.use('fivethirtyeight')
%matplotlib inline
```

```
In [49]:
```

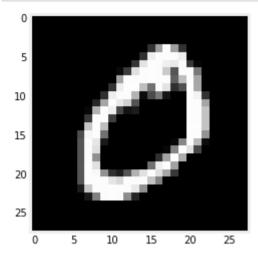
```
from load_data import load_mnist

MNIST = load_mnist('./')
images, labels = MNIST['data'], MNIST['target']
```

Now, let's plot a digit from the dataset:

In [50]:

```
plt.figure(figsize=(4,4))
plt.imshow(images[0].reshape(28,28), cmap='gray');
plt.grid(False)
```



PCA

Now we will implement PCA. Before we do that, let's pause for a moment and think about the steps for performing PCA. Assume that we are performing PCA on some dataset \boldsymbol{X} for \boldsymbol{M} principal components. We then need to perform the following steps, which we break into parts:

- 1. Data normalization (normalize).
- 2. Find eigenvalues and corresponding eigenvectors for the covariance matrix S. Sort by the largest eigenvalues and the corresponding eigenvectors (eig).
- 3. Compute the orthogonal projection matrix and use that to project the data onto the subspace spanned by the eigenvectors.

Data normalization normalize

We will first implement the data normalization mentioned above.

Before we implement the main steps of PCA, we will need to do some data preprocessing.

To preprocess the dataset for PCA, we will make sure that the dataset has zero mean. Given a dataset X, we will subtract the mean vector from each row of the dataset to obtain a zero-mean dataset \overline{X} . In the first part of this notebook, you will implement normalize to do that.

To work with images, it's also a common practice to convert the pixels from unsigned interger 8 (uint8) encoding to a floating point number representation between 0-1. We will do this conversion for you for the MNIST dataset so that you don't have to worry about it.

Data normalization is a common practice. More details can be found in <u>Data Normalization or Feature Scaling (https://en.wikipedia.org/wiki/Feature_scaling)</u>.

In [51]:

```
# GRADED FUNCTION: DO NOT EDIT THIS LINE
def normalize(X):
    """Normalize the given dataset X to have zero mean.
    Args:
        X: ndarray, dataset of shape (N,D)
    Returns:
        (Xbar, mean): tuple of ndarray, Xbar is the normalized dataset
        with mean 0; mean is the sample mean of the dataset.
    # YOUR CODE HERE
    # Note that D is the columns, so
    ### Uncomment and modify the code below
    N, D = X.shape
    mu = X.mean(axis = 0)
    #print(mu.shape)
    Xbar = X - mu
    #print(Xbar)
    return Xbar, mu
```

```
"""Test data normalization"""
from numpy.testing import assert_allclose
X0 = np.array([[0, 0.0],
               [1.0, 1.0],
               [2.0, 2.0]])
X0_normalize, X0_mean = normalize(X0)
# Test that normalized data has zero mean
assert allclose(np.mean(X0 normalize, 0), np.zeros((2,)))
assert_allclose(X0_mean, np.array([1.0, 1.0]))
assert allclose(normalize(X0 normalize)[0], X0 normalize)
X0 = np.array([[0, 0.0],
               [1.0, 0.0],
               [2.0, 0.0]])
X0 normalize, X0 mean = normalize(X0)
# Test that normalized data has zero mean and unit variance
assert_allclose(np.mean(X0_normalize, 0), np.zeros((2,)))
assert allclose(X0 mean, np.array([1.0, 0.0]))
assert_allclose(normalize(X0_normalize)[0], X0_normalize)
# Some hidden tests below
# ...
```

Compute eigenvalues and eigenvectors eig

```
# GRADED FUNCTION: DO NOT EDIT THIS LINE
def eiq(S):
    """Compute the eigenvalues and corresponding eigenvectors
        for the covariance matrix S.
   Args:
        S: ndarray, covariance matrix
   Returns:
        (eigvals, eigvecs): ndarray, the eigenvalues and eigenvectors
    Note:
        the eigenvals and eigenvecs should be sorted in descending
       order of the eigen values
   # YOUR CODE HERE
   # Uncomment and modify the code below
     # Compute the eigenvalues and eigenvectors
     # You can use library routines in `np.linalg.*`
#
     # https://numpy.org/doc/stable/reference/routines.linalg.html
#
      # for this
   eigvals, eigvecs = np.linalg.eig(S)
#
     # The eigenvalues and eigenvectors need to be
#
      # sorted in descending order according to the eigenvalues
#
     # We will use `np.argsort` (https://docs.scipy.org/doc/numpy/reference/gen
erated/numpy.argsort.html)
#
     # to find a permutation of the indices
#
      # of eigvals that will sort eigvals in ascending order and
#
     # then find the descending order via [::-1], which reverse
     # the indices
   sort_indices = np.argsort(eigvals)[::-1]
      # Notice that we are sorting the columns (not rows) of
      # eigvecs since the columns represent the eigenvectors.
   return eigvals[sort indices], eigvecs[:, sort indices]
```

Some test cases for implementing eig.

```
def _flip_eigenvectors(B):
    """Flip the eigenvectors.
    signs = np.sign(B[np.argmax(np.abs(B), axis=0), range(B.shape[1])])
    return B * signs
def normalize eigenvectors(B):
    # Normalize eigenvectors to have unit length
    # Also flip the direction of the eigenvector based on
    # the first element
    B normalized = B / np.linalg.norm(B, axis=0)
    for i in range(B.shape[1]):
        if (B_normalized[0, i] < 0):</pre>
            B normalized[:, i] = -B normalized[:, i]
    return B normalized
A = np.array([[3, 2], [2, 3]])
expected eigenvalues = np.array([5., 1.])
expected eigenvectors = np.array(
    [[0.70710678, -0.70710678],
     [ 0.70710678, 0.70710678]]
actual_eigenvalues, actual_eigenvectors = eig(A)
# Check that the eigenvalues match
assert allclose(actual eigenvalues, expected eigenvalues)
# Check that the eigenvectors match
assert allclose(
    normalize eigenvectors(actual eigenvectors),
    _normalize_eigenvectors(expected_eigenvectors),
)
```

Compute projection matrix

Next given a orthonormal basis spanned by the eigenvectors, we will compute the projection matrix. This should be the same as what you have done last week.

In [55]:

```
# GRADED FUNCTION: DO NOT EDIT THIS LINE

def projection_matrix(B):
    """Compute the projection matrix onto the space spanned by `B`
    Args:
        B: ndarray of dimension (D, M), the basis for the subspace M

Returns:
        P: the projection matrix
    """

# YOUR CODE HERE
# Uncomment and modify the code below
inv = np.linalg.inv(B.T @ B)
PM = B @ inv @ B.T
return PM # <--- EDIT THIS to compute the projection matrix</pre>
```

```
In [56]:
```

Compute principal component analysis

In [65]:

```
# GRADED FUNCTION: DO NOT EDIT THIS LINE
def PCA(X, num components):
   Args:
        X: ndarray of size (N, D), where D is the dimension of the data,
           and N is the number of datapoints
        num components: the number of principal components to use.
        the reconstructed data, the sample mean of the X, principal values
        and principal components
    # YOUR CODE HERE
    # your solution should take advantage of the functions you have implemented
 above.
   ### Uncomment and modify the code below
     # first perform normalization on the digits so that they have zero mean an
d unit variance
   #print ("X.shape=", X.shape)
   X, mean = normalize(X) # EDIT THIS
   #print ("mean.shape= ", mean.shape)
   # Then compute the data covariance matrix S
   S = np.cov(X, rowvar = False, bias=True)
   #print ("S.shape = ", S.shape)
    #Third, get the eigen decomposition of the cov matrix
   vals, vecs = eig(S)
   pvals = vals[:num components]; pvecs = vecs[:,:num components]
   #Then, reconstruct projection matrix from some of the eigen vectors
   P = projection_matrix(vecs[:, :num_components]) # projection matrix
   #Finally, reconstruct X
   reconstX = (P @ X.T).T + mean
   #print("pvals.shape=", pvals.shape)
   #print("pvecs.shape=", pvecs.shape)
   #print("reconstX.shape = ", reconstX.shape)
   return reconstX, mean, pvals, pvecs
```

```
In [58]:
```

Some test cases that check the implementation of PCA

```
In [66]:
```

```
D = 2
N = 10
# Generate a dataset X from a 2D Gaussian distribution
mvn = scipy.stats.multivariate normal(
    mean=np.ones(D, dtype=np.float64),
    cov=np.array([[1, 0.8], [0.8, 1]], dtype=np.float64)
)
X = mvn.rvs((N,), random state=np.random.RandomState(0))
reconst, m, pv, pc = PCA(X, 1)
# Check the shape returned by the PCA implementation matches the specification.
assert reconst.shape == X.shape
assert m.shape == (D, )
assert pv.shape == (1, )
assert pc.shape == (D, 1)
# Check that PCA with num components == D gives identical reconstruction
reconst, m, pv, pc = PCA(X, D)
assert reconst.shape == X.shape
assert m.shape == (D, )
assert pv.shape == (2, )
assert pc.shape == (D, 2)
assert allclose(reconst, X)
```

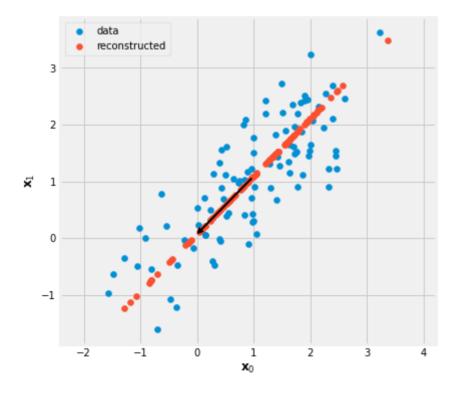
Visualize PCA

We will first visualize what PCA does on a 2D toy dataset. You can use the visualization below to get better intuition about what PCA does and use it to debug your code above.

In [60]:

```
mvn = scipy.stats.multivariate normal(
    mean=np.ones(2),
    cov=np.array([[1, 0.8], [0.8, 1]])
)
X = mvn.rvs((100,), random state=np.random.RandomState(0))
num components = 1
X reconst, mean, principal values, principal components = PCA(X, num components)
fig, ax = plt.subplots(figsize=(6, 6))
# eig vals, eig vecs = eig vals[:num components], eig vecs[:, :num components]
ax.scatter(X[:, 0], X[:, 1], label='data')
for (princial variance, principal component) in (zip(principal values, principal
_components.T)):
    draw vector(
        mean, mean + np.sqrt(princial variance) * principal component,
ax.scatter(X_reconst[:, 0], X_reconst[:, 1], label='reconstructed')
plt.axis('equal');
plt.legend();
ax.set(xlabel='\mbox{mathbf}(x) 0$', ylabel='<math>\mbox{mathbf}(x) 1$');
```

```
X.shape= (100, 2)
mean.shape= (2,)
S.shape = (2, 2)
pvals.shape= (1,)
pvecs.shape= (2, 1)
reconstX.shape = (100, 2)
```



We can also compare our PCA implementation with the implementation in scikit-learn (a popular machine learning library in Python that includes implementation of PCA) to see if we get identical results.

```
In [61]:
```

```
X.shape=(10, 5)
mean.shape= (5,)
S.shape = (5, 5)
pvals.shape= (1,)
pvecs.shape=(5, 1)
reconstX.shape = (10, 5)
difference in reconstruction for num components = 1: 2.6439936648525
73e-28
X.shape=(10, 5)
mean.shape= (5,)
S.shape = (5, 5)
pvals.shape= (2,)
pvecs.shape=(5, 2)
reconstX.shape = (10, 5)
difference in reconstruction for num components = 2: 4.4773576383227
25e-28
X.shape=(10, 5)
mean.shape= (5,)
S.shape = (5, 5)
pvals.shape= (3,)
pvecs.shape= (5, 3)
reconstX.shape = (10, 5)
difference in reconstruction for num_components = 3: 7.8676356751157
41e-29
```

PCA for MNIST digits

Once you have implemented PCA correctly, it's time to apply to the MNIST dataset. First, we will do some preprocessing of the data to get it into a good shape.

```
In [67]:
```

```
## Some preprocessing of the data
NUM_DATAPOINTS = 1000
X = (images.reshape(-1, 28 * 28)[:NUM_DATAPOINTS]) / 255.
```

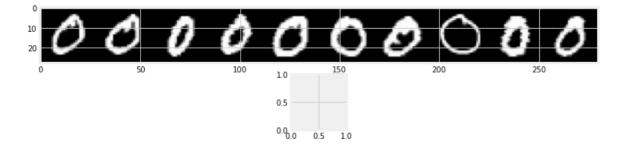
In [69]:

```
reconst, _, _, _ = PCA(X, num_components=10)
num_images_to_show = 10
reconst_images = np.reshape(reconst[:num_images_to_show], (-1, 28, 28))
reconst_images.astype("float64")
print("reconst_images.type= ", reconst_images.dtype)
fig, ax = plt.subplots(2, 1, figsize=(num_images_to_show * 3, 3))
ax[0].imshow(np.concatenate(np.reshape(X[:num_images_to_show], (-1, 28, 28)), -1), cmap="gray")
ax[1].imshow(np.concatenate(reconst_images, -1), cmap="gray");
```

reconst_images.type= complex128

```
Traceback (most recent cal
TypeError
l last)
<ipython-input-69-d8255584c92d> in <module>
      6 fig, ax = plt.subplots(2, 1, figsize=(num images to show * 3
, 3))
      7 ax[0].imshow(np.concatenate(np.reshape(X[:num images to show
], (-1, 28, 28)), -1), cmap="gray")
----> 8 ax[1].imshow(np.concatenate(reconst images, -1), cmap="gray"
);
/opt/conda/lib/python3.7/site-packages/matplotlib/ init .py in inn
er(ax, data, *args, **kwargs)
            def inner(ax, *args, data=None, **kwargs):
   1563
   1564
                if data is None:
-> 1565
                    return func(ax, *map(sanitize sequence, args), *
*kwargs)
   1566
   1567
                bound = new sig.bind(ax, *args, **kwargs)
/opt/conda/lib/python3.7/site-packages/matplotlib/cbook/deprecation.
py in wrapper(*args, **kwargs)
    356
                        f"%(removal)s. If any parameter follows {na
me!r}, they "
    357
                        f"should be pass as keyword, not positionall
y.")
                return func(*args, **kwargs)
--> 358
    359
    360
            return wrapper
/opt/conda/lib/python3.7/site-packages/matplotlib/cbook/deprecation.
py in wrapper(*args, **kwargs)
    356
                        f"%(removal)s. If any parameter follows {na
me!r}, they "
                        f"should be pass as keyword, not positionall
    357
y.")
                return func(*args, **kwargs)
--> 358
    359
    360
            return wrapper
/opt/conda/lib/python3.7/site-packages/matplotlib/axes/ axes.py in i
mshow(self, X, cmap, norm, aspect, interpolation, alpha, vmin, vmax,
origin, extent, shape, filternorm, filterrad, imlim, resample, url,
 **kwarqs)
   5613
                                       resample=resample, **kwargs)
   5614
-> 5615
                im.set data(X)
   5616
                im.set_alpha(alpha)
                if im.get clip path() is None:
/opt/conda/lib/python3.7/site-packages/matplotlib/image.py in set da
ta(self, A)
    692
                        not np.can_cast(self._A.dtype, float, "same_
kind")):
                    raise TypeError("Image data of dtype {} cannot b
    693
e converted to "
--> 694
                                     "float".format(self. A.dtype))
    695
    696
                if not (self. A.ndim == 2
```

TypeError: Image data of dtype complex128 cannot be converted to flo at



The greater number of of principal components we use, the smaller will our reconstruction error be. Now, let's answer the following question:

How many principal components do we need in order to reach a Mean Squared Error (MSE) of less than 10.0 for our dataset?

We have provided a function in the next cell which computes the mean squared error (MSE), which will be useful for answering the question above.

In [70]:

```
def mse(predict, actual):
    """Helper function for computing the mean squared error (MSE)"""
    return np.square(predict - actual).sum(axis=1).mean()
```

In [71]:

```
loss = []
reconstructions = []
# iterate over different number of principal components, and compute the MSE
for num_component in range(1, 100, 5):
    reconst, _, _, _ = PCA(X, num_component)
    error = mse(reconst, X)
    reconstructions.append(reconst)
    # print('n = {:d}, reconstruction_error = {:f}'.format(num_component, error))
    loss.append((num_component, error))

reconstructions = np.asarray(reconstructions)
reconstructions = reconstructions
loss = np.asarray(loss)
```

In [81]:

```
import pandas as pd
# create a table showing the number of principal components and MSE
df = pd.DataFrame(loss, columns=['no. of components', 'mse'])
newdf = df[df['mse']<10.0]
newdf['no. of components'] = [str(x).split(".")[0] for x in newdf['no. of components']]
newdf</pre>
```

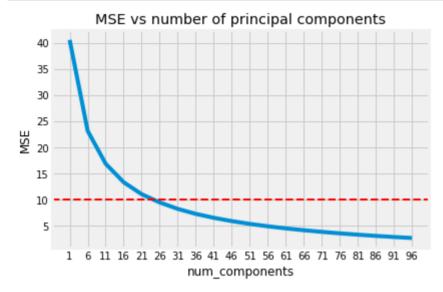
Out[81]:

	no. of components	mse
5	(26+0j)	9.498890+0.000000j
6	(31+0j)	8.267745+0.000000j
7	(36+0j)	7.313488+0.000000j
8	(41+0j)	6.558018+0.000000j
9	(46+0j)	5.927011+0.000000j
10	(51+0j)	5.393007+0.000000j
11	(56+0j)	4.937360+0.000000j
12	(61+0j)	4.533004+0.000000j
13	(66+0j)	4.179846+0.000000j
14	(71+0j)	3.865891+0.000000j
15	(76+0j)	3.583798+0.000000j
16	(81+0j)	3.327250+0.000000j
17	(86+0j)	3.096546+0.000000j
18	(91+0j)	2.886497+0.000000j
19	(96+0j)	2.692053+0.000000j

We can also put these numbers into perspective by plotting them.

In [82]:

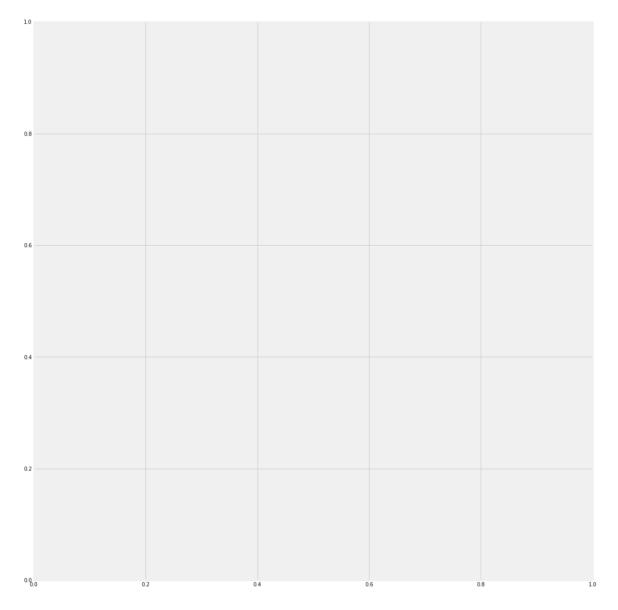
```
fig, ax = plt.subplots()
ax.plot(loss[:,0], loss[:,1]);
ax.axhline(10, linestyle='--', color='r', linewidth=2)
ax.xaxis.set_ticks(np.arange(1, 100, 5));
ax.set(xlabel='num_components', ylabel='MSE', title='MSE vs number of principal components');
```



But *numbers dont't tell us everything*! Just what does it mean *qualitatively* for the loss to decrease from around 45.0 to less than 10.0?

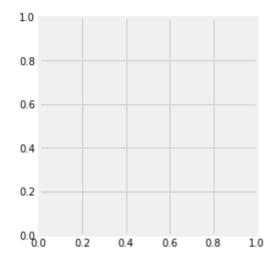
Let's find out! In the next cell, we draw the the leftmost image is the original dight. Then we show the reconstruction of the image on the right, in descending number of principal components used.

```
In [83]:
```



We can also browse through the reconstructions for other digits. Once again, interact becomes handy for visualing the reconstruction.

```
@interact(i=(0, 10))
def show_pca_digits(i=1):
    """Show the i th digit and its reconstruction"""
    plt.figure(figsize=(4,4))
    actual_sample = X[i].reshape(28,28)
    reconst_sample = (reconst[i, :]).reshape(28, 28)
    plt.imshow(np.hstack([actual_sample, reconst_sample]), cmap='gray')
    plt.grid(False)
    plt.show()
```



PCA for high-dimensional datasets

Sometimes, the dimensionality of our dataset may be larger than the number of samples we have. Then it might be inefficient to perform PCA with your implementation above. Instead, as mentioned in the lectures, you can implement PCA in a more efficient manner, which we call "PCA for high dimensional data" (PCA_high_dim).

Below are the steps for performing PCA for high dimensional dataset

- 1. Normalize the dataset matrix X to obtain \overline{X} that has zero mean.
- 2. Compute the matrix $\overline{X}\overline{X}^T$ (a N by N matrix with N << D)
- 3. Compute eigenvalues λ s and eigenvectors V for $\overline{X}\overline{X}^T$ with shape (N, N). Compare this with computing the eigenspectrum of $\overline{X}^T\overline{X}$ which has shape (D, D), when N << D, computation of the eigenspectrum of $\overline{X}\overline{X}^T$ will be computationally less expensive.
- 4. Compute the eigenvectors for the original covariance matrix as $\overline{X}^{1}V$. Choose the eigenvectors associated with the n largest eigenvalues to be the basis of the principal subspace U.
 - A. Notice that \overline{X}^TV would give a matrix of shape (D, N) but the eigenvectors beyond the Dth column will have eigenvalues of 0, so it is safe to drop any columns beyond the D'th dimension.
 - B. Also note that the columns of U will not be unit-length if we pre-multiply V with \overline{X}^I , so we will have to normalize the columns of U so that they have unit-length to be consistent with the PCA implementation above.
- 5. Compute the orthogonal projection of the data onto the subspace spanned by columns of *U*.

Functions you wrote for earlier assignments will be useful.

```
# GRADED FUNCTION: DO NOT EDIT THIS LINE
def normalize eigenvectors(B):
   # Normalize eigenvectors to have unit length
   # Also flip the direction of the eigenvector based on
   # the first element
   B normalized = B / np.linalg.norm(B, axis=0)
    for i in range(B.shape[1]):
        if (B normalized[0, i] < 0):
            B normalized[:, i] = -B normalized[:, i]
   return B normalized
def PCA high dim(X, num components):
    """Compute PCA for small sample size but high-dimensional features.
   Args:
        X: ndarray of size (N, D), where D is the dimension of the sample,
           and N is the number of samples
        num components: the number of principal components to use.
        X reconstruct: (N, D) ndarray. the reconstruction
        of X from the first `num components` pricipal components.
    # YOUR CODE HERE
    # Uncomment and modify the code below
   N, D = X.shape
   # Normalize the dataset
   X, mean = normalize(X)
      # Find the covariance matrix
   # Remember now N is smaller than D! So the covariance matrix
   # will be of dimension DxD.
   S = X @ X.T ## X has already been normalised here.
      # Next find eigenvalues and corresponding eigenvectors for S
      # Make sure that you only take the first D eigenvalues/vectors
     # You can also take a look at the eigenvalues beyond column (D-1) and they
should be
      # zero (or a very small number due to finite floating point precision)
   vals, vecs = eig(S)
   vecs = normalize eigenvectors(vecs)
   vals = vals[:D] ; vecs = vecs[:, :D]
   print("vals.shape = ", vals.shape)
   print("vecs.shape = ", vecs.shape)
   # Compute the eigenvalues and eigenvectors for the original system
   evecs = X.T @ vecs
   print("evecs.shape=", evecs.shape)
   evecs = evecs[:, :D]
   print("New evecs.shape=",evecs.shape)
     # Normalize the eigenvectors to have unit-length
   evecs = normalize eigenvectors(evecs)
      # Take the top `num components` of the eigenvalues / eigenvectors
#
      # as the principal values and principal components
   pvals = vals[:num components]
   pvecs = evecs[:, :num components]
   print("pvals.shape = ", pvals.shape)
   print("pvecs.shape = ", pvecs.shape)
     # reconstruct the images from the lower dimensional representation
   P = projection matrix(pvecs)
   reconst = (P @ X.T).T + mean
      # Remember to add back the sample mean
   return reconst, mean, pvals, pvecs
```

```
In [ ]:
```

```
# YOUR CODE HERE
```

In []:

```
# Some hidden tests below ### ...
```

Given the same dataset, PCA_high_dim and PCA should give the same output. Assuming we have implemented PCA, correctly, we can then use PCA to test the correctness of PCA_high_dim. Given the same dataset, PCA and PCA_high_dim should give identical results.

We can use this **invariant** to test our implementation of PCA_high_dim, assuming that we have correctly implemented PCA.

In [95]:

```
random = np.random.RandomState(0)
# Generate some random data
X = random.randn(5, 4)
pca_rec, pca_mean, pca_pvs, pca_pcs = PCA(X, 2)
pca_hd_rec, pca_hd_mean, pca_hd_pvs, pca_hd_pcs = PCA_high_dim(X, 2)
# Check that the results returned by PCA and PCA_high_dim are identical
np.testing.assert_allclose(pca_rec, pca_hd_rec)
np.testing.assert_allclose(pca_mean, pca_hd_mean)
np.testing.assert_allclose(pca_pvs, pca_pvs)
np.testing.assert_allclose(pca_pcs, pca_pcs)
```

```
vals.shape = (4,)
vecs.shape = (5, 4)
evecs.shape= (4, 4)
New evecs.shape= (4, 4)
pvals.shape = (2,)
pvecs.shape = (4, 2)
```

Congratulations! You have now learned how PCA works!