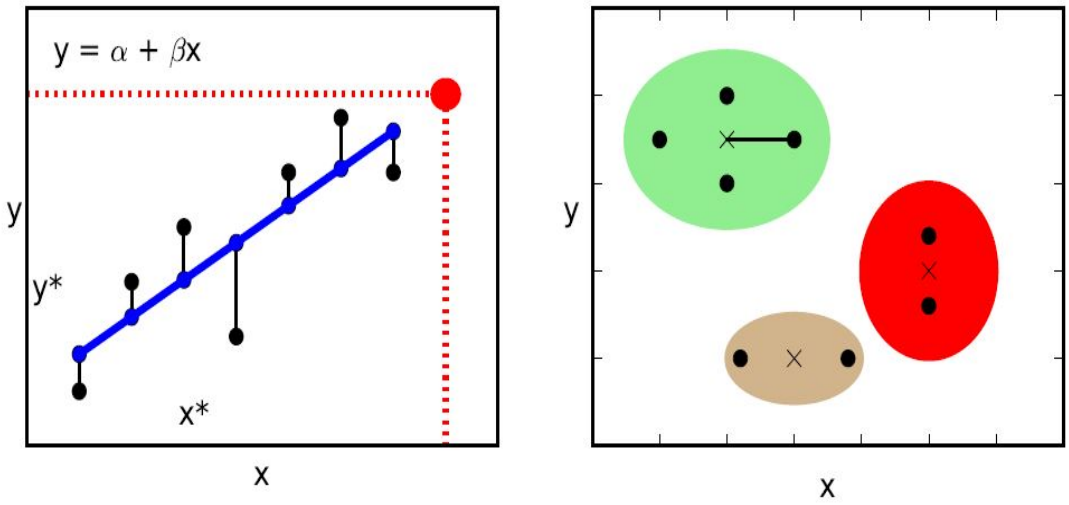
# $k$-means

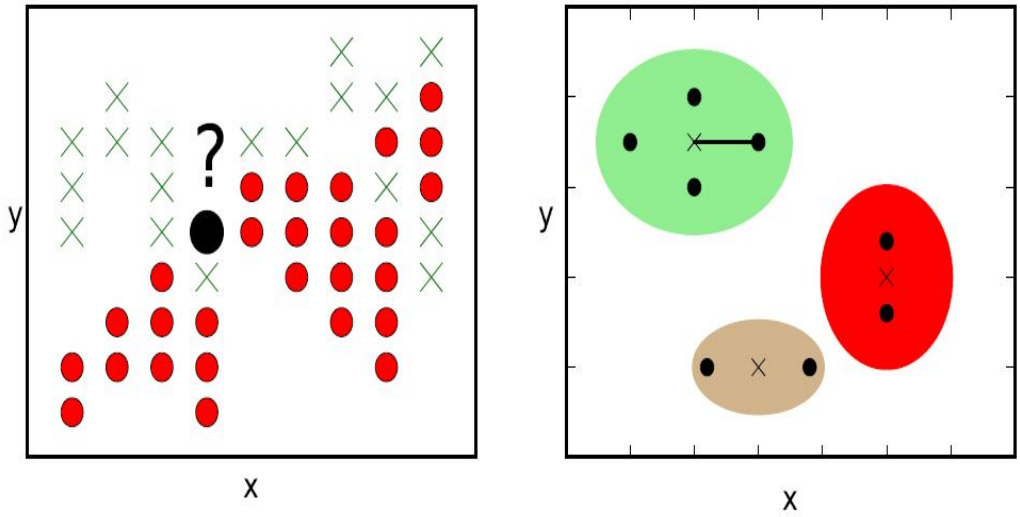
# Clustering

# Prediction vs. Classification




- two main goals in machine learning

# Classification with Clustering

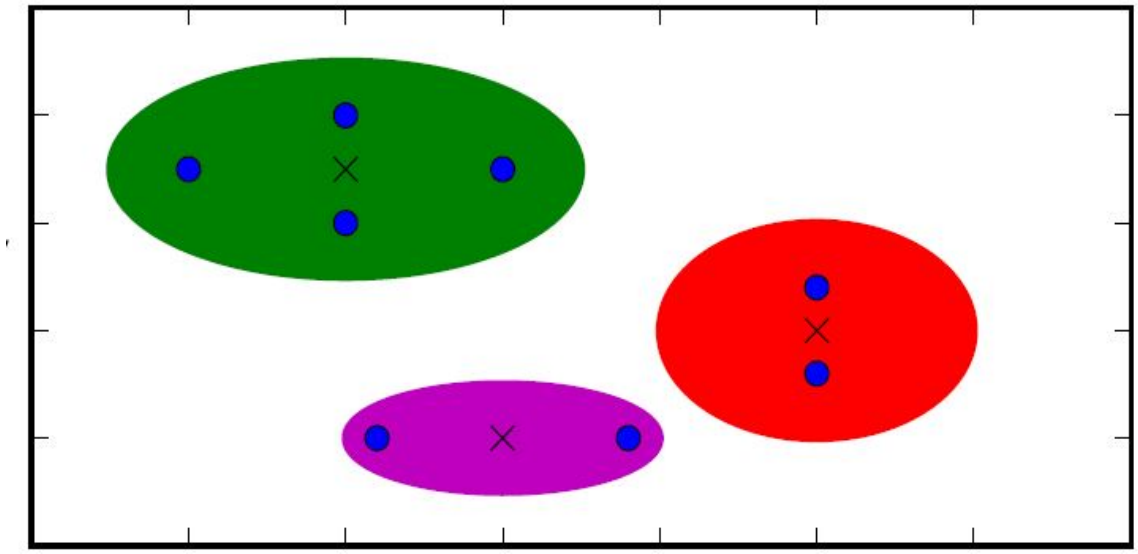



- split objects into clusters
- describe clusters by centroids
- need similarity (distance)
- most widely used: $k$-means

# $k$-means Clustering

- unlabeled data
- assume distances between points
- goal: split data into $k$ disjoint groups
- points in each cluster are closer to its center than to other centers
- computes allocation by iteration

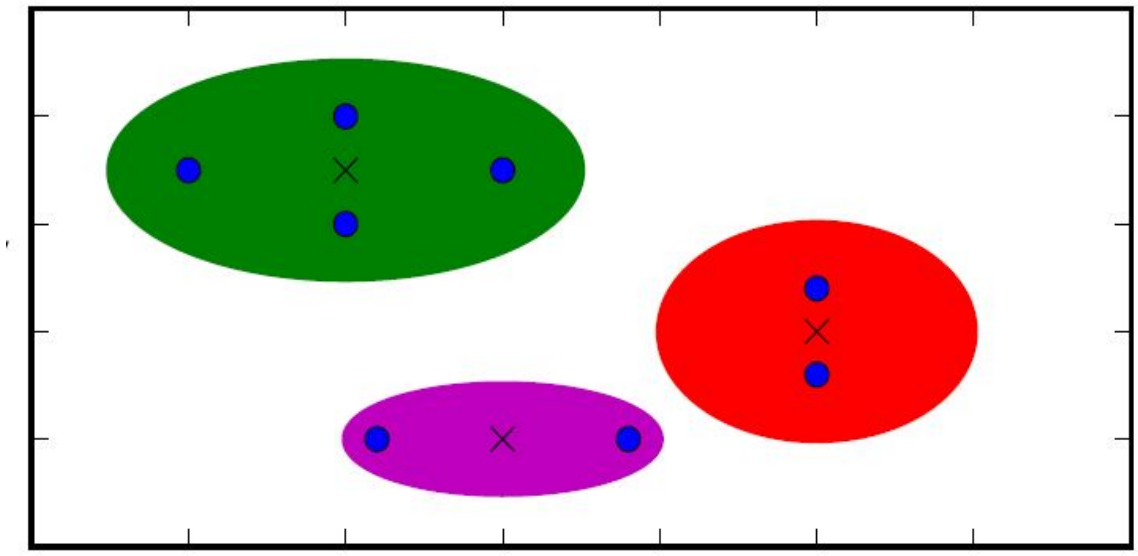
# Formal Description



- $N$ data points $x_1, \ldots, x_N$
- $k$ clusters $C_1, \ldots, C_k$
- want to minimize "inertia"

$$E = \sum_{j=1}^{k} \left( \sum_{x \in C_i} ||x - \mu(C_i)||^2 \right)$$

# Formal Description



- point $x$ is assigned to $C_i$ with min. distance to $\mu(C_i)$
- default distance is Euclidean

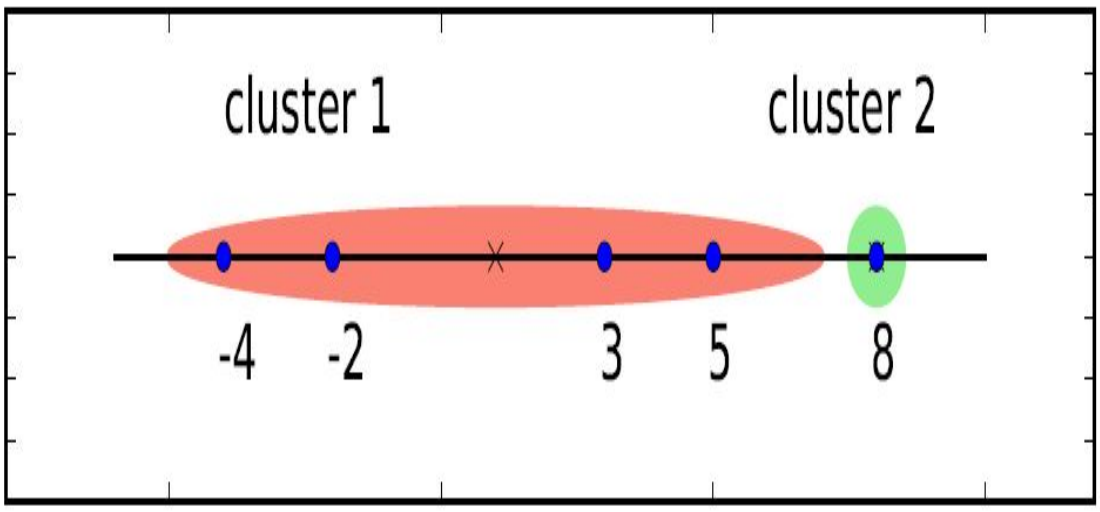
# $k$-means Algorithm

1. choose $k$ initial centroids
2. assign points to nearest centroids
3. recalculate centroids
4. repeat steps 2 and 3 until no more updates to clusters are possible

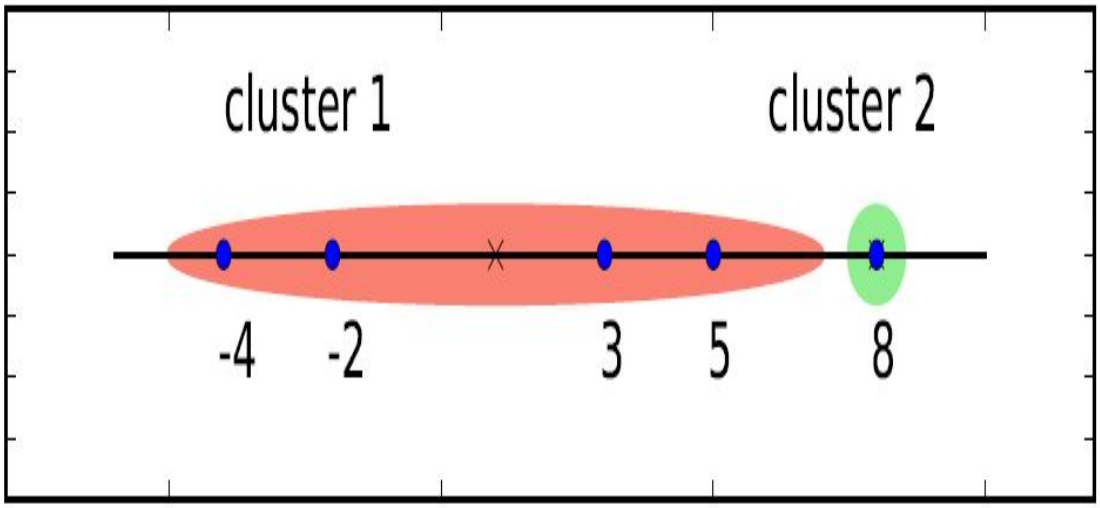
- $k$-means algorithm is guaranteed to converge

# A Simple Example

- 5 points: $-4, -2, 3, 5, 8$
- choose initial clusters:
  $c_1 = \{-4, -2, 3, 5\}, \quad c_2 = \{8\}$



# Initial Centers & Inertia

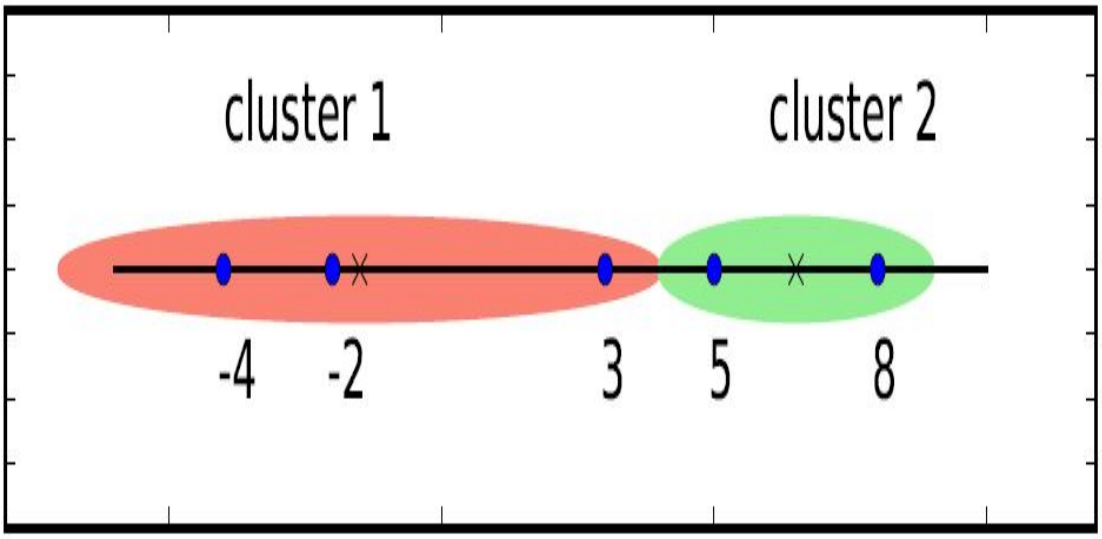



$$\mu_1 = \frac{(-4-2+3+5)}{4} = 0.5$$

$$\mu_2 = 8$$

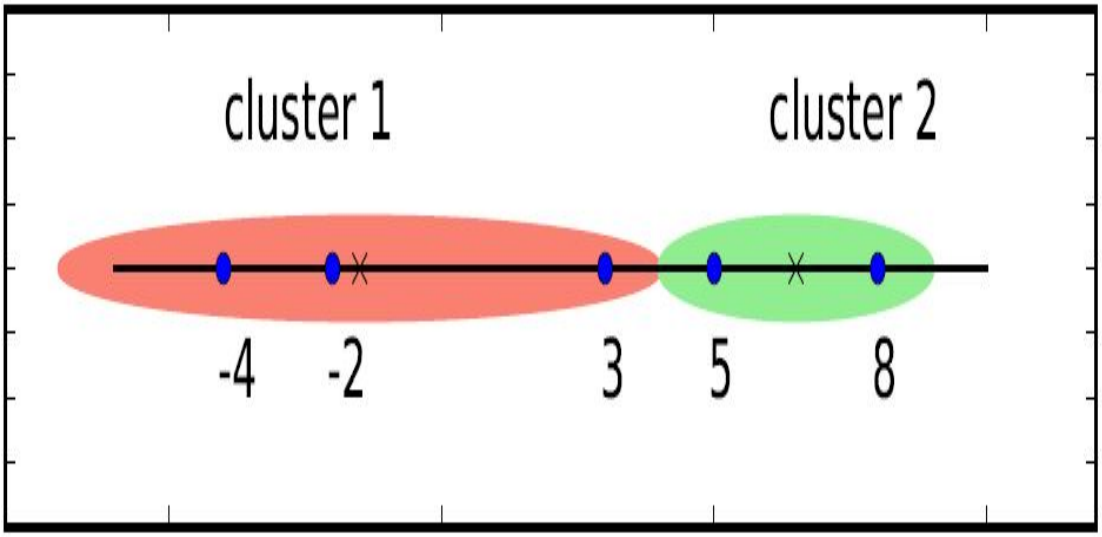
$$E = [(-4-0.5)^2 + (-2-0.5)^2 + (3-0.5)^2 + (5-0.5)^2] + [(8-8)^2] = 53$$

# Updating Clusters




- 5 is closer to $\mu_2 = 8$ than to $\mu_1 = 0.5$
- re-assign 5 to cluster $C_2$
- need to update $\mu_1$ and $\mu_2$

# New Centers & Inertia

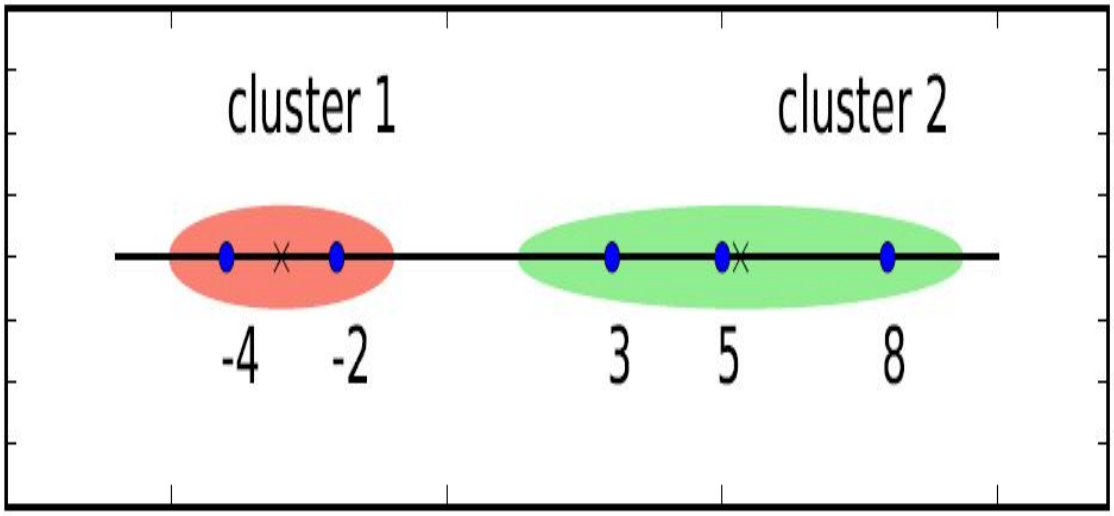



$$\mu_1 = \frac{(-4-2+3)}{3} = -1$$

$$\mu_2 = \frac{(5+8)}{2} = 6.5$$

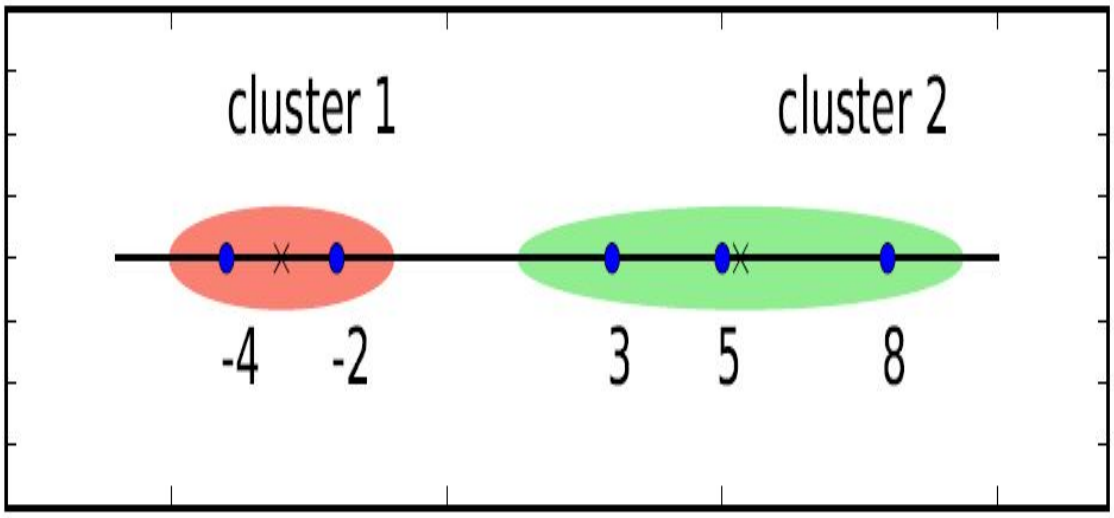
$$\begin{aligned} E = &[(-4-(-1))^2 + (-2-(-1))^2 \\ &+ (3-(-1))^2] + [(5-6.5)^2] \\ &+ [(8-6.5)^2] = 30.5 \end{aligned}$$

# Updating Clusters




- 3 is closer to $\mu_2 = 6.5$ than to $\mu_1 = -1$
- re-assign 3 to cluster $C_2$
- need to update $\mu_1$ and $\mu_2$

# New Centers & Inertia

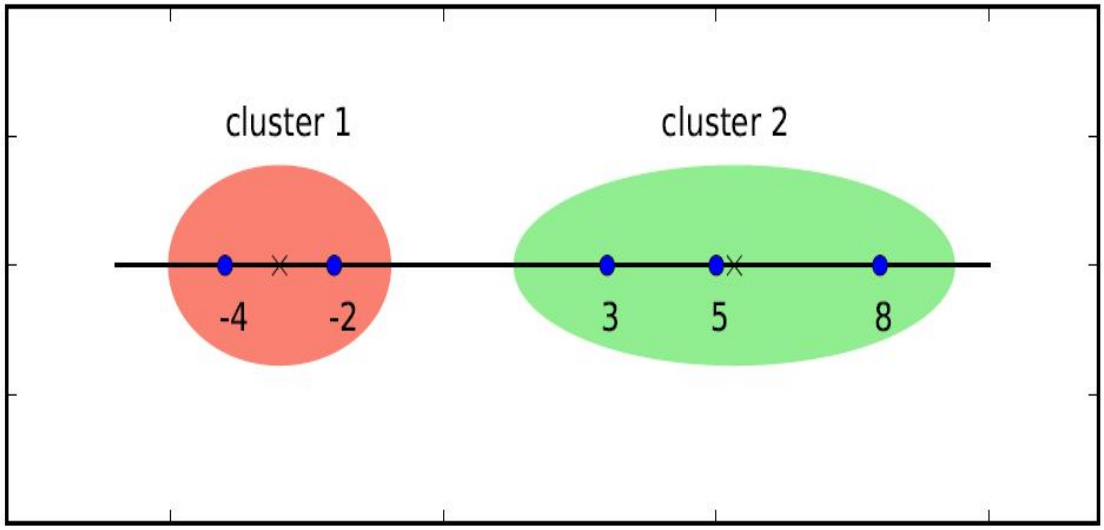



$$\mu_1 = \frac{(-4-2)}{2} = -3$$

$$\mu_2 = \frac{(3+5+8)}{3} = 5.3$$

$$\begin{aligned} E = &[(-4-(-3))^2 + (-2-(-3))^2] \\ &+ [(3-5.3)^2] + (5-5.3)^2] \\ &+ [(8-5.3)^2] = 14.7 \end{aligned}$$

# Final Allocation



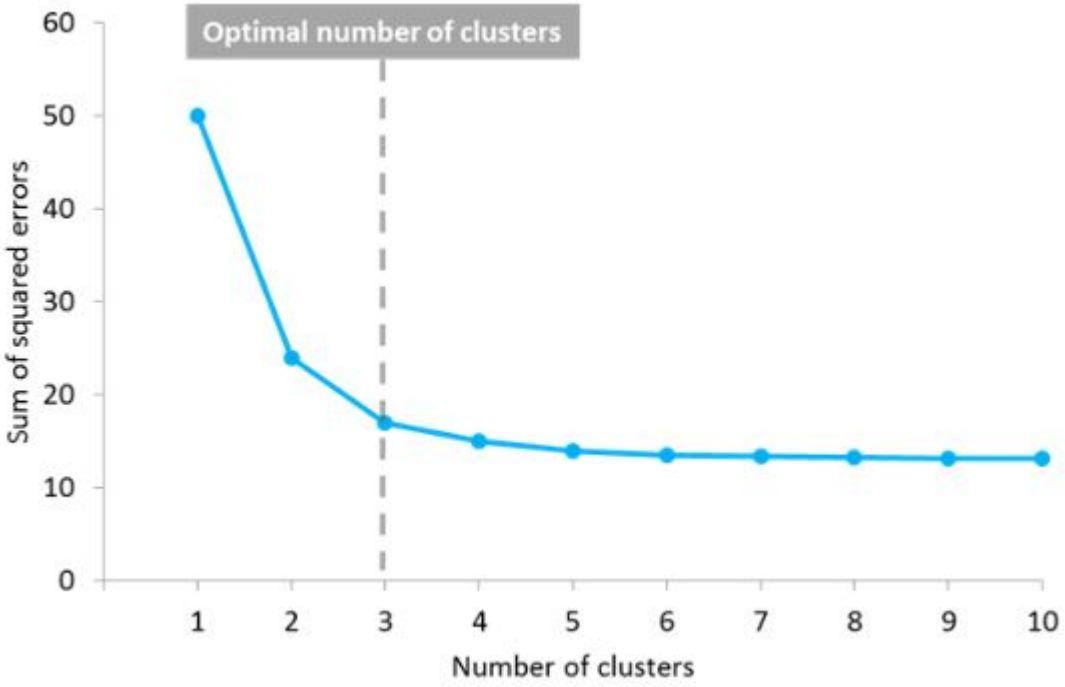

- no points need to be re-allocated
- this is final allocation

$$c_1 = \{-4, -2\}, \quad c_2 = \{3, 5, 8\}$$

# Notes on the Algorithm

- optimal solution is intractable
- allocation depends on the choice of initial clusters
- want moderate values of $k$
- $k$ is typically chosen visually by the "knee" method

# "Knee" Method




- visual inspection
- no significant decrease in "loss" function beyond some $k$

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# Initial Centroids

- allocation depends on the choice of initial clusters
- how do we choose?

(a) random $k$ data points

(b) $k$-means++: choose first at random, assign others as far from chosen centraoids as possible

# A Numerical Dataset

| object $x_i$ | Height (H) | Weight (W) | Foot (F) | Label (L) |
|---|---|---|---|---|
| $x_1$ | 5.00 | 100 | 6 | green |
| $x_2$ | 5.50 | 150 | 8 | green |
| $x_3$ | 5.33 | 130 | 7 | green |
| $x_4$ | 5.75 | 150 | 9 | green |
| $x_5$ | 6.00 | 180 | 13 | red |
| $x_6$ | 5.92 | 190 | 11 | red |
| $x_7$ | 5.58 | 170 | 12 | red |
| $x_8$ | 5.92 | 165 | 10 | red |

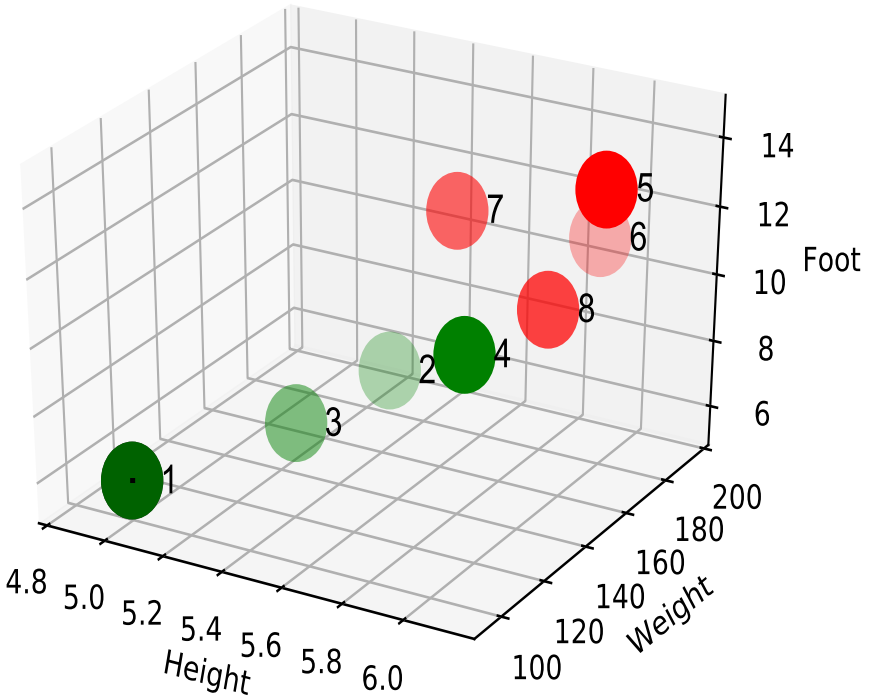
- $N = 8$ items
- $M = 3$ (unscaled) attributes

# Code for the Dataset

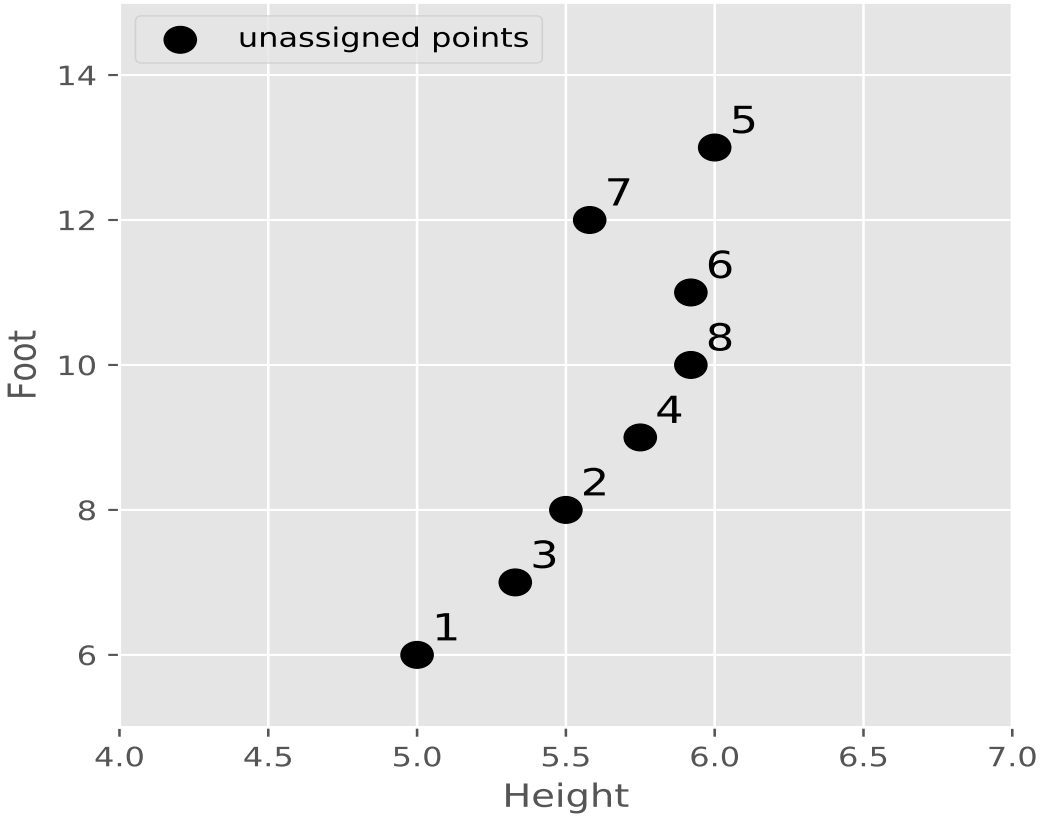
```
import pandas as pd
data = pd.DataFrame(
        {'id': [ 1,2,3,4,5,6,7,8],
        'Label': ['green','green','green','green',
                  'red','red','red','red'],
        'Height': [5, 5.5, 5.33, 5.75,
                   6.00, 5.92,  5.58, 5.92],
        'Weight': [100, 150, 130, 150,
                   180, 190, 170, 165],
        'Foot': [6, 8, 7, 9, 13, 11, 12, 10]},
         columns = ['id', 'Height', 'Weight',
                    'Foot', 'Label'] )
```

```
ipdb> data
  id Height Weight Foot Label
0  1   5.00    100    6  green
1  2   5.50    150    8  green
2  3   5.33    130    7  green
3  4   5.75    150    9  green
4  5   6.00    180   13    red
5  6   5.92    190   11    red
6  7   5.58    170   12    red
7  8   5.92    165   10    red
```

# A Dataset Illustration

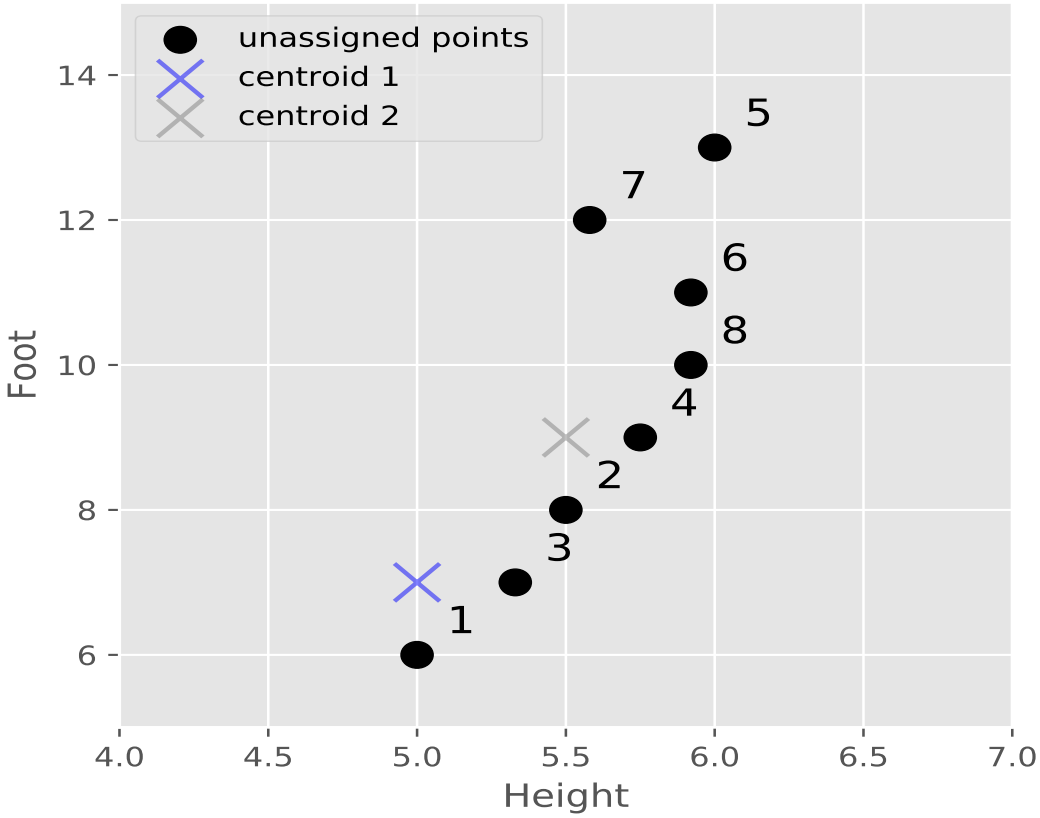


# Initial Dataset



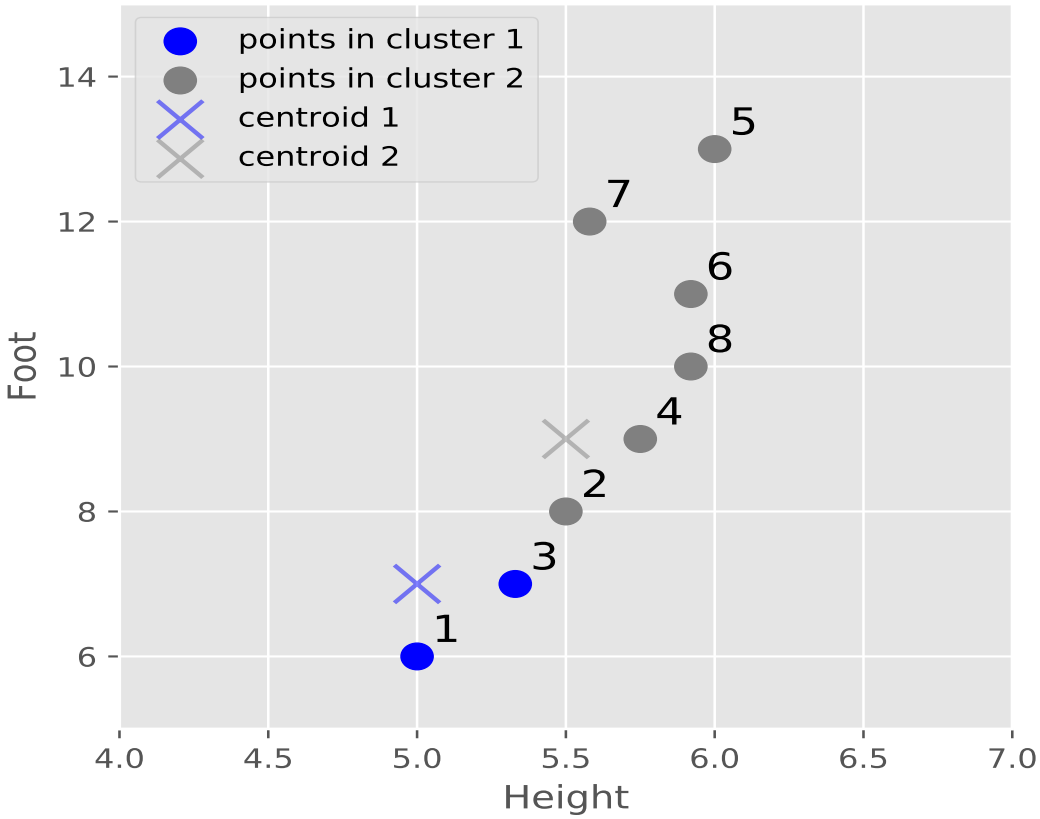

- points are not labelled
- want to split into $k = 2$ clusters

# Initial Centroids




- difficult problem to choose
- solution may depend on this choice

# Initial Assignment




- can assign at random

$$C_1 = (5.0,\ 7.0), \quad C_2 = (5.5,\ 9.0)$$

# A Initial Assignment

$$C_1 = (5.0,\ 7.0), \quad C_2 = (5.5,\ 9.0)$$

| $x_i$ | Height (H) | Foot (F) | Cluster $C_k$ |
|---|---|---|---|
| $x_1$ | 5.00 | 6 | 1 |
| $x_2$ | 5.50 | 8 | 2 |
| $x_3$ | 5.33 | 7 | 1 |
| $x_4$ | 5.75 | 9 | 2 |
| $x_5$ | 6.00 | 13 | 2 |
| $x_6$ | 5.92 | 11 | 2 |
| $x_7$ | 5.58 | 12 | 2 |
| $x_8$ | 5.92 | 10 | 2 |

# Distances for Initial Assignment

| $x_i$ | H | F | $C$ | $d(x_i, C_1)$ | $d(x_i, C_2)$ | $C'$ |
|---|---|---|---|---|---|---|
| $x_1$ | 5.00 | 6 | 1 | 1.00 | 3.04 | 1 |
| $x_2$ | 5.50 | 8 | 2 | 1.12 | 1.00 | 2 |
| $x_3$ | 5.33 | 7 | 1 | 0.33 | 2.01 | 1 |
| $x_4$ | 5.75 | 9 | 2 | 2.13 | 0.25 | 2 |
| $x_5$ | 6.00 | 13 | 2 | 6.08 | 4.03 | 2 |
| $x_6$ | 5.92 | 11 | 2 | 4.10 | 2.04 | 2 |
| $x_7$ | 5.58 | 12 | 2 | 5.03 | 3.00 | 2 |
| $x_8$ | 5.92 | 10 | 2 | 3.14 | 1.08 | 2 |

- need to compute $\mu(C_1)$, $\mu(C_2)$
- may need to update $C_1$, $C_2$

# Updating Centroids for Initial Assignment

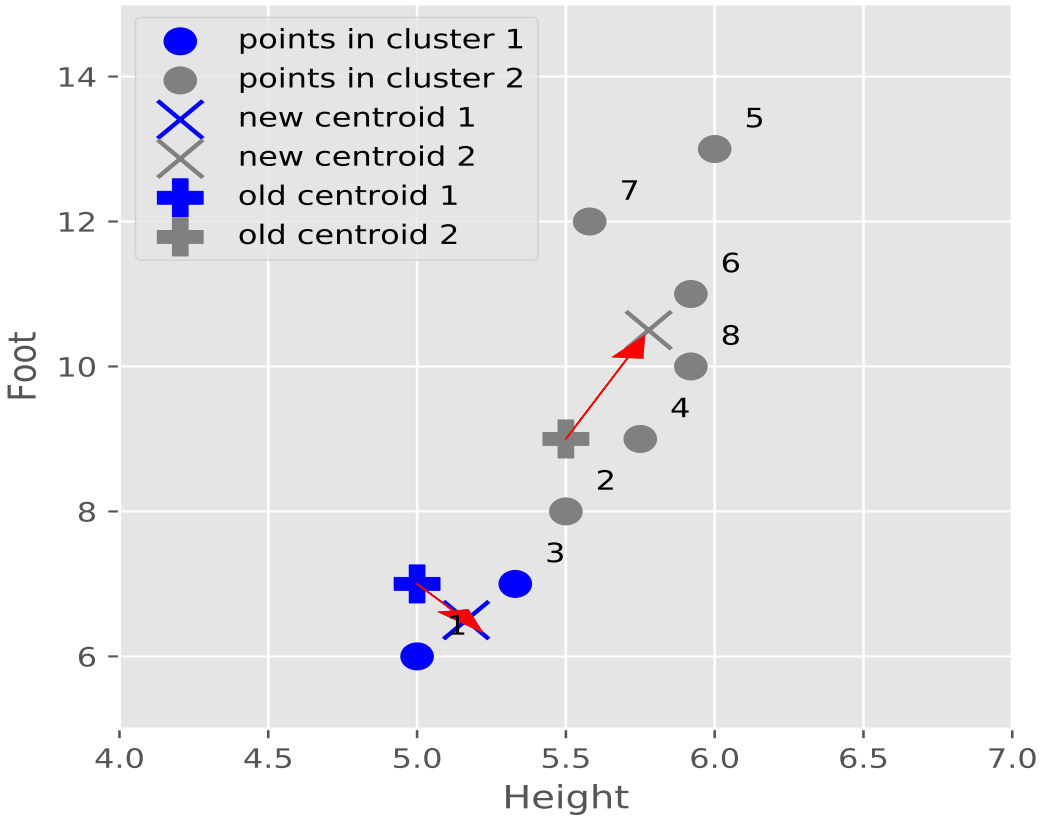
- cluster 1 has two points: $x_1, x_3$

$$C_1 = \frac{(x_1 + x_3)}{2} = \frac{(5, 6) + (5.33, 7)}{2}$$
$$= (5.17,\ 6.5)$$

- cluster 2 has 6 points: $x_2, x_4, x_5, x_6, x_7, x_8$

$$C_2 = \frac{(x_2 + x_4 + x_5 + x_6 + x_7 + x_8)}{6}$$
$$= (5.78,\ 10.5)$$

# Updating Centroids




$$C_1 : \ (5.0,\ 7) \mapsto (5.17,\ 6.5)$$
$$C_2 : \ (5.5,\ 9) \mapsto (5.78,\ 10.5)$$

# How to re-assign Points to Clusters

- $C_1 = (5.17,\ 6.5)$, $C_2 = (5.78,\ 10.5)$
- for each $x_i$, assign it to cluster $C_k$ with minimum $d(x_i, C_k)$
- for point $x_1 = (5,\ 6)$:

$$d(x_1, C_1) = \sqrt{(5 - 5.17)^2 + (6 - 6.5)^2} = 0.53$$
$$d(x_1, C_2) = \sqrt{(5 - 5.78)^2 + (6 - 10.5)^2} = 4.57$$

$\Rightarrow x_1$ remains in cluster 1

- for point $x_2 = (5.5,\ 8)$:

$$d(x_2, C_1) = \sqrt{(5.5 - 5.17)^2 + (8 - 6.5)^2} = 1.54$$
$$d(x_2, C_2) = \sqrt{(5.5 - 5.78)^2 + (8 - 10.5)^2} = 2.52$$

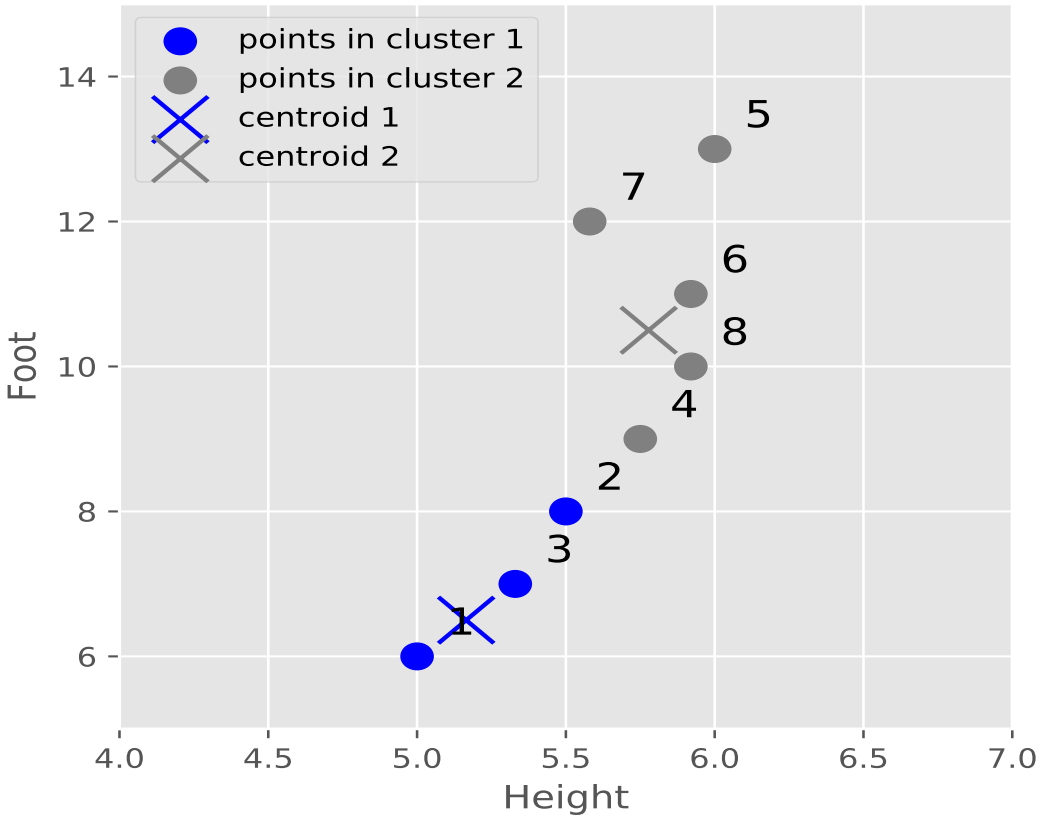
$\Rightarrow x_2$ is re-assigned to cluster 1

# Re-assigning Points to Clusters

| $x_i$ | H | F | $C$ | $d(x_i, C_1)$ | $d(x_i, C_2)$ | $C'$ | updated |
|---|---|---|---|---|---|---|---|
| $x_1$ | 5.00 | 6 | 1 | 0.53 | 4.57 | 1 | no |
| $x_2$ | 5.50 | 8 | 2 | 1.54 | 2.52 | 1 | yes |
| $x_3$ | 5.33 | 7 | 1 | 0.53 | 3.53 | 1 | no |
| $x_4$ | 5.75 | 9 | 2 | 2.57 | 1.50 | 2 | no |
| $x_5$ | 6.00 | 13 | 2 | 6.55 | 2.51 | 2 | no |
| $x_6$ | 5.92 | 11 | 2 | 4.56 | 0.52 | 2 | no |
| $x_7$ | 5.58 | 12 | 2 | 5.52 | 1.51 | 2 | no |
| $x_8$ | 5.92 | 10 | 2 | 3.58 | 0.52 | 2 | no |

- if some points are re-assigned to new cluster(s) then we need to compute new centroids

# New Assignment




- compute distances to each center
- re-assign points to clusters

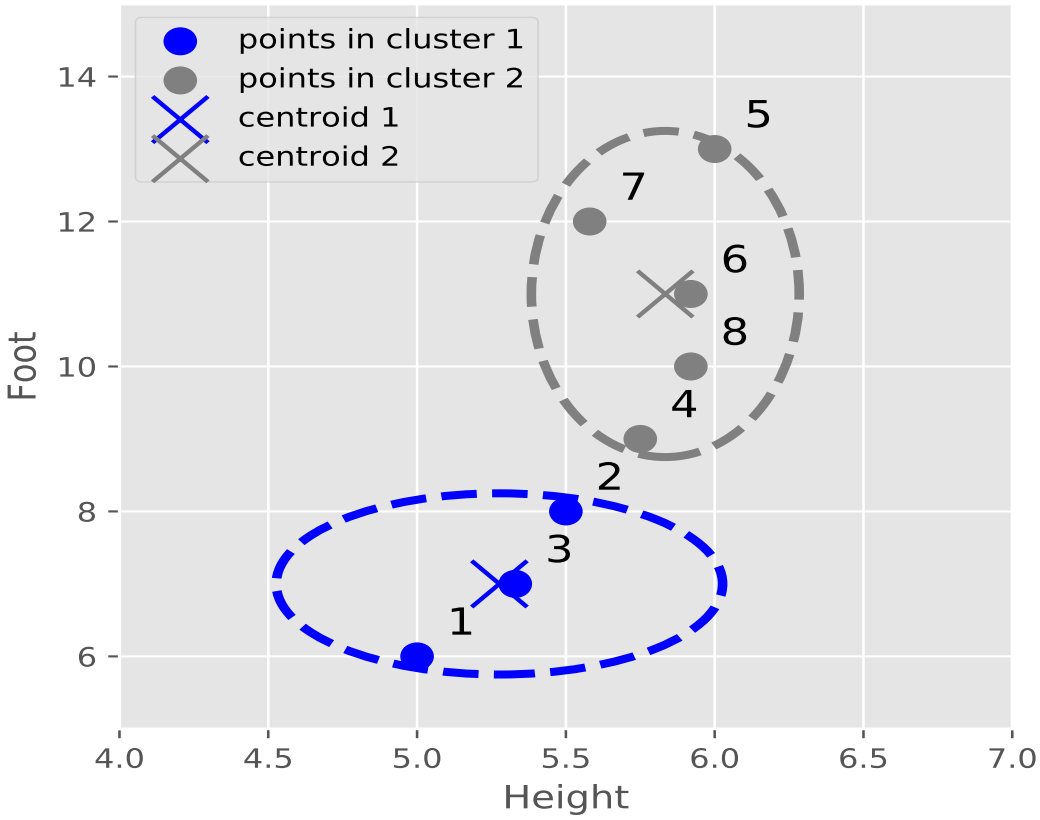
# Final Assignment

- $C_1 = (5.28,\ 7), C_2 = (5.83,\ 11)$

| $x_i$ | H | F | $C$ | $d(x_i, C_1)$ | $d(x_i, C_2)$ | $C'$ | updated |
|---|---|---|---|---|---|---|---|
| $x_1$ | 5.00 | 6 | 1 | 1.04 | 5.07 | 1 | no |
| $x_2$ | 5.50 | 8 | 1 | 1.02 | 3.02 | 1 | no |
| $x_3$ | 5.33 | 7 | 1 | 0.05 | 4.03 | 1 | no |
| $x_4$ | 5.75 | 9 | 2 | 2.06 | 2.00 | 2 | no |
| $x_5$ | 6.00 | 13 | 2 | 6.04 | 2.01 | 2 | no |
| $x_6$ | 5.92 | 11 | 2 | 4.05 | 0.09 | 2 | no |
| $x_7$ | 5.58 | 12 | 2 | 5.01 | 1.03 | 2 | no |
| $x_8$ | 5.92 | 10 | 2 | 3.07 | 1.00 | 2 | no |

- points cannot be updated
- this is the final clustering

# Final Assignment




- points allocated to right cluster
- no more updates are possible

# $k$-means in Python

- many parameters
- can specify number of clusters and initial centroids
- computes the cluster labels, centroids and inertia
- can choose best algorithm out of n_init different initalizations

# Python Code

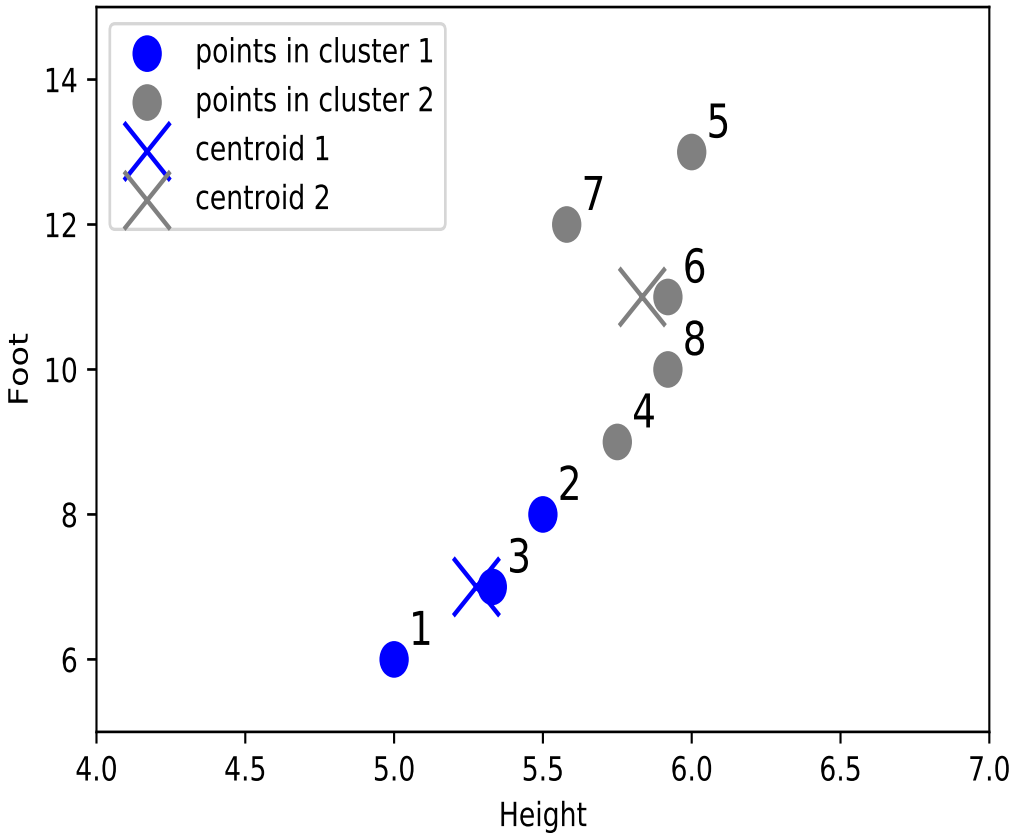
```
import pandas as pd
import numpy as np
from sklearn.cluster import KMeans

data = pd.DataFrame(
    {'id': [ 1,2,3,4,5,6,7,8],
     'Label': ['green', 'green', 'green', 'green', 'red',
                                          'red', 'red', 'red'],
     'Height': [5, 5.5, 5.33, 5.75, 6.00, 5.92,  5.58, 5.92],
     'Weight': [100, 150, 130, 150, 180, 190, 170, 165],
     'Foot': [6, 8, 7, 9, 13, 11, 12, 10]},
      columns = ['id', 'Height', 'Weight', 'Foot', 'Label']
        )
init_centers = np.array([[5.0,7.0],[5.5, 9.0]])
colmap = {0: 'blue', 1: 'grey'}
x = data[['Height', 'Foot']].values
kmeans_classifier = KMeans(n_clusters=n_clusters,init=init_centers)
y_means=kmeans_classifier.fit_predict(x)
```

```
>>> centroids
array([[  5.28, 7.0],
       [  5.83, 11.0]])
>>> y_kmeans
array([0, 0, 0, 1, 1, 1, 1, 1])
```

# Python Code for Plotting

```
import matplotlib.pyplot as plt

fig = plt.figure()

for i in range(n_clusters):
    new_df = data[data['cluster']==i]
    plt.scatter(new_df['Height'],new_df['Foot'], color=colmap[i],
                s=100, label='points in cluster ' + str(i+1))

for i in range(n_clusters):
    plt.scatter(centroids[i][0], centroids[i][1], color=colmap[i],
                marker='x', s=300,label='centroid ' + str(i+1))

for i in range(len(data)):
    x_text = data['Height'].iloc[i] + 0.05
    y_text = data['Foot'].iloc[i] + 0.2
    id_text = data['id'].iloc[i]
    plt.text(x_text, y_text, str(id_text), fontsize=14)

plt.legend(loc='upper left')
plt.xlim(4, 7)
plt.ylim(5, 15)
plt.xlabel('Height')
plt.ylabel('Foot')
plt.show()
```

# Python Code for Plotting



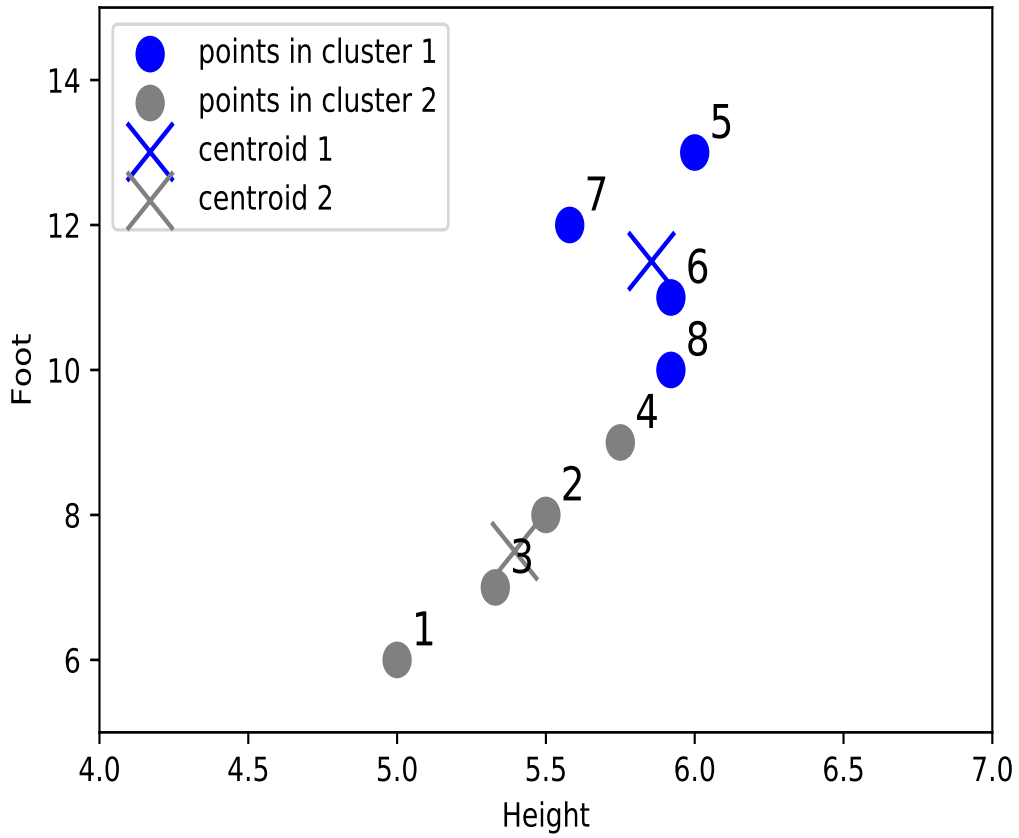
# Python Code

- random initial centroids

```
import pandas as pd
from sklearn.cluster import KMeans

data = pd.DataFrame(
    {'id': [ 1,2,3,4,5,6,7,8],
     'Label': ['green', 'green', 'green', 'green', 'red',
                                              'red', 'red', 'red'],
     'Height': [5, 5.5, 5.33, 5.75, 6.00, 5.92,  5.58, 5.92],
     'Weight': [100, 150, 130, 150, 180, 190, 170, 165],
     'Foot': [6, 8, 7, 9, 13, 11, 12, 10]},
     columns = ['id', 'Height', 'Weight', 'Foot', 'Label']
        )
colmap = {0: 'blue', 1: 'grey'}
x = data[['Height', 'Foot']].values
kmeans_classifier = KMeans(n_clusters=n_clusters)
y_means=kmeans_classifier.fit_predict(x)
centroids = kmeans_classifier.cluster_centers_
```

```
>>> centroids
array([[  5.395,   7.5  ],
       [  5.855,  11.5  ]])
>>> y_kmeans
array([0, 0, 0, 0, 1, 1, 1, 1])
```

# Results for Random Initialization



# Python Code for IRIS

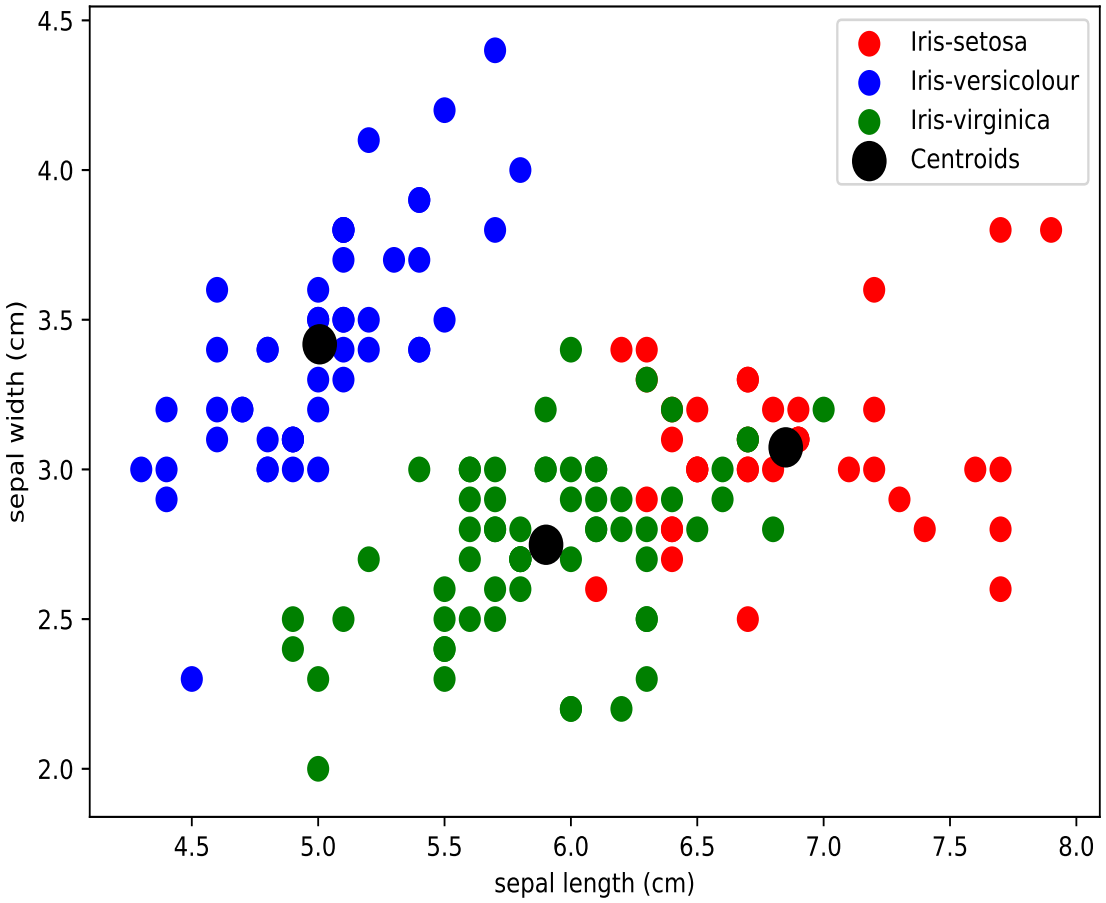
```
from sklearn import datasets
from sklearn.cluster import KMeans

iris = datasets.load_iris()
x = iris.data

kmeans_classifier = KMeans(n_clusters=3)
y_kmeans = kmeans_classifier.fit_predict(x)
centroids = kmeans_classifier.cluster_centers_
```

```
>>> centroids
array([[ 5.90, 2.75, 4.39, 1.43],
       [ 5.01, 3.42, 1.46, 0.24],
       [ 6.85, 3.07, 5.74, 2.07]])
```

# Python Code for Plotting

```
import matplotlib.pyplot as plt

fig, ax = plt.subplots(1,figsize=(7,5))
plt.scatter(x[y_kmeans == 0, 0], x[y_kmeans == 0, 1],
                s = 75, c = 'red', label = 'Iris-setosa')
plt.scatter(x[y_kmeans == 1, 0], x[y_kmeans == 1, 1],
                s = 75, c = 'blue', label = 'Iris-versicolour')
plt.scatter(x[y_kmeans == 2, 0], x[y_kmeans == 2, 1],
                s = 75, c = 'green', label = 'Iris-virginica')
plt.scatter(centroids[:, 0], centroids[:,1],
                s = 200, c = 'black', label = 'Centroids')

x_label = iris.feature_names[0]
y_label = iris.feature_names[1]

plt.legend()
plt.xlabel(x_label)
plt.ylabel(y_label)
plt.tight_layout()
plt.show()
```

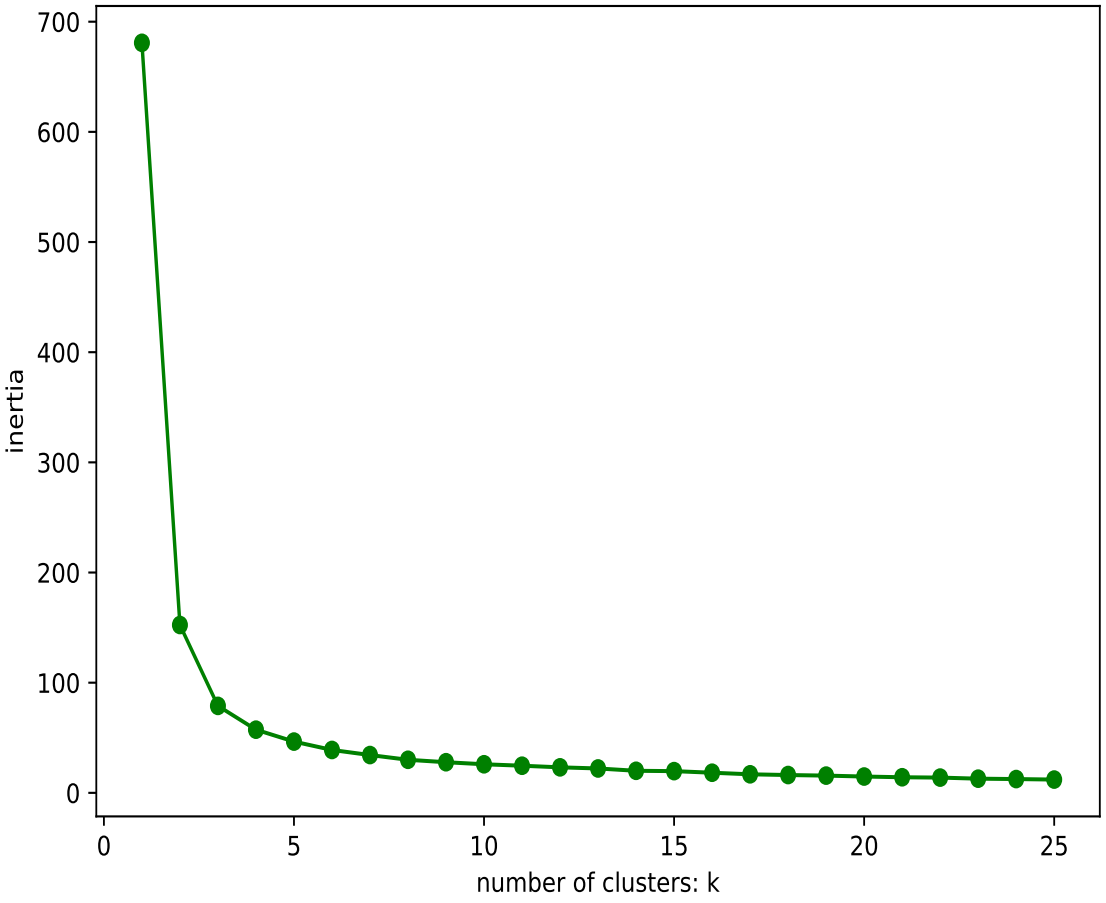
# $k$-means for IRIS



# Code to Compute $k$

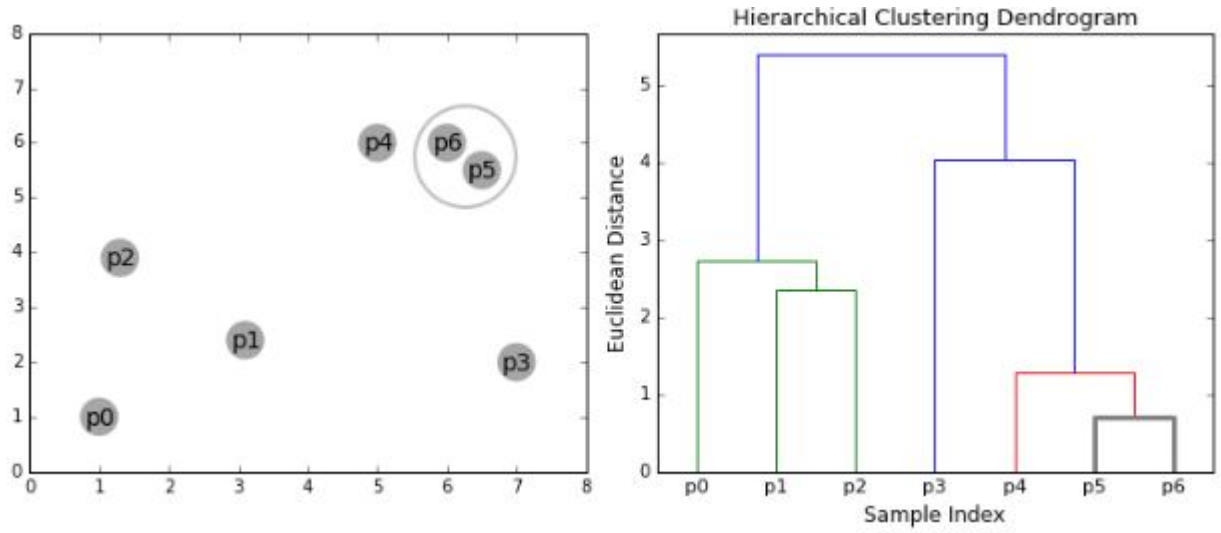
```
from sklearn import datasets
import matplotlib.pyplot as plt
from sklearn.cluster import KMeans

iris = datasets.load_iris()

x = iris.data
inertia_list = []
for k in range(1,26):
    kmeans_classifier = KMeans(n_clusters=k)
    y_kmeans = kmeans_classifier.fit_predict(x)
    inertia = kmeans_classifier.inertia_
    inertia_list.append(inertia)

fig, ax = plt.subplots(1,figsize=(7,5))
plt.plot(range(1, 26), inertia_list, marker='o',
         color='green')

plt.legend()
plt.xlabel('number of clusters: k')
plt.ylabel('inertia')
plt.tight_layout()

plt.show()
```

# Computing $k$ for IRIS




- choose $k$ visually - no more significant decline in inertia

# Hierarchical Clustering




- agglomerative hierarchical clustering (HAC)
- bottom-up clustering
- initially: each point is one cluster

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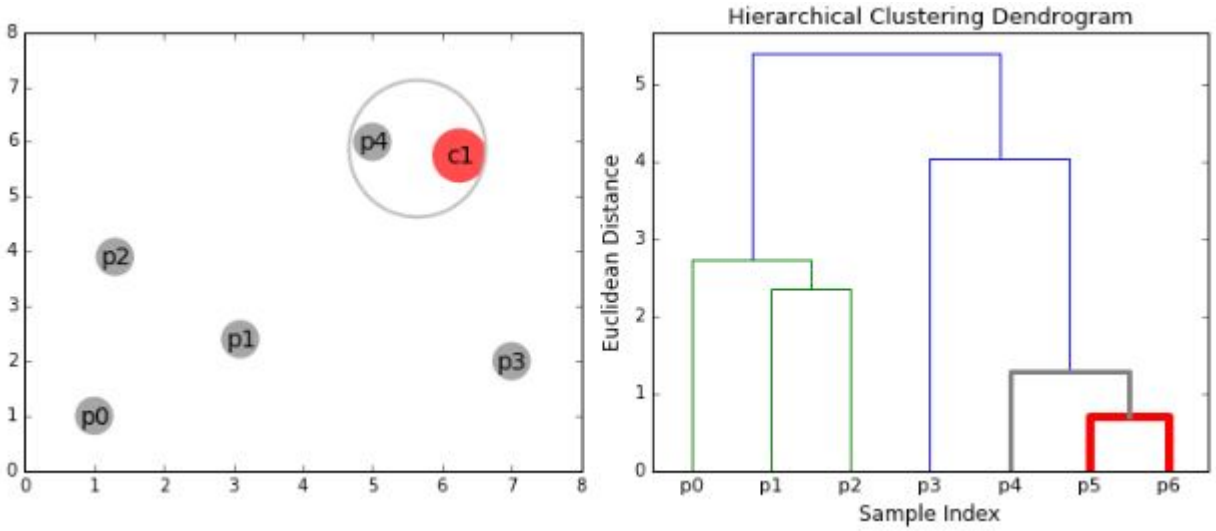
# Hierarchical Clustering (cont'd)




- define distance between clusters ("linkage")
- combine clusters based on linkage

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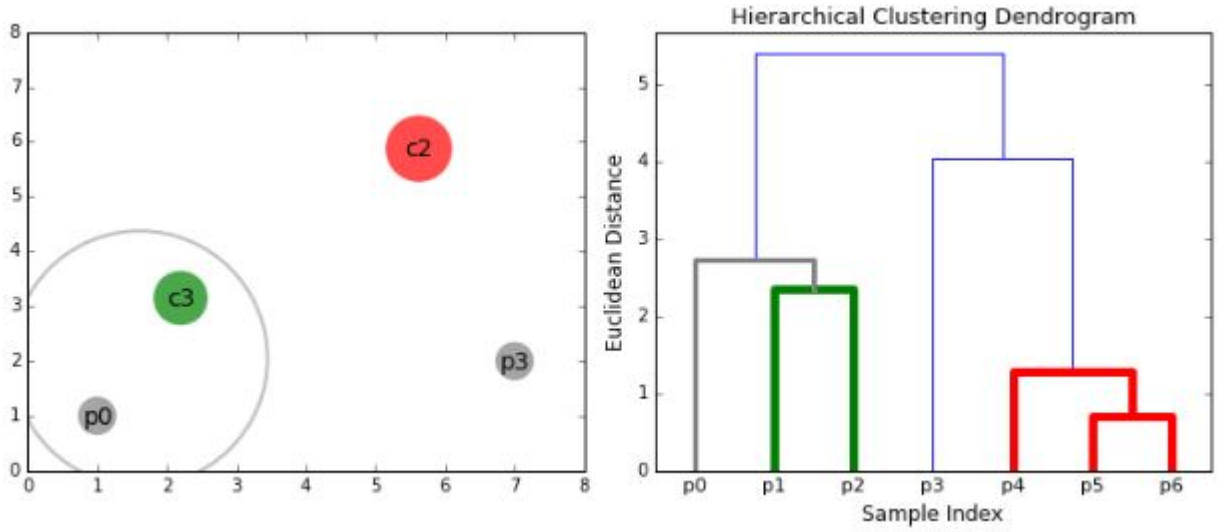
# Hierarchical Clustering (cont'd)




- continue combining clusters

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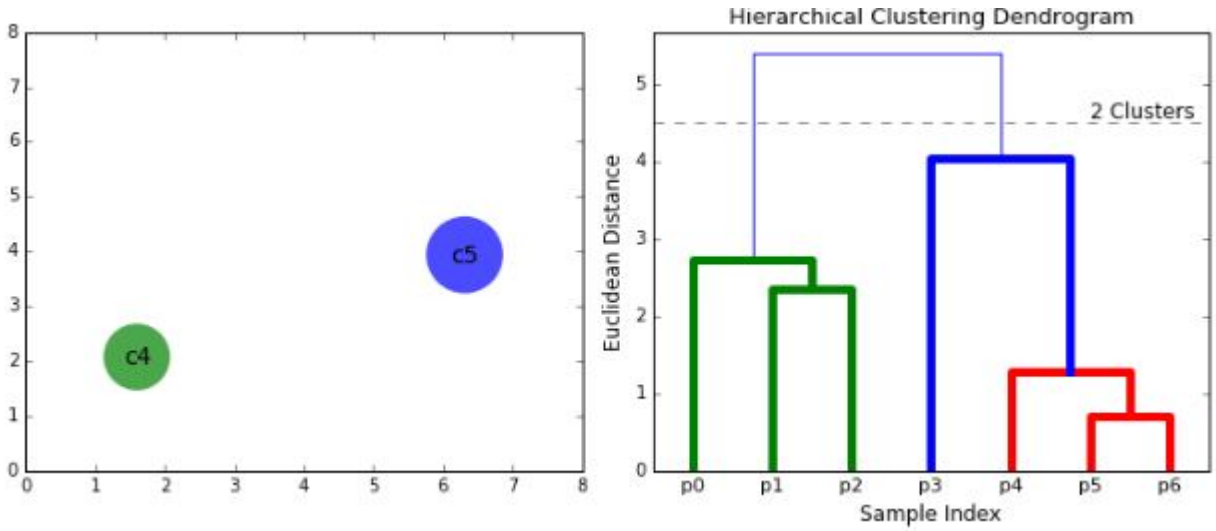
# Hierarchical Clustering (cont'd




- build a "tree" (hierarchy)

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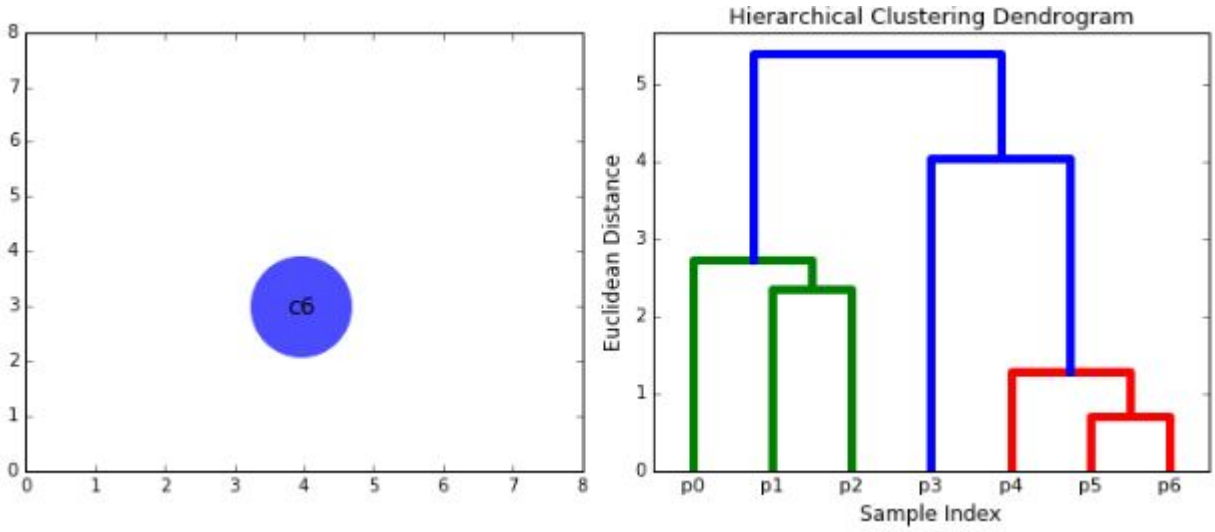
# Hierarchical Clustering (cont'd)




- result is a "dendogram"

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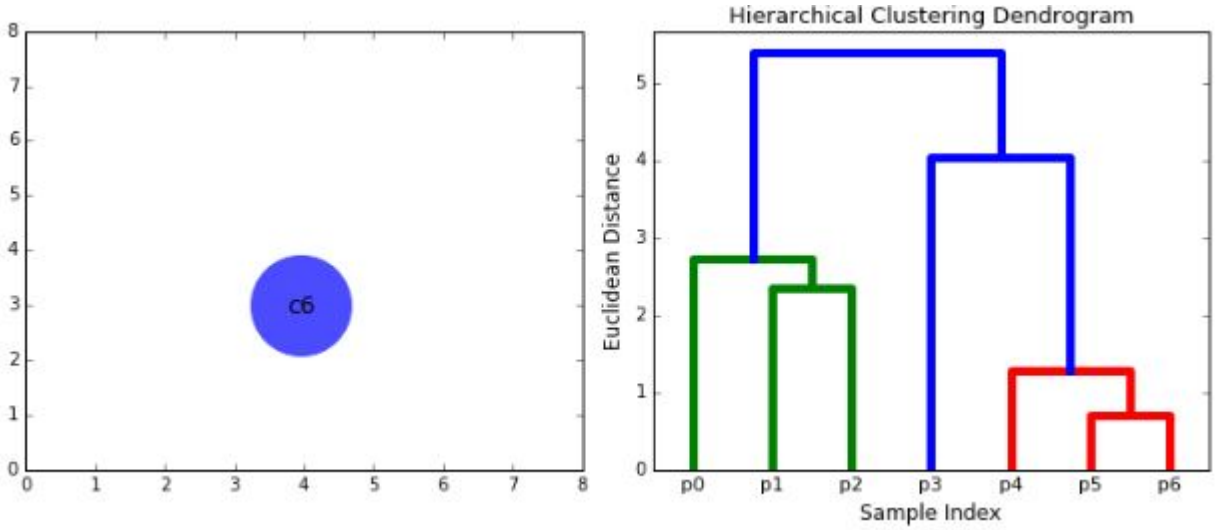
# Notes on Hierarchical Clustering




- do not specify number of clusters
- can decide at stop at any $k$ as build dendogram
- useful to cluster hierachical data

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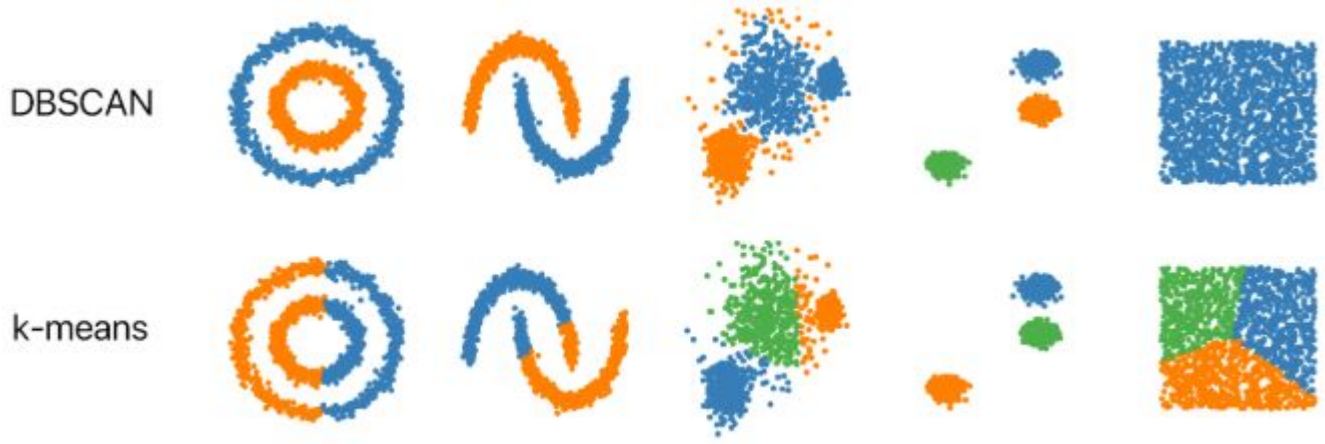
# Density Based Clustering (DBSCAN)




- $k$-means - need to know $k$ and may cluster unrelated points
- DBSCAN - cluster "dense" regions into clusters

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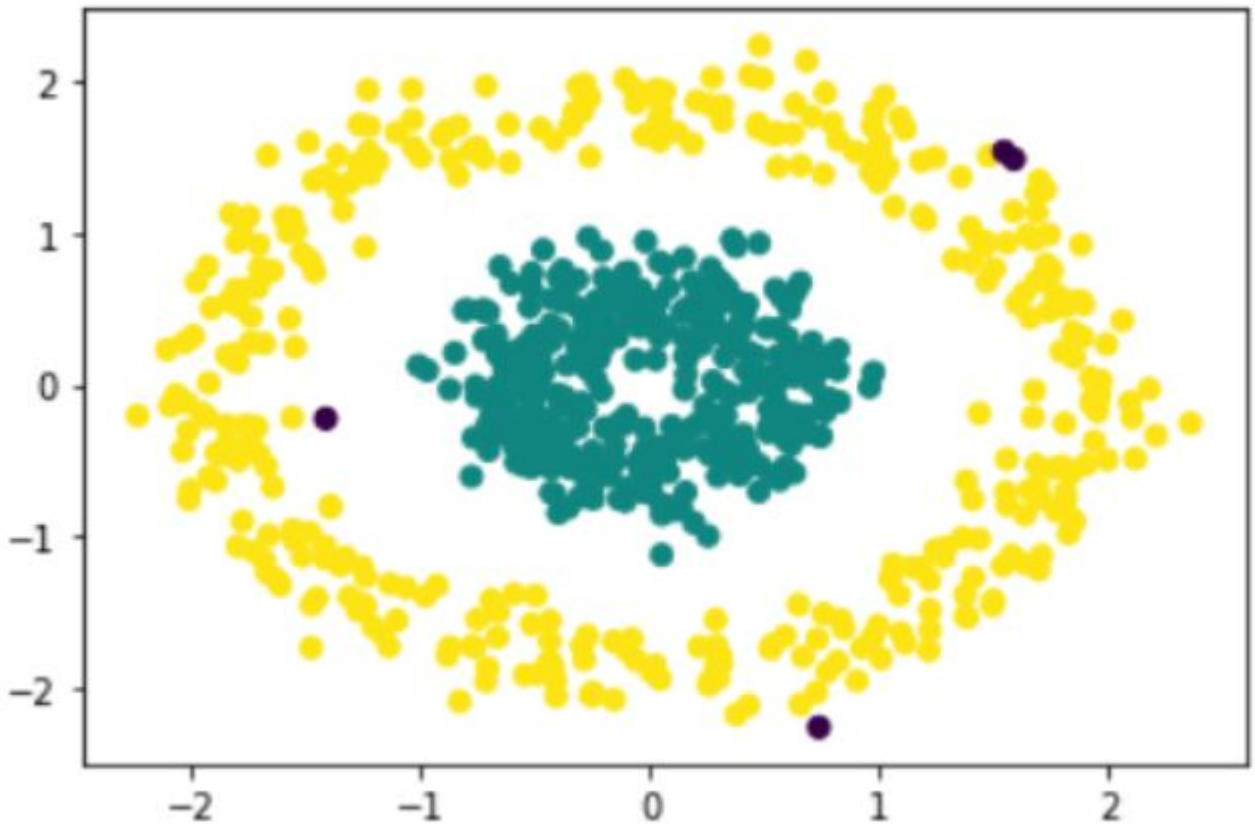
# DBSCAN vs. $k$-means




- clusters reflect distribution of objects

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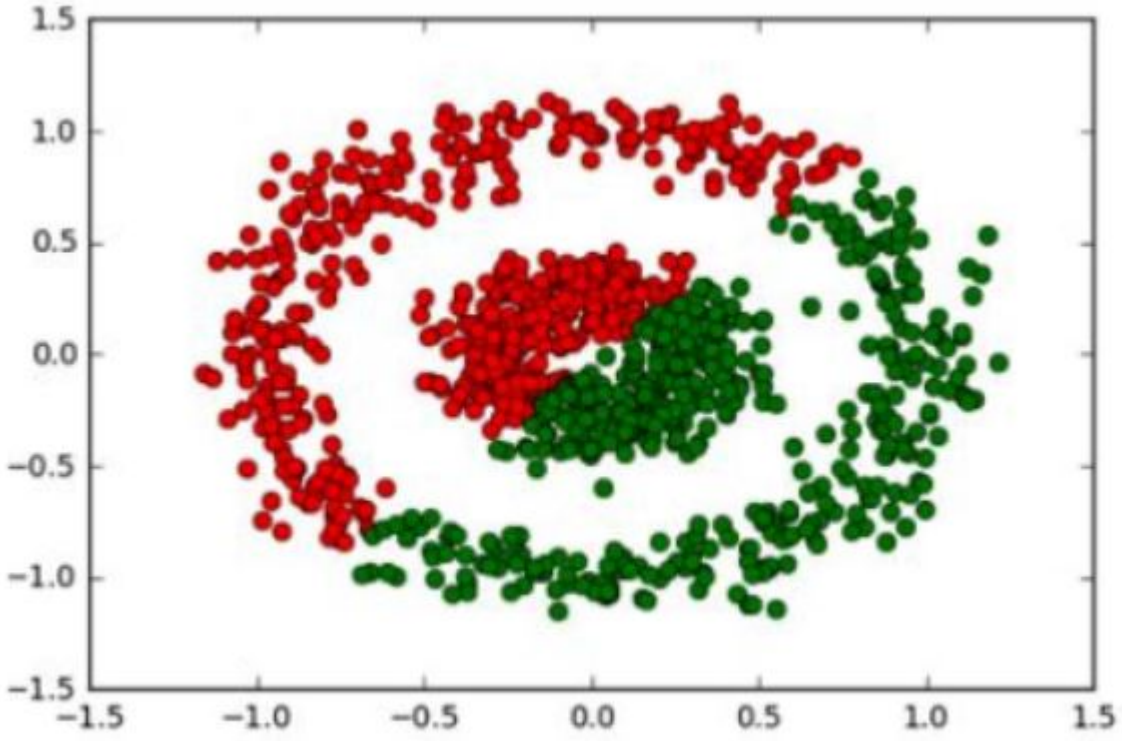
# DBSCAN vs. $k$-means (cont'd)




- $k$-means does not reflect distribution of objects

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# Concepts Check:

(a) inertia

(b) centroid

(c) knee method

(d) hierarchical clustering

(e) dendogram

(f) density-based clustering