CS224 - Fall 2024

PROGRAMMING ASSIGNMENT 1 - Principal Component Analysis (PCA) & K-means Clustering

Due: November 5, 2024 @ 11:59pm PDT

Submission Method: Submit both the .ipynb and the PDF file on **Gradescope**. (For more details, see the Assignment Guidelines.)

Maximum points: 15

Overview

In this assignment, We will implement PCA, apply it to the **MNIST** dataset, and observe how the reconstruction changes as we change the number of principal components used.

For this assignment we will use the functionality of Numpy, and Matplotlib.

- Before you start, make sure you have installed all those packages in your local Jupyter instance.
- If you are asked to implement a particular functionality, you should **not** use an existing implementation from the libraries above (or some other library that you may find). When in doubt, **please just ASK**.
- It's okay to use functions in `numpy.linalg` to calculate matrix decomposition (e.g., `la.eig()`, `la.svd()`), but using built-in functions like `sklearn.decomposition.PCA()` will **not** get you any points.

Please read **all** cells carefully and answer **all** parts (both text and missing code). You will need to complete all the code marked `YOUR CODE HERE` and answer descriptive/derivation questions.

```
!pip install numpy
!pip install matplotlib
!pip install scikit-learn
```

```
Requirement already satisfied: numpy in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (2.1.3)
Requirement already satisfied: matplotlib in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (3.9.2)
Requirement already satisfied: contourpy>=1.0.1 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from matplotlib) (1.3.0)
Requirement already satisfied: cycler>=0.10 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
```

```
site-packages (from matplotlib) (0.12.1)
Requirement already satisfied: fonttools>=4.22.0 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from matplotlib) (4.54.1)
Requirement already satisfied: kiwisolver>=1.3.1 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from matplotlib) (1.4.7)
Requirement already satisfied: numpy>=1.23 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from matplotlib) (2.1.3)
Requirement already satisfied: packaging>=20.0 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from matplotlib) (24.1)
Requirement already satisfied: pillow>=8 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from matplotlib) (11.0.0)
Requirement already satisfied: pyparsing>=2.3.1 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from matplotlib) (3.2.0)
Requirement already satisfied: python-dateutil>=2.7 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from matplotlib) (2.9.0.post0)
Requirement already satisfied: six>=1.5 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from python-dateutil>=2.7->matplotlib) (1.16.0)
Requirement already satisfied: scikit-learn in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (1.5.2)
Requirement already satisfied: numpy>=1.19.5 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from scikit-learn) (2.1.3)
Requirement already satisfied: scipy>=1.6.0 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from scikit-learn) (1.14.1)
Requirement already satisfied: joblib>=1.2.0 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from scikit-learn) (1.4.2)
Requirement already satisfied: threadpoolctl>=3.1.0 in
/Users/berserker/.pyenv/versions/3.11.6/envs/ml_course/lib/python3.11/
site-packages (from scikit-learn) (3.5.0)
```

```python
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
from sklearn.datasets import load_digits

np.random.seed(42)
# DO NOT REMOVE THE CODE ABOVE
```

Question 1 [8 points]

Preliminaries

The **MNIST** database (Modified National Institute of Standards and Technology database) is a large database of handwritten digits that is commonly used for training various image processing systems.

First, Let's import the images and vectorize each image in the dataset.

```
# Data Preparation
mnist = load_digits()
data = mnist.data
# Display the shape of the data
print("Data shape:", data.shape)
```

```
Data shape: (1797, 64)
```

```
data[0]
```

```
array([ 0.,  0.,  5., 13.,  9.,  1.,  0.,  0.,  0.,  0., 13., 15.,
10.,
       15.,  5.,  0.,  0.,  3., 15.,  2.,  0., 11.,  8.,  0.,  0.,
4.,
       12.,  0.,  0.,  8.,  8.,  0.,  0.,  5.,  8.,  0.,  0.,  9.,
8.,
        0.,  0.,  4., 11.,  0.,  1., 12.,  7.,  0.,  0.,  2., 14.,
5.,
       10., 12.,  0.,  0.,  0.,  0.,  6., 13., 10.,  0.,  0.,  0.])
```

(a) [1 point] Compute the mean and variance of the images and standardize the dataset.

```
# Step 1: Standardize the Data
def standardize(data):
    """
    Standardize the dataset.

    Parameters:
    data (numpy array): Original data array.

    Returns:
    standardized_data (numpy array): Data after standardization.
    """
    # TODO: Compute the mean and standard deviation of the data.
    mean = np.mean(data, axis=0)# YOUR CODE HERE
    std = np.std(data, axis=0) + 1e-10 # 1e-10 added to avoid division
by zero error

    # TODO: Return the standardized data.
    standardized_data = (data - mean)/std# YOUR CODE HERE
```

```
    # print(mean, mean.shape)
    # print(std, std.shape)
    return standardized_data, mean, std

# Standardize the data and print the first 2 rows
data_standardized, mean, std = standardize(data)
print("Shape of data_standardized: ", data_standardized.shape)
print("Shape of mean vector: ", mean.shape)
# print(np.mean(data_standardized, axis=0))

Shape of data_standardized:  (1797, 64)
Shape of mean vector:  (64,)
```

(b) [1 point] Calculate the covariance matrix for the standardized dataset and calculate the eigenvalues and eigenvectors.

```
# Step 2: Calculate the covariance matrix for the features in the
dataset.
def compute_covariance_matrix(data):
    """
    Compute the covariance matrix of the standardized data.

    Parameters:
    data (numpy array): Standardized data array.

    Returns:
    covariance_matrix (numpy array): Covariance matrix of the data.
    """
    covariance_matrix = np.cov(data, rowvar=False)# YOUR CODE HERE;
    covariance_matrix = data.T @ data / (data.shape[0]-1)# YOUR CODE
HERE;
    # You can use the numpy function for this; however, if you write
your own code to implement it and show that the result is similar to
what numpy provides, you can get 1 extra point credit.
    return covariance_matrix

# Compute the covariance matrix
covariance_matrix = compute_covariance_matrix(data_standardized)
print("Shape of Covariance Matrix", covariance_matrix.shape)

Shape of Covariance Matrix (64, 64)

def compute_eigen(covariance_matrix):
    """
    Compute the eigenvalues and eigenvectors of the covariance matrix.

    Parameters:
    covariance_matrix (numpy array): Covariance matrix of the data.

    Returns:
```

```
    eigenvalues (numpy array): Eigenvalues in descending order.
    eigenvectors (numpy array): Corresponding eigenvectors.
    """

    # Step 3: Calculate the eigenvalues and eigenvectors for the
covariance matrix.
    eigenvalues, eigenvectors = np.linalg.eig(covariance_matrix)# YOUR
CODE HERE
    # print(eigenvalues.shape, eigenvectors.shape)
    # print(eigenvalues)

    # Step 4: Sort eigenvalues and their corresponding eigenvectors
(in descending order.)
    sorted_indices = np.argsort(eigenvalues)[::-1]# YOUR CODE HERE
    print(sorted_indices)
    eigenvalues = np.array([eigenvalues[x] for x in sorted_indices]) #
YOUR CODE HERE
    eigenvectors = np.array([eigenvectors[x] for x in sorted_indices])
# YOUR CODE HERE

    return eigenvalues, eigenvectors

# Compute eigenvalues and eigenvectors
eigenvalues, eigenvectors = compute_eigen(covariance_matrix)
print(eigenvalues)
print("Shape of Eigenvalues: ", eigenvalues.shape)
print("Shape of Eigenvectors:", eigenvectors.shape)
```

```
[ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22
23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 41 42 43 54 57 59 60 58
56
 55 53 52 51 50 49 48 47 46 45 44 40 39 61 62 63]
[7.34477606 5.83549054 5.15396118 3.96623597 2.96634519 2.57204442
 2.40600941 2.06867355 1.82993314 1.78951739 1.69784615 1.57287888
 1.38870781 1.35933609 1.32152536 1.16829176 1.08368677 0.99977861
 0.97438293 0.90891242 0.82271926 0.77631014 0.71155675 0.64552365
 0.59527399 0.5765018  0.52673155 0.5106363  0.48686381 0.45560107
 0.44285155 0.42230086 0.3991063  0.39110111 0.36094517 0.34860306
 0.3195963  0.29406627 0.27692285 0.258273   0.24783029 0.2423566
 0.217582   0.20799593 0.2000909  0.18983516 0.17612894 0.16875236
 0.15818474 0.14311427 0.13321081 0.12426371 0.11932898 0.11188655
 0.10250434 0.09840876 0.09018543 0.08246812 0.07635394 0.06328961
 0.05037444 0.         0.         0.        ]
Shape of Eigenvalues:  (64,)
Shape of Eigenvectors: (64, 64)
```

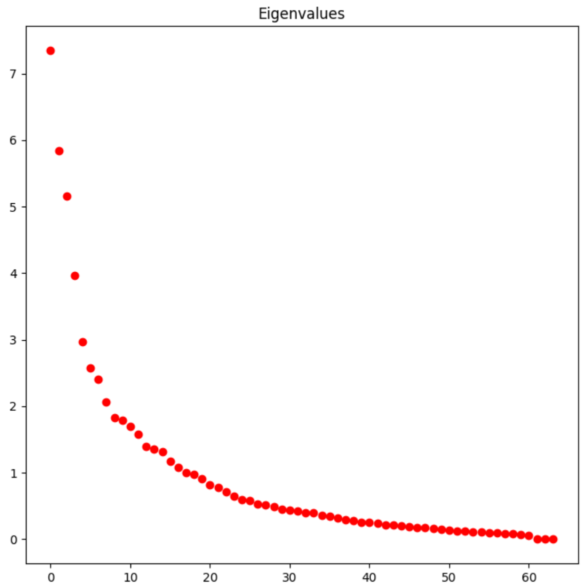
(c) [2 points] Analyze the eigenvalues in Λ and decide which eigenvalues to retain and which can be set to zero.

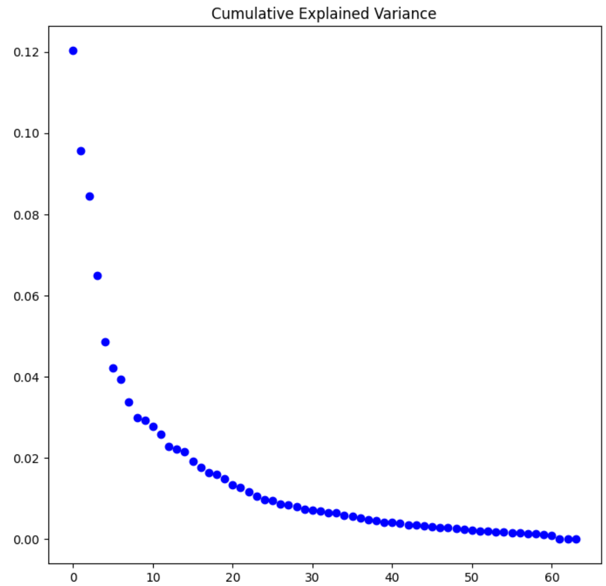
- You may want to plot the eigenvalues, the fraction of variance explained, AIC, or BIC to help decide on a threshold.
- Ensure your plots are clearly labeled with titles and axes labels, which is critical for understanding the visualized data.

```
def draw(eigenvalues, eigenvectors):
    # TODO: Add your plotting code here
    # Example plots you may consider include:
    # - Plotting the eigenvalues
    # - Plotting the cumulative explained variance
    cumulative_variance = [x/np.sum(eigenvalues) for x in eigenvalues]
    print(cumulative_variance)
    figure, axis = plt.subplots(1, 2, figsize=(18, 8))
    axis[0].plot(eigenvalues, 'ro')
    axis[0].set_title("Eigenvalues")
    axis[1].plot(cumulative_variance, 'bo')
    axis[1].set_title("Cumulative Explained Variance")
    plt.show()
    # - Any additional analysis (AIC, BIC, etc.)

    # YOUR CODE HERE
    pass

draw(eigenvalues, eigenvectors)
```

```
[np.float64(0.12033916102799788), np.float64(0.09561054407310768),
np.float64(0.08444414896481628), np.float64(0.06498407910328302),
np.float64(0.04860154877407397), np.float64(0.042141198681765 5),
np.float64(0.03942082804878714), np.float64(0.03389380925855059 5),
np.float64(0.02998221010554150 5), np.float64(0.02932002549105000 2),
np.float64(0.02781805461636938 8), np.float64(0.02577055090357863 2),
np.float64(0.02275303315257608), np.float64(0.02227179739008725),
np.float64(0.02165229430705492 2), np.float64(0.01914166605688979 3),
np.float64(0.01775547081927488 6), np.float64(0.01638069271122277 4),
np.float64(0.01596460166718235), np.float64(0.01489191186281565 1),
np.float64(0.01347969565951893 6), np.float64(0.01271931368951408 2),
np.float64(0.01165837350584530 1), np.float64(0.01057646598842375 3),
np.float64(0.00975315947304111 8), np.float64(0.00944558990058499 4),
np.float64(0.00863013827109151 3), np.float64(0.00836642853646099 6),
np.float64(0.00797693248697255 7), np.float64(0.00746471371173467 7),
np.float64(0.00725582151528697 9), np.float64(0.00691911244921238),
np.float64(0.00653908535722340 7), np.float64(0.00640792572898046 3),
np.float64(0.00591384111895530 8), np.float64(0.00571162405026001 1),
np.float64(0.00523636802894210 8), np.float64(0.00481807586469533 6),
np.float64(0.00453719259989183 7), np.float64(0.00423162753384676 6),
np.float64(0.00406053070134172 3), np.float64(0.00397084808417377 2),
np.float64(0.0035649330329631432), np.float64(0.0034078718162224306),
np.float64(0.0032783533541580387), np.float64(0.0031103200748033993),
np.float64(0.0028857529423145425), np.float64(0.0027648926362603154),
np.float64(0.00259174940991830 6), np.float64(0.00234483005626975 8),
```

```
np.float64(0.0021825685780481646), np.float64(0.0020359763460414022),
np.float64(0.001955124261040471), np.float64(0.00183318499277946),
np.float64(0.0016794638755460072), np.float64(0.0016123606230980057),
np.float64(0.0014776269417368544), np.float64(0.0013511841139844417),
np.float64(0.0012510074255517234), np.float64(0.0010369573020414834),
np.float64(0.0008253509451987544), np.float64(0.0), np.float64(0.0),
np.float64(0.0)]
```





(d) [1 point] Reconstruct an approximation of each X after removing some of the small eigenvalues. (Display only a couple of the reconstructed **images**, and you will need to restore the reconstructed data to its original scale using the mean and standard deviation.)

```
# Step 5: Pick k eigenvalues and form a matrix of eigenvectors.
def find_optimal_k(eigenvalues, eigenvectors):
    """
    Analyze eigenvalues and decide which to retain.

    Parameters:
    eigenvalues (numpy array): Eigenvalues in descending order.
    eigenvectors (numpy array): Corresponding eigenvectors.

    Returns:
    n_components (int): Number of principal components to retain.
    """

    # TODO: Determine the number of components needed to reach the
threshold.
    # YOUR CODE HERE
    # I will not use the last 3 eigen vectors who have cumulative
eigen value equals 0
    n_components = 61 # YOUR CODE HERE
```

```
    return n_components

def choose_principal_components(n_components, eigenvectors):
    """
    Choose the principal components based on the number selected.

    Parameters:
    n_components (int): Number of components to retain.
    eigenvectors (numpy array): The original eigenvectors.

    Returns:
    selected_eigenvectors (numpy array): Eigenvectors corresponding to
the top k components.
    """
    selected_eigenvectors = eigenvectors[:, :n_components]# YOUR CODE
HERE
    return selected_eigenvectors

n_components = find_optimal_k(eigenvalues, eigenvectors)
selected_eigenvectors = choose_principal_components(n_components,
eigenvectors)
print(f"Selected {n_components} eigenvectors.")
print(f"Shape of selected eigenvectors:
{selected_eigenvectors.shape}")
```

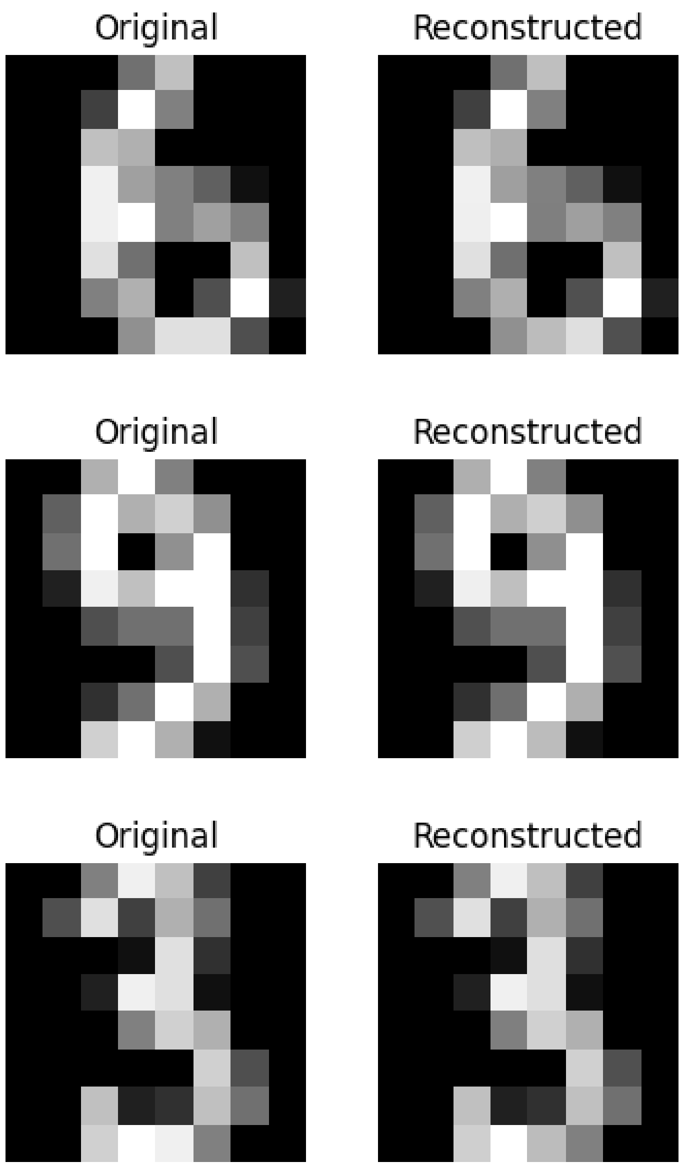
```
Selected 61 eigenvectors.
Shape of selected eigenvectors: (64, 61)
```

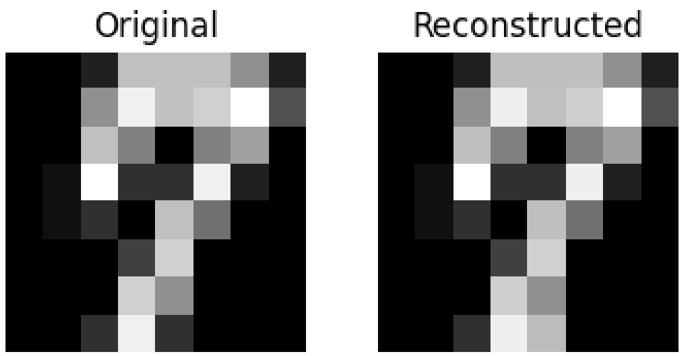
```
# Step 6: Reconstruct Data from Principal Components
def reconstruct_data(data_standardized, selected_eigenvectors):
    """
    Reconstruct the original data using selected eigenvectors.

    Parameters:
    data_standardized (numpy array): The standardized data matrix.
    selected_eigenvectors (numpy array): Eigenvectors corresponding to
the top k components.

    Returns:
    data_reconstructed (numpy array): Reconstructed approximation of
the original data.
    """
    # Project the original data onto the selected principal components
    data_projected = data_standardized @ selected_eigenvectors# YOUR
CODE HERE

    # Reconstruct the data by projecting back into the original space
    data_reconstructed = data_projected @ selected_eigenvectors.T#
YOUR CODE HERE
```

```
    return data_reconstructed

def restore_original_scale(X_reconstructed, mean_vector, std_vector):
    """
    Restore the reconstructed data to its original scale using the
mean and standard deviation.

    Parameters:
    X_reconstructed (numpy array): Reconstructed data (standardized
scale).
    mean_vector (numpy array): Mean vector used during
standardization.
    std_vector (numpy array): Standard deviation vector used during
standardization.

    Returns:
    X_restored (numpy array): Reconstructed data in its original
scale.
    """
    X_restored = X_reconstructed * std + mean# YOUR CODE HERE

    return X_restored

def display_reconstruct_data(data_standardized, data_reconstructed,
num_examples=4):
    image_shape = (8, 8)
    random_indices = np.random.choice(data_standardized.shape[0],
size=num_examples, replace=False)

    for idx in random_indices:
        plt.figure(figsize=(4, 2))

        # Original image
        plt.subplot(1, 2, 1)
        plt.imshow(data_standardized[idx].reshape(image_shape),
cmap='gray')
        plt.title("Original")
        plt.axis('off')

        # Reconstructed image
        plt.subplot(1, 2, 2)
        plt.imshow(data_reconstructed[idx].reshape(image_shape),
cmap='gray')
        plt.title("Reconstructed")
        plt.axis('off')

        plt.tight_layout()
        plt.show()
```

```python
# Transform the data using the selected components
data_reconstructed = reconstruct_data(data_standardized,
selected_eigenvectors)
print("Shape of reconstructed data:", data_reconstructed.shape)

display_reconstruct_data(restore_original_scale(data_standardized,
mean, std),
                         restore_original_scale(data_reconstructed,
mean, std))
```

```
Shape of reconstructed data: (1797, 64)
```





(e) [2 points] Compute the error between the reconstructed X and original image. (The mean of the original data should **not** be included in the error.)

```
def compute_reconstruction_error(data_standardized,
data_reconstructed):
    """
    Compute the mean squared error (MSE) between the standardized
original data
    and the reconstructed data.

    Parameters:
    data_standardized (numpy array): The standardized original data
matrix.
    data_reconstructed (numpy array): Reconstructed approximation of
the standardized data.

    Returns:
    error (float): Mean squared error between original and
reconstructed data.
    """
    # TODO: Calculate the MSE between the standardized original data
and reconstructed data
    error = (np.square(data_reconstructed -
data_standardized)).mean(axis=0)# YOUR CODE HERE
    error = np.linalg.norm(error)/error.shape[0]

    return error

reconstruction_error = compute_reconstruction_error(data_standardized,
data_reconstructed)
with np.printoptions(precision=3):
    print(f"Reconstruction error (MSE): {reconstruction_error}")

Reconstruction error (MSE): 0.015624999999936636
```

(f) [1 points] Analyze by choosing different numbers of eigenvalues to be zeroed out. Provide a short summary of your conclusions based on this analysis.

```python
# TODO: YOUR CODE HERE
for i in range(data.shape[1]+1):
    trial_selected_eigenvectors = choose_principal_components(i,
eigenvectors)
    print(f"Selected {i} eigenvectors.")
    print(f"Shape of selected eigenvectors:
{trial_selected_eigenvectors.shape}")
    trial_data_reconstructed = reconstruct_data(data_standardized,
trial_selected_eigenvectors)
    trial_reconstruction_error =
compute_reconstruction_error(data_standardized,
trial_data_reconstructed)
    with np.printoptions(precision=3):
        print(f"Reconstruction error (MSE) for number of components
{i}: {trial_reconstruction_error}")
```

```
Selected 0 eigenvectors.
Shape of selected eigenvectors: (64, 0)
Reconstruction error (MSE) for number of components 0:
0.12203515112460833
Selected 1 eigenvectors.
Shape of selected eigenvectors: (64, 1)
Reconstruction error (MSE) for number of components 1:
0.1165027033862443
Selected 2 eigenvectors.
Shape of selected eigenvectors: (64, 2)
Reconstruction error (MSE) for number of components 2:
0.11027365413459407
Selected 3 eigenvectors.
Shape of selected eigenvectors: (64, 3)
Reconstruction error (MSE) for number of components 3:
0.10569112328755628
Selected 4 eigenvectors.
Shape of selected eigenvectors: (64, 4)
Reconstruction error (MSE) for number of components 4:
0.10186565146095734
Selected 5 eigenvectors.
Shape of selected eigenvectors: (64, 5)
Reconstruction error (MSE) for number of components 5:
0.09812172169831605
Selected 6 eigenvectors.
Shape of selected eigenvectors: (64, 6)
Reconstruction error (MSE) for number of components 6:
0.09496933177724225
Selected 7 eigenvectors.
Shape of selected eigenvectors: (64, 7)
Reconstruction error (MSE) for number of components 7:
0.09140924489037566
Selected 8 eigenvectors.
Shape of selected eigenvectors: (64, 8)
```

```
Reconstruction error (MSE) for number of components 8:
0.08828301401659545
Selected 9 eigenvectors.
Shape of selected eigenvectors: (64, 9)
Reconstruction error (MSE) for number of components 9:
0.0855539328748038
Selected 10 eigenvectors.
Shape of selected eigenvectors: (64, 10)
Reconstruction error (MSE) for number of components 10:
0.08240087164883658
Selected 11 eigenvectors.
Shape of selected eigenvectors: (64, 11)
Reconstruction error (MSE) for number of components 11:
0.08016103435707536
Selected 12 eigenvectors.
Shape of selected eigenvectors: (64, 12)
Reconstruction error (MSE) for number of components 12:
0.0777719346271376
Selected 13 eigenvectors.
Shape of selected eigenvectors: (64, 13)
Reconstruction error (MSE) for number of components 13:
0.07552587966358028
Selected 14 eigenvectors.
Shape of selected eigenvectors: (64, 14)
Reconstruction error (MSE) for number of components 14:
0.07296796022363092
Selected 15 eigenvectors.
Shape of selected eigenvectors: (64, 15)
Reconstruction error (MSE) for number of components 15:
0.07078157249764067
Selected 16 eigenvectors.
Shape of selected eigenvectors: (64, 16)
Reconstruction error (MSE) for number of components 16:
0.06863502554266183
Selected 17 eigenvectors.
Shape of selected eigenvectors: (64, 17)
Reconstruction error (MSE) for number of components 17:
0.06636092673381318
Selected 18 eigenvectors.
Shape of selected eigenvectors: (64, 18)
Reconstruction error (MSE) for number of components 18:
0.06485416091413085
Selected 19 eigenvectors.
Shape of selected eigenvectors: (64, 19)
Reconstruction error (MSE) for number of components 19:
0.06342432665030132
Selected 20 eigenvectors.
Shape of selected eigenvectors: (64, 20)
Reconstruction error (MSE) for number of components 20:
```

```
0.06199854946911831
Selected 21 eigenvectors.
Shape of selected eigenvectors: (64, 21)
Reconstruction error (MSE) for number of components 21:
0.060819475137742184
Selected 22 eigenvectors.
Shape of selected eigenvectors: (64, 22)
Reconstruction error (MSE) for number of components 22:
0.05957115088621587
Selected 23 eigenvectors.
Shape of selected eigenvectors: (64, 23)
Reconstruction error (MSE) for number of components 23:
0.058067509879198446
Selected 24 eigenvectors.
Shape of selected eigenvectors: (64, 24)
Reconstruction error (MSE) for number of components 24:
0.05731598043268359
Selected 25 eigenvectors.
Shape of selected eigenvectors: (64, 25)
Reconstruction error (MSE) for number of components 25:
0.0560949744839143
Selected 26 eigenvectors.
Shape of selected eigenvectors: (64, 26)
Reconstruction error (MSE) for number of components 26:
0.05388183309792983
Selected 27 eigenvectors.
Shape of selected eigenvectors: (64, 27)
Reconstruction error (MSE) for number of components 27:
0.05270945950055712
Selected 28 eigenvectors.
Shape of selected eigenvectors: (64, 28)
Reconstruction error (MSE) for number of components 28:
0.05076765499225945
Selected 29 eigenvectors.
Shape of selected eigenvectors: (64, 29)
Reconstruction error (MSE) for number of components 29:
0.04821402822558926
Selected 30 eigenvectors.
Shape of selected eigenvectors: (64, 30)
Reconstruction error (MSE) for number of components 30:
0.047520327206708665
Selected 31 eigenvectors.
Shape of selected eigenvectors: (64, 31)
Reconstruction error (MSE) for number of components 31:
0.04554503419693811
Selected 32 eigenvectors.
Shape of selected eigenvectors: (64, 32)
Reconstruction error (MSE) for number of components 32:
0.04464309507103537
```

```
Selected 33 eigenvectors.
Shape of selected eigenvectors: (64, 33)
Reconstruction error (MSE) for number of components 33:
0.043853297626950914
Selected 34 eigenvectors.
Shape of selected eigenvectors: (64, 34)
Reconstruction error (MSE) for number of components 34:
0.042833555395672976
Selected 35 eigenvectors.
Shape of selected eigenvectors: (64, 35)
Reconstruction error (MSE) for number of components 35:
0.04184964743198816
Selected 36 eigenvectors.
Shape of selected eigenvectors: (64, 36)
Reconstruction error (MSE) for number of components 36:
0.039964326202471034
Selected 37 eigenvectors.
Shape of selected eigenvectors: (64, 37)
Reconstruction error (MSE) for number of components 37:
0.03948876014940888
Selected 38 eigenvectors.
Shape of selected eigenvectors: (64, 38)
Reconstruction error (MSE) for number of components 38:
0.0381830683545873
Selected 39 eigenvectors.
Shape of selected eigenvectors: (64, 39)
Reconstruction error (MSE) for number of components 39:
0.03631360670855527
Selected 40 eigenvectors.
Shape of selected eigenvectors: (64, 40)
Reconstruction error (MSE) for number of components 40:
0.03379590578669933
Selected 41 eigenvectors.
Shape of selected eigenvectors: (64, 41)
Reconstruction error (MSE) for number of components 41:
0.03207710888454537
Selected 42 eigenvectors.
Shape of selected eigenvectors: (64, 42)
Reconstruction error (MSE) for number of components 42:
0.030250464863641642
Selected 43 eigenvectors.
Shape of selected eigenvectors: (64, 43)
Reconstruction error (MSE) for number of components 43:
0.02951597343629718
Selected 44 eigenvectors.
Shape of selected eigenvectors: (64, 44)
Reconstruction error (MSE) for number of components 44:
0.02865260947239254
Selected 45 eigenvectors.
```

```
Shape of selected eigenvectors: (64, 45)
Reconstruction error (MSE) for number of components 45:
0.027948628349657875
Selected 46 eigenvectors.
Shape of selected eigenvectors: (64, 46)
Reconstruction error (MSE) for number of components 46:
0.02717917182777194
Selected 47 eigenvectors.
Shape of selected eigenvectors: (64, 47)
Reconstruction error (MSE) for number of components 47:
0.025885498972274157
Selected 48 eigenvectors.
Shape of selected eigenvectors: (64, 48)
Reconstruction error (MSE) for number of components 48:
0.02380022665150514
Selected 49 eigenvectors.
Shape of selected eigenvectors: (64, 49)
Reconstruction error (MSE) for number of components 49:
0.02329023295247534
Selected 50 eigenvectors.
Shape of selected eigenvectors: (64, 50)
Reconstruction error (MSE) for number of components 50:
0.02278566726805045
Selected 51 eigenvectors.
Shape of selected eigenvectors: (64, 51)
Reconstruction error (MSE) for number of components 51:
0.02194995743678517
Selected 52 eigenvectors.
Shape of selected eigenvectors: (64, 52)
Reconstruction error (MSE) for number of components 52:
0.021347524576309562
Selected 53 eigenvectors.
Shape of selected eigenvectors: (64, 53)
Reconstruction error (MSE) for number of components 53:
0.01959407288802084
Selected 54 eigenvectors.
Shape of selected eigenvectors: (64, 54)
Reconstruction error (MSE) for number of components 54:
0.017853079659981227
Selected 55 eigenvectors.
Shape of selected eigenvectors: (64, 55)
Reconstruction error (MSE) for number of components 55:
0.01739260183547541
Selected 56 eigenvectors.
Shape of selected eigenvectors: (64, 56)
Reconstruction error (MSE) for number of components 56:
0.01710944597961311
Selected 57 eigenvectors.
Shape of selected eigenvectors: (64, 57)
```

```
Reconstruction error (MSE) for number of components 57:
0.016512098581989074
Selected 58 eigenvectors.
Shape of selected eigenvectors: (64, 58)
Reconstruction error (MSE) for number of components 58:
0.016243658316347463
Selected 59 eigenvectors.
Shape of selected eigenvectors: (64, 59)
Reconstruction error (MSE) for number of components 59:
0.015900289319927634
Selected 60 eigenvectors.
Shape of selected eigenvectors: (64, 60)
Reconstruction error (MSE) for number of components 60:
0.015726789321378727
Selected 61 eigenvectors.
Shape of selected eigenvectors: (64, 61)
Reconstruction error (MSE) for number of components 61:
0.01562499999936636
Selected 62 eigenvectors.
Shape of selected eigenvectors: (64, 62)
Reconstruction error (MSE) for number of components 62:
0.01562499999936636
Selected 63 eigenvectors.
Shape of selected eigenvectors: (64, 63)
Reconstruction error (MSE) for number of components 63:
0.01562499999936636
Selected 64 eigenvectors.
Shape of selected eigenvectors: (64, 64)
Reconstruction error (MSE) for number of components 64:
1.68101868015422e-29
```

After displaying the reconstructed error, it is clear that as we intake more n_components the reconstruction is more accurate to the original.

[TODO: YOUR SUMMARY HERE]

Question 2 [7 points]

After implementing PCA, use k-means clustering on the PCA-transformed data.

- To enable effective visualization in a 2D space, we choose the first 2 components of your PCA-transformed data for further (visual) analysis.

```
def transform_data_with_pca(data_standardized, eigenvectors,
n_components):
    X = data_standardized @ choose_principal_components(n_components,
eigenvectors)
    return X

X = transform_data_with_pca(data_standardized, eigenvectors,
```

```python
n_components=2)
print("Shape of X: ", X.shape)

true_labels = mnist.target
print("Shape of true_labels: ", true_labels.shape)
```

```
Shape of X:  (1797, 2)
Shape of true_labels:  (1797,)
```

(a)[3 points] Implement k-means from scratch. Please refrain from using libraries like `scikit-learn` for the k-means functionality.

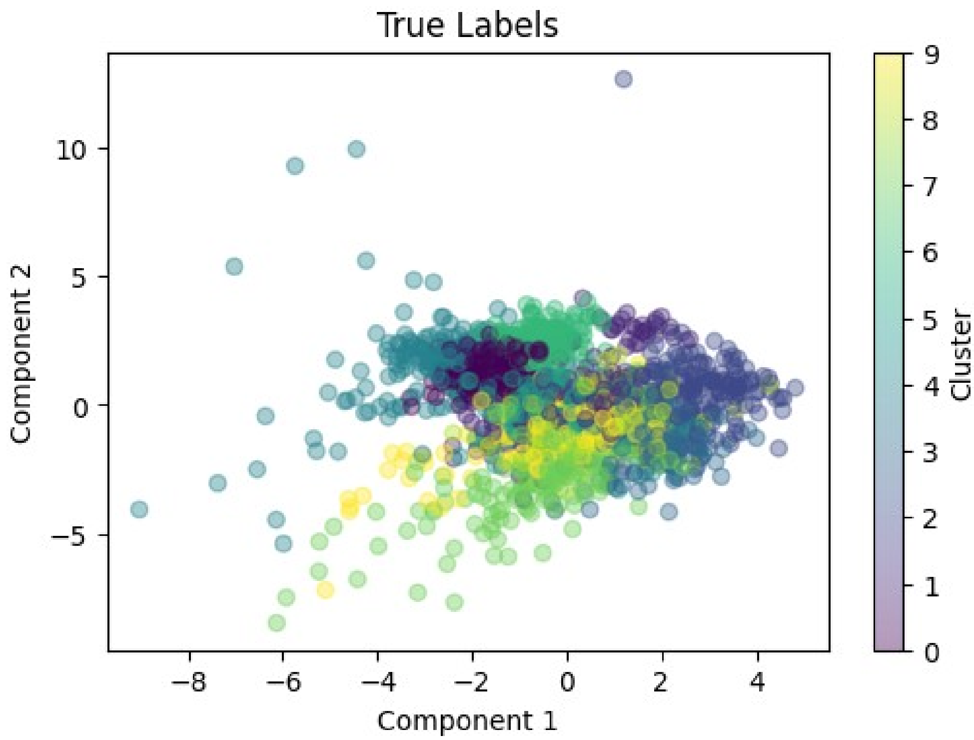
```python
# Apply K-means Clustering to PCA-transformed Data
def k_means(X, k, max_iter=300):
    """
    Implement K-means clustering from scratch.

    Parameters:
    X (numpy array): Data to be clustered (n_samples, n_features).
    k (int): Number of clusters.
    max_iter (int): Maximum number of iterations for convergence.

    Returns:
    cluster_labels (numpy array): Cluster labels for each data point.
    centroids (numpy array): Coordinates of the cluster centers.
    """
    np.random.seed(0)  # For reproducibility
    # Randomly initialize the centroids by selecting k random samples
from X
    centroids = X[np.random.choice(X.shape[0], size=k,
replace=False)]# YOUR CODE HERE
    # print('centroid shape', centroids.shape)

    for iteration in range(max_iter):
        # Assign each data point to the nearest centroid
        # YOUR CODE HERE
        labels = []# YOUR CODE HERE
        for vec in np.array(X):
            distances = []
            for i in range(k):
                distances.append(np.linalg.norm(vec - centroids[i]))
            labels.append(np.argmin(distances))
        # Calculate new centroids as the mean of assigned points
        # print(X.shape)
        labels = np.array(labels)
        # print('labels shape ', labels.shape)
        new_centroids = np.empty((k, X.shape[1]))# YOUR CODE HERE
        # print(new_centroids.shape)
        for i in range(k):
```

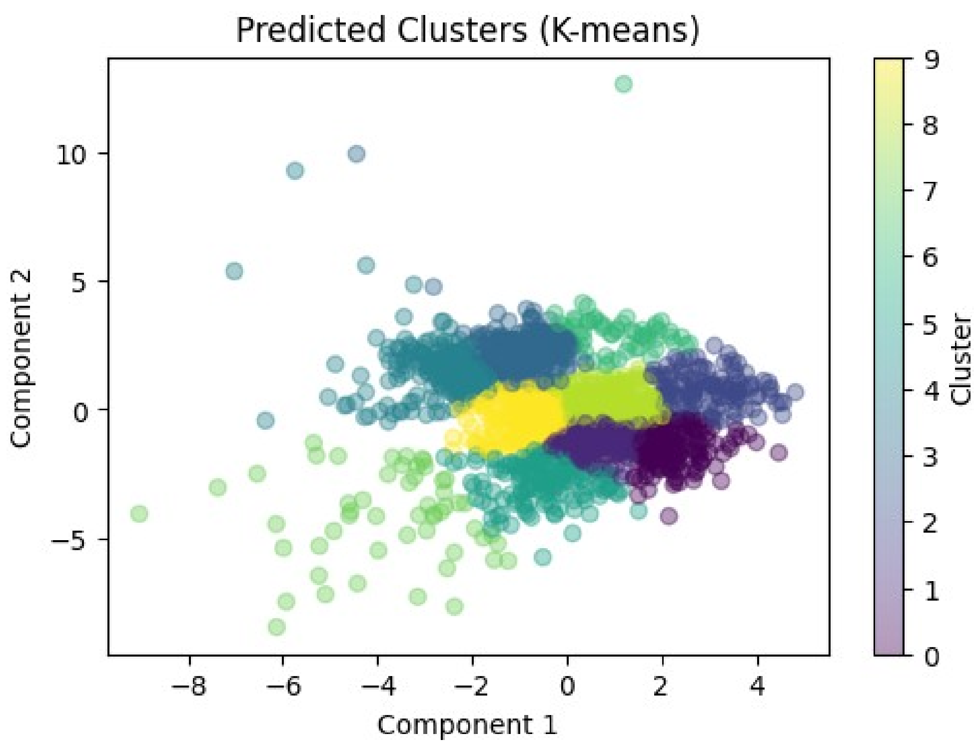
```
            points = X[labels == i]
            # print(points.shape)
            new_centroids[i] = np.mean(points, axis=0)

        # Check for convergence (if centroids don't change)
        if np.all(centroids == new_centroids):
            break

        centroids = new_centroids

    return labels, centroids


k = 10 # Number of clusters (digits 0-9)
cluster_labels, centroids = k_means(X, k)
print("Shape of centroids: ", centroids.shape)
```

```
Shape of centroids:  (10, 2)
```

Plot the clustering results on the PCA-reduced data using different colors for each cluster(digit).

```
# Visualize Clusters
def plot_clusters(data, labels, title):
    plt.figure(figsize=(6, 4))
    plt.scatter(data[:, 0], data[:, 1], c=labels, cmap='viridis',
alpha=0.4)
    plt.title(title)
    plt.xlabel('Component 1')
    plt.ylabel('Component 2')
    plt.colorbar(label='Cluster')
    plt.show()


# Plot the ground truth clusters
plot_clusters(X, true_labels, "True Labels")
# Plot the predicted clusters on PCA-transformed data
plot_clusters(X, cluster_labels, "Predicted Clusters (K-means)")
```





After applying k-means on the PCA-reduced data, let's evaluate how well the clustering algorithm performed by checking the accuracy for each digit.

(b)[3 points] Analyze the accuracy of clustering for each digit.

```python
from collections import Counter
def analyze_clustering_accuracy(true_labels, cluster_labels,
num_clusters):
    """
    Analyze the accuracy of clustering for each digit based on true
labels.

    Parameters:
    - true_labels: array-like, shape (n_samples,)
        The true labels of the samples (0-9 for digits).
    - cluster_labels: array-like, shape (n_samples,)
        The predicted cluster labels from k-means.
    - num_clusters: int
        The number of clusters (should match the number of unique
digits, usually 10).

    Returns:
    - accuracy_per_digit: dict
        A dictionary mapping each digit to its accuracy.
    - total_accuracy: float
        The overall accuracy of the clustering.
    - cluster_to_digit: dict
        A dictionary mapping each cluster to the assigned digit class.
    """

    # Initialize accuracy dictionary for digits 0-9
    accuracy_per_digit = {digit: 0.0 for digit in range(10)}

    # Initialize total correct predictions
    total_correct_predictions = 0
    total_samples = len(true_labels)

    # Create a mapping from cluster to digit
    cluster_to_digit = {}

    # Count correct predictions for each cluster
    for cluster in range(num_clusters):
        cluster_mask = (cluster_labels == cluster)  # Mask for the
current cluster
        if np.any(cluster_mask):  # Only proceed if the cluster has
members
            predicted_labels = true_labels[cluster_mask]  # True
labels for this cluster
            # TODO: Find the most common true label in this cluster
            # value, counts = np.unique(predicted_labels,
return_counts=True)
            most_common_label =
Counter(predicted_labels).most_common(1)[0][0]# YOUR CODE HERE
            cluster_to_digit[cluster] = most_common_label  # Map the
cluster to the most common label
```

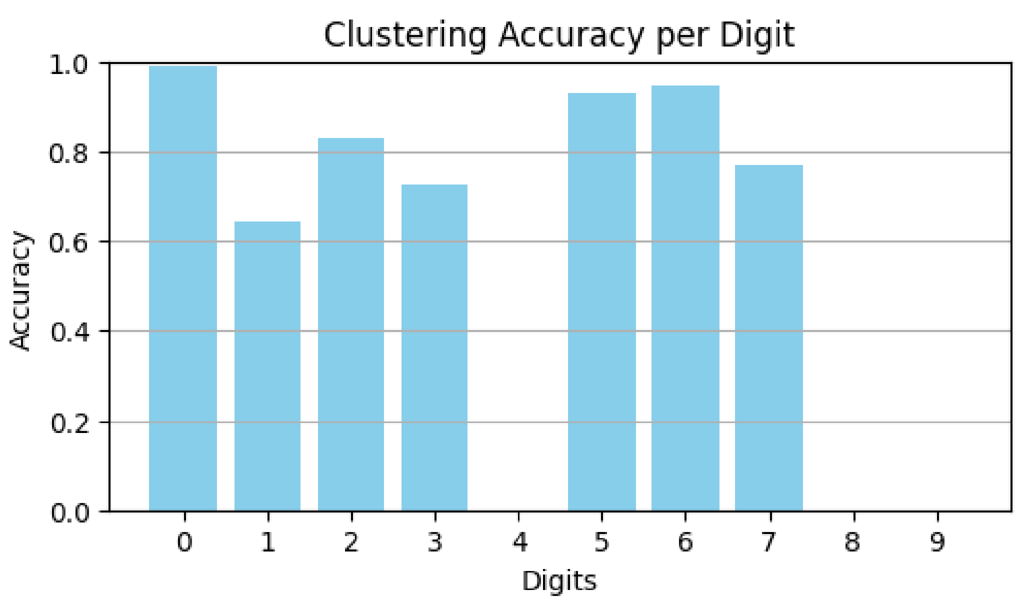
```
            # Update total correct predictions
            total_correct_predictions += np.sum(predicted_labels ==
most_common_label)  # Count correct predictions

            # Accumulate accuracy for the most common label
            accuracy_per_digit[most_common_label] +=
np.sum(predicted_labels == most_common_label)

    # Normalize the accuracy by the number of instances for each digit
    for digit in range(10):
        total_count = np.sum(true_labels == digit)
        if total_count > 0:
            accuracy_per_digit[digit] /= total_count

    # Calculate total accuracy
    total_accuracy = total_correct_predictions / total_samples if
total_samples > 0 else 0.0

    # Assign new predicted labels based on the cluster-to-digit
mapping
    final_predicted_labels = np.vectorize(cluster_to_digit.get)
(cluster_labels)

    return accuracy_per_digit, total_accuracy, cluster_to_digit,
final_predicted_labels

# TODO: Try changing this value to see how it affects the clustering
n_components = 12 # YOUR CODE HERE

X = transform_data_with_pca(data_standardized, eigenvectors,
n_components=n_components)

cluster_labels, centroids = k_means(X, k)
accuracy_per_digit, total_accuracy, cluster_to_digit,
final_predicted_labels = analyze_clustering_accuracy(true_labels,
cluster_labels, num_clusters=k)

print("n_components: ", n_components)
print("Shape of X: ", X.shape)
[print(f"Digit {digit}: {accuracy:.4f}") for digit, accuracy in
accuracy_per_digit.items()]
```

```
n_components:  12
Shape of X:  (1797, 12)
Digit 0: 0.9888
Digit 1: 0.6429
Digit 2: 0.8305
Digit 3: 0.7268
Digit 4: 0.0000
```

```
Digit 5: 0.9286
Digit 6: 0.9448
Digit 7: 0.7709
Digit 8: 0.0000
Digit 9: 0.0000
```

```
[None, None, None, None, None, None, None, None, None, None]
```

```
def plot_accuracy_per_digit(accuracy_per_digit):
    """
    Plot a bar chart for the accuracy of each digit.

    Parameters:
    - accuracy_per_digit: dict
        A dictionary mapping each digit to its accuracy.
    """
    digits = list(accuracy_per_digit.keys())
    accuracies = list(accuracy_per_digit.values())

    plt.figure(figsize=(6, 3))
    plt.bar(digits, accuracies, color='skyblue')
    plt.xlabel('Digits')
    plt.ylabel('Accuracy')
    plt.title('Clustering Accuracy per Digit')
    plt.xticks(digits)  # Ensure each digit is shown on the x-axis
    plt.ylim(0, 1)  # Set y-axis limits to [0, 1]
    plt.grid(axis='y')  # Add grid lines for better readability
    plt.show()

plot_accuracy_per_digit(accuracy_per_digit)
```



(c)[1 point] Provide a short summary of your observations based on this analysis.

- Better to use some standard library for AIC or BIC instead of implementing manually.
- For matrix multiplication its good to use numpy operations and numpy data formats to store matrices as they are both space and efficiency optimized.
- The larger size of MNIST dataset (60,000 images) can get a better dimensionality reduction of PCA.
- Identifying image 0 was the most easiest for a large variation of the principal components used.
- Instead of K means we can also use another clustering algorithm to evaluate PCA.
- PCA visualization can get a little messy especially when we have used a large value of n_components but we are only using the top 2 for visualizing.
- More images for specific digits such as 4 can improve the PCA dimensionality reduction as well as accuracy in K-means