In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
```

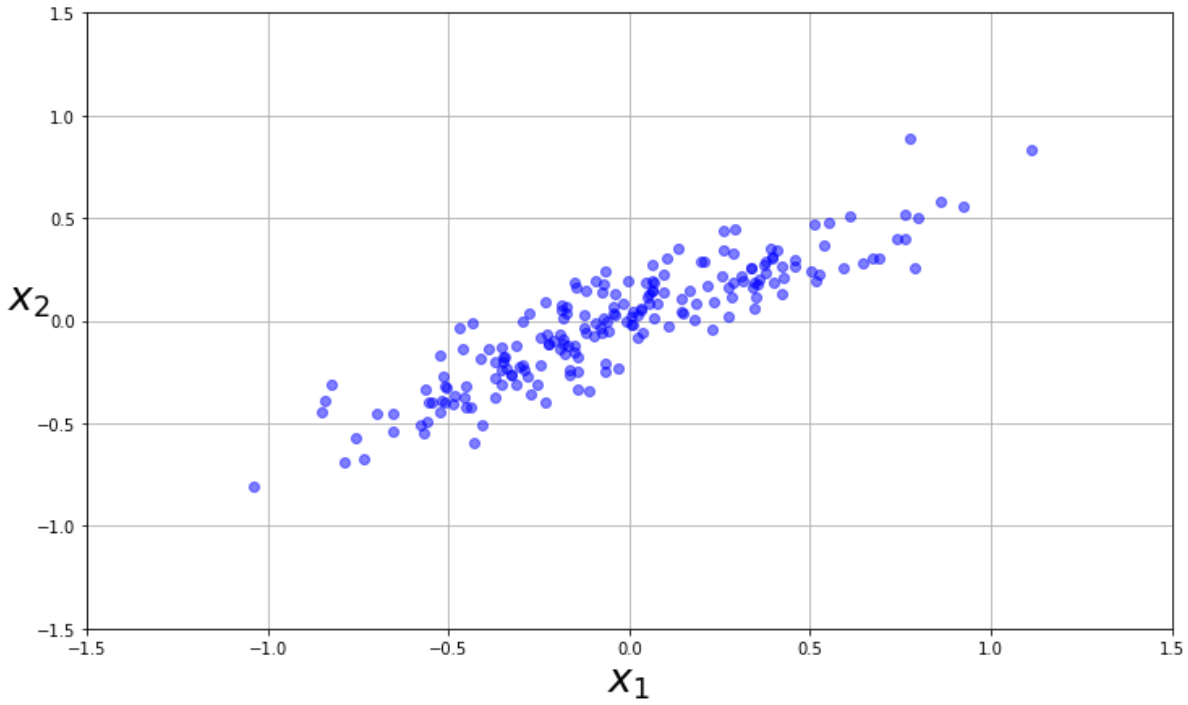
11.2 Principal Component Analysis (PCA)

In most real-world problems, dataset points are not spread out uniformly across all dimensions. Many features are almost constant, while others are highly correlated. As a result, all points lie within (or close to) a much **lower-dimensional subspace** of the high-dimensional space.

Principal Component Analysis (PCA) is the oldest and, by far, the most popular algorithm to project a dataset into a low-dimensional subspace. First, PCA identifies the subspace that lies closest to the data, and then it projects the data onto it.

Example: Let us consider the following 2-dimensional dataset

In [2]:
```
# dataset parameters:
m = 200
angle = np.pi / 5
stretch = 5

# dataset
X = np.random.randn(m, 2) / 10
X[:,0] = stretch*X[:,0]
X = X@np.array([[np.cos(angle), np.sin(angle)], [-np.sin(angle), np.cos(angle
)]]) # rotate

plt.figure(figsize=(12,7))
# plot dataset
plt.plot(X[:, 0], X[:, 1], "bo", alpha=0.5)

#
plt.axis([-1.5, 1.5, -1.5, 1.5]) # axes ranges#
plt.xlabel("$x_1$", fontsize=25)
plt.ylabel("$x_2$", fontsize=25, rotation=0)
plt.grid(True)
```

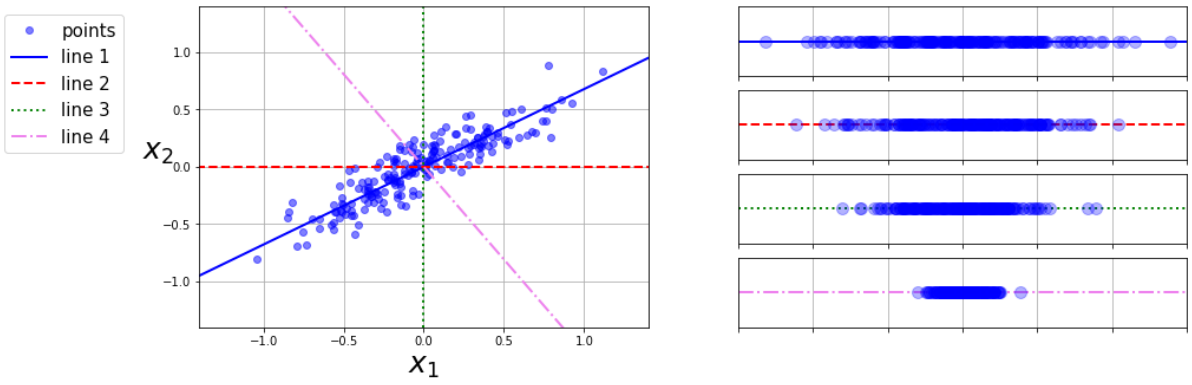


Suppose we want to project this dataset onto a 1-dimensional subspace (a line). How do we find the "right line"?

In the plot below, we have our original dataset, along with four different lines (1-dimensional subspaces). On the right is the result of the projection of the dataset onto each of these lines.

In [3]:
```
# angles
angle1 = np.pi/5
angle2 = np.pi
angle3 = np.pi/2
angle4 = np.pi-np.pi/3

# unit vectors along the lines
u1 = np.array([np.cos(angle1), np.sin(angle1)])
u2 = np.array([np.cos(angle2), np.sin(angle2)])
u3 = np.array([np.cos(angle3), np.sin(angle3)])
u4 = np.array([np.cos(angle4), np.sin(angle4)])

# projections onto the lines
X_proj1 = X@u1[:,None]
X_proj2 = X@u2[:,None]
X_proj3 = X@u3[:,None]
X_proj4 = X@u4[:,None]

# plot size
plt.figure(figsize=(15,5))

# plot dataset
plt.subplot2grid((4,2), (0, 0), rowspan=4)
plt.plot(X[:, 0], X[:, 1], "bo", alpha=0.5, label = 'points')
plt.axis([-1.4, 1.4, -1.4, 1.4]) # axes ranges#

# plot the lines on the interval [-1.5, 1.5]
plt.plot([-1.5, 1.5], [-1.4*u1[1]/u1[0], 1.4*u1[1]/u1[0]], "k-", color='blue',
linewidth=2, label = 'line 1')
plt.plot([-1.5, 1.5], [-1.4*u2[1]/u2[0], 1.4*u2[1]/u2[0]], "k--", color='red',
linewidth=2, label = 'line 2')
plt.plot([-1.5, 1.5], [-1.4*u3[1]/u3[0], 1.4*u3[1]/u3[0]], "k:", color='green'
, linewidth=2, label = 'line 3')
plt.plot([-1.5, 1.5], [-1.4*u4[1]/u4[0], 1.4*u4[1]/u4[0]], "k-.", color='viole
t', linewidth=2, label = 'line 4')

# plot options
plt.xlabel("$x_1$", fontsize=25)
plt.ylabel("$x_2$", fontsize=25, rotation=0)
plt.legend(fontsize=15, bbox_to_anchor=(-0.15, 1))
plt.grid(True)

# plot projections

# projection 1
plt.subplot2grid((4,2), (0, 1))
plt.plot([-1.5, 1.5], [0, 0], "k-", color='blue', linewidth=2)
plt.plot(X_proj1[:, 0], np.zeros(m), "bo", markersize=10, alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.gca().get_xaxis().set_ticklabels([])
plt.axis([-1.5, 1.5, -1, 1])
plt.grid(True)

# projection 2
plt.subplot2grid((4,2), (1, 1))
plt.plot([-1.5, 1.5], [0, 0], "k--", color='red', linewidth=2)
```

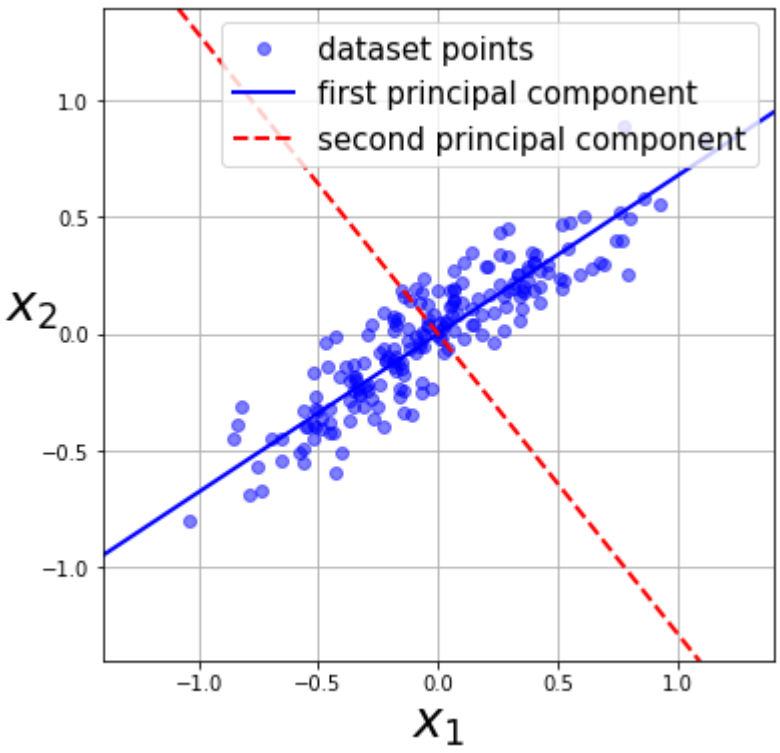
```
plt.plot(X_proj2[:, 0], np.zeros(m), "bo", markersize=10, alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.gca().get_xaxis().set_ticklabels([])
plt.axis([-1.5, 1.5, -1, 1])
plt.grid(True)

# projection 3
plt.subplot2grid((4,2), (2, 1))
plt.plot([-1.5, 1.5], [0, 0], "k:", color='green', linewidth=2)
plt.plot(X_proj3[:, 0], np.zeros(m), "bo", markersize=10, alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.gca().get_xaxis().set_ticklabels([])
plt.axis([-1.5, 1.5, -1, 1])
plt.grid(True)

# projection 4
plt.subplot2grid((4,2), (3, 1))
plt.plot([-1.5, 1.5], [0, 0], "k-.", color='violet', linewidth=2)
plt.plot(X_proj4[:, 0], np.zeros(m), "bo", markersize=10, alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.gca().get_xaxis().set_ticklabels([])
plt.axis([-1.5, 1.5, -1, 1])
plt.grid(True)
```



It seems reasonable to select the line that preserves the maximum amount of variance (in the example, the solid blue line), as it will most likely lose less information than the other projections. In mathematical terms, we want to select the line that minimizes the mean squared distance between the original dataset and its projection onto the axis. This is the idea behind PCA.

PCA identifies the line that accounts for the largest amount of variance in the dataset. In our previous example, it is the solid blue line. It also finds a second line, orthogonal to the first one, that accounts for the largest amount of remaining variance. These axes/lines are called **principal components**.

In [4]:
```
# principal component angles
angle1 = np.pi/5 # first principal component
angle2 = angle1 + np.pi/2 # second principal component


# unit vectors
u1 = np.array([np.cos(angle1), np.sin(angle1)])
u2 = np.array([np.cos(angle2), np.sin(angle2)])

# plot dataset
plt.figure(figsize=(6,6))
plt.plot(X[:, 0], X[:, 1], "bo", alpha=0.5, label = 'dataset points')
plt.axis([-1.4, 1.4, -1.4, 1.4]) # axes ranges#

# plot principal components
plt.plot([-1.5, 1.5], [-1.4*u1[1]/u1[0], 1.4*u1[1]/u1[0]], "k-", color='blue',
linewidth=2, label = 'first principal component')
plt.plot([-1.5, 1.5], [-1.4*u2[1]/u2[0], 1.4*u2[1]/u2[0]], "k--", color='red',
linewidth=2, label = 'second principal component')

# plot options
plt.xlabel("$x_1$", fontsize=25)
plt.ylabel("$x_2$", fontsize=25, rotation=0)
plt.legend(fontsize=15, loc='upper right')
plt.grid(True)
```



If the dataset were a higher-dimensional dataset, PCA would also find a third axis, orthogonal to both previous axes, and a fourth, a fifth, and so on --as many axes as the number of dimensions in the dataset.

11.2.1 Principal Components -- The Singular Value Decomposition (SVD)

How can we find the principal components of a dataset? If the dataset is centered around the origin, The **Singular Value Decomposition (SVD)** can find the principal components and the projections onto them!!

Recall that the SVD of the dataset matrix X decomposes X as the product of three matrices

$$X = U\Sigma V.$$

The matrix U has orthonormal columns, the matrix V has orthonormal rows, and the matrix Σ is diagonal. The diagonal elements of Σ are called the singular values of X. You can find the svd of a matrix by using NumPy's svd function.

In [5]:
```
u,s,v = np.linalg.svd(X)
```

Here is an amazing fact. The rows of V are the principal components: row 1 is the first principal component, row 2 is the second principal component, row 3 is the third principal component, and so on.

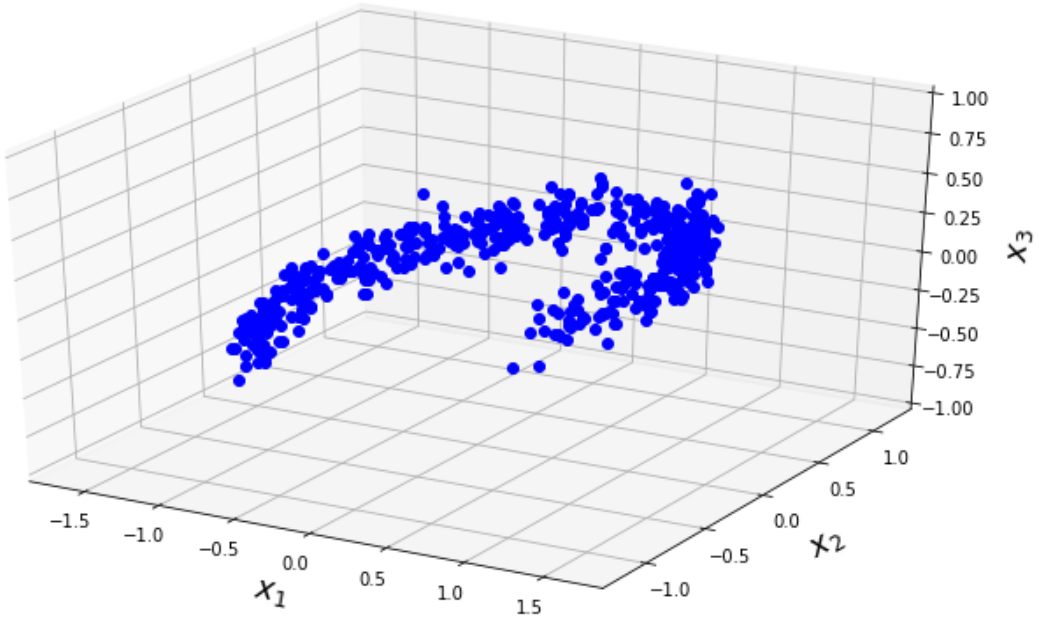
The projection of X onto the subspace spanned by the first k principal components is:

In [6]:
```
k = 2
X_reduced = X@v[:k].T
```

Example: Let us consider the following 3-dimensional dataset

In [7]:
```
# build the 3d dataset
m = 500
w1, w2 = 0.1, 0.3
noise = 0.1
axes = [-1.8, 1.8, -1.3, 1.3, -1.0, 1.0]


angles = np.random.rand(m) * 3 * np.pi / 2 - 0.5
X = np.empty((m, 3))
X[:, 0] = np.cos(angles) + np.sin(angles)/2 + noise * np.random.randn(m) / 2
X[:, 1] = np.sin(angles) * 0.7 + noise * np.random.randn(m) / 2
X[:, 2] = X[:, 0] * w1 + X[:, 1] * w2 + noise * np.random.randn(m) # the z-com
ponents are almost a linear combination of the x and y components

# plot the dataset
from mpl_toolkits.mplot3d import proj3d
plt.figure(figsize=(12,7))
ax = plt.axes(projection='3d')
plt.plot(X[:,0],X[:,1],X[:,2],'bo')

ax.set_xlabel("$x_1$", fontsize=18, labelpad=10)
ax.set_ylabel("$x_2$", fontsize=18, labelpad=10)
ax.set_zlabel("$x_3$", fontsize=18, labelpad=10)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])
```

Out[7]: (-1.0, 1.0)



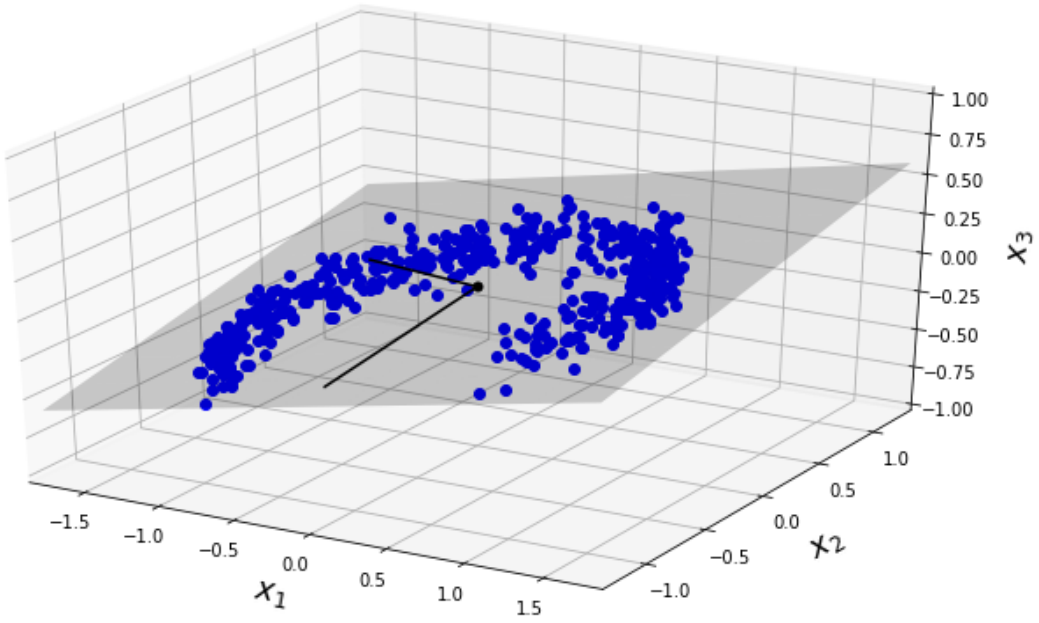
All the points lie close to a plane (although it's not evident from the image itself). Let us use PCA to find this plane and project every point onto it.

In [8]:
```
'PCA'

# center the dataset
X_centered = X - np.mean(X,axis=0)

# Singular Value Decomposition
u,s,v = np.linalg.svd(X_centered)

# principal components
c1 = v[:,0] # first principal component
c2 = v[:,1] # second principal component
```

Let us plot the plane spanned by the first two principal components

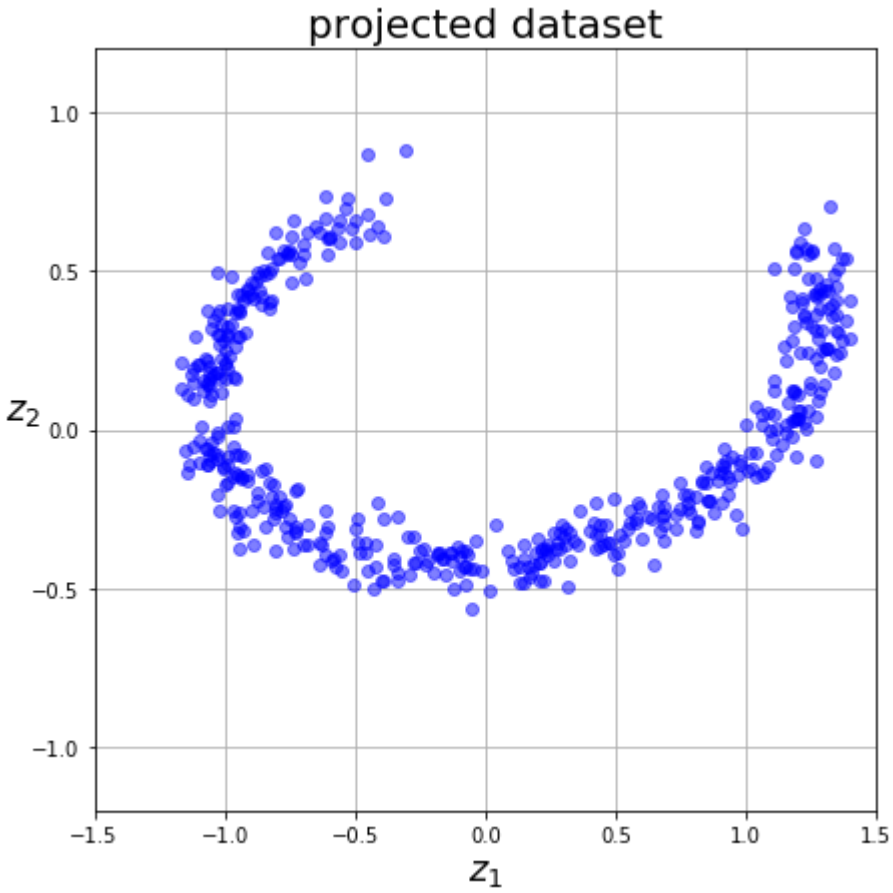
In [9]:
```
# plot the centered dataset
plt.figure(figsize=(12,7))
ax = plt.axes(projection='3d')
plt.plot(X_centered[:,0],X_centered[:,1],X_centered[:,2],'bo')

# origin
ax.plot([0],[0],[0],'ko',markersize=5)

# plot c1 and c2
ax.plot([0,c1[0]],[0,c1[1]],[0,c1[2]],'k-')
ax.plot([0,c2[0]],[0,c2[1]],[0,c2[2]],'k-')

# plot the plane
x1s = np.linspace(axes[0], axes[1], 10)
x2s = np.linspace(axes[2], axes[3], 10)
x1, x2 = np.meshgrid(x1s, x2s)
n = np.cross(c1,c2) # plane's normal vector
x3 = -(n[0]*x1+n[0]*x2)/n[2]
ax.plot_surface(x1, x2, x3, alpha=0.2, color="k")

# plot options
ax.set_xlabel("$x_1$", fontsize=18, labelpad=10) # axes labels
ax.set_ylabel("$x_2$", fontsize=18, labelpad=10)
ax.set_zlabel("$x_3$", fontsize=18, labelpad=10)
ax.set_xlim(axes[0:2]) # axes limits
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])
```

Out[9]: (-1.0, 1.0)



Finally, let us project the dataset onto the plane spanned by the first two principal components.

In [11]:
```
# projection
k = 2
X_reduced = X_centered@v[:k].T

# plot the projected dataset
plt.figure(figsize=(7,7))
plt.plot(X_reduced[:,0],X_reduced[:,1],'bo',alpha=0.5)
plt.xlabel("$z_1$", fontsize=18)
plt.ylabel("$z_2$", fontsize=18, rotation=0)
plt.axis([-1.5, 1.5, -1.2, 1.2])
plt.title('projected dataset',fontsize=20)
plt.grid(True)
```



We have just reduced the dataset's dimensionality from 3D to 2D, without losing too much information.

11.2.2 Choosing the Right Number of Dimensions

Let us load the MNist dataset

In [12]:
```
from sklearn.datasets import fetch_openml

mnist = fetch_openml('mnist_784', version=1)
mnist.target = mnist.target.astype(np.uint8)
X = mnist["data"][:5000] # we'll use the first 5000 digits
y = mnist["target"][:5000]
```

In [13]:
```
y = y.astype(np.uint8)
```

In [14]:
```
m,n = X.shape
print('the dimension of the data set is '+str(n))
```

```
the dimension of the data set is 784
```

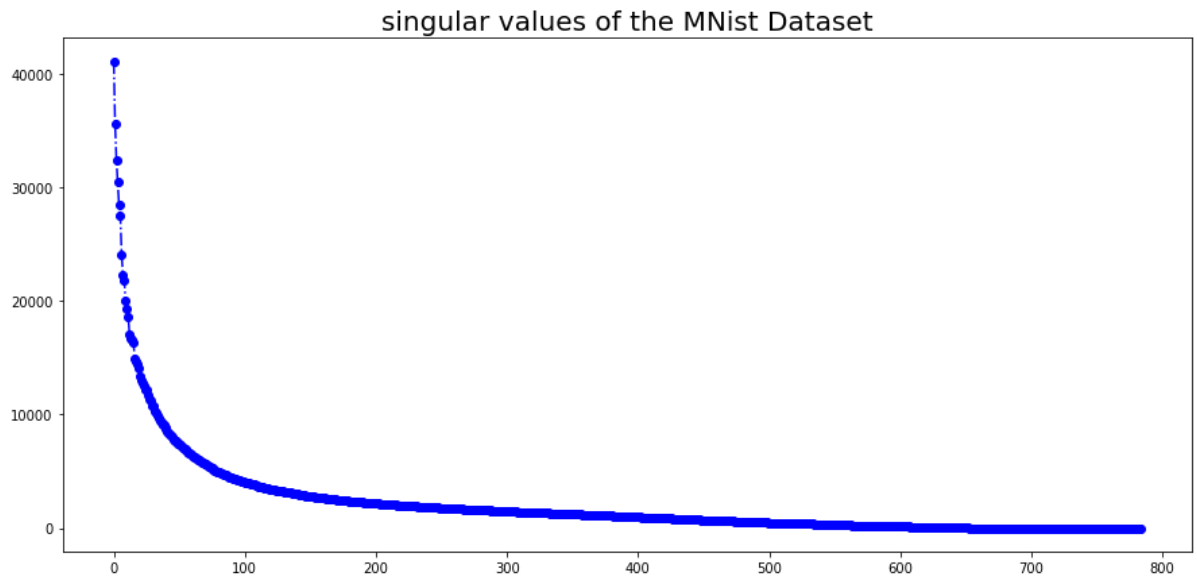
and compute its principal components

In [15]:
```
X_centered = X - np.mean(X,axis=0)
u,s,v = np.linalg.svd(X_centered,full_matrices=False) # full_matrices = False
 will save some memory
```

The singular values produced are in order from largest to smallest

In [16]:
```
plt.figure(figsize=(15,7))
plt.plot(s,'bo-.')
plt.title('singular values of the MNist Dataset',fontsize=20)
```

Out[16]:
```
Text(0.5, 1.0, 'singular values of the MNist Dataset')
```

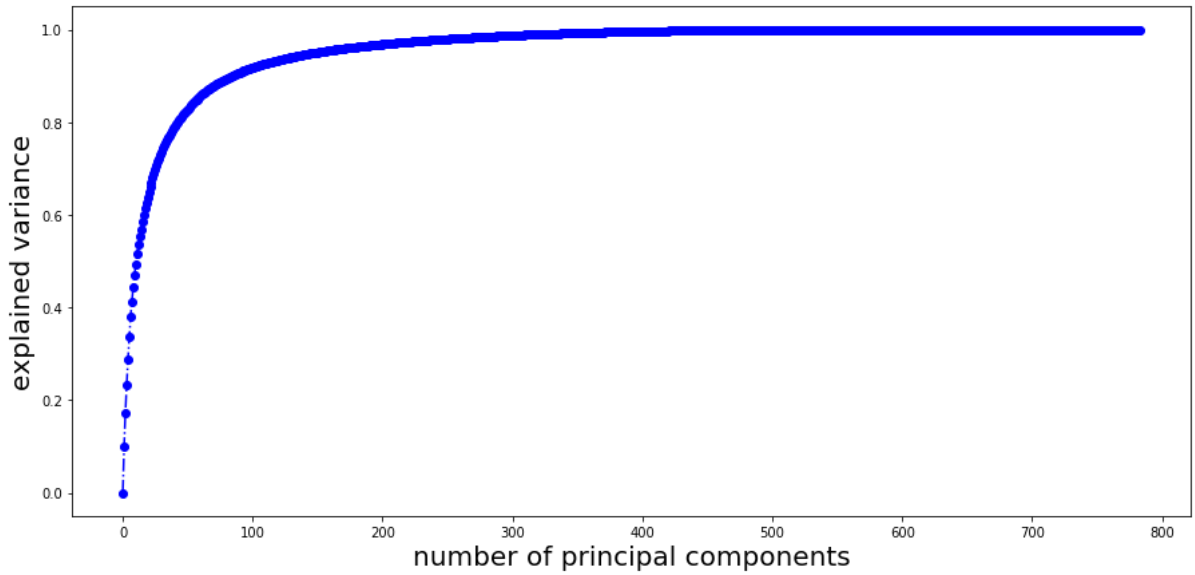


and when squared are proportional to the amount of variance explained by a given principal component

In [17]:
```
# explained variance
s_squared = np.square(s)
explained_variance = np.array([np.sum(s_squared[:k])/np.sum(np.square(s)) for
k in range(n)])
```

In [18]:
```
plt.figure(figsize=(15,7))
plt.plot(explained_variance,'bo-.')
plt.xlabel('number of principal components', fontsize=20)
plt.ylabel('explained variance', fontsize=20)
```

Out[18]:
```
Text(0, 0.5, 'explained variance')
```



Instead of arbitrarily choosing the number of dimensions to reduce down to, it is simple to choose the number of dimensions that add up to a sufficiently large portion of the variance (for example, 95%).

In our example, reducing the dimensionality down to about $k = 150$ wouldn't lose too much explained variance.

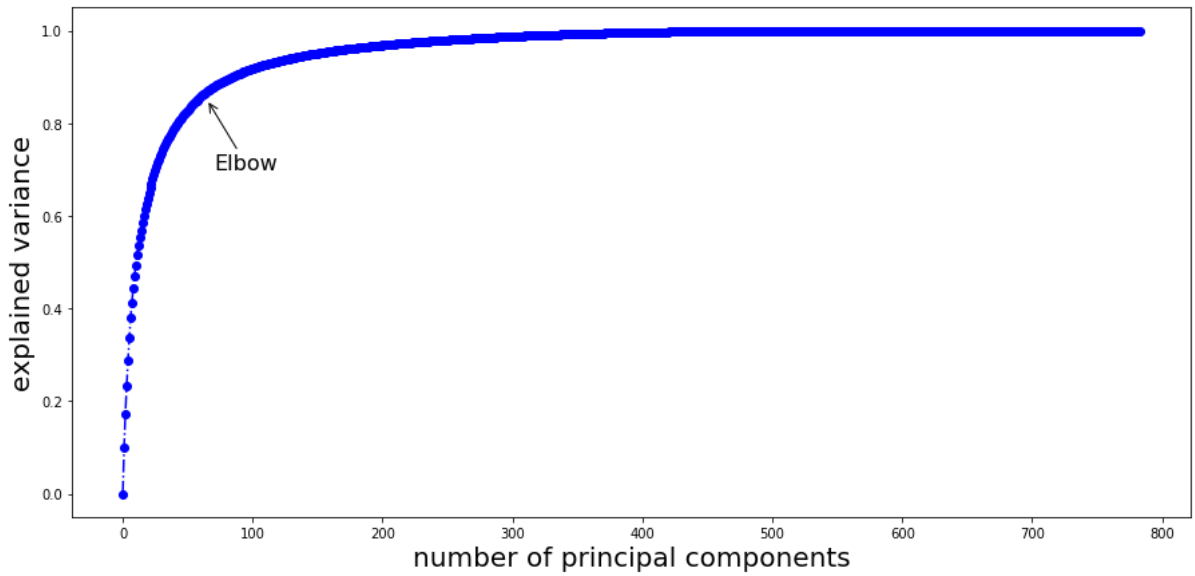
In [19]:
```
explained_variance[150]
```

Out[19]:
```
0.9510446077847862
```

Another option is to plot the explained variance as a function of the number of dimensions. There will usually be an elbow in the curve, where the explained variance stops growing fast:

In [20]:
```
plt.figure(figsize=(15,7))
plt.plot(explained_variance,'bo-.')
plt.annotate("Elbow", xy=(65, 0.85), xytext=(70, 0.7),
             arrowprops=dict(arrowstyle="->"), fontsize=16)
plt.xlabel('number of principal components', fontsize=20)
plt.ylabel('explained variance', fontsize=20)
```

Out[20]:
```
Text(0, 0.5, 'explained variance')
```



11.2.3 PCA for Visualization

PCA can also be used to visualize high-dimensional data.

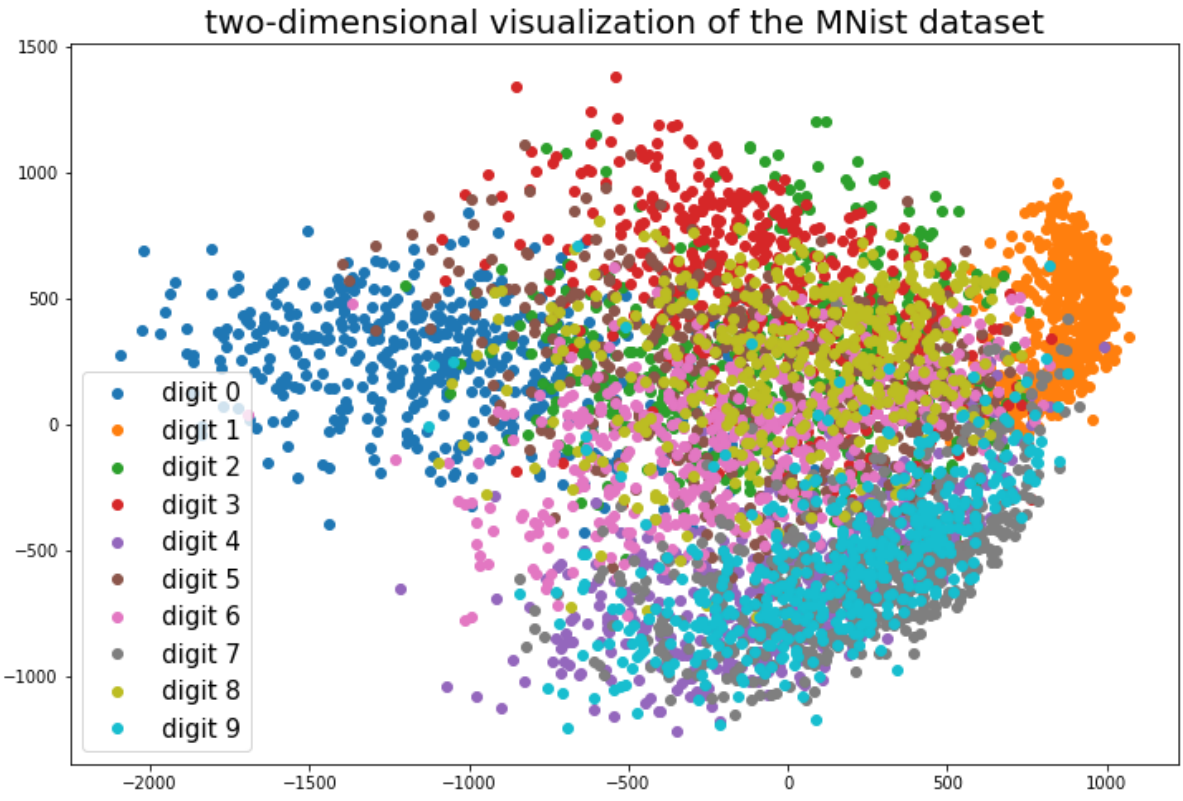
Let's visualize the MNIST dataset

two-dimensional visualization

In [21]:
```
k = 2 # two-dimensional visualization
X_reduced = X_centered@v[:k].T
```

In [22]:
```
import matplotlib.cm as cm
colors = cm.tab10(np.linspace(0, 1, 10))

plt.figure(figsize=(12,8))
for i in range(10):
    plt.plot(X_reduced[y==i,0],X_reduced[y==i,1],'o',color=colors[i],label='di
git '+str(i))
    plt.legend(fontsize=15)
plt.title('two-dimensional visualization of the MNist dataset',fontsize=20)
```

Out[22]: Text(0.5, 1.0, 'two-dimensional visualization of the MNist dataset')



Observe that some of the digits (for example, digits 0, 1 and 3) are separated from the other digits.

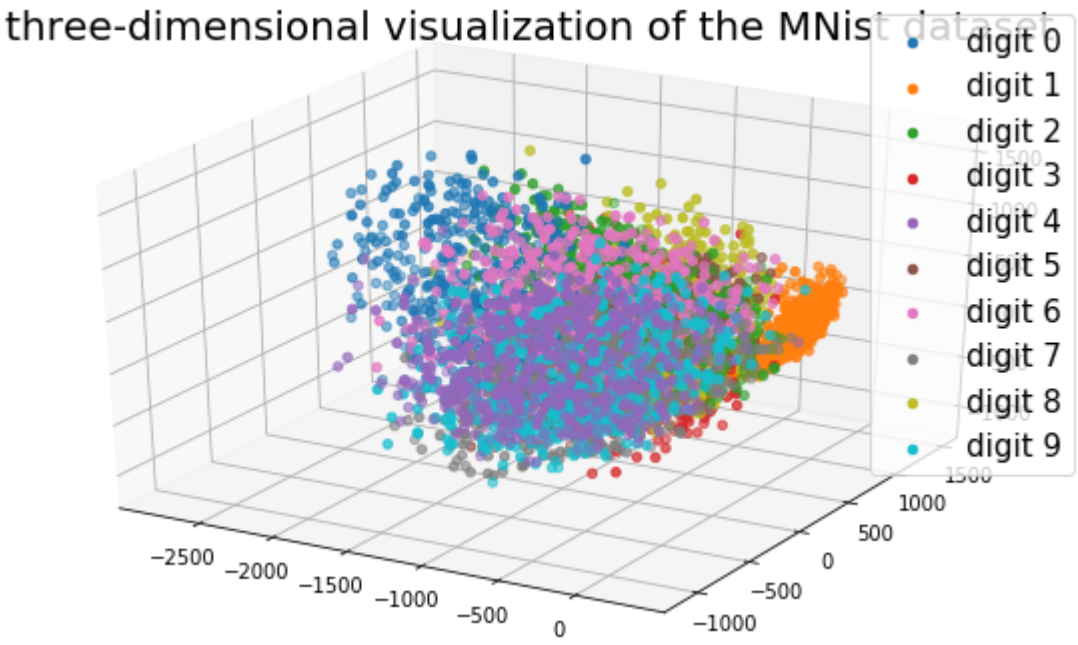
three-dimensional visualization

In [23]:
```
k = 3 # three-dimensional visualization
X_reduced = X@v[:k].T
```

In [24]:
```
colors = cm.tab10(np.linspace(0, 1, 10))
fig = plt.figure(figsize=(10,6))
ax = plt.axes(projection='3d')
for i in range(10):
    ax.scatter(X_reduced[y==i,0],X_reduced[y==i,1],X_reduced[y==i,2],c=colors[
i], label='digit '+str(i))
    plt.legend(fontsize=15)
plt.title('three-dimensional visualization of the MNist dataset',fontsize=20)
```

```
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
'c' argument looks like a single numeric RGB or RGBA sequence, which should b
e avoided as value-mapping will have precedence in case its length matches wi
th 'x' & 'y'.  Please use a 2-D array with a single row if you really want to
specify the same RGB or RGBA value for all points.
```

Out[24]:
```
Text(0.5, 0.92, 'three-dimensional visualization of the MNist dataset')
```



11.2.4 PCA for Speeding-up Clustering

First, let us load the Olivetti dataset

In [25]:
```
from sklearn.datasets import fetch_olivetti_faces
olivetti = fetch_olivetti_faces()
```

In [26]:
```
images, labels = olivetti.images, olivetti.target
```

In [27]:
```
X = images.reshape(400,64*64)
print('the dimension of the data set is '+str(n))
```

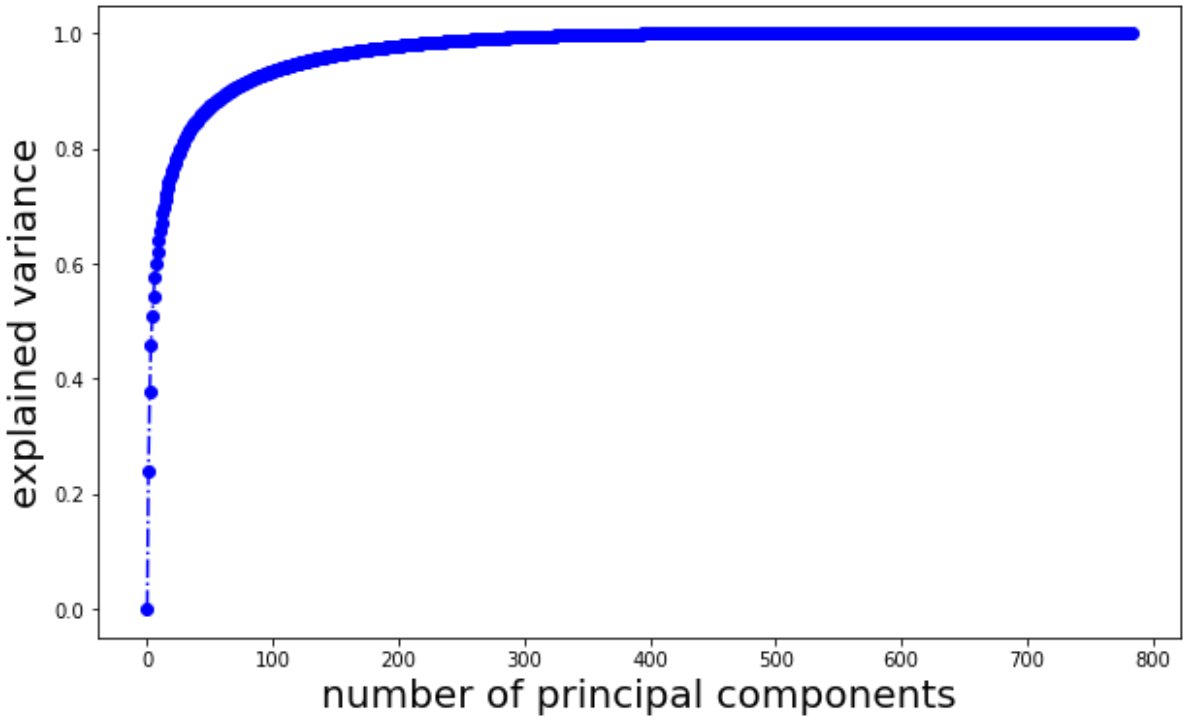
```
the dimension of the data set is 784
```

We are going to cluster the dataset by using k-means. To speed up the algorithm, we will reduce the dataset's dimensionality (using PCA, preserving 95% of the variance).

In [28]:
```
'PCA'

# center the dataset
X_centered = X - np.mean(X,axis=0)
# svd
u,s,v = np.linalg.svd(X_centered,full_matrices=False) # full_matrices = False
 will save some memory
# explaned variance
s_squared = np.square(s)
explained_variance = np.array([np.sum(s_squared[:k])/np.sum(np.square(s)) for
k in range(n)])
```

In [29]:
```
plt.figure(figsize=(10,6))
plt.plot(explained_variance,'bo-.')
plt.xlabel('number of principal components', fontsize=20)
plt.ylabel('explained variance', fontsize=20)
```

Out[29]:
```
Text(0, 0.5, 'explained variance')
```



Reducing the dimensionality down to about k=150 wouldn't lose too much explained variance.

In [30]:
```
explained_variance[150]
```

Out[30]:
```
0.9632106
```

In [31]:
```
k = 150 # three-dimensional visualization
X_reduced = X@v[:k].T
X_reduced.shape
```

Out[31]:
```
(400, 150)
```

Finally, we can cluster the projected dataset by using Hierarchical Clustering.

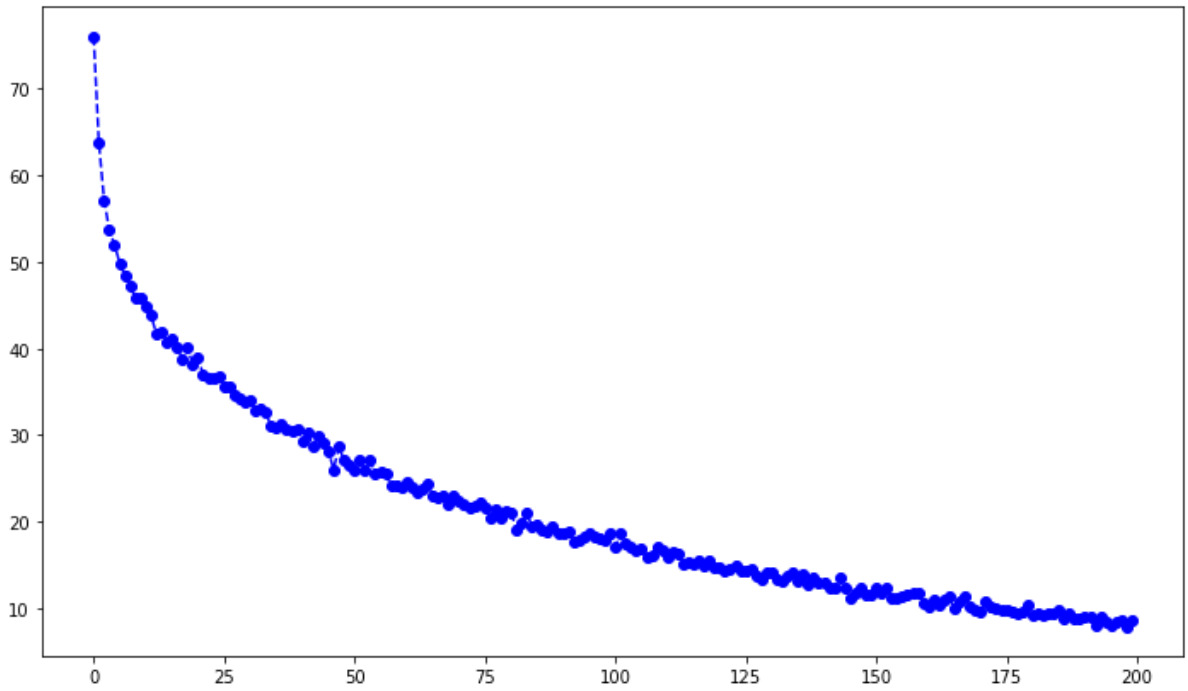
In [32]:
```
def k_means(X,k,max_it=1000000):
    it = 0
    m,n = X.shape #dataset size, number of features
    repeat = True
    'random initialization of clusters'
    clusters = np.random.randint(k,size=len(X)) # random assignment
    'means initialization'
    means = np.zeros((k,n))
    while repeat and it<=max_it: # repeat until clusters do not change or iter
ations > max_it
        it = it + 1
        'step 1: update means'
        for i in range(k):
            if len(X[clusters==i])!=0:
                means[i] = np.mean(X[clusters==i],axis=0)
            else: # if any of the cluster centers has no data points associate
d with it, replace it with a random data point
                idx = np.random.randint(m)
                means[i] = X[idx]
        'step 2: update clusters'
        new_clusters = np.argmin(np.array([np.linalg.norm(X-means[i],axis=1) f
or i in range(k)]),axis=0)
        'check whether clusters and new_clusters are equal or not'
        if sum(clusters!=new_clusters)==0:
            repeat = False
        clusters = new_clusters
    return clusters, means

def inertia(X,k,clusters,means):
    m = X.shape[0] #dataset size
    inertia = 0
    for i in range(k): # iterate over clusters
        distances = np.square(np.linalg.norm(X[clusters==i]-means[i],axis=1))
# distances from points in cluster i to cluster i mean
        inertia = inertia + np.sum(distances)
    inertia = inertia/m
    return inertia
```

In [33]:
```
'run k-means with different values for k'
largest_k = 200
k_list = [k+1 for k in range(largest_k)] # [1,2,3,...,largest_k]
inertia_list = []
for k in k_list:
    if k % 10 == 0:
        print(k)
    clusters, means = k_means(X_reduced,k)
    inertia_list.append(inertia(X_reduced,k,clusters,means))
```

```
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
```

In [34]:
```
plt.figure(figsize=(12,7))
plt.plot(inertia_list,'bo--')
```

Out[34]:
```
[<matplotlib.lines.Line2D at 0x1ed2e3d08c8>]
```



The optimal number of clusters is not clear on this inertia diagram, as there is no obvious elbow, so let's take k=100

In [35]:
```
k_best = 100
clusters,_ = k_means(X_reduced, k = k_best)
```

Let us visualize the clusters

In [36]:
```
for i in range(k_best):
    print("Cluster", i)
    n_faces = sum(clusters==i)
    n_cols = 5
    n_rows = (n_faces - 1) // n_cols + 1
    cluster_faces = X[clusters==i]
    #plt.figure(figsize=(10,10))
    for j in range(n_faces):
        face = cluster_faces[j].reshape(64,64)
        plt.subplot(n_rows, n_cols,j+1)
        plt.imshow(face,cmap='gray')
        plt.axis('off')
        plt.tight_layout()
    plt.show()
```

Cluster 0

Cluster 1

Cluster 2

Cluster 3

Cluster 4

Cluster 5

Cluster 6

Cluster 7

Cluster 8

Cluster 9

Cluster 10

Cluster 11

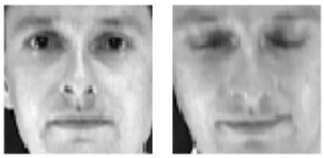
Cluster 12

Cluster 13

Cluster 14

Cluster 15

Cluster 16

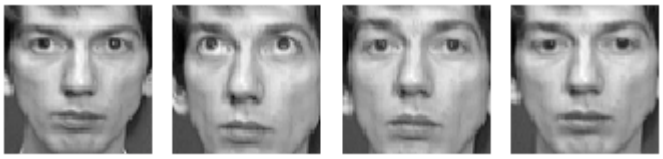


Cluster 17

Cluster 18

Cluster 19

Cluster 20



Cluster 21

Cluster 22

Cluster 23

Cluster 24

Cluster 25

Cluster 26

Cluster 27

Cluster 28

Cluster 29

Cluster 30

Cluster 31

Cluster 32

Cluster 33

Cluster 34

Cluster 35

Cluster 36

Cluster 37

Cluster 38

Cluster 39

Cluster 40

Cluster 41

Cluster 42

Cluster 43

Cluster 44

Cluster 45

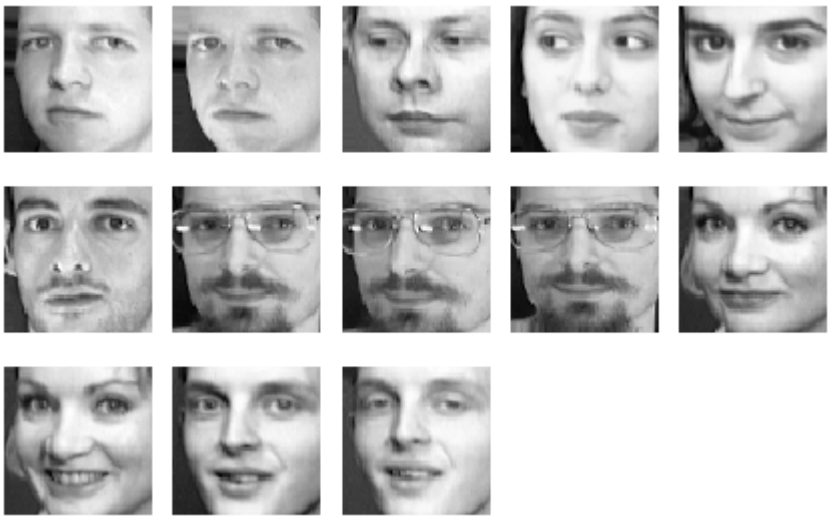
Cluster 46

Cluster 47

Cluster 48

Cluster 49

Cluster 50



Cluster 51

Cluster 52

Cluster 53

Cluster 54


Cluster 55




Cluster 56

Cluster 57

Cluster 58

Cluster 59

Cluster 60

Cluster 61

Cluster 62

Cluster 63

Cluster 64

Cluster 65

Cluster 66

Cluster 67

Cluster 68

Cluster 69

Cluster 70

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Cluster 92

Cluster 93

Cluster 94

Cluster 95

Cluster 96

Cluster 97

Cluster 98

```
Cluster 99
```

You should see similar faces in each cluster

In [ ]: