Unsupervised Learning : K-means Clustering and PCA

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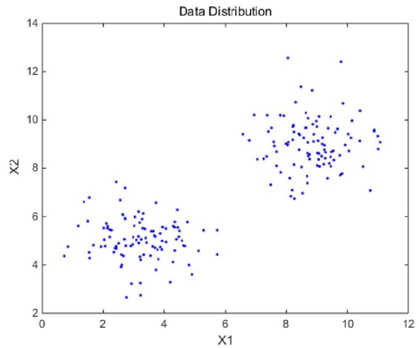
1. K-means Clustering

To see how it works, click here (http://i-systems.github.io/HSE545/machine%20learning%20all/05%20Clustering/iSystems_01_K-means_Clustering.html)

Unsupervised Learning

- Data clustering is an unsupervised learning problem
- Given:
  - m unlabeled examples $\{x^{(1)}, x^{(2)} \cdots, x^{(m)}\}$
  - the number of partitions k
- Goal: group the examples into k partitions



$$\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\} \quad \Rightarrow \quad \text{Clustering}$$

- the only information clustering uses is the similarity between examples
- clustering groups examples based of their mutual similarities
- A good clustering is one that achieves:
  - high within-cluster similarity
  - low inter-cluster similarity

1.1. (Iterative) Algorithm

Randomly initialize k cluster centroids $\mu_1, \mu_2, \cdots, \mu_k \in \mathbb{R}^n$

Repeat{
  for $i = 1$ to m
    $c_i :=$ index (from 1 to k) of cluster centroid closest to $x^{(i)}$
  for $k = 1$ to k
    $\mu_k :=$ average (mean) of points assigned to cluster k
}

1.2. Python code

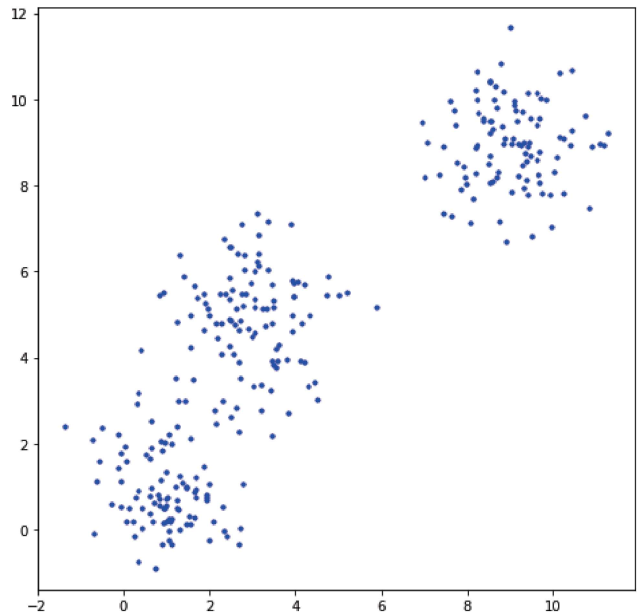
Data Load

- kmeans_example 예제 데이터는 아래 링크에서 다운로드
  - kmeans_example.pkl (data_files/kmeans_example.pkl)

```
In [1]: import matplotlib.pyplot as plt
        from six.moves import cPickle

        X = cPickle.load(open('./data_files/kmeans_example.pkl','rb'))

        plt.figure(figsize=(8,8))
        plt.plot(X[:,0],X[:,1],'b.')
        plt.axis('equal')
        plt.show()
```



K-means clustering

```
In [2]: from sklearn.cluster import KMeans

        kmeans = KMeans(n_clusters = 3, random_state = 0)
        kmeans.fit(X)
```

```
Out[2]: KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
            n_clusters=3, n_init=10, n_jobs=1, precompute_distances='auto',
            random_state=0, tol=0.0001, verbose=0)
```

```
In [3]: print(kmeans.labels_)
```

```
[2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
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 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1]
```
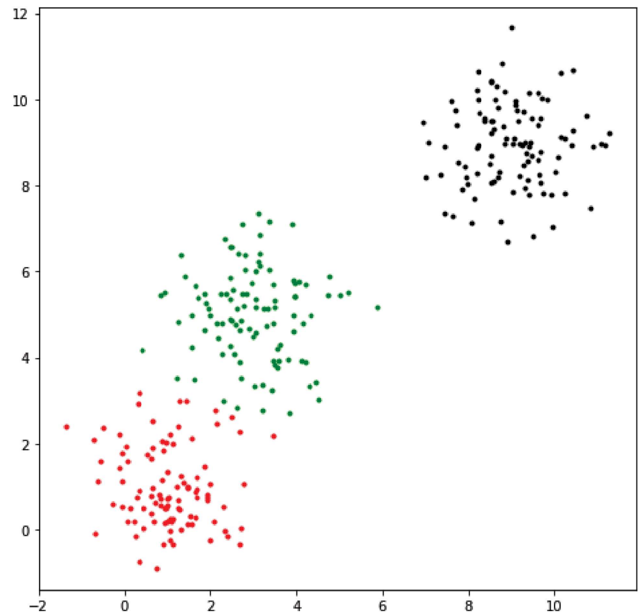
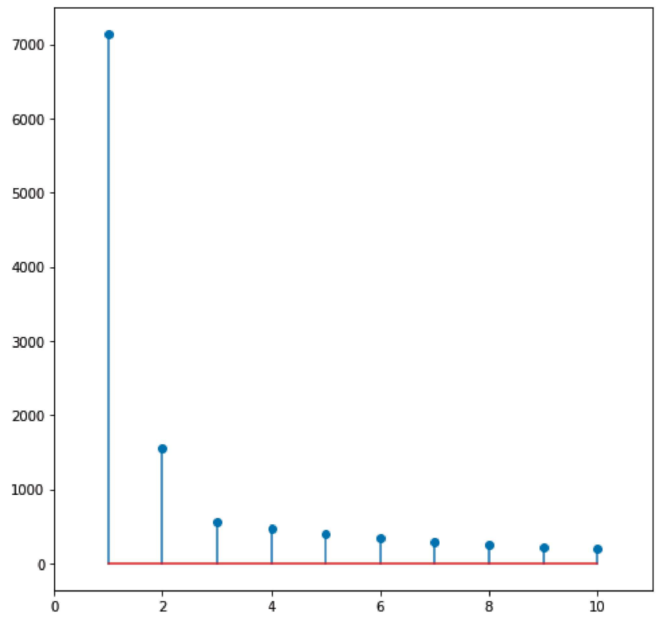

```
In [4]: plt.figure(figsize=(8,8))
        # plt.hold(True)

        plt.plot(X[kmeans.labels_ == 0,0],X[kmeans.labels_ == 0,1],'g.')
        plt.plot(X[kmeans.labels_ == 1,0],X[kmeans.labels_ == 1,1],'k.')
        plt.plot(X[kmeans.labels_ == 2,0],X[kmeans.labels_ == 2,1],'r.')

        plt.axis('equal')
        plt.show()
```



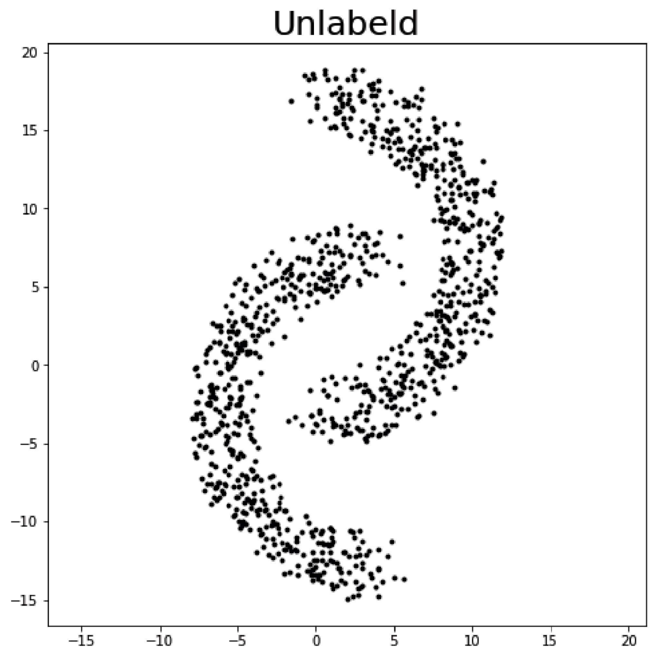
1.3. Choosing the Number of Clusters

- Idea: when adding another cluster does not give much better modeling of the data
- One way to select k for the K-means algorithm is to try different values of k, plot the K-means objective versus k, and look at the 'elbow-point' in the plot

In [5]:
```
cost = []
for i in range(1,11):
    kmeans = KMeans(n_clusters=i, random_state=0).fit(X)
    cost.append(abs(kmeans.score(X)))

plt.figure(figsize=(8,8))
plt.stem(range(1,11),cost)
plt.xlim([0, 11])
plt.show()
```



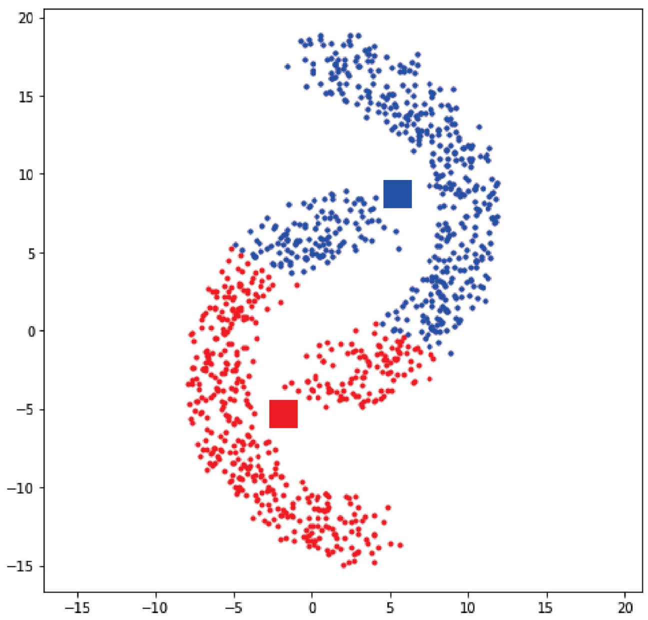
In [6]:
```
from six.moves import cPickle
X = cPickle.load(open('./data_files/kmeans_lim.pkl','rb'))

plt.figure(figsize=(8,8))
plt.axis('equal')
plt.plot(X[:,0], X[:,1],'k.')
plt.title('Unlabeld', fontsize='25')
plt.show()
```



1.4. K-means: Limitations

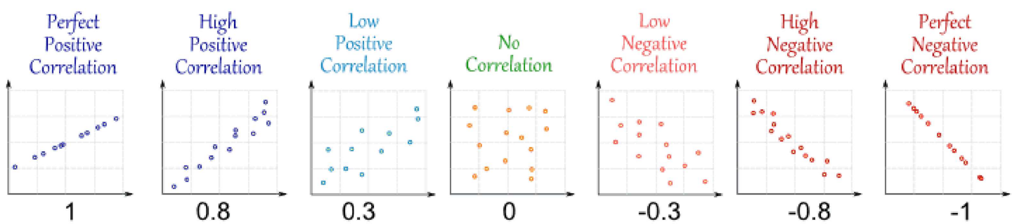
- kmeans_lim 예제 데이터는 아래 링크에서 다운로드
  - kmeans_lim.pkl (data_files/kmeans_lim.pkl)

In [7]:
```
kmeans = KMeans(n_clusters=2, random_state=0).fit(X)

plt.figure(figsize=(8,8))
# plt.hold(True)

plt.axis('equal')
plt.plot(X[kmeans.labels_ == 0,0],X[kmeans.labels_ == 0,1],'r.')
plt.plot(kmeans.cluster_centers_[0][0], kmeans.cluster_centers_[0]
[1],'rs',markersize=20)

plt.plot(X[kmeans.labels_ == 1,0],X[kmeans.labels_ == 1,1],'b.')
plt.plot(kmeans.cluster_centers_[1][0], kmeans.cluster_centers_[1]
[1],'bs',markersize=20)
plt.show()
```

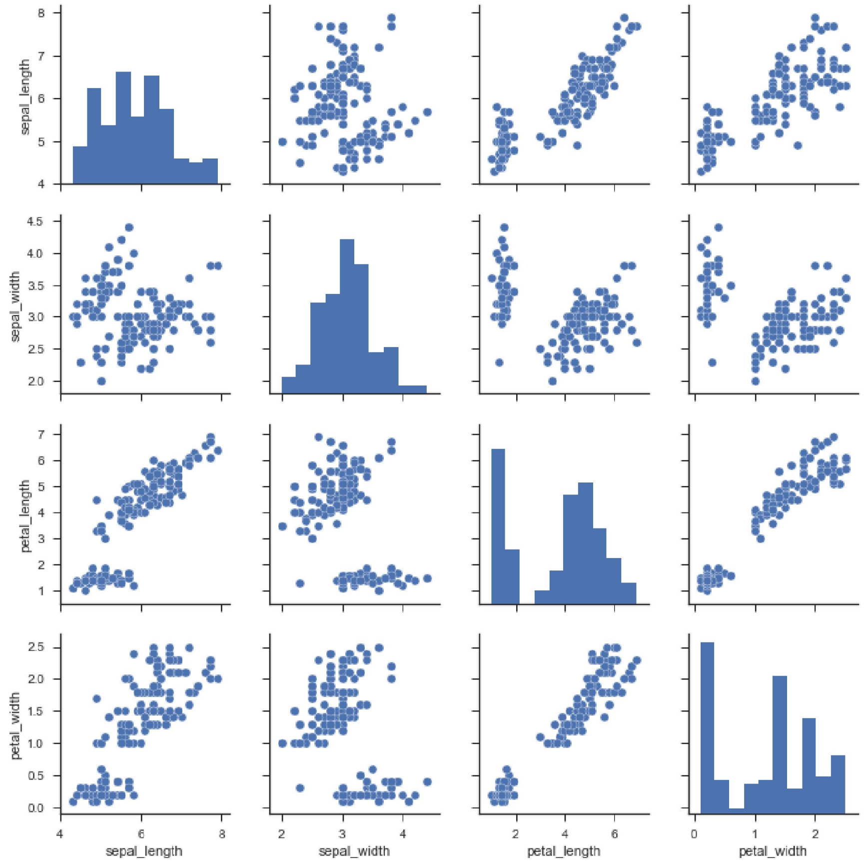


2. Correlation Analysis

- Statistical relationship between two sets of data
- http://rpsychologist.com/d3/correlation/ (http://rpsychologist.com/d3/correlation/)



In [8]:
```
import numpy as np
import seaborn as sns
%matplotlib inline

sns.set(style="ticks", color_codes=True)
iris = sns.load_dataset("iris")

g = sns.pairplot(iris)
# sns.plt.show()
```



3. Principal Component Analysis (PCA)

Motivation: Can we describe high-dimensional data in a "simpler" way?

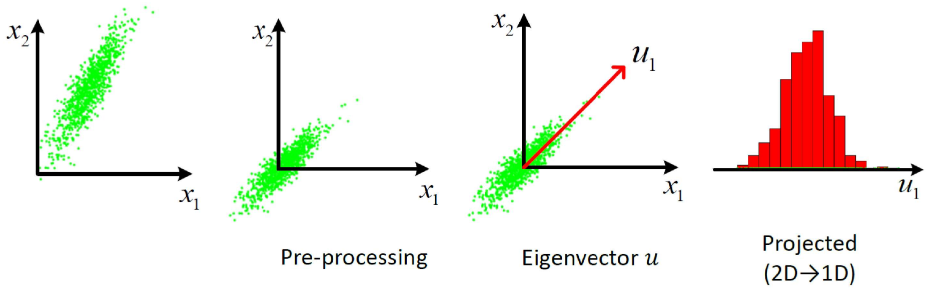
→ Dimension reduction without losing too much information
→ Find a low-dimensional, yet useful representation of the data

3.1. Dimension Reduction method ($n \to k$)

1. Choose top k (orthonormal) eigenvectors, $U = [u_1, u_2, \cdots, u_k]$
2. Project x_i onto span $\{u_1, u_2, \cdots, u_k\}$

$$z^{(i)} = \begin{bmatrix} u_1^T x^{(i)} \\ u_2^T x^{(i)} \\ \vdots \\ u_k^T x^{(i)} \end{bmatrix} \quad \text{or} \quad z = U^T x$$

- Pictorial summary of PCA



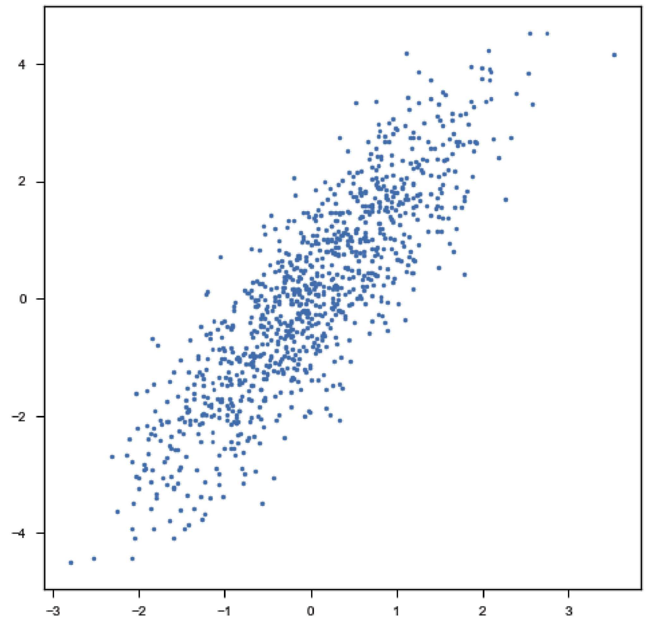
$x^{(i)} \to$ projection onto unit vector $u \implies u^T x^{(i)} =$ distance from the origin along u

3.2. Python code

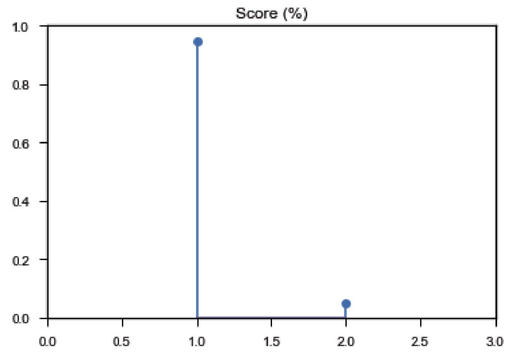
- pca_example 예제 데이터는 아래 링크를 통해 받을 수 있습니다.
  - pca_example.pkl (data_files/pca_example.pkl)

In [9]:

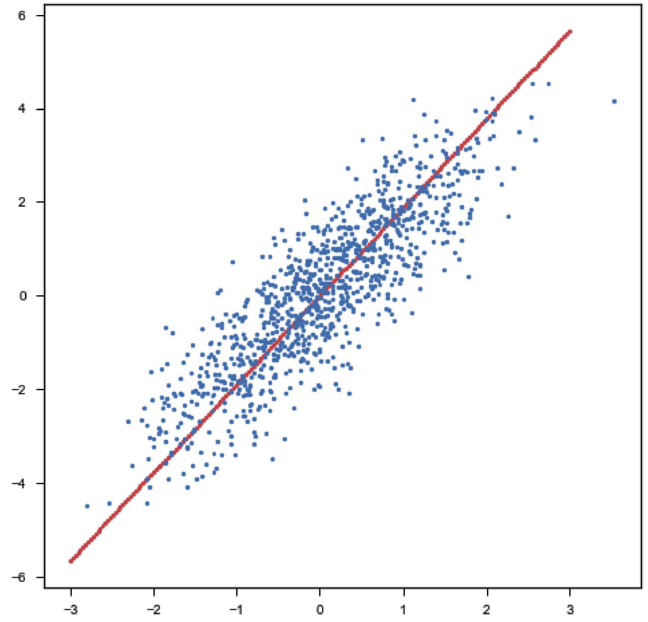
```
import numpy as np
import matplotlib.pyplot as plt
from six.moves import cPickle
%matplotlib inline

X = cPickle.load(open('./data_files/pca_example.pkl','rb'))
plt.figure(figsize=(8, 8))
plt.plot(X[:, 0], X[:, 1],'b.')
plt.show()
```



In [10]:
```
from sklearn.decomposition import PCA

# Apply PCA
pca = PCA(n_components=2)
pca.fit(X)

plt.figure()
plt.stem(range(1,3), pca.explained_variance_ratio_)
plt.xlim([0, 3])
plt.ylim([0, 1])
plt.title('Score (%)')
plt.show()
```



In [11]:
```
# Nomalization and calculate gradient
principal_axis = pca.components_[0, :]
u1 = principal_axis/(np.linalg.norm(principal_axis))
h = u1[1]/u1[0]

x = np.linspace(-3,3,200)
plt.figure(figsize=(8, 8))
# plt.hold(True)
plt.plot(x,x.dot(h),'r.')
plt.plot(X[:, 0], X[:, 1],'b.')
plt.show()
```



In [12]:
```
pca = PCA(n_components=1)
pca.fit(X)
reduced_coordinate = pca.fit_transform(X)
plt.hist(reduced_coordinate, 15)
plt.show()
```