04_assignment_pca

April 20, 2025

Assignment 4: Principal Component Analysis

CPSC 381/581: Machine Learning

Yale University

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Prerequisites:

1. Enable Google Colaboratory as an app on your Google Drive account
2. Create a new Google Colab notebook, this will also create a "Colab Notebooks" directory under "MyDrive" i.e.

```
/content/drive/MyDrive/Colab Notebooks
```

3. Create the following directory structure in your Google Drive

```
/content/drive/MyDrive/Colab Notebooks/CPSC 381-581: Machine Learning/Assignments
```

4. Move the 04_assignment_pca.ipynb into

```
/content/drive/MyDrive/Colab Notebooks/CPSC 381-581: Machine Learning/Assignments
```

so that its absolute path is

```
/content/drive/MyDrive/Colab Notebooks/CPSC 381-581: Machine Learning/Assignments/04_assignmen
```

In this assignment, we will use principal component analysis (PCA) to compress data. We will first train PCA to find the linear transformation that will preserve variance within a dataset. We will measure loss by reconstruction. We will also use PCA to synthesize new examples.

We will work with two datasets: the handwritten digits dataset and the Olivetti faces dataset, to explore how PCA performs on different types of image data.

Submission:

1. Implement all TODOs in the code blocks below.
2. List any collaborators.

```
Collaborators: None.
```

Import packages

```
[1]: import numpy as np
import sklearn.datasets as skdata
import sklearn.metrics as skmetrics
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
import warnings

warnings.filterwarnings(action='ignore')
np.random.seed(42)  # Set a fixed seed for reproducibility
```

Plotting functions

```
[2]: def plot(x, y, title, xlabel, ylabel):
    '''
    Plots x against y with plot title

    Arg(s):
        x : numpy[float32]
            array of values
        y : numpy[float32]
            array of values
        title : str
            (super)title of plot
        xlabel : str
            label of x axis
        ylabel : str
            label of y axis
    '''

    # Create a 1 x 1 figure
    fig = plt.figure()
    ax = fig.add_subplot(1, 1, 1)

    # DONE: Plot y against x, set marker to 'o', color to 'b'
    ax.plot(x, y, marker='o', color='b')

    # DONE: Create super title for figure
    fig.suptitle(title)

    # DONE: Set x and y axis with labels
    ax.set_xlabel(xlabel)
    ax.set_ylabel(ylabel)


def plot_images(X, n_row, n_col, title, cmap='gray'):
    '''
    Creates n_row by n_col panel of images
```

```
    Args:
        X : numpy[float32]
            N x h x w numpy array
        n_row : int
            number of rows in figure
        n_col : list[str]
            number of columns in figure
        title : str
            title of plot
        cmap : str
            colormap to use for visualizing images
    '''

    fig = plt.figure(figsize=(10, 10))

    # DONE: Set title as figure super title
    fig.suptitle(title)


    # DONE?: Iterate through X and plot the first n_row x n_col elements as␣
 ↪figures
    # visualize using the specified 'gray' colormap
    # use plt.box(False) and plt.axis('off') to turn off borders and axis
    for i in range(0, n_row * n_col):
        ax = fig.add_subplot(n_row, n_col, i + 1)
        ax.imshow(X[i], cmap='gray')
        plt.box(False)
        plt.axis('off')
```

Implementation of Principal Component Analysis (PCA) for dimensionality reduction

[3]:
```
class PrincipalComponentAnalysis(object):

    def __init__(self, d):
        # Number of eigenvectors to keep
        self.__d = d

        # Mean of the dataset
        self.__mean = None

        # Linear weights or transformation to project to lower subspace
        self.__weights = None

        # Eigenvalues of the dataset
        self.__eigenvalues = None

    def __center(self, X):
```

```python
        '''
        Centers the data to zero-mean

        Args:
            X : numpy[float32]
                N x D feature vectors
        Returns:
            numpy[float32] : N x D centered feature vectors
        '''

        # DONE: Center the data

        return X - self.__mean

    def __covariance_matrix(self, X):
        '''
        Computes the covariance matrix of feature vectors

        Args:
            X : numpy[float32]
                N x D feature vectors
        Returns:
            numpy[float32] : D x D covariance matrix
        '''

        # DONE?: Compute the covariance matrix
        N = X.shape[0]
        return (1 / (N-1)) * np.dot(X.T, X)

    def fit(self, X):
        '''
        Obtains the top d eigenvectors (weights) from the input feature vectors

        Arg(s):
            X : numpy[float32]
                N x D feature vector
        '''

        # DONE?: Implement the fit function

        # Make sure that d is less or equal D
        assert self.__d <= X.shape[1]

        # DONE: Compute mean
        self.__mean = np.mean(X, axis=0)

        # DONE: Compute the covariance matrix
```

```python
        X = self.__center(X)
        cov = self.__covariance_matrix(X)


        # DONE: Eigen decomposition
        eigenvalues, eigenvectors = np.linalg.eig(cov)

        # DONE?: Store the top d eigenvalues
        self.__eigenvalues = eigenvalues[:self.__d]

        # DONE?: Select the top d eigenvectors
        self.__weights = eigenvectors[:, :self.__d]

    def project_to_subspace(self, X):
        '''
        Project data X to lower dimension subspace using the top d eigenvectors

        Arg(s):
            X : numpy[float32]
                N x D feature vectors
        Returns:
            numpy[float32] : N x d feature vectors
        '''

        # DONE: Computes transformation to lower dimension and project to␣
↪subspace

        return np.dot(X - self.__mean, self.__weights)

    def get_eigenvalues(self):
        '''
        Returns eigenvalues

        Returns:
            numpy[float32] : eigenvalues
        '''

        return self.__eigenvalues

    def get_weights(self):
        '''
        Returns weights (eigenvectors)

        Returns:
            numpy[float32] : weights
        '''
```

```
        return self.__weights

    def get_mean(self):
        '''
        Returns mean

        Returns:
            numpy[float32] : mean
        '''

        return self.__mean

    def reconstruct_from_subspace(self, Z):
        '''
        Reconstruct the original feature vectors from the latent vectors

        Arg(s):
            Z : numpy[float32]
                N x d latent vectors
        Returns:
            numpy[float32] : N x D feature vectors
        '''

        # DONE: Reconstruct the original feature vector

        return np.dot(Z, self.__weights.T) + self.__mean

    def generate_new_samples(self, m):
        '''
        Generates new data points by sampling from a normal distribution

        Arg(s):
            m : int
                number of samples to generate
        Returns:
            numpy[float32] : m x D samples
        '''

        # DONE: Generate new samples

        return np.dot(np.random.randn(m, self.__d), self.__weights.T) + self.
↪__mean
```

0.1 Part 1: Handwritten Digits Dataset

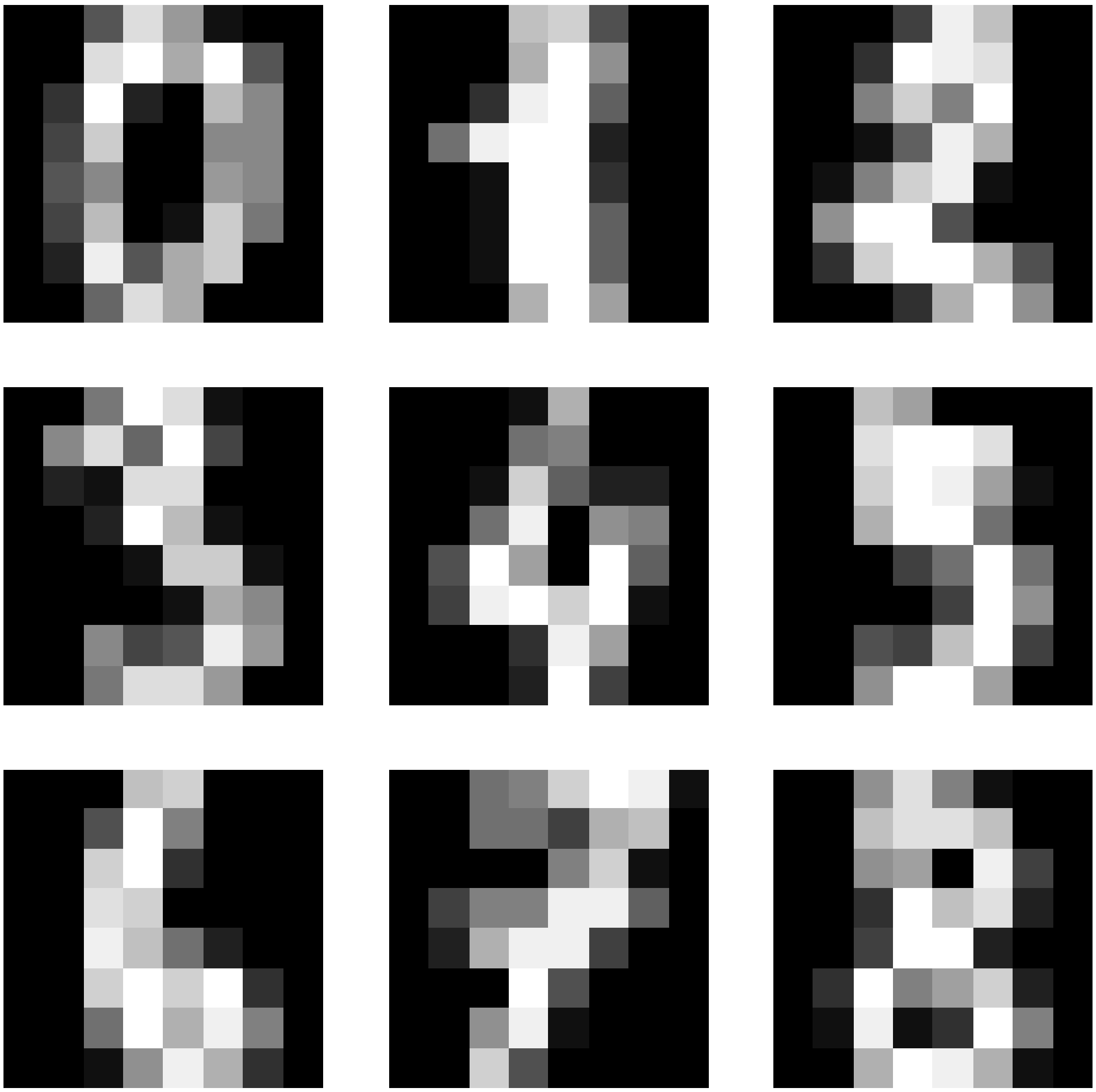
Load digits dataset

[4]:
```
# Load digits dataset
dataset = skdata.load_digits()

# Dataset of image, currently vectorized as (N, 64) shape
X = dataset.data
y = dataset.target
```

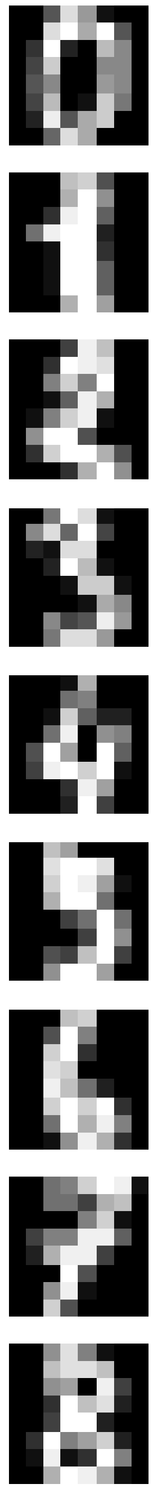
Visualize digits dataset as images

[ ]:
```
# DONE: Get the number of dimensions in the dataset
n_dim = X.shape[1]

# DONE: Reshape handwritten digits dataset to N x 8 x 8
X_reshaped = X.reshape(-1, 8, 8)

# DONE: Plot 3 x 3 panel of handwritten digits with title 'Handwritten digits␣
 ↪dataset'
plot_images(X_reshaped, 3, 3, 'Handwritten digits dataset')

# DONE: Vectorize handwritten digits dataset to N x D
X_vec = X_reshaped.reshape(-1, n_dim)

# DONE: Plot 9 x 1 panel of handwritten digits with title 'Vectorized␣
 ↪handwritten digits dataset'
X_vec_reshaped = X_vec.reshape(-1, 8, 8)
plot_images(X_vec_reshaped, 9, 1, 'Vectorized handwritten digits dataset')
```

Handwritten digits dataset

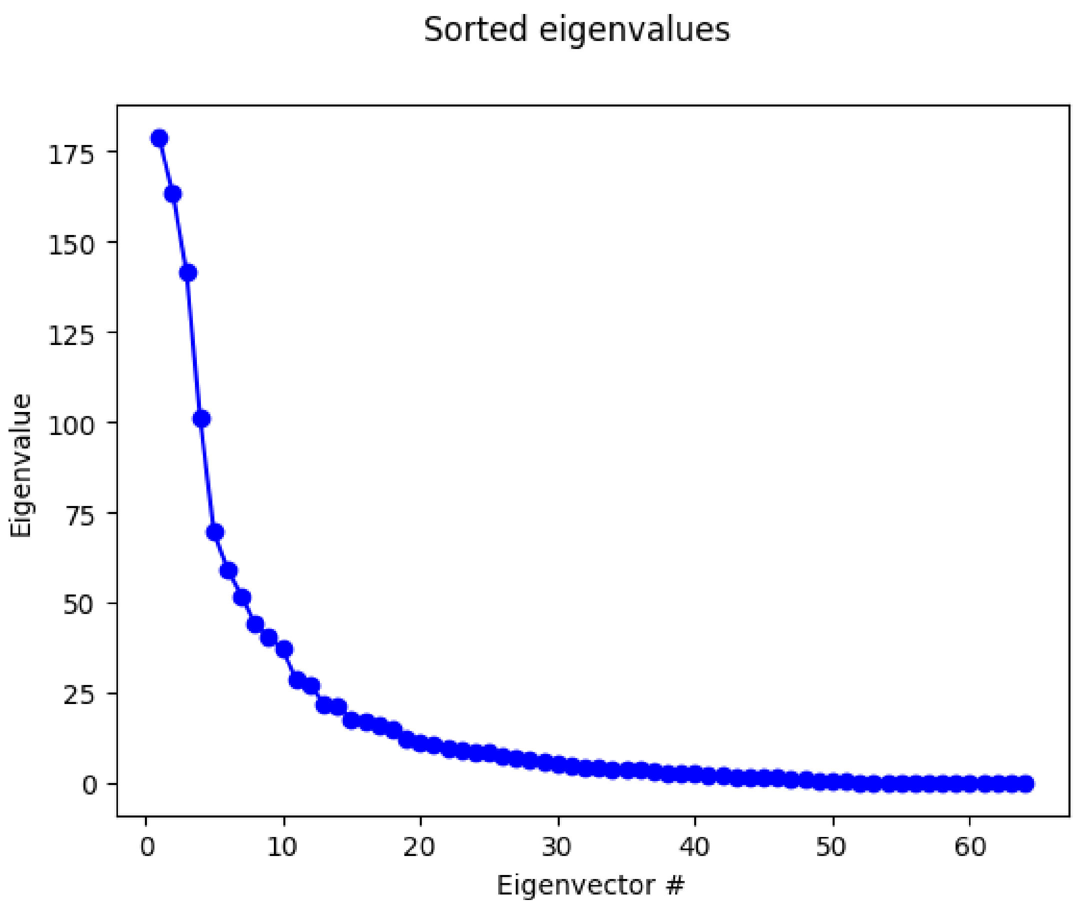


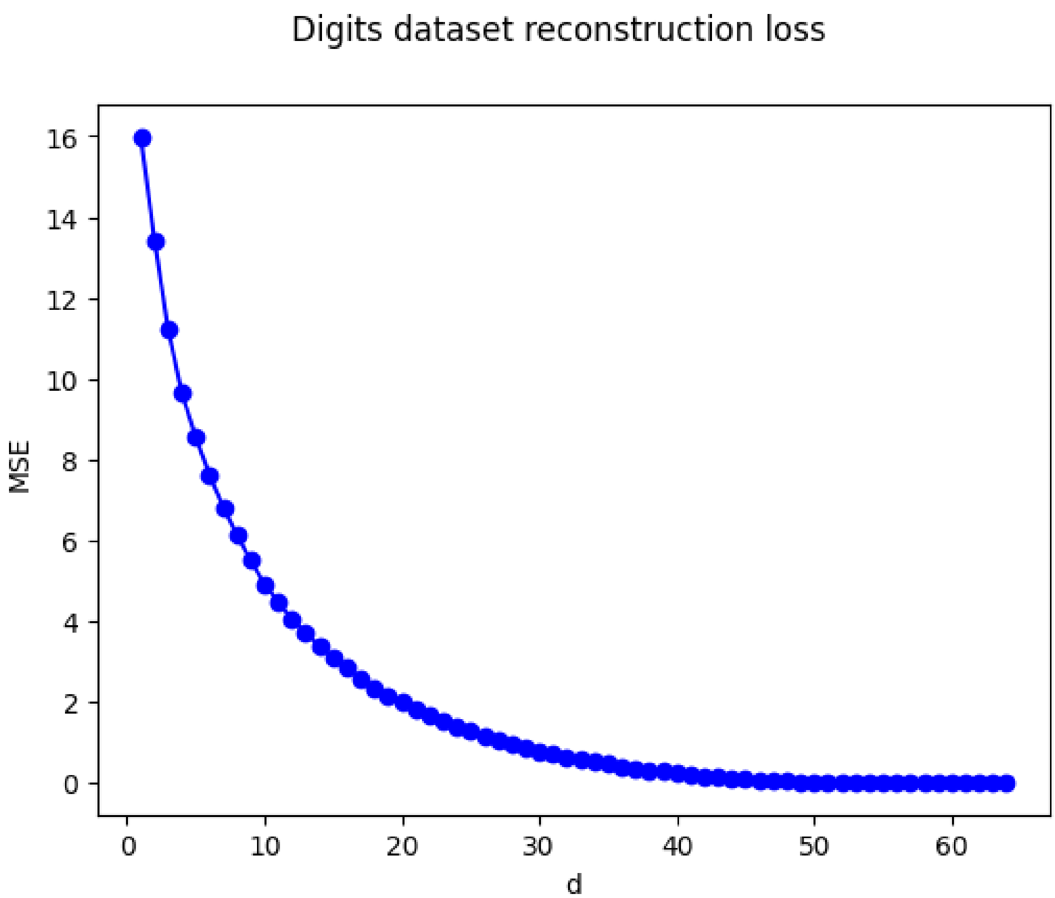
Vectorized handwritten digits dataset



Compressing and reconstructing with principal component analysis (PCA)

```
[8]: # DONE: Plot full set of eigenvalues for dataset
# set title of plot 'Sorted eigenvalues' with xlabel of 'Eigenvector #' and␣
↪ylabel of 'Eigenvalue'
pca = PrincipalComponentAnalysis(n_dim)
pca.fit(X_vec)
eigenvalues = pca.get_eigenvalues()
plot(np.arange(1, n_dim + 1), eigenvalues, 'Sorted eigenvalues', 'Eigenvector␣
↪#', 'Eigenvalue')

# MSE scores to keep track of loss from compression
mse_scores = []

# Test reconstruction error using top d number of eigenvectors
for d in range(1, n_dim + 1):

    # DONE: Fit PCA to data
    pca = PrincipalComponentAnalysis(d)
    pca.fit(X_vec)

    # DONE: Project the data to subspace
    Z = pca.project_to_subspace(X_vec)

    # DONE: Reconstruct the original data
    X_hat = pca.reconstruct_from_subspace(Z)

    # DONE: Measures mean squared error between original data and reconstructed␣
↪data
    mse_score = skmetrics.mean_squared_error(X_vec, X_hat)

    # DONE: Save MSE score
    mse_scores.append(mse_score)

# DONE: Create plot for number of top eigenvectors used and their MSE for␣
↪reconstruction
# set title of plot 'Digits dataset reconstruction loss' with xlabel of 'd' and␣
↪ylabel of 'MSE'
plot(np.arange(1, n_dim + 1), mse_scores, 'Digits dataset reconstruction loss',␣
↪'d', 'MSE')
```


Sorted eigenvalues
175
150
125
100
75
50
25
0
Eigenvalue
0
10
20
30
40
50
60
Eigenvector #



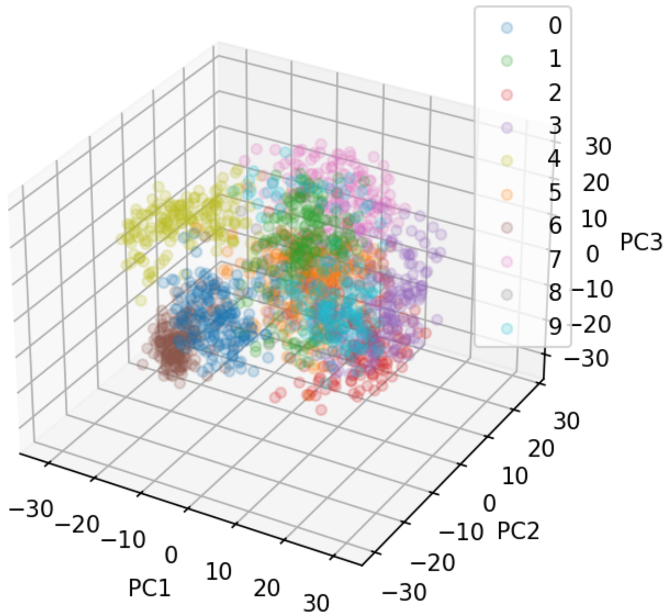
Visualize data using PCA

```
[ ]: # Set colors
colors = [
    'tab:blue',
    'tab:green',
    'tab:red',
    'tab:purple',
    'tab:olive',
    'tab:orange',
    'tab:brown',
    'tab:pink',
    'tab:gray',
    'tab:cyan'
]

# DONE?: Project the data into 3-dimensional subspace
pca = PrincipalComponentAnalysis(3)
pca.fit(X_vec)
```

```
Z = pca.project_to_subspace(X_vec)

fig = plt.figure(dpi=150)
fig.suptitle('Visualization of digits projected from {} dimensions to␣
↪3-dimensional subspace'.format(n_dim))
ax = fig.add_subplot(1, 1, 1, projection='3d')

# Iterate through each class and plot them into the figure as scatter plot with␣
↪different colors
for label, color in zip(np.sort(np.unique(y)), colors):

    # DONE?: Select from projected points the ones belonging to current class
    Z_class = Z[y == label]

    # DONE: Plot using scatter for selected points with associated color
    # set the plot label as label, set alpha to 0.2
    ax.scatter(Z_class[:, 0], Z_class[:, 1], Z_class[:, 2], c=color,␣
↪label=label, alpha=0.2)

# DONE: Turn on legend and set loc to best
ax.legend(loc='best')

# DONE: set xlabel, ylabel and zlabel to their respective principal component␣
↪(PC#)
ax.set_xlabel('PC1')
ax.set_ylabel('PC2')
ax.set_zlabel('PC3')
```

[ ]: Text(0.5, 0, 'PC3')

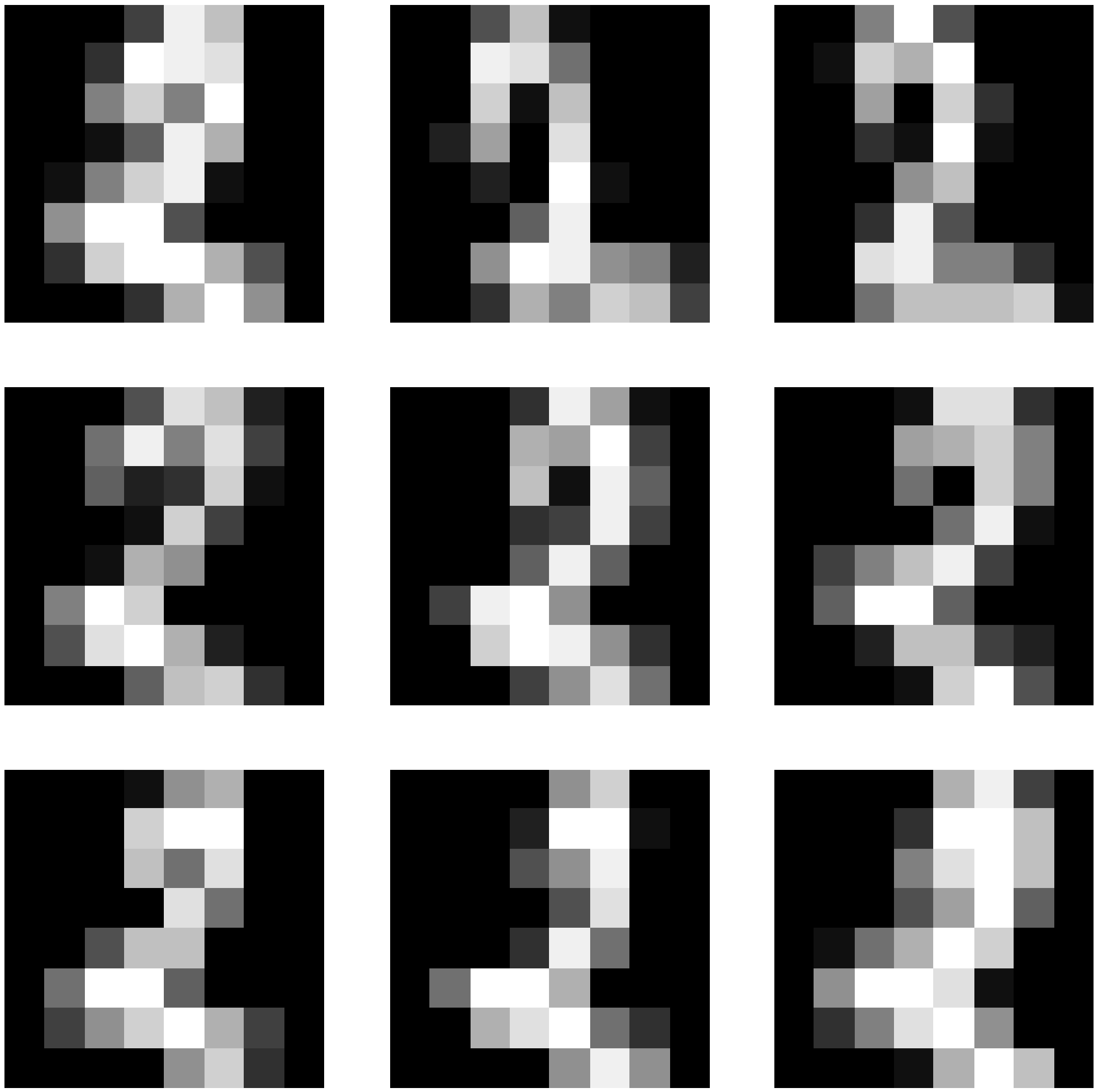
Visualization of digits projected from 64 dimensions to 3-dimensional subspace



Select 2s from digits dataset

[20]:
```
# DONE: Select all 2's from the digit dataset
X_2s = X_vec[y == 2]

# DONE: Reshape handwritten digits dataset of 2s to (N, 8, 8)
X_2s_reshaped = X_2s.reshape(-1, 8, 8)

# DONE: Plot 3 x 3 panel of handwritten digits and name is 'Handwritten digits␣
↪dataset of 2s'
plot_images(X_2s_reshaped, 3, 3, 'Handwritten digits dataset of 2s')
```

Handwritten digits dataset of 2s



PCA as a generative model

[24]:
```
# DONE: Vectorize handwritten digits dataset of 2s
X_2s_vec = X_2s_reshaped.reshape(-1, n_dim)

# DONE: Compute PCA and with 5 dimensions
pca_2s = PrincipalComponentAnalysis(5)
pca_2s.fit(X_2s_vec)
```

```python
# DONE: Generate 25 novel examples
X_2s_hat = pca_2s.generate_new_samples(25)

# DONE: Plot 5 x 5 panel of handwritten digits and name is 'Synthesized␣
↪handwritten digits dataset'
plot_images(X_2s_hat.reshape(-1, 8, 8), 5, 5, 'Synthesized handwritten digits␣
↪dataset')
```

0.2 Part 2: Olivetti Faces Dataset

[25]:
```python
# Load Olivetti faces dataset
from sklearn.datasets import fetch_olivetti_faces
faces_dataset = fetch_olivetti_faces(shuffle=True)

# Dataset of face images with shape (N, 64, 64)
X_faces = faces_dataset.images
y_faces = faces_dataset.target

print('Faces dataset shape: {}'.format(X_faces.shape))
print('Number of unique individuals: {}'.format(len(np.unique(y_faces))))
```

```
downloading Olivetti faces from https://ndownloader.figshare.com/files/5976027
to /Users/haileyrobertson/scikit_learn_data
Faces dataset shape: (400, 64, 64)
Number of unique individuals: 40
```

Visualize faces dataset

[ ]:
```python
# DONE: Get the dimensions of a face image
face_height, face_width = X_faces.shape[1], X_faces.shape[2]

# DONE: Plot 3 x 3 panel of face images with title 'Olivetti faces dataset'
plot_images(X_faces, 3, 3, 'Olivetti faces dataset')

# DONE: Vectorize face images to N x D
X_faces_vec = X_faces.reshape(X_faces.shape[0], -1)

# DONE: Plot 9 x 1 panel of vectorized face images with title 'Vectorized␣
↪Olivetti faces dataset'
plot_images(X_faces_vec.reshape(-1, face_height, face_width), 9, 1, 'Vectorized␣
↪Olivetti faces dataset')
```

Olivetti faces dataset

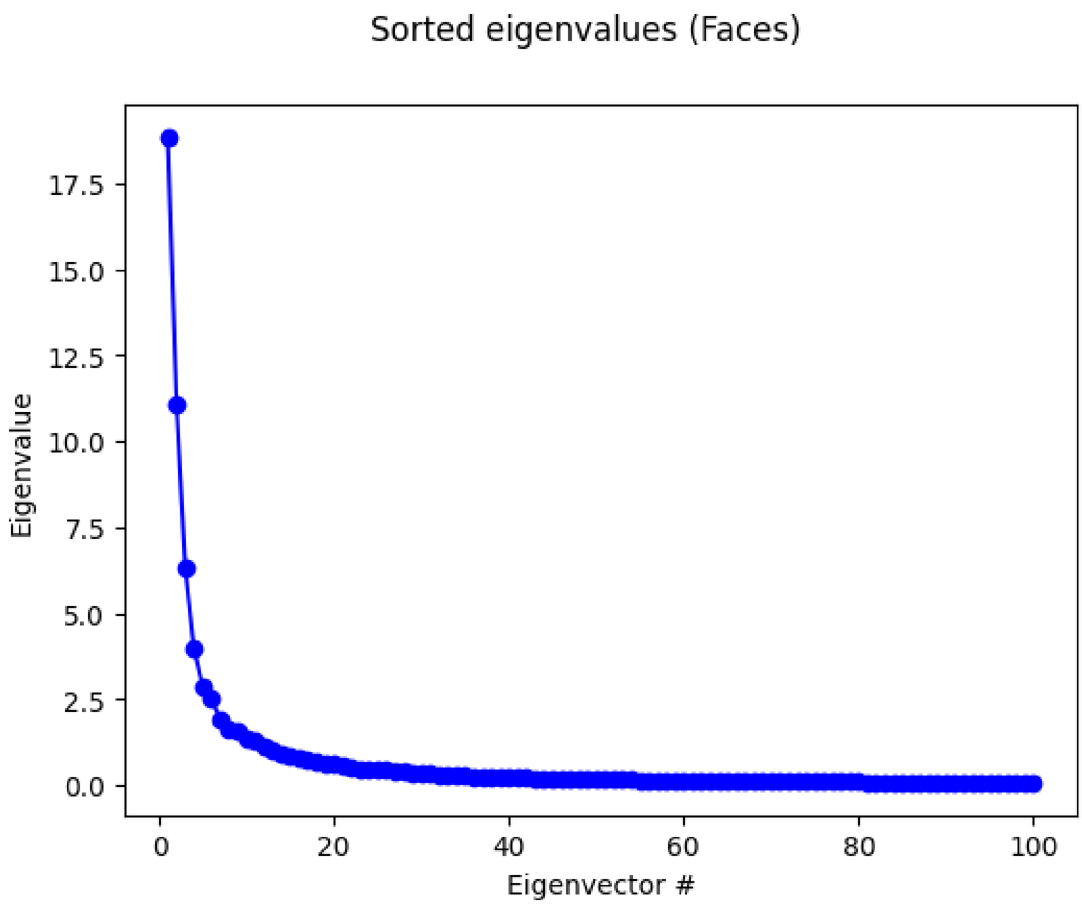
Vectorized Olivetti faces dataset

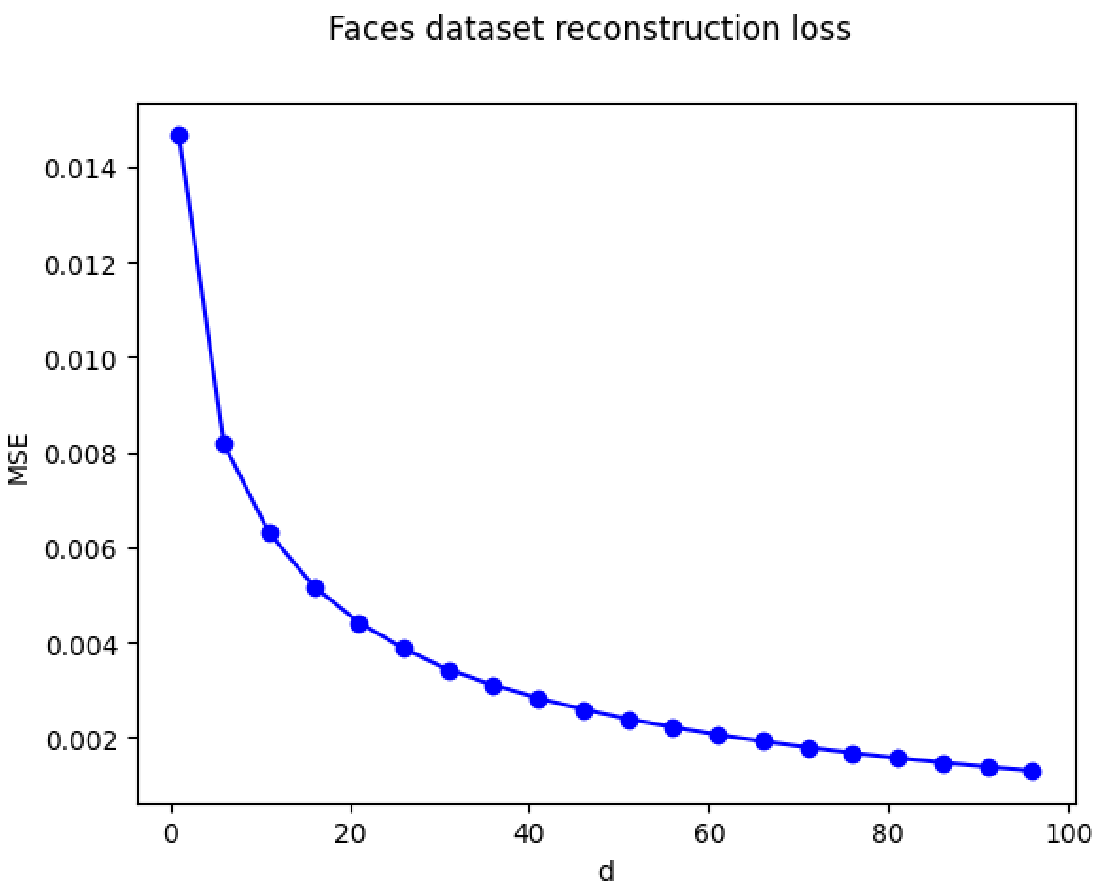
Compressing and reconstructing faces with PCA

```
[29]: # Get the number of dimensions in the faces dataset
n_dim_faces = X_faces_vec.shape[1] if X_faces_vec is not None else 0

# DONE: Plot full set of eigenvalues for faces dataset
# set title of plot 'Sorted eigenvalues (Faces)' with xlabel of 'Eigenvector #'␣
 ↪and ylabel of 'Eigenvalue'
# Note: Computing all eigenvalues would be computationally expensive
# Let's compute a reasonable number, say 100
n_components_to_compute = 100
pca_faces = PrincipalComponentAnalysis(n_components_to_compute)
pca_faces.fit(X_faces_vec)

eigenvalues_faces = pca_faces.get_eigenvalues()
plot(np.arange(1, n_components_to_compute + 1), eigenvalues_faces, 'Sorted␣
 ↪eigenvalues (Faces)', 'Eigenvector #', 'Eigenvalue')

# MSE scores to keep track of loss from compression
mse_scores_faces = []

# Test reconstruction error using top d number of eigenvectors
# Use a reasonable range to save computation
d_values = np.arange(1, 101, 5)  # [1, 6, 11, ..., 96]
for d in d_values:
    # DONE: Fit PCA to face data
    pca_faces = PrincipalComponentAnalysis(d)
    pca_faces.fit(X_faces_vec)

    # DONE: Project the data to subspace
    Z_faces = pca_faces.project_to_subspace(X_faces_vec)

    # DONE: Reconstruct the original data
    X_faces_hat = pca_faces.reconstruct_from_subspace(Z_faces)

    # DONE: Measures mean squared error between original data and reconstructed␣
 ↪data
    mse_score_faces = skmetrics.mean_squared_error(X_faces_vec, X_faces_hat)

    # DONE: Save MSE score
    mse_scores_faces.append(mse_score_faces)

    # Print progress
    print('Completed PCA with {d} components'.format(d=d))
```

```
# DONE: Create plot for number of top eigenvectors used and their MSE for␣
↪reconstruction
# set title of plot 'Faces dataset reconstruction loss' with xlabel of 'd' and␣
↪ylabel of 'MSE'
plot(d_values, mse_scores_faces, 'Faces dataset reconstruction loss', 'd',␣
↪'MSE')
```

```
Completed PCA with 1 components
Completed PCA with 6 components
Completed PCA with 11 components
Completed PCA with 16 components
Completed PCA with 21 components
Completed PCA with 26 components
Completed PCA with 31 components
Completed PCA with 36 components
Completed PCA with 41 components
Completed PCA with 46 components
Completed PCA with 51 components
Completed PCA with 56 components
Completed PCA with 61 components
Completed PCA with 66 components
Completed PCA with 71 components
Completed PCA with 76 components
Completed PCA with 81 components
Completed PCA with 86 components
Completed PCA with 91 components
Completed PCA with 96 components
```


Sorted eigenvalues (Faces)
Eigenvalue
Eigenvector #
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
0
20
40
60
80
100

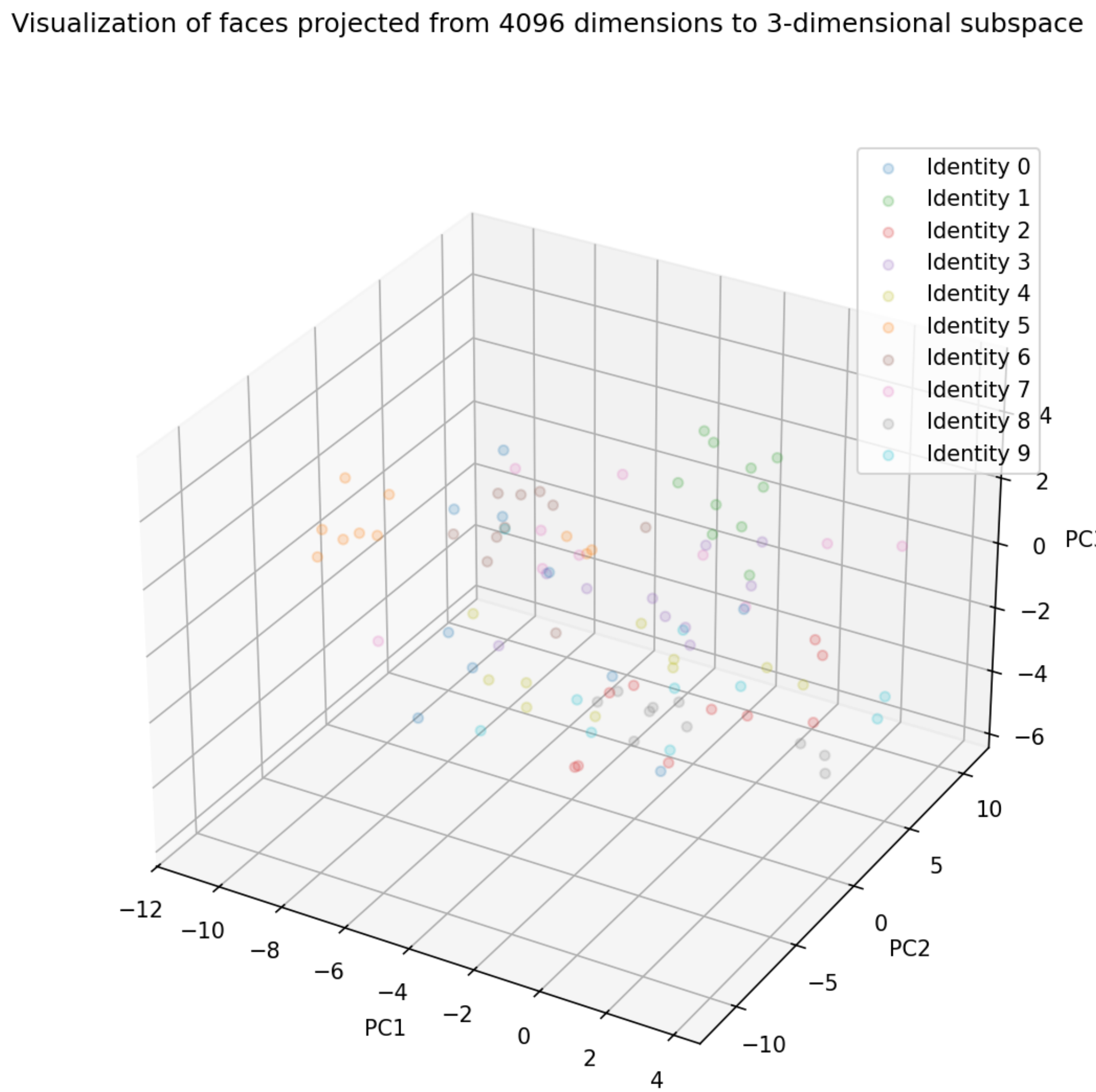


Visualizing Faces in 3D Space

```
[ ]: # DONE?: Project the face data into 3-dimensional subspace
pca_faces_3d = PrincipalComponentAnalysis(3)
pca_faces_3d.fit(X_faces_vec) #maybe don't need this?
Z_faces_3d = pca_faces_3d.project_to_subspace(X_faces_vec)

fig = plt.figure(dpi=150, figsize=(10, 8))
fig.suptitle('Visualization of faces projected from {} dimensions to␣
 ↪3-dimensional subspace'.format(n_dim_faces))
ax = fig.add_subplot(1, 1, 1, projection='3d')

# For clarity, let's select a subset of identities
selected_identities = np.arange(10)  # First 10 identities
identity_colors = colors[:len(selected_identities)]

# DONE: Plot each identity with a different color
# Hint: Use indices = np.where(y_faces == identity)[0] to find indices for each␣
 ↪identity
```

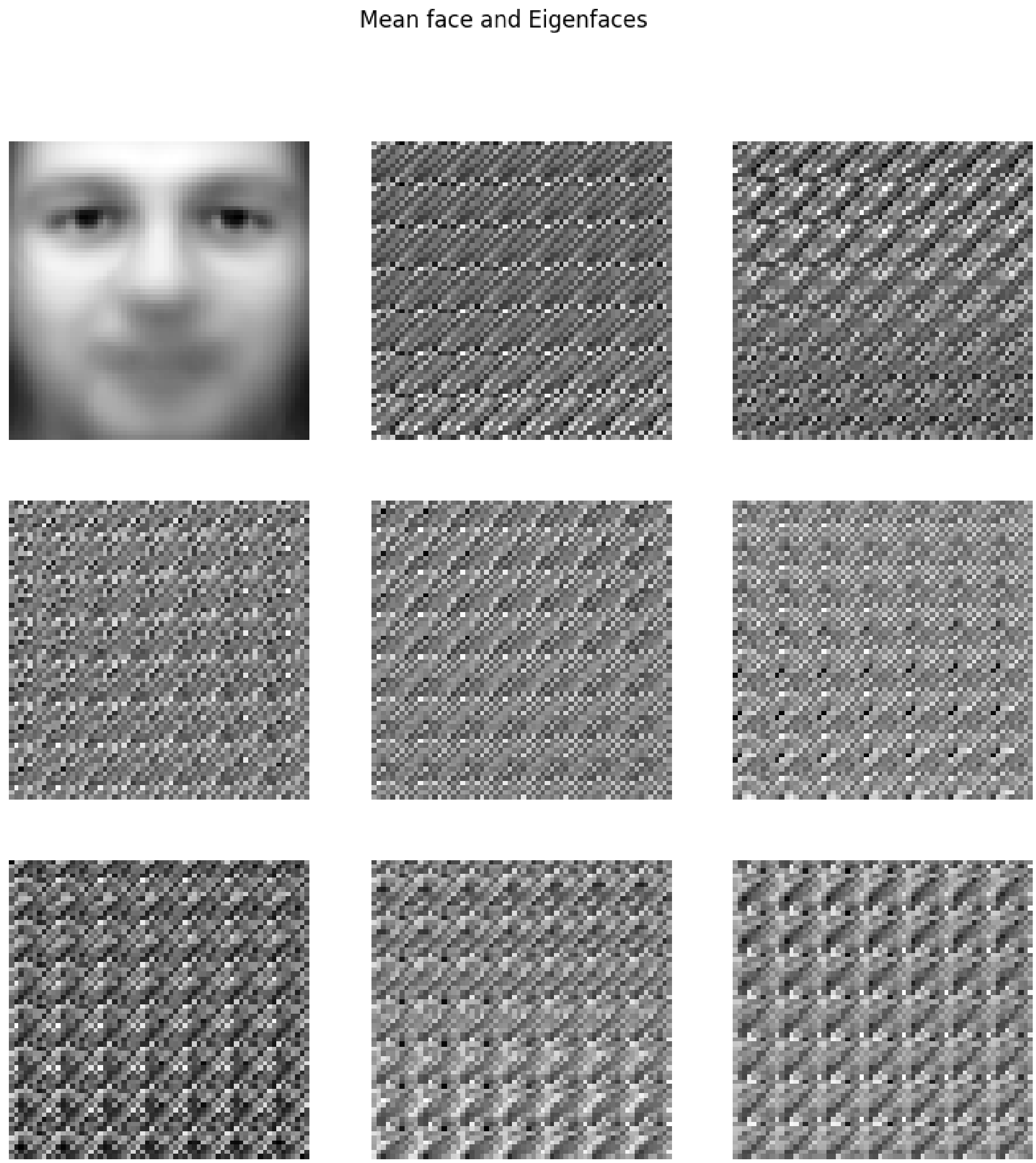
```
# Then use ax.scatter to plot the corresponding points from Z_faces_3d
for identity, color in zip(selected_identities, identity_colors):
    indices = np.where(y_faces == identity)[0]
    Z_identity = Z_faces_3d[indices]
    ax.scatter(Z_identity[:, 0], Z_identity[:, 1], Z_identity[:, 2], c=color,␣
 ↪label=f'Identity {identity}', alpha=0.2)

# DONE: Add legend, labels for the axes (PC1, PC2, PC3)
ax.legend(loc='best')
ax.set_xlabel('PC1')
ax.set_ylabel('PC2')
ax.set_zlabel('PC3')
```

[ ]: Text(0.5, 0, 'PC3')



Visualizing Eigenfaces

```
[ ]: # DONE: Fit PCA to face data with 9 components
pca_eigenfaces = PrincipalComponentAnalysis(9)
pca_eigenfaces.fit(X_faces_vec)

# DONE: Get the eigenfaces by reshaping the components to (n_components,␣
↪face_height, face_width)
# Hint: Also get the mean face by reshaping the mean
mean_face = pca_eigenfaces.get_mean().reshape(face_height, face_width)
eigenfaces = pca_eigenfaces.get_weights().reshape(-1, face_height, face_width)

# DONE?: Plot the mean face and the first 8 eigenfaces in a 3 x 3 grid
# First subplot should be the mean face, remaining 8 should be the eigenfaces
# Hint: Use plt.subplots(3, 3) to create the grid
faces_to_plot = np.concatenate((mean_face[np.newaxis, :, :], eigenfaces[:8]),␣
↪axis=0)
plot_images(faces_to_plot, 3, 3, 'Mean face and Eigenfaces')
```



Face Reconstruction with Different Numbers of Components

[ ]:
```python
# DONE: Create a function to visualize original and reconstructed faces
def plot_face_reconstruction(X_original, X_reconstructed, n_components,␣
↪n_faces=5):
    '''
    Plot original and reconstructed faces

    Args:
```

```
        X_original: Original face images (n_samples, height, width)
        X_reconstructed: Reconstructed face images (n_samples, height, width)
        n_components: Number of principal components used for reconstruction
        n_faces: Number of faces to display
    '''

    # DONE: Implement the function
    X_combined = np.concatenate((X_original, X_reconstructed), axis=0)
    plot_images(X_combined, 2, n_faces, f'Original and Reconstructed Faces␣
↪(d={n_components})')

# DONE: Generate reconstructions with different numbers of components (e.g., 5,␣
↪15, 30, 50, 100)
n_faces_to_show = 5
components_to_try = [5, 15, 30, 50, 100]

# DONE: Visualize the original and reconstructed faces side by side
for n_components in components_to_try:
    pca_faces = PrincipalComponentAnalysis(n_components)
    pca_faces.fit(X_faces_vec)

    Z_faces = pca_faces.project_to_subspace(X_faces_vec)
    X_faces_hat = pca_faces.reconstruct_from_subspace(Z_faces)

    # Select a subset of faces to visualize
    X_original_subset = X_faces[:n_faces_to_show]
    X_reconstructed_subset = X_faces_hat[:n_faces_to_show].
↪reshape(n_faces_to_show, face_height, face_width)

    plot_face_reconstruction(X_original_subset, X_reconstructed_subset,␣
↪n_components, n_faces=n_faces_to_show)
```

Original and Reconstructed Faces (d=5)


Original and Reconstructed Faces (d=15)

Original and Reconstructed Faces (d=30)

Original and Reconstructed Faces (d=50)

Original and Reconstructed Faces (d=100)

Face Generation for a Single Identity

```
[ ]: identity_idx = 30  # Choose identity

     # DONE: Select all faces from a single identity
     X_single_identity = X_faces[y_faces == identity_idx]

     # Show the original faces for this identity
     X_single_identity_images = X_faces[y_faces == identity_idx] if X_faces is not␣
      ↪None else None
     if X_single_identity_images is not None:
         plot_images(X_single_identity_images, 2, 5, 'Original faces of person {}'.
      ↪format(identity_idx))
```

```
# DONE: Compute PCA with 5 dimensions on this subset
pca_identity = PrincipalComponentAnalysis(5)
pca_identity.fit(X_single_identity.reshape(-1, face_height * face_width))

# DONE: Generate 25 novel face examples for this identity
X_generated_faces = pca_identity.generate_new_samples(25)

# DONE: Plot 5 x 5 panel of generated faces and name it 'Synthesized faces␣
 ↪dataset'
# Hint: Don't forget to reshape the generated faces back to 2D images
X_generated_faces_reshaped = X_generated_faces.reshape(-1, face_height,␣
 ↪face_width)
plot_images(X_generated_faces_reshaped, 5, 5, 'Synthesized faces dataset')

# Show plots
plt.show()
```

Original faces of person 30

Synthesized faces dataset

```
[ ]:
```