

Clustering: K-means

Industrial AI Lab.

Prof. Seungchul Lee



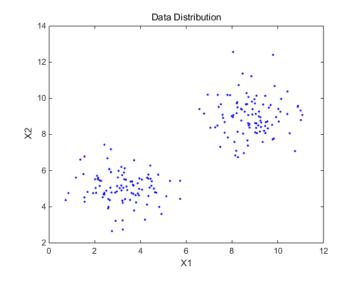
Supervised vs. Unsupervised Learning

Supervised Learning	Unsupervised Learning
Building a model from labeled data	Clustering from unlabeled data
Data Distribution 14 12 10 8 X 6 4 4 2 -8 -6 -4 -2 0 2 4 6 8 10 12 X1	Data Distribution 14
$\{x^{(1)},x^{(2)},\cdots,x^{(m)}\}\ \{y^{(1)},y^{(2)},\cdots,y^{(m)}\}$ \Rightarrow Classification	$\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\} \Rightarrow ext{Clustering}$



Data Clustering

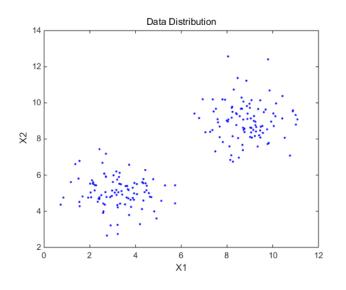
- Data clustering is an unsupervised learning problem
- Given:
 - -m unlabeled examples $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$
 - the number of partitions k
- Goal: group the examples into k partitions



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



Data Clustering: Similarity



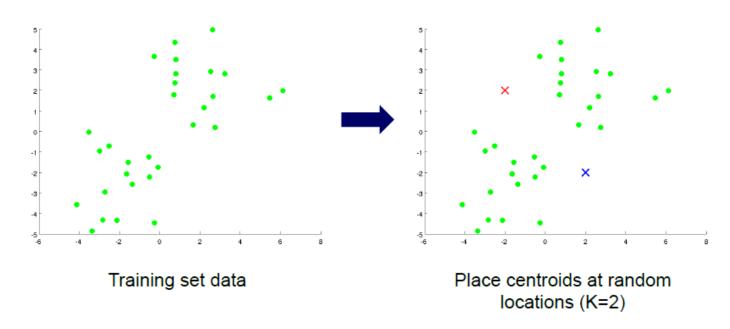
$$\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\} \quad \Rightarrow \quad ext{Clustering}$$

- The only information clustering uses is the mutual similarity between samples
- A good clustering is one that achieves:
 - high within-cluster similarity
 - low inter-cluster similarity

K-means: (Iterative) Algorithm

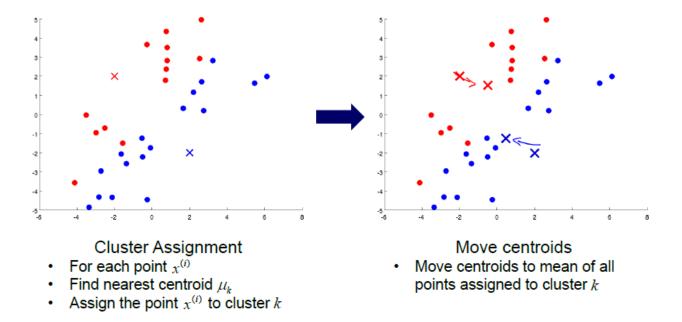
1) Initialization

- Input
 - -k: the number of clusters
 - Training set $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$
- Randomly initialize cluster centers anywhere in \mathbb{R}^n



K-means: (Iterative) Algorithm

2) Iteration



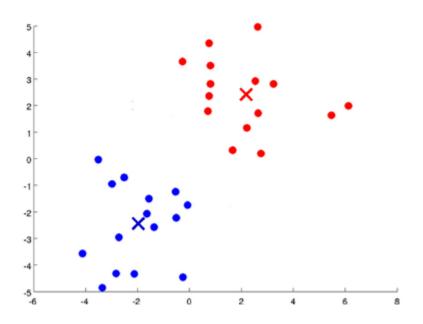
- Repeat until convergence
 - A possible convergence criteria: cluster centers do not change anymore



K-means: (Iterative) Algorithm

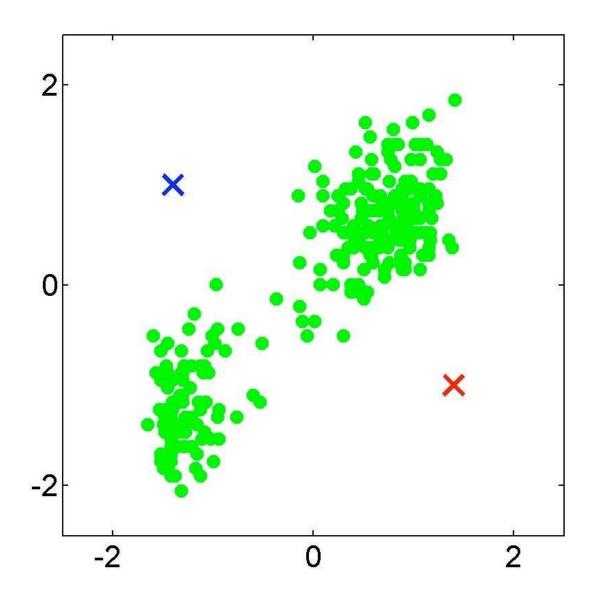
3) Output

- c (label): index (1 to k) of cluster centroid (centers)
- μ : averages (mean) of points assigned to cluster $\{\mu_1, \mu_2, \cdots, \mu_k\}$

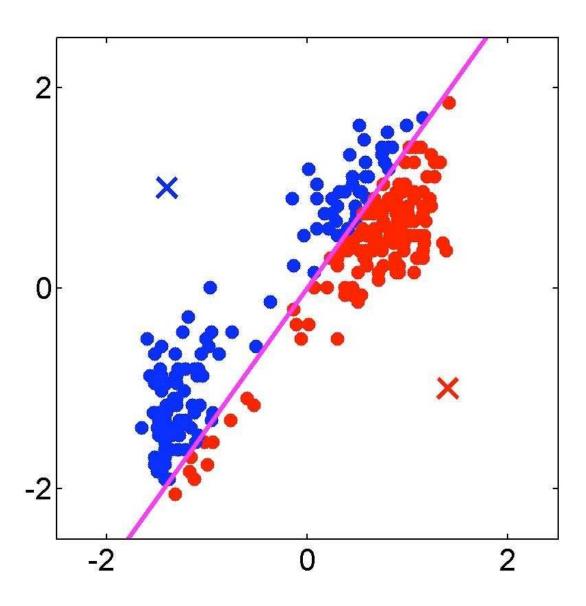




Initialization (k = 2)

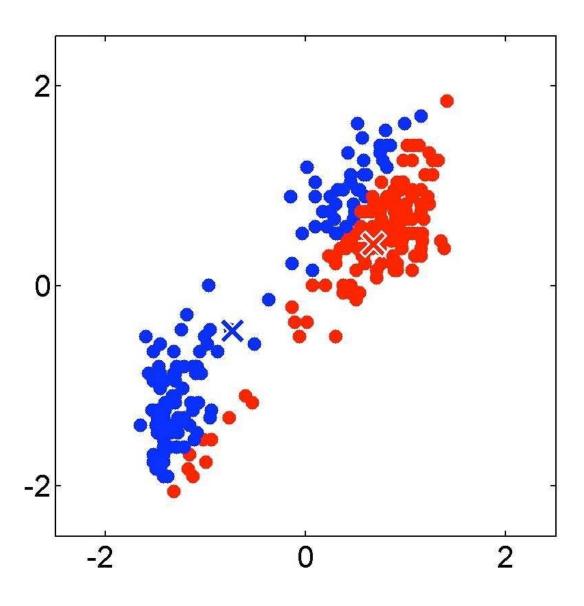


Assigning Points



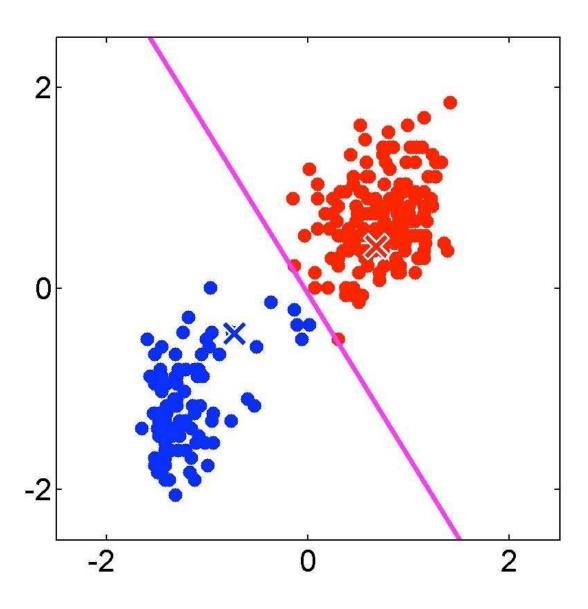


Recomputing the Cluster Centers



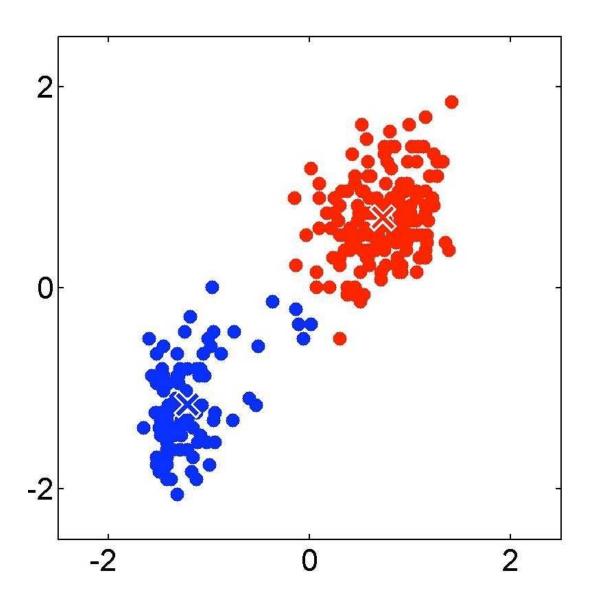


Assigning Points

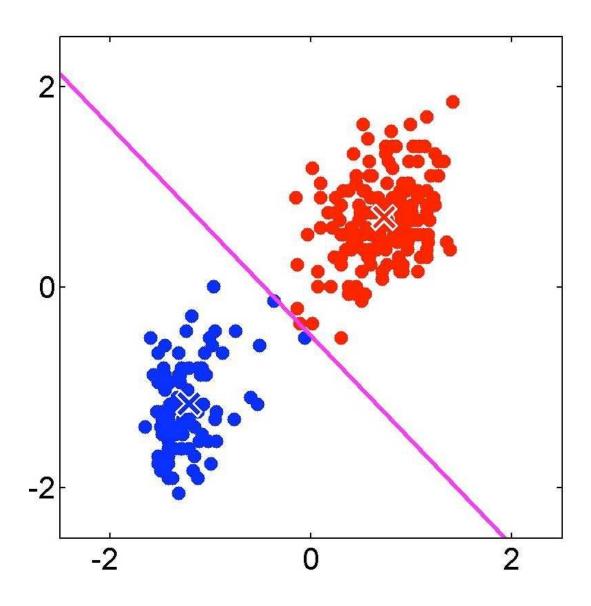




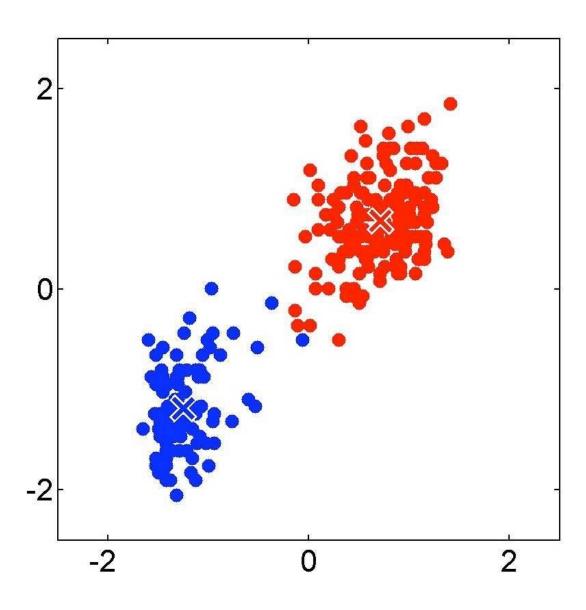
Recomputing the Cluster Centers



Assigning Points

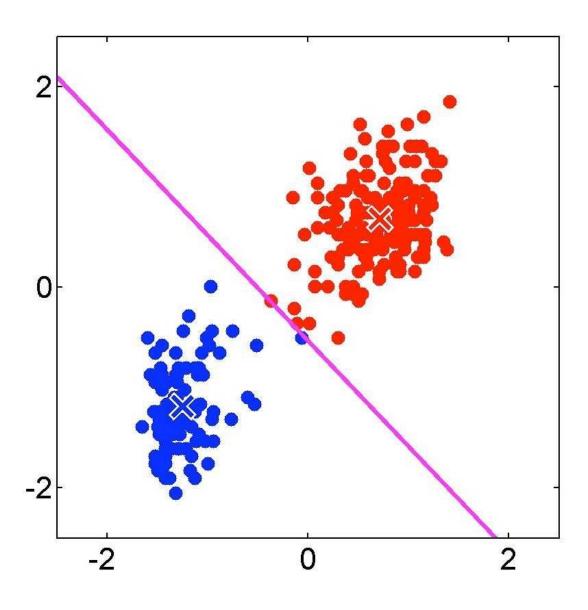


Recomputing the Cluster Centers

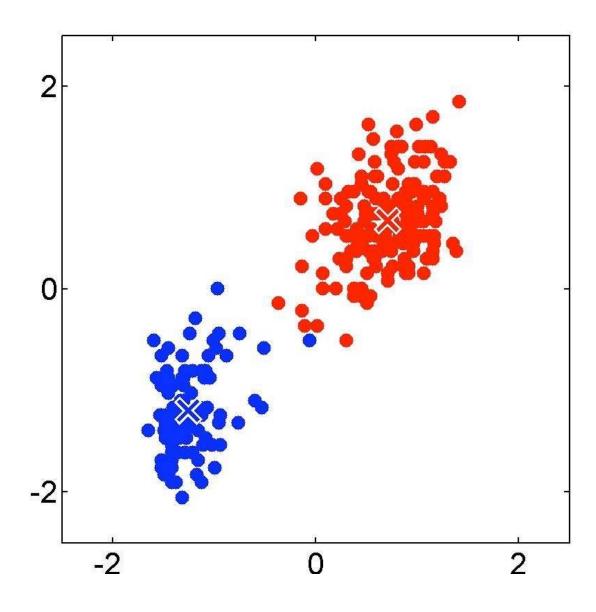




Assigning Points



Recomputing the Cluster Centers





Summary: K-means Clustering

• (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 := \operatorname{index} (\operatorname{from} 1 \text{ to } k) \text{ of cluster centroid closest to } x^{(i)}
for k=1 to k
\mu_k := \operatorname{average} (\operatorname{mean}) \text{ of points assigned to cluster } k
\}
```



K-means: Optimization Point of View (Optional)

- c_i = index of cluster $(1, 2, \dots, k)$ to which example $x^{(i)}$ is currently assigned
- μ_k = cluster centroid
- μ_{c_i} = cluster centroid of cluster to which example $\chi^{(i)}$ has been assigned
- Optimization objective:

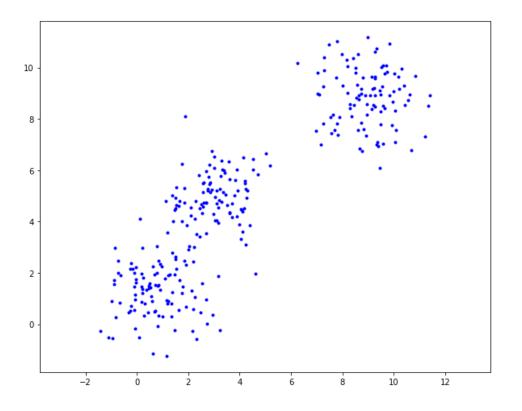
$$J(c_1,\cdots,c_m,\mu_1,\cdots,\mu_k) = rac{1}{m} \sum_{i=1}^m \lVert x^{(i)} - \mu_{c_i}
Vert^2 \ \min_{c_1,\cdots,c_m,\; \mu_1,\cdots,\mu_k} J(c_1,\cdots,c_m,\mu_1,\cdots,\mu_k)$$

Expectation Maximization (EM) Algorithm

- It is a "chicken and egg" problem (dilemma)
 - Q: if we knew c_i s, how would we determine which points to associate with each cluster center?
 - A: for each point $x^{(i)}$, choose closest c_i
 - Q: if we knew the cluster memberships, how do we get the centers?
 - A: choose c_i to be the mean of all points in the cluster
- Extension of K-means algorithm
 - A special case of Expectation Maximization (EM) algorithm
 - A special case of Gaussian Mixture Model (GMM)
 - Won't be discussed in this course

Python: Data Generation

```
# data generation
G0 = np.random.multivariate_normal([1, 1], np.eye(2), 100)
G1 = np.random.multivariate_normal([3, 5], np.eye(2), 100)
G2 = np.random.multivariate_normal([9, 9], np.eye(2), 100)
X = np.vstack([G0, G1, G2])
```



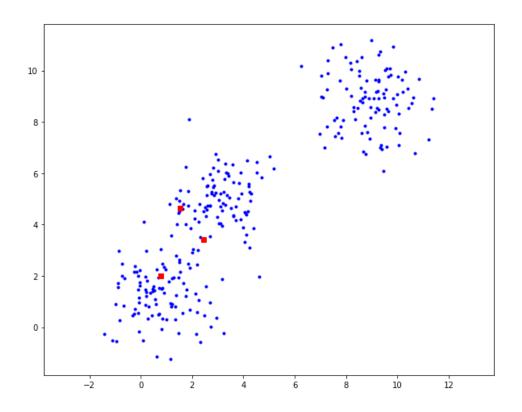


Python: Data Generation and Random Initialization

```
# data generation
G0 = np.random.multivariate_normal([1, 1], np.eye(2), 100)
G1 = np.random.multivariate_normal([3, 5], np.eye(2), 100)
G2 = np.random.multivariate_normal([9, 9], np.eye(2), 100)
X = np.vstack([G0, G1, G2])
```

```
# The number of clusters and data
k = 3
m = X.shape[0]

# ramdomly initialize mean points
mu = X[np.random.randint(0, m, k), :]
```



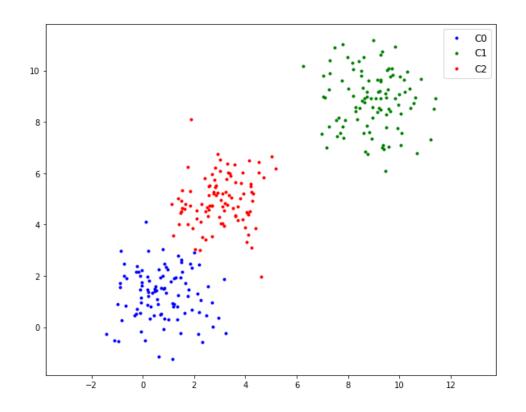


Python: K-Means

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

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

```
y = np.empty([m,1])
# Run K-means
for n iter in range(500):
   for i in range(m):
       d\theta = np.linalg.norm(X[i,:] - mu[0,:], 2)
       d1 = np.linalg.norm(X[i,:] - mu[1,:], 2)
       d2 = np.linalg.norm(X[i,:] - mu[2,:], 2)
       y[i] = np.argmin([d0, d1, d2])
   err = 0
   for i in range(k):
       mu[i,:] = np.mean(X[np.where(y == i)[0]], axis = 0)
       err += np.linalg.norm(pre mu[i,:] - mu[i,:], 2)
   pre_mu = mu.copy()
   if err < 1e-10:
        print("Iteration:", n_iter)
        break
```



Python: K-Means in Scikit-learn

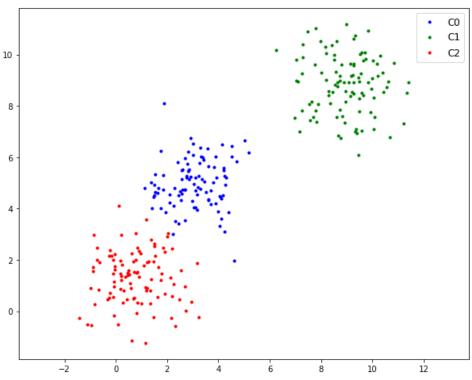


```
# use kmeans from the scikit-learn module

from sklearn.cluster import KMeans

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

plt.figure(figsize = (10,8))
plt.plot(X[kmeans.labels_ == 0, 0],X[kmeans.labels_ == 0, 1], 'b.', label = 'C0')
plt.plot(X[kmeans.labels_ == 1, 0],X[kmeans.labels_ == 1, 1], 'g.', label = 'C1')
plt.plot(X[kmeans.labels_ == 2, 0],X[kmeans.labels_ == 2, 1], 'r.', label = 'C2')
plt.axis('equal')
plt.legend(fontsize = 12)
plt.show()
```





Initialization Issues

- k-means is extremely sensitive to cluster center initialization
- Bad initialization can lead to
 - Poor convergence speed
 - Bad overall clustering
- Safeguarding measures:
 - Choose first center as one of the examples, second which is the farthest from the first, third which is the farthest from both, and so on.
 - Try multiple initialization and choose the best result

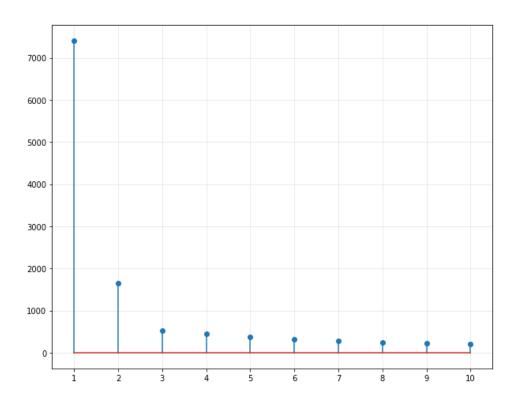
Choosing the Number of Clusters

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

Choosing the Number of Clusters

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





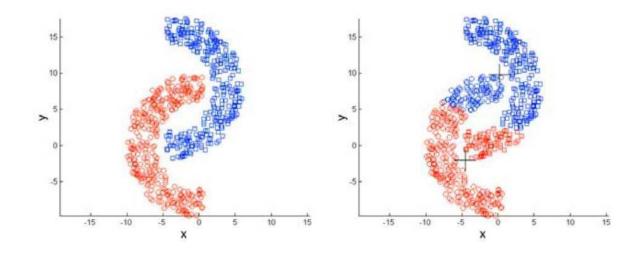
- Make hard assignments of points to clusters
 - A point either completely belongs to a cluster or not belongs at all
 - No notion of a soft assignment (i.e., probability of being assigned to each cluster)
 - Gaussian mixture model (we will study later) and Fuzzy K-means allow soft assignments
- Sensitive to outlier examples
 - K-medians algorithm is a more robust alternative for data with outliers



- Works well only for round shaped, and of roughly equal sizes/density cluster
- Does badly if the cluster have non-convex shapes
 - Spectral clustering (we will study later) and Kernelized K-means can be an alternative



• Non-convex/non-round-shaped cluster: standard K-means fails!



• (optional) Connectivity → networks → spectral partitioning

• Clusters with different densities

