Rules:

- Unless otherwise stated, all answers must be mathematically justified.
- Partial answers will be graded.
- Your submission has to be uploaded to Gradescope. In Gradescope, indicate the page on which each problem is written.
- You can work in groups but each student must write his/her/their own solution based on his/her/their own understanding of the problem. Please list on your submission the students you work with for the homework (this will not affect your grade).
- Problems with a ($\star$) are extra credit, they will not (directly) contribute to your score of this homework. However, for every 4 extra credit questions successfully answered your lowest homework score get replaced by a perfect score.
- If you have any questions, feel free to ask them on Ed Discussion (so that everyone can benefit from the answer) or stop at the office hours.

Problem 7.1 (3 points)**.** *We say that a symmetric matrix $M \in \mathbb{R}^{n\times n}$ is positive semi-definite if for all $x \in \mathbb{R}^n$, $x^\intercal Mx \geq 0$.*

(a) *Let $D \in \mathbb{R}^{n\times n}$ be a diagonal matrix. When is D positive semi-definite?*

We first give the claim: When all the diagonal entries are bigger than or equal to zero, D is PSD.

Proof. *$\forall \vec{x} \in \mathbb{R}^n$, we have $\vec{x}^\top D\vec{x} = \sum_{i=1}^n D_{i,i}x_i^2 \geq 0$, which implies that D is PSD.* □

(b) *Let $M \in \mathbb{R}^{n\times n}$ be a symmetric matrix. Show that M is positive semi-definite* ***if and only if*** *its eigenvalues are all non-negative.*

Proof.

(a) ($\implies$): Since M is symmetric, we know from the spectrum theorem that $M = PDP^\top$ for some orthogonal matrix P and diagonal matrix D. Then we have that $\vec{x}^\top PDP^\top\vec{x} = \vec{y}^\top D\vec{y}$ where $\vec{y} = P^\top\vec{x}$. Since $\vec{y}^\top D\vec{y} = \sum_{i=1}^n D_{i,i}y_i^2 = \sum_{i=1}^n \lambda_i y_i^2 \geq 0$ by definition of PSD. Since the above inequality holds for all $\vec{y} \in \mathbb{R}^n$, we have that $\lambda_i \geq 0$.

(b) ($\impliedby$): If all eigenvalues of M are non-negative, we have $\lambda_i \geq 0, \forall i = 1, 2, \cdots, n$(Note that there could be some i, j such that $\lambda_i = \lambda_j$).We have that $\forall \vec{x} \in \mathbb{R}^n$, $\vec{x}^\top M\vec{x} = \vec{y}^\top D\vec{y} = \sum_{i=1}^n \lambda_i y_i^2$ as shown in the forward direction. Since $\lambda_i \geq 0$, we have $\sum_{i=1}^n \lambda_i y_i^2 \geq 0$, which implies that $\vec{x}^\top M\vec{x} \geq 0, \forall \vec{x} \in \mathbb{R}^n$, which implies that M is PSD.

□

(c) *Let $A \in \mathbb{R}^{n\times m}$ be any rectangular matrix. Show that $A^\top A$ and $AA^\top$ are positive semi-definite. (This shows that these matrices have non-negative eigenvalues.)*

(a) For $A^\top A$ we have $\forall \vec{x} \in \mathbb{R}^n$, $\vec{x}^\top A^\top A\vec{x} = \|A\vec{x}\|_2^2 \geq 0$, which implies that $A^\top A \in \mathbb{S}_+^n$.

(b) For $AA^\top$ we have $\forall \vec{x} \in \mathbb{R}^n$, $\vec{x}^\top AA^\top\vec{x} = \|A^\top\vec{x}\|_2^2 \geq 0$, which implies that $AA^\top \in \mathbb{S}_+^n$.

Problem 7.2 (3 points). *Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix.*

(a) *Let $A = PDP^\top$ with P orthogonal and D diagonal. Show that for any $k \in \mathbb{N}$, $A^k = PD^kP^\top$.*

We show it through mathematical induction, where the inductive hypothesis is $P(n) : A^n = PD^nD^\top$.

Proof.

(a) Base Step: When $k = 0$, we have $I = A^0 = PIP^\top = I$, which is true.

(b) Inductive Step: Suppose $P(k), k \geq 0$ is true, then $A^k = PD^kP^\top$. Then for $n = k + 1$, $A^{k+1} = PD^kP^\top PDP^\top = PD^{k+1}P^\top$, which shows that $P(k + 1)$ is true.

By mathematical induction, we have that $P(n)$ is true $\forall n \in \mathbb{N}$. $\square$

(b) *Same question when k is a negative integer.*

We show it through mathematical induction, where the inductive hypothesis is $P(n) : A^{-n} = PD^{-n}D^\top$.

Proof.

(a) Base Step: When $k = 1$, we have $A^{-1} = (PDP^\top)^{-1} = PD^{-1}P^\top$, which is true.

(b) Inductive Step: Suppose $P(k), k \geq 0$ is true, then $A^{-k} = PD^{-k}P^\top$. Then for $n = k+1$, $A^{-(k+1)} = PD^{-k}P^\top PD^{-1}P^\top = PD^{-(k+1)}P^\top$, which shows that $P(k + 1)$ is true.

By mathematical induction, we have that $P(n)$ is true $\forall n \in \mathbb{N}$. $\square$

(c) *Assume that A is positive semi-definite. Prove that there exists a symmetric positive semi-definite matrix $B \in \mathbb{R}^{n\times n}$ such that $A = B^2$. (Hint: in some sense, $B = A^{1/2}$. Can you guess how to define B?)*

The claim would be: there exists a PSD matrix $B = PD^{\frac{1}{2}}P^\top$ such that $A = B^2$ where P is the eigenvectors of A and the diagonal entries of D are eigenvalues of A.

Proof. *Since A is PSD, by spectrum theorem we have $A = PDP^\top = PD^{\frac{1}{2}}P^\top PD^{\frac{1}{2}}P^\top$ and we let $B = PD^{\frac{1}{2}}P^\top$. Note that since A is PSD and we have proved that all the eigenvalues of A are non-negative, so $D^{\frac{1}{2}}$ is still a real matrix(no complex numbers on the diagonal). Moreover, $B^\top = (PD^{\frac{1}{2}}P^\top)^\top = P(D^{\frac{1}{2}})^\top P^\top = PD^{\frac{1}{2}}P^\top = B$, so B is symmetric. Since $\forall \vec{x} \in \mathbb{R}^n, \vec{x}^\top B\vec{x} = \vec{x}^\top PD^{\frac{1}{2}}P^\top\vec{x} = \vec{y}^\top D^{\frac{1}{2}}\vec{y} = \sum_{i=1}^n \lambda_i^{\frac{1}{2}} y_i^2 \geq 0$, which implies that B is PSD, which finishes our proof.* $\square$

Problem 7.3 (2 points). *Consider a dataset $x_1, \dots, x_n \in \mathbb{R}^d$ with mean $\mu \in \mathbb{R}^d$ nd covariance $\Sigma \in \mathbb{R}^{d\times d}$*

(a) *Let $A \in \mathbb{R}^{m\times d}$ and $b \in \mathbb{R}^m$. Define $y_i = Ax_i + b$ for $i = 1, \dots, n$. Calculate the mean μ' and covariance Σ' of the dataset $y_1, \dots, y_n$.*

We have the following:

(a) $\mu' = \frac{1}{n}\sum_{i=1}^n y_i = \frac{1}{n}\sum_{i=1}^n (Ax_i + b) = \frac{1}{n}(A\sum_{i=1}^n x_i + nb) = \frac{1}{n}A\sum_{i=1}^n x_i + \frac{nb}{n} = A\mu + b.$

(b) *We have the following derivations:*

$$\begin{aligned}
\Sigma' &= \frac{1}{n}\sum_{i=1}^n (y_i - \mu')(y_i - \mu')^\top && \text{(By Definition)}\\
&= \frac{1}{n}\sum_{i=1}^n A(x_i - \mu)(A(x_i - \mu))^\top && \text{(From part(a))}\\
&= \frac{1}{n}\sum_{i=1}^n A(x_i - \mu)(x_i - \mu)^\top A^\top && \text{(Properties of Transpose)}\\
&= A\frac{1}{n}\sum_{i=1}^n (x_i - \mu)(x_i - \mu)^\top A^\top && \text{(Linearity of linear map)}\\
&= A\Sigma A^\top
\end{aligned}$$

(b) *Find A and b as a function of μ and Σ so that $\mu' = 0$ and $\Sigma' = \mathrm{Id}$ (there are several solutions for A, you do not have to find all of them). We call such an operation "whitening". (Hint: search for A of the form $PD'P^\top$, where $\Sigma = PDP^\top$ using the spectral theorem.)*

In other words, we have to find A, b that satisfies the following: $\begin{cases} A\mu + b = 0 \\ A\Sigma A^\top = I \end{cases}$

If we let $A = PD^{'}P^\top$ where $\Sigma = PDP^\top$ then we would have $\begin{cases} PD^{'}P^\top u + b = 0 \\ PD^{'}P^\top PDP^\top PD^{'}P^\top = I \end{cases}$,

that is $\begin{cases} D^{'}P^\top u + P^\top b = 0 & \text{,If we times } P^\top \text{ on both sides} \\ (D^{'})^2 D = P^\top P = I & \text{,If we times } P^\top \text{ on the left side and } P \text{ on the right side} \end{cases}$

Then one possible solution would be: $\begin{cases} D^{'} = D^{-\frac{1}{2}} \\ b = -(P^\top)^{\frac{1}{2}}u \end{cases}$. *Note that this can be constructed since P is invertible(orthogonal)and the solution b came from the least square procedure where $P^\top b = -D^{-\frac{1}{2}}P^\top u$.*

Finally we assemble the result and get $A = PD^{-\frac{1}{2}}P^\top = P^{\frac{1}{2}}\Sigma^{-\frac{1}{2}}(P^\top)^{\frac{1}{2}}$ and $b = -D^{-\frac{1}{2}}u$.

Alternatively, we could construct $\begin{cases} A = (P\Sigma^{\frac{1}{2}})^{-1} \\ b = -(P\Sigma^{\frac{1}{2}})^{-1}u \end{cases}$ *that satisfies the above equations.*

Problem 7.4 (3 points). *Complete the* `mnist_pca.ipynb` *Jupyter notebook to compute the mean, covariance, and PCA of the MNIST dataset. Please only submit a pdf version of your notebook (right-click → 'print' → 'Save as pdf').*
Jupyter notebook pdf link
Jupyter notebook link

In [1]:

```
import numpy as np
from matplotlib import pyplot as plt
%matplotlib inline
```

The MNIST dataset

The MNIST dataset is composed of 70,000 28×28 grayscale images of handwritten digits. It is represented as a $70000 \times 28 \times 28$ numpy array (a "3d matrix").

In [2]:

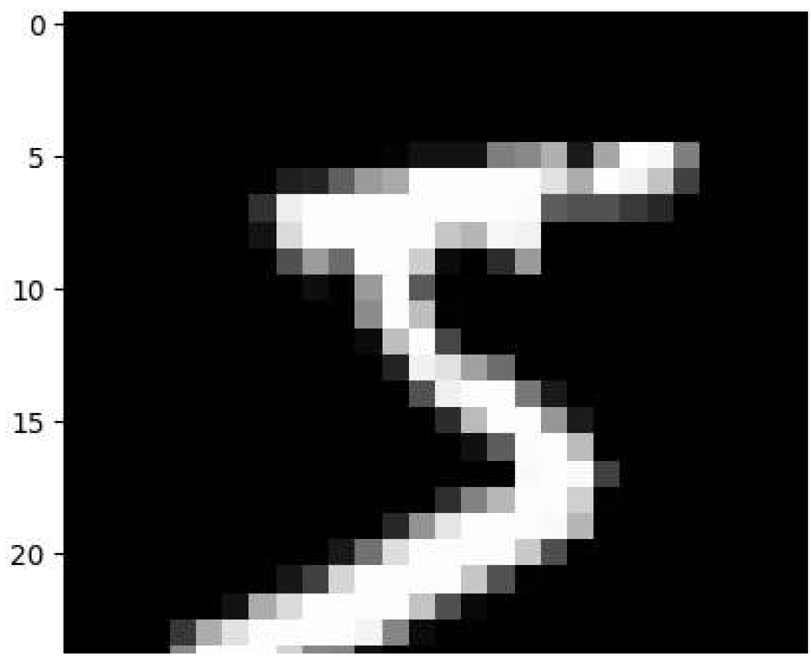
```
x = np.load("mnist.npy")
print(x.shape)
```

```
(70000, 28, 28)
```

Display the first few digits in the dataset.

In [3]:

```
for i in range(5):
    plt.imshow(x[i], cmap="gray")
    plt.show()
```



Computing and diagonalizing the covariance of MNIST

We will interpret each image as a vector in $\mathbb{R}^d$ with $d = 28^2 = 768$. The dataset can thus be seen as a matrix $in \mathbb{R}^{n \times d}$ where $n = 70000$.

In [4]:

```
xx = x.reshape((x.shape[0], -1))
xx
```

Out[4]:

```
array([[0, 0, 0, ..., 0, 0, 0],
       [0, 0, 0, ..., 0, 0, 0],
       [0, 0, 0, ..., 0, 0, 0],
       ...,
       [0, 0, 0, ..., 0, 0, 0],
       [0, 0, 0, ..., 0, 0, 0],
       [0, 0, 0, ..., 0, 0, 0]], dtype=uint8)
```

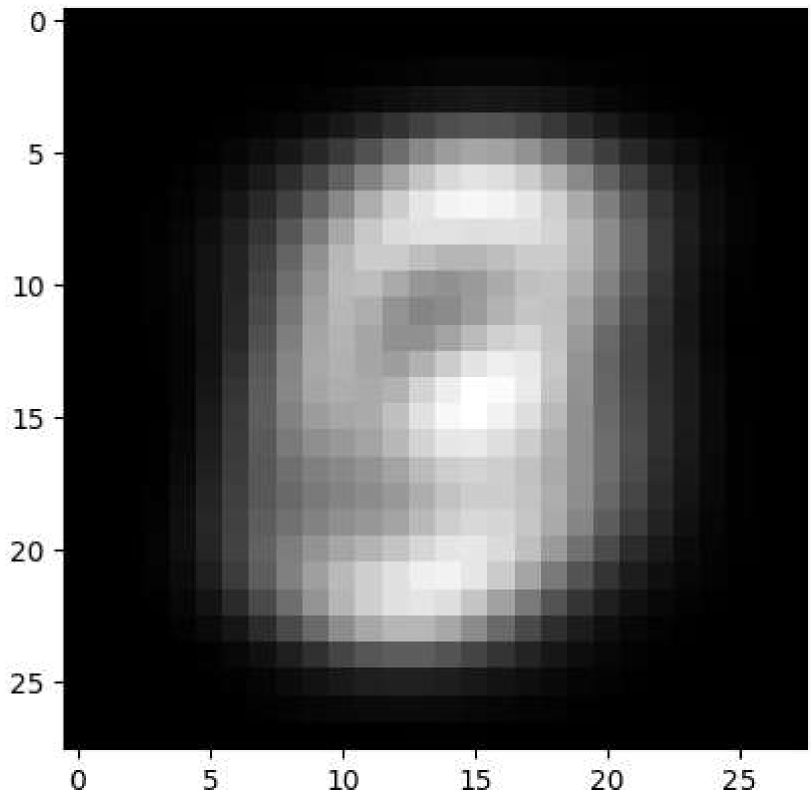
1. Compute the mean $\mu \in \mathbb{R}^d$ of the MNIST dataset and plot it as a 28×28 image.

In [5]:

```
# Your answer here
mean_vector = xx.mean(axis=0)
mean_image = mean_vector.reshape((28,28))
plt.imshow(mean_image, cmap="gray")
```

Out[5]:

```
<matplotlib.image.AxesImage at 0x21641d28130>
```



2. Compute the covariance $\Sigma \in \mathbb{R}^{d \times d}$ of the MNIST dataset and diagonalize it using the function `np.linalg.eigh`.

In [11]:

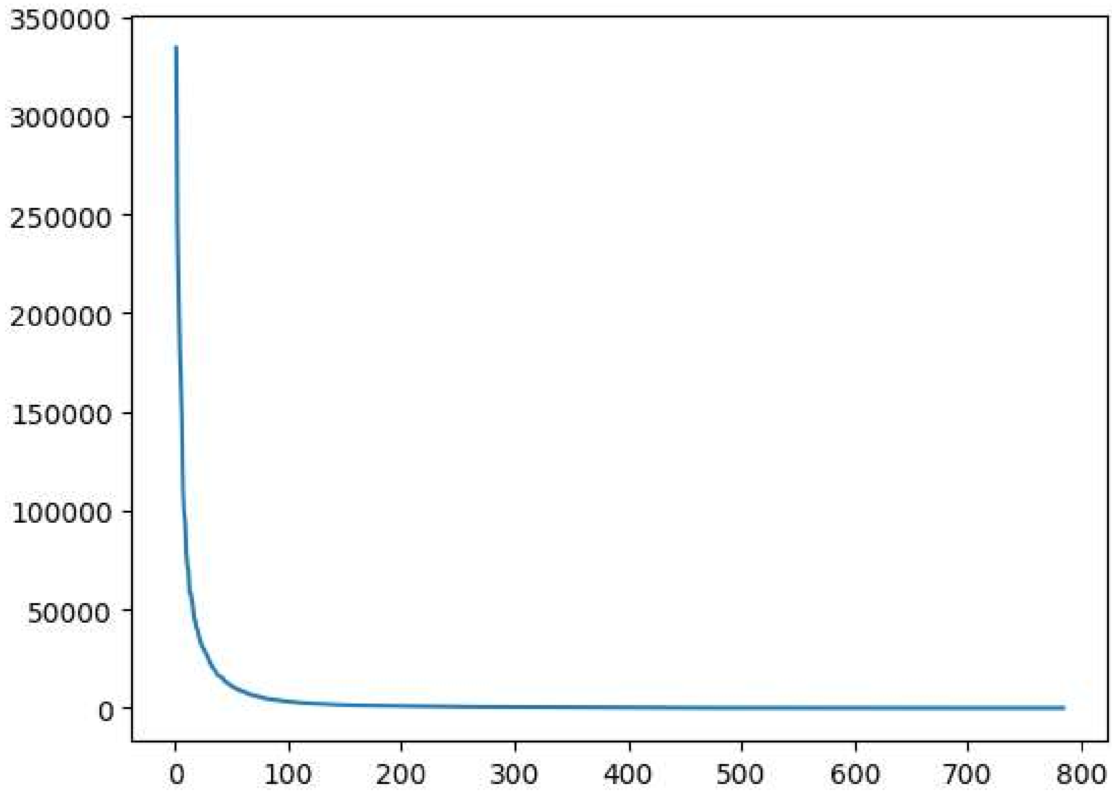
```
# Your answer here
cov_matrix = (1 / x.shape[0]) * (xx - mean_vector).T @ (xx - mean_vector)
eigenvalues, eigenvectors = np.linalg.eigh(cov_matrix)
eigenvalues, eigenvectors
```

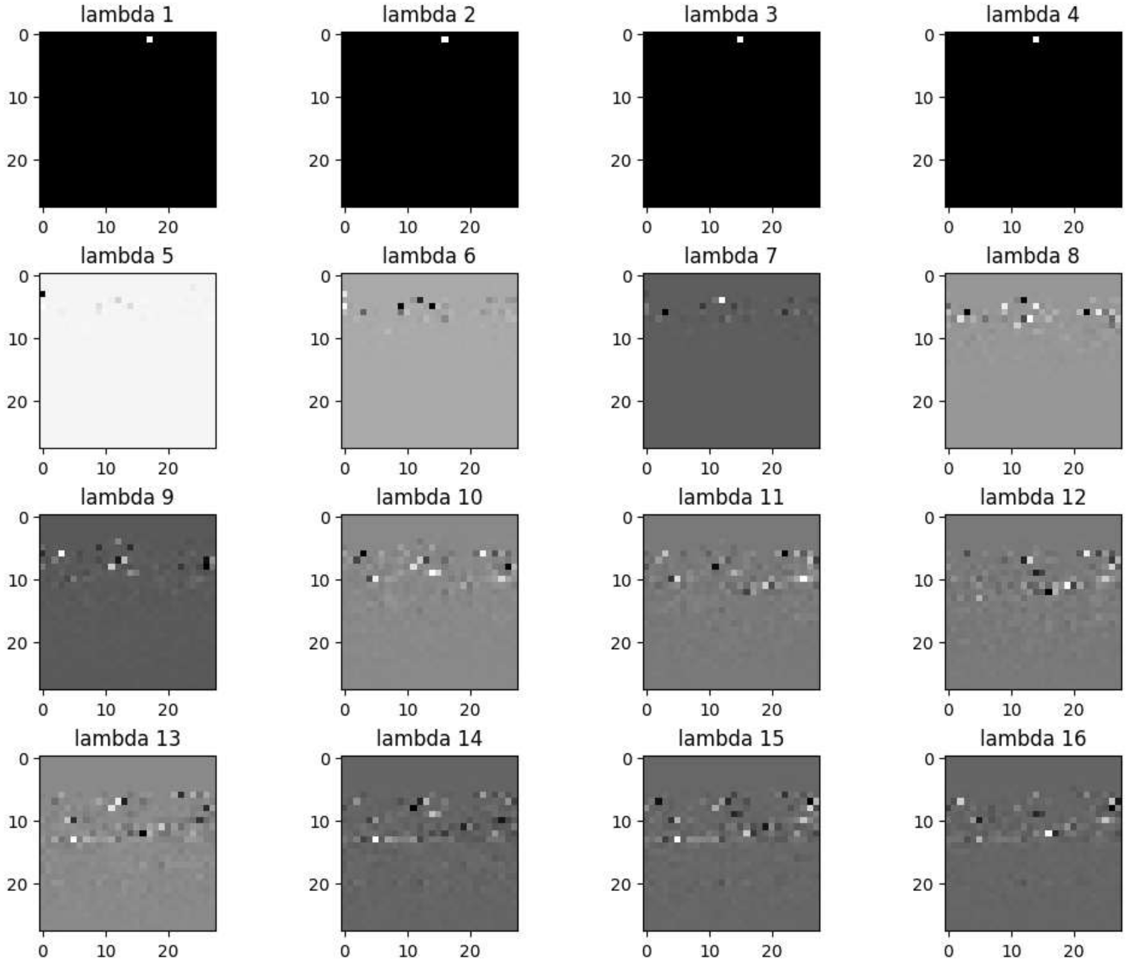
```
        9.24113022e+03,   9.69015100e+03,   9.84750631e+03,   1.01692003e+04,
        1.06378912e+04,   1.08680122e+04,   1.09654969e+04,   1.16184074e+04,
        1.19714546e+04,   1.23968292e+04,   1.28893227e+04,   1.31610777e+04,
        1.35883208e+04,   1.43447224e+04,   1.52605741e+04,   1.55847279e+04,
        1.60383427e+04,   1.64280388e+04,   1.67066997e+04,   1.73116665e+04,
        1.86409047e+04,   1.94395023e+04,   2.00863333e+04,   2.06079485e+04,
        2.21394661e+04,   2.25055712e+04,   2.36673094e+04,   2.53908053e+04,
        2.69499231e+04,   2.77770236e+04,   2.87712502e+04,   3.02965122e+04,
        3.12002508e+04,   3.28986421e+04,   3.46356878e+04,   3.65648922e+04,
        3.95454343e+04,   4.07231430e+04,   4.38698621e+04,   4.52536592e+04,
        5.09812503e+04,   5.43096063e+04,   5.81044457e+04,   5.85518694e+04,
        6.98875556e+04,   7.22588790e+04,   8.03348093e+04,   9.46111872e+04,
        9.91139674e+04,   1.12443533e+05,   1.47668187e+05,   1.67689177e+05,
        1.85334709e+05,   2.10927341e+05,   2.45429921e+05,   3.34289286e+05]),
 array([[0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        ...,
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
```

3. Plot the ordered eigenvalues $\lambda_1 \geq \cdots \geq \lambda_k \geq \cdots$ as a function $k = 1, \ldots, d$ with the x axis in log scale, and the first few eigenvectors $u_1, \ldots, u_k, \ldots$ as 28×28 images.

In [47]:

```
# Your answer here
eigenvalues_tuples = [(i, eigenvalues[i]) for i in range(len(eigenvalues))]
sorted_eigenvalues = sorted(eigenvalues_tuples, key = lambda x: x[1], reverse=True)
sorted_eigenvectors = eigenvectors[list(map(lambda x: x[0], sorted_eigenvalues))]

plt.plot(range(1,len(eigenvalues)+1),sorted(eigenvalues,reverse=True))
fig, axes = plt.subplots(4,4, layout='constrained', figsize=(10, 8))
for i in range(4):
    for j in range(4):
        index = 4 * i + j
        axes[i][j].imshow(sorted_eigenvectors[index].reshape(28, 28), cmap="gray")
        axes[i][j].set_title(f"lambda {index + 1}")
```



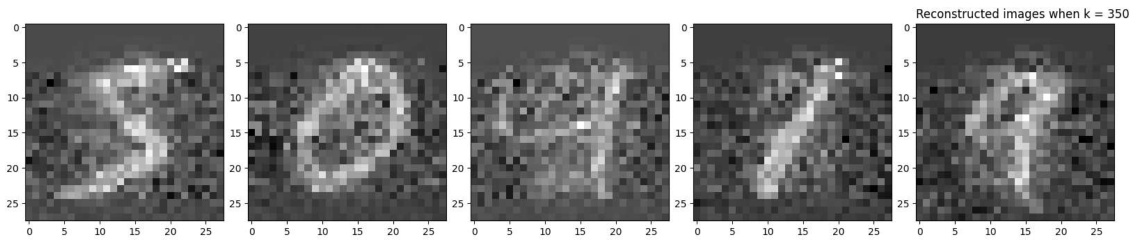


ataset using the
$\cdots + z_{i,k} u_k$,
, u_k). Display
ecognizing the

In [123]:

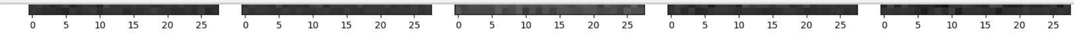
```
# Your answer here
# Compute the dimension of each data point
def dim_data(data):
    return data.shape[1]

# Compute the mean of the sample
def mean_data(data):
    return np.mean(data, axis=0)


# Compute the standard deviation of the sample
def sd_data(data):
    return (data - np.mean(data, axis=0)) / np.svd(data, axis=0)


# Centerize the data for further computation of the covariance matrix
def centerize_data(data):
    # Centerize the data
    return data - np.mean(data, axis=0)

# Compute the eigenbasis with k eigenvectors
def compute_eigenbasis_k(centered_data, k):
    # Compute the top k eigenvectors for our eigenbasis
    cov_matrix = 1 / len(centered_data) * centered_data.T @ centered_data
    eigenvalues, eigenvectors = np.linalg.eigh(cov_matrix)

    sorted_eigenvalues = sorted([(i, eigenvalues[i]) for i in range(len(eigenvalues))], key = l
    sorted_eigenvectors = eigenvectors[list(map(lambda x: x[0], sorted_eigenvalues))][:k]

    return sorted_eigenvectors.T


# Main Procedure: PCA
def PCA_procedure(data, k):
    centered_data = centerize_data(data)
    V_k = compute_eigenbasis_k(centered_data, k)

    # Find PCA coordinates
    Z_k = V_k.T @ centered_data.T

    # Z_k is a matrix with (k, 70000), where the coordinates for each data point is organized in
    return Z_k, V_k


# Main Procesure: Inverse PCA
def inverse_PCA_procedure(Z_k, V_k, data, k):
    centered_data = centerize_data(data)
    mu = data.mean(axis=0)

    # Revert to origin
    RC_k = V_k @ Z_k + mu.reshape(dim_data(data),1)


    # RC_k is a matrix with (784, 70000), where the reconstructed coordinates for each data poin
    return RC_k

# Display the reconstructed images
def show_first_five_reconstructed(data, k):
    # Draw the first five reconstructed images
```

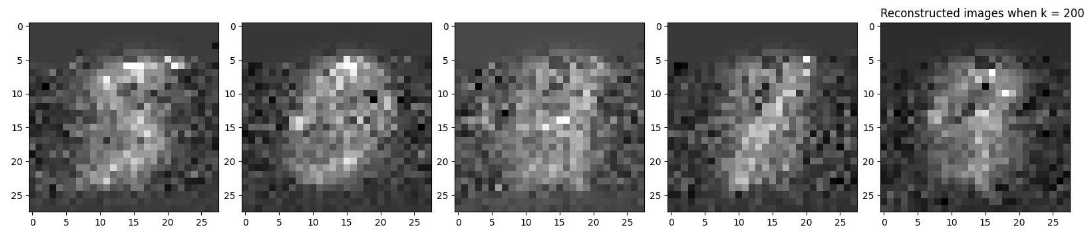
```
    fig, axes = plt.subplots(1, 5, figsize=(16,16), constrained_layout=True)

    Z_k, V_k = PCA_procedure(data, k)
    RC_k = inverse_PCA_procedure(Z_k, V_k, data, k)

    for i in range(5):
        axes[i].imshow(RC_k[:,i].reshape(28,28), cmap="gray")

    plt.title(f"Reconstructed images when k = {k}", loc = "left")


def problem_1(data):
    k = 350
    show_first_five_reconstructed(data, k)


def problem_2(data):
    k_list = [150, 200, 220, 240, 250, 260, 270, 280, 290, 300]
    for k in k_list:
        show_first_five_reconstructed(data, k)


# xx is (70000, 784)
problem_1(xx) # We pick 350, when we could recognize the reconstructed digits by raw eyes, which
```

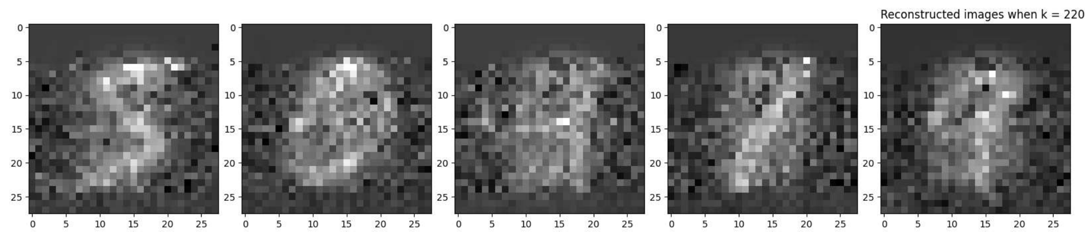


In [124]:

```
problem_2(xx) # We find that 300 is minimum number of eigenvectors that are needed to reconstruc
```







In [ ]:

Problem 7.5 ($\star$)**.** *Let $A \in \mathbb{R}^{n\times m}$ a rectangular matrix. Show that there exists an orthonormal basis $u_1, \dots, u_m$ of $\mathbb{R}^m$ such that $Au_1, \dots, Au_m$ is an orthogonal family (its vectors are pairwise orthogonal but not necessarily of norm one). (Hint: apply the spectral theorem to $A^\top A$.)*

Assume $U = \begin{bmatrix} \vec{u}_1 & \vec{u}_2 & \cdots & \vec{u}_m \end{bmatrix} \in \mathbb{R}^{m\times m}$ is the orthonormal basis that satisfies the problem statement. Then we must have $(AU)^\top AU = U^\top A^\top AU = D$, where D is a diagonal matrix. This has to hold since if AU is orthogonal family, $(A\vec{u}_i)^\top A\vec{v}_j = 0, \forall i \neq j$ and $(A\vec{u}_i)^\top A\vec{v}_i = \|A\vec{v}_i\|_2^2$, which is some non-zero value and is different across i. Now since we should have $U^\top A^\top AU = D$, we rearrange it and could get $A^\top A = UDU^\top$, which is just the spectrum decomposition of matrix $A^\top A$. Thus there exists the orthonormal basis U, which is just the eigenvectors of $A^\top A$ such that $A\vec{u}_i$'s is an orthogonal family.