COMP5211: Machine Learning

Lecture 17

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Clustering

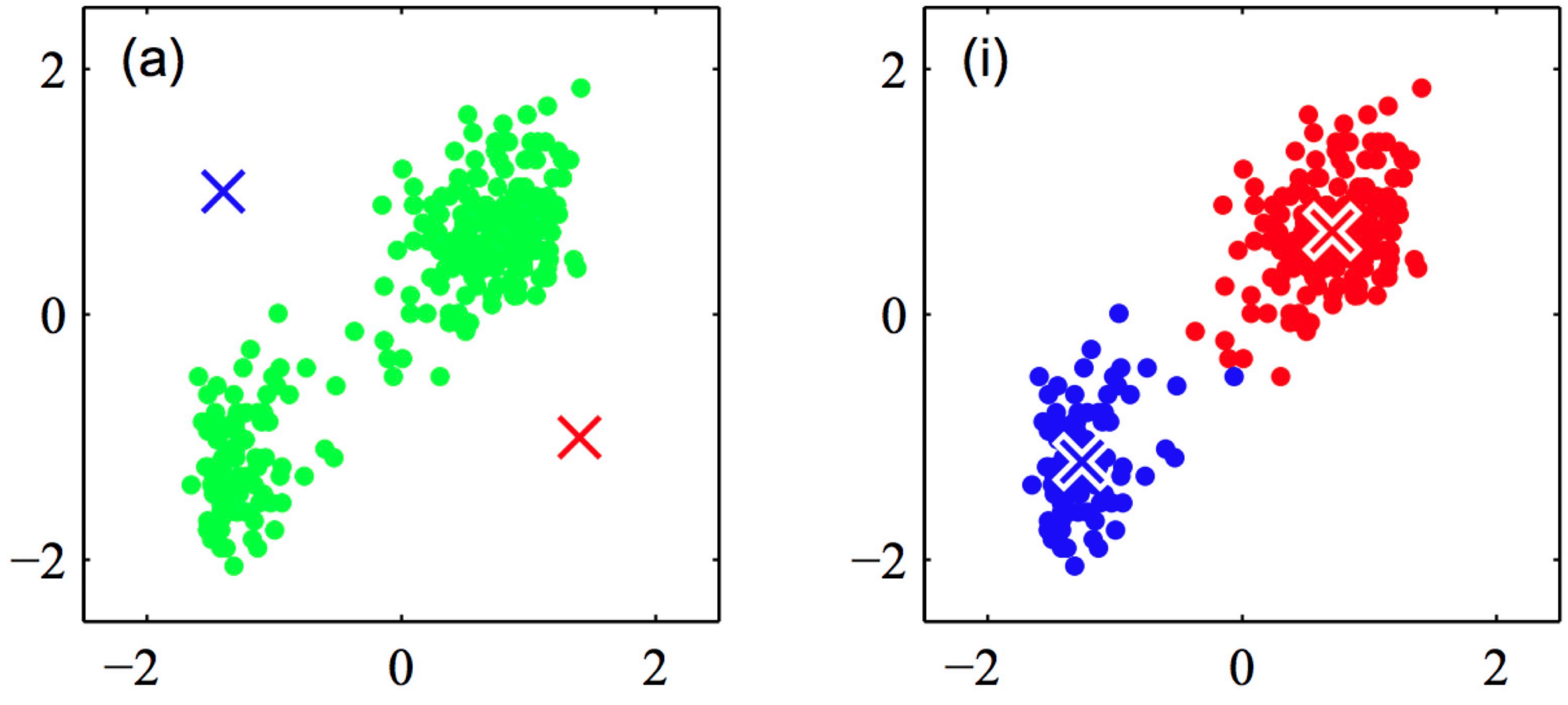
Supervised versus unsupervised learning

- Supervised learning:
  - Learning from labeled observations
  - Classification, regression
- Unsupervised learning:
  - Learning from unlabeled observations
  - Discover hidden patterns
  - Clustering (today)

Clustering

Definition

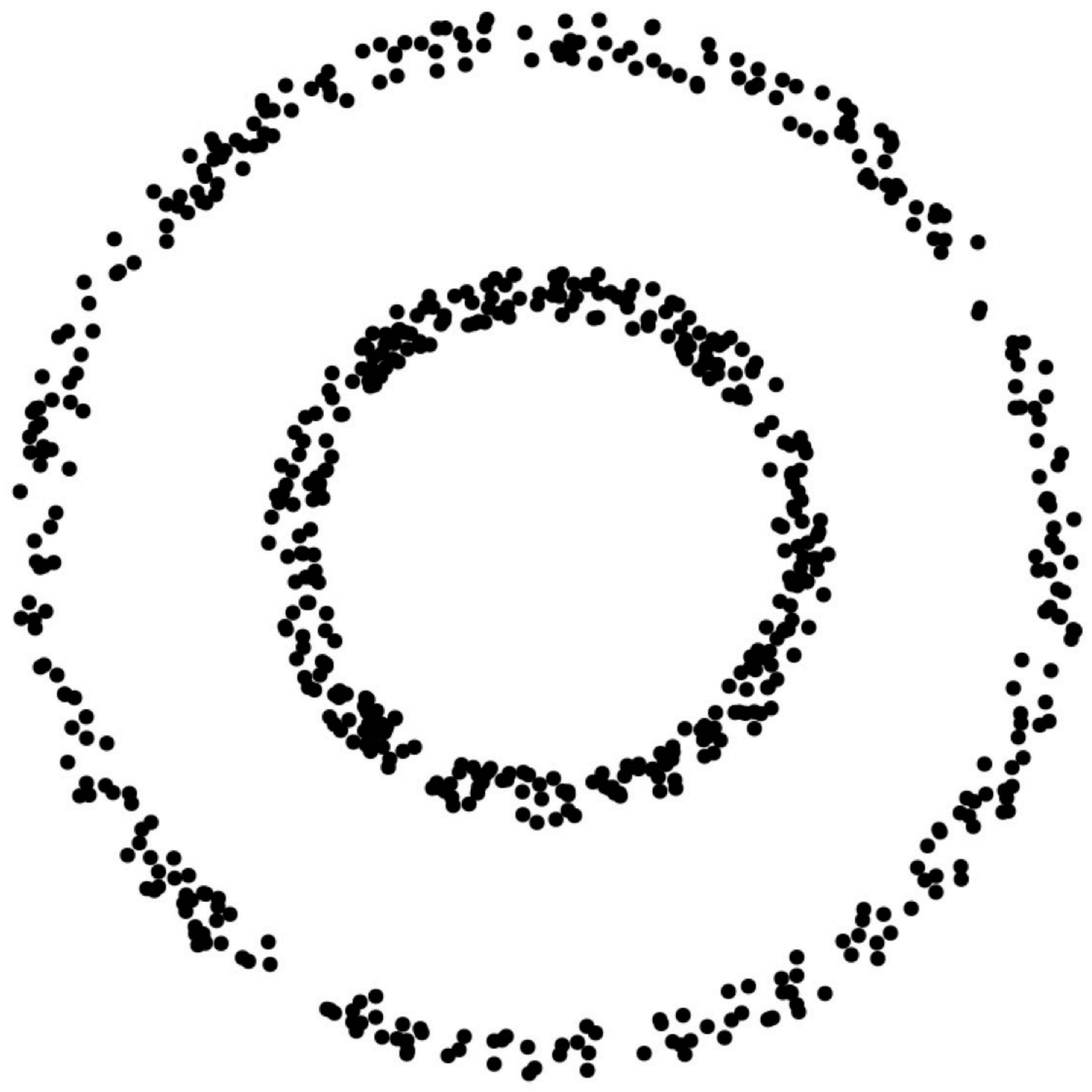
- Given $\{x_1, x_2, \ldots, x_n\}$ and K (number of clusters)
- Output $A(x_i) \in \{1,2,\ldots,K\}$ (cluster membership)



Clustering

Two circles

- Can we split the data into two clusters?



Clustering

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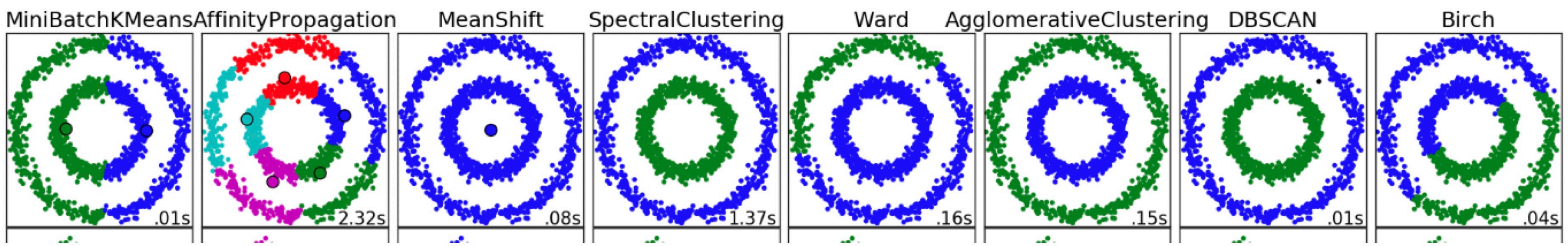
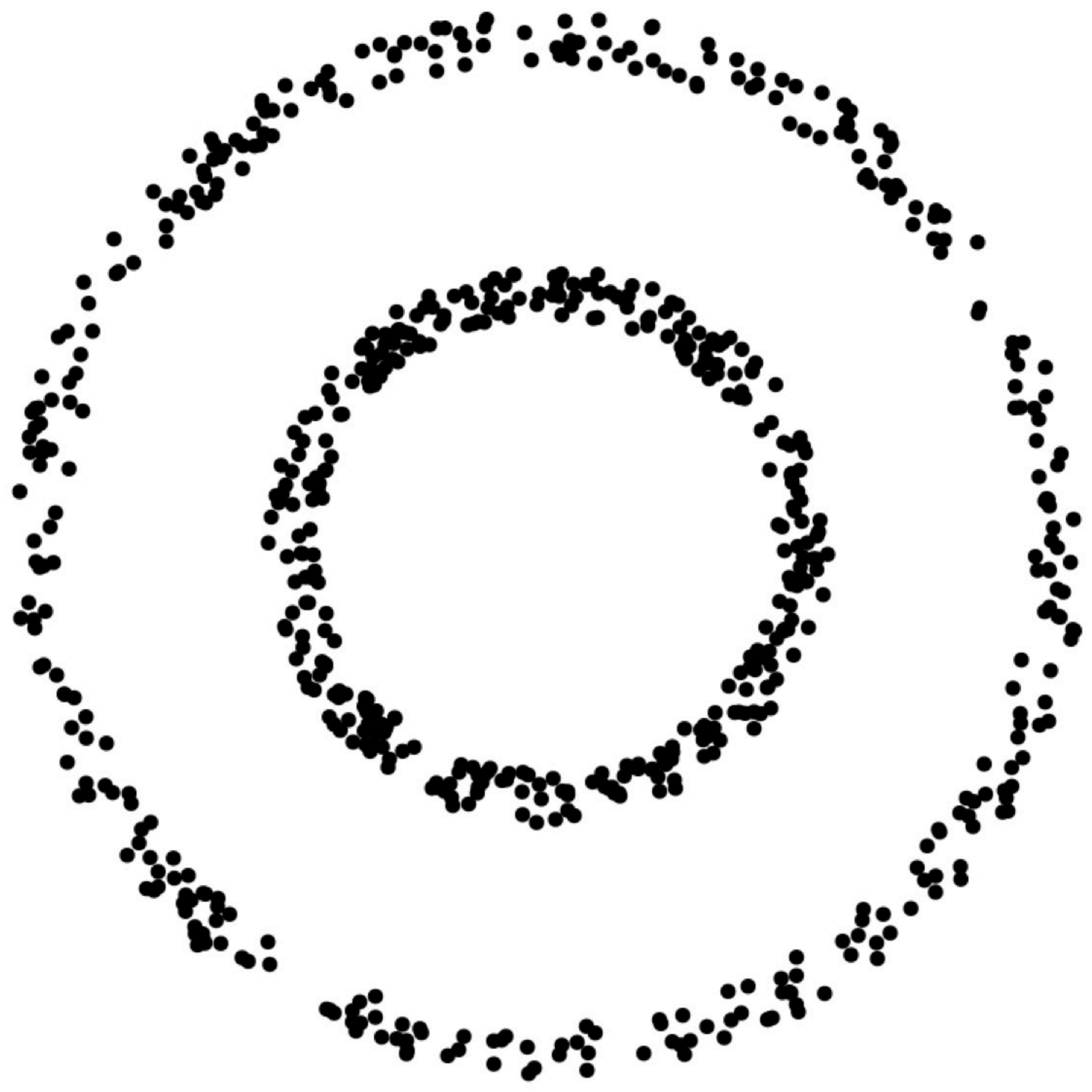
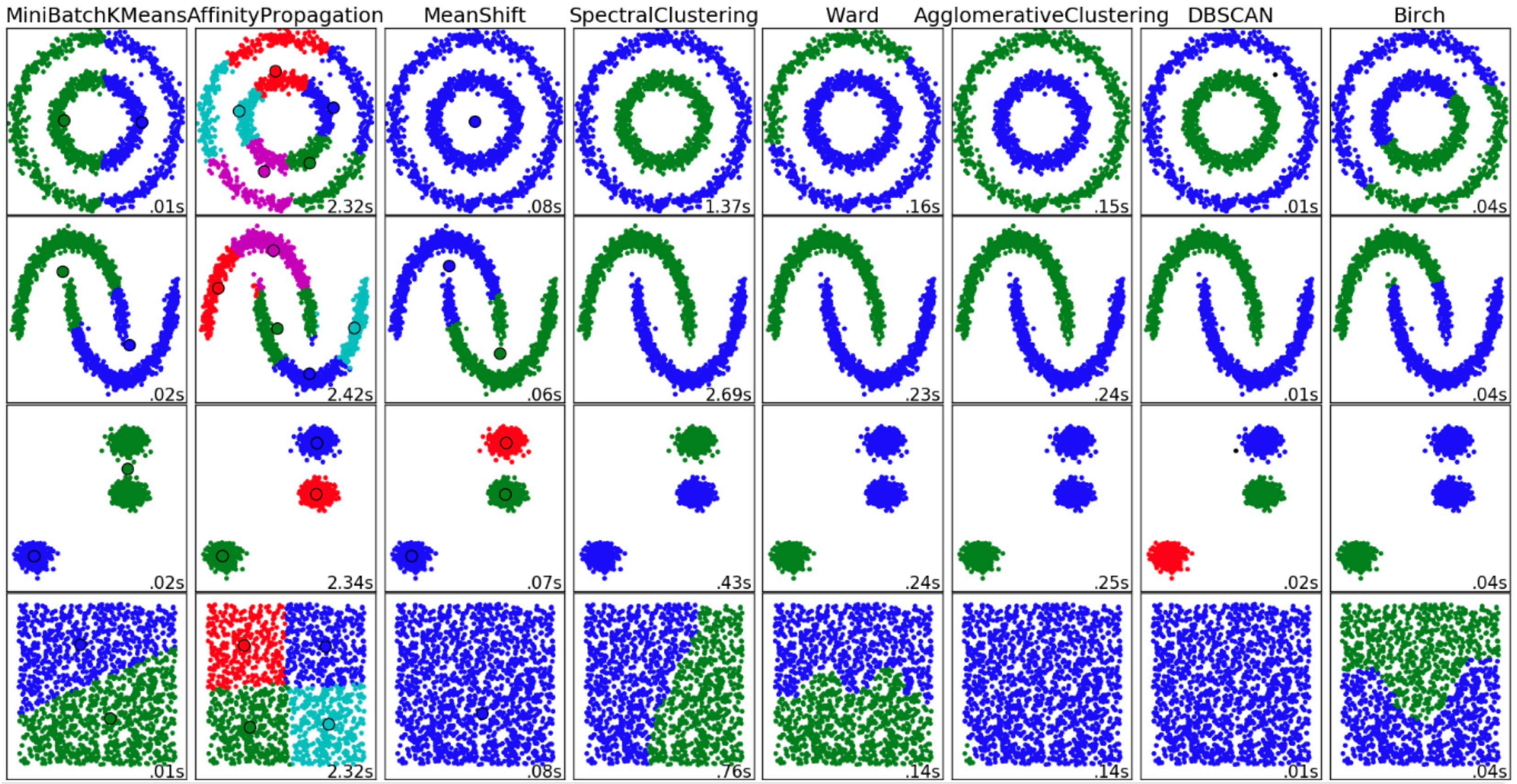




Clustering

Clustering is subjective

- Non-trivial to say on partition is better than others
- Each algorithm has two parts:
    - Define the objective function
    - Design an algorithm to minimize this objective function



Clustering

K-means

- Partition datasets into $C_1, C_2, \ldots, C_k$ to minimize the following objective:
- $J = \sum_{k=1}^{K} \sum_{x \in C_k} \|x - m_k\|_2^2$
    - Where m_k is the mean of C_k

Clustering

K-means

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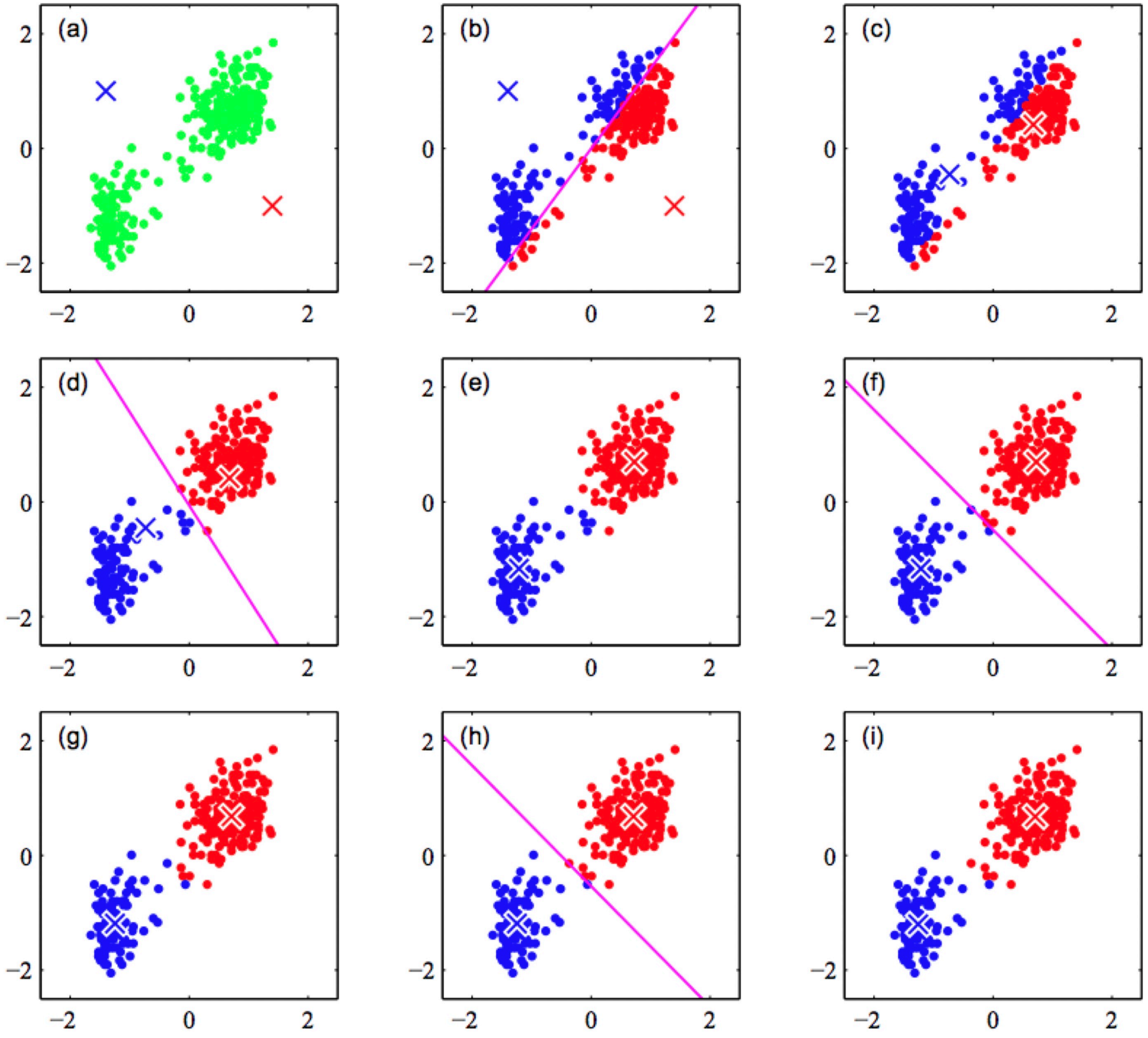
    - $J = \sum_{k=1}^{K} \sum_{x \in C_k} \|x - m_k\|_2^2$
    - Where m_k is the mean of C_k
- Multiple ways to minimize this objective
    - Hierarchical Agglomerative Clustering
    - Kmeans Algorithm (Today)
    - …

Clustering

K-means



Clustering

K-means Algorithm

- Re-write objective:
  - $J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|x_n - m_k\|_2^2$
  - Where $r_{nk} \in \{0,1\}$ is an indicator variable
    - $r_{nk} = 1$ if and only if $x_n \in C_k$
- Alternative optimization between $\{r_{nk}\}$ and $\{m_k\}$
  - Fix $\{m_k\}$ and update $\{r_{nk}\}$
  - Fix $\{r_{nk}\}$ and update $\{m_k\}$

Clustering

K-means Algorithm

- Step 0: initialize $\{m_k\}$ to some values

Clustering

K-means Algorithm

- Step 0: initialize $\{m_k\}$ to some values
- Step 1: Fix $\{m_k\}$ and minimize over $\{r_{nk}\}$:
  - $r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|x_n - m_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$

Clustering

K-means Algorithm

- Step 0: initialize $\{m_k\}$ to some values
- Step 1: Fix $\{m_k\}$ and minimize over $\{r_{nk}\}$:
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- Step 2: Fix $\{r_{nk}\}$ and minimize over $\{m_k\}$:
  - $m_k = \dfrac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$

Clustering

K-means Algorithm

- Step 0: initialize $\{m_k\}$ to some values
- Step 1: Fix $\{m_k\}$ and minimize over $\{r_{nk}\}$:
  - $r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|x_n - m_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$
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  - $m_k = \dfrac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$
- Step 3: Return to step 1 unless stopping criterion is met

Clustering

K-means Algorithm

- Equivalent to the following procedure:
  - Step 0: initialize centers $\{m_k\}$ to some values
  - Step 1: Assign each x_n to the nearest center:
    - $A(x_n) = \arg\min_j \|x_n - m_j\|_2^2$
    - Update cluster:
      - $C_k = \{x_n : A(x_n) = k\} \ \forall k = 1,\ldots,K$
  - Step 2: Calculate mean of each cluster C_k:
    - $m_k = \dfrac{1}{|C_k|} \sum_{x_n \in C_k} x_n$
  - Step 3: Return to step 1 unless stopping criterion is met

Clustering

More on K-means Algorithm

- Always decrease the objective function for each update
- Objective function will remain unchanged when step 1 doesn't change cluster assignment ⇒ Converged

Clustering

More on K-means Algorithm

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- May not convene to global minimum
    - Sensitive to initial values

Clustering

More on K-means Algorithm

- Always decrease the objective function for each update
- Objective function will remain unchanged when step 1 doesn't change cluster assignment $\Rightarrow$ Converged
- May not convene to global minimum
  - Sensitive to initial values
- Kmeans++: A better way to initialize the clusters

Clustering

Graph Clustering

- Given a graph $G = (V, E, W)$
  - V : nodes $\{v_1, \ldots, v_n\}$
  - E : edges $\{e_1, \ldots, e_m\}$
  - W : weight matrix
  - $W_{ij} = \begin{cases} w_{ij}, & \text{if } (i, j) \in E \\ 0, & \text{otherwise} \end{cases}$
- Goal: Partition V into k clusters of nodes
  - $V = V_1 \cup V_2 \cup \ldots \cup V_k, \quad V_i \cap V_j = \varphi, \forall i, j$

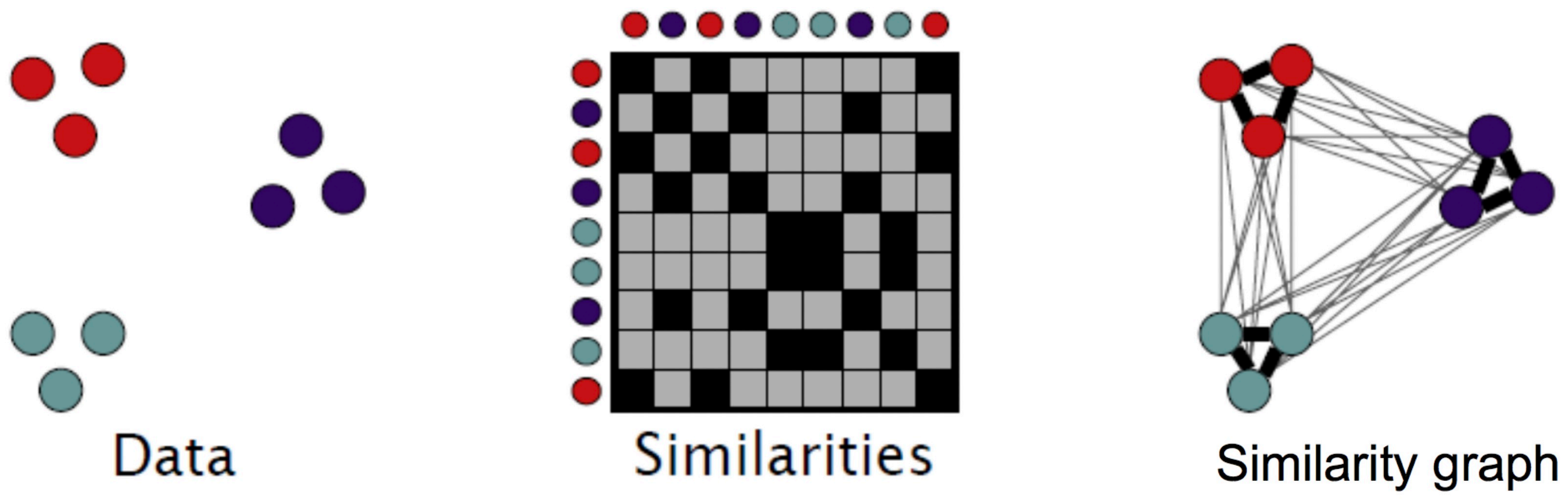
Clustering

Similarity Graph

- Example: similarity graph
- Given samples $x_1, \ldots, x_n$
- Weight (similarities) indicates "closeness of samples"

Similarity Graph: G(V,E,W)

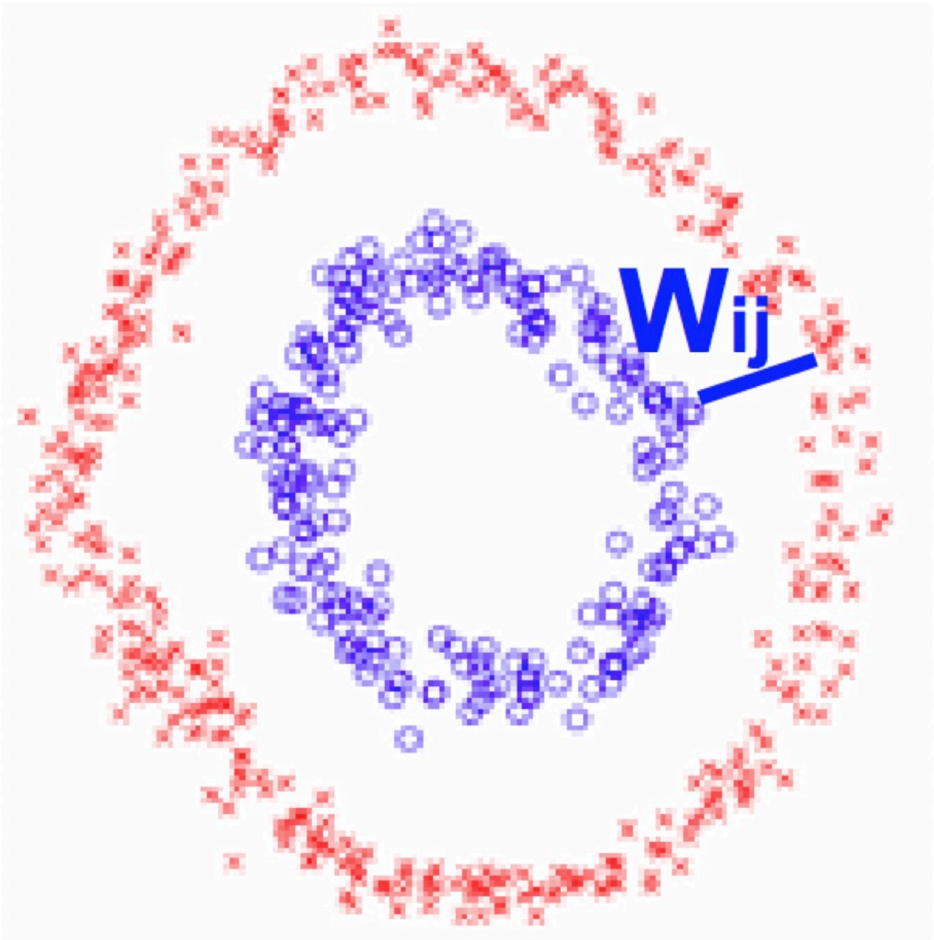
V – Vertices (Data points)
E – Edge if similarity > 0
W - Edge weights (similarities)



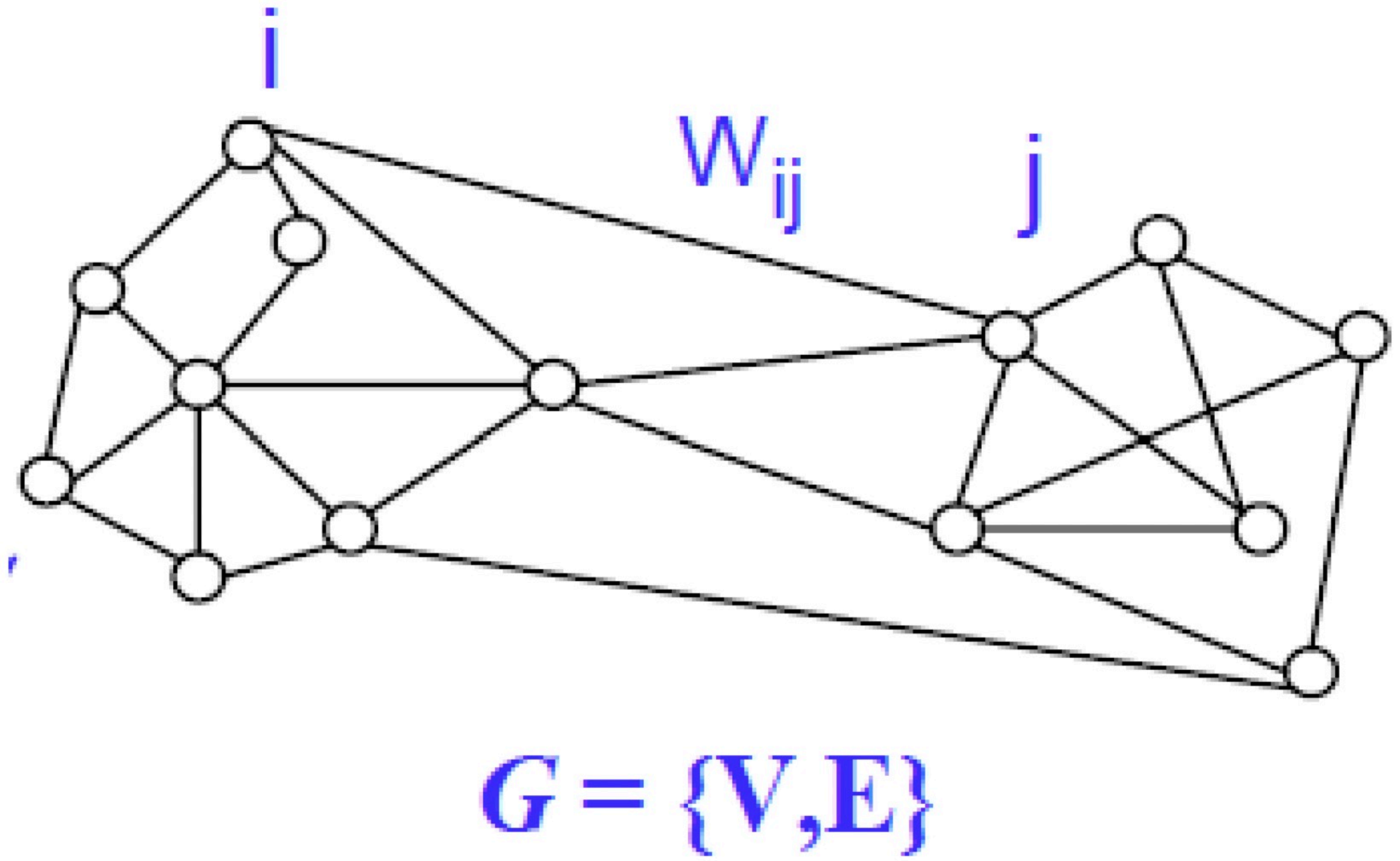
Partition the graph so that edges within a group have large weights and edges across groups have small weights.

Clustering
Similarity graph

- E.g., Gaussian kernel $W_{ij} = e^{-\|x_i - x_j\|^2/\sigma^2}$



Data clustering

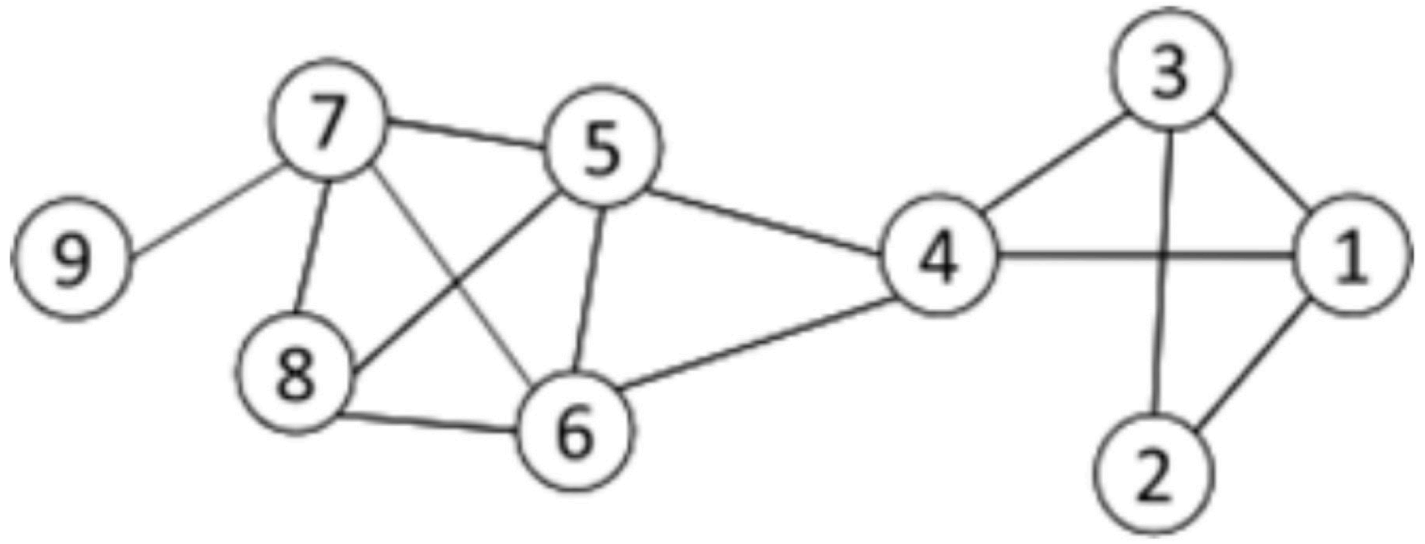


Clustering

Social graph

- Nodes: users in social network
- Edges: $W_{ij} = 1$ if user i and j are friends, otherwise $W_{ij} = 0$

Graph Representation



Matrix Representation

Node	1	2	3	4	5	6	7	8	9
1	-	1	1	1	0	0	0	0	0
2	1	-	1	0	0	0	0	0	0
3	1	1	-	1	0	0	0	0	0
4	1	0	1	-	1	1	0	0	0
5	0	0	0	1	-	1	1	1	0
6	0	0	0	1	1	-	1	1	0
7	0	0	0	0	1	1	-	1	1
8	0	0	0	0	1	1	1	-	0
9	0	0	0	0	0	0	1	0	-

Clustering

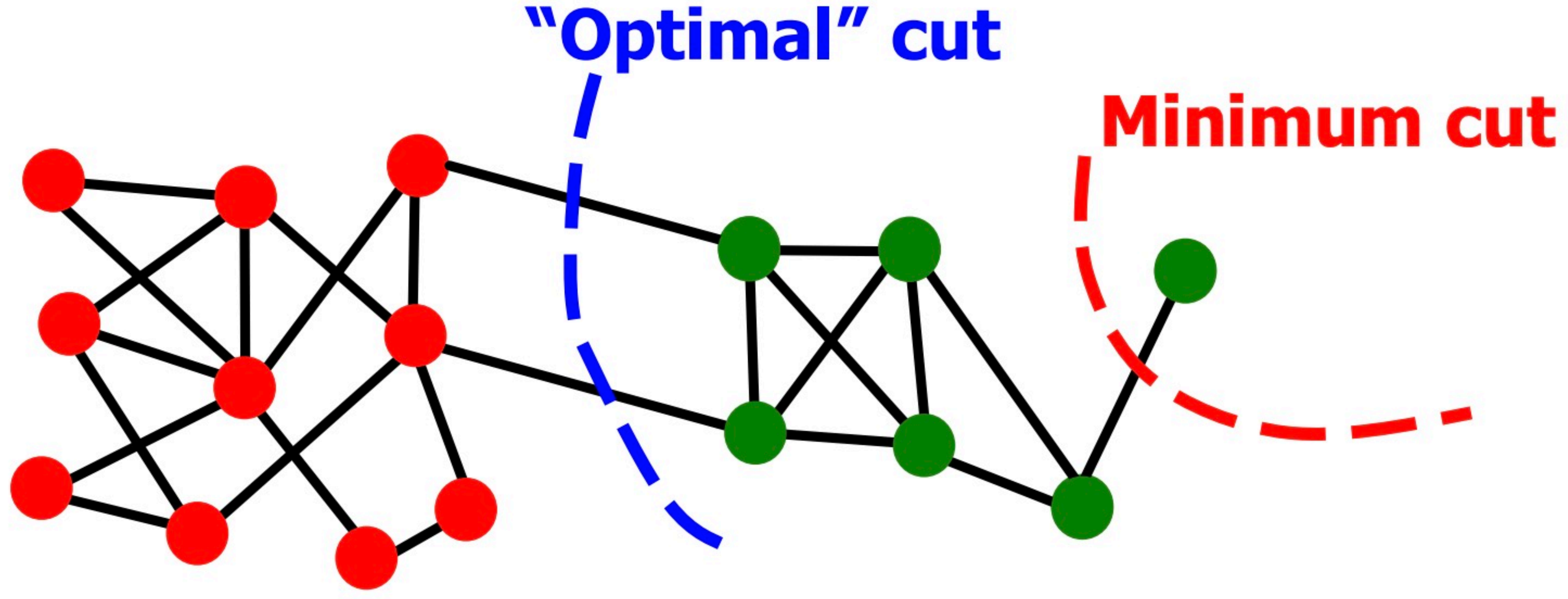
Partitioning into two clusters

- Partition graph into two sets V_1, V_2 to minimize the cut value:
- $$\text{cut}(V_1, V_2) = \sum_{v_i \in V_1, v_j \in V_2} W_{ij}$$

Clustering

Partitioning into two clusters

- Partition graph into two sets V_1, V_2 to minimize the cut value:
- $$\text{cut}(V_1, V_2) = \sum_{v_i \in V_1, v_j \in V_2} W_{ij}$$
- Also, the size of V_1, V_2 needs to be similar (balance)



Clustering

Partitioning into two clusters

- Partition graph into two sets V_1, V_2 to minimize the cut value:
  - $\text{cut}(V_1, V_2) = \sum_{v_i \in V_1, v_j \in V_2} W_{ij}$
- Also, the size of V_1, V_2 needs to be similar (balance)
- One classical way of enforcing balance:
  - $\min_{V_1, V_2} \text{cut}(V_1, V_2)$
    s.t. $|V_1| = |V_2|, V_1 \cup V_2 = \{1, \ldots, n\}, V_1 \cap V_2 = \varphi$
  - $\Rightarrow$ This is NP-hard (cannot be solved in polynomial time)

Clustering

Kernaghan-Lin Algorithm

- Start with some partitioning V_1, V_2
- Calculate change in cut if 2 vertices are swapped
- Swap the vertices (1 in V_1 & 1 in V_2) that decease the cut the most
- Iterate until convergence

Clustering

Kernaghan-Lin Algorithm

- Start with some partitioning V_1, V_2
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- Iterate until convergence
- Used when we need exact balanced clusters (e.g. circuit design)

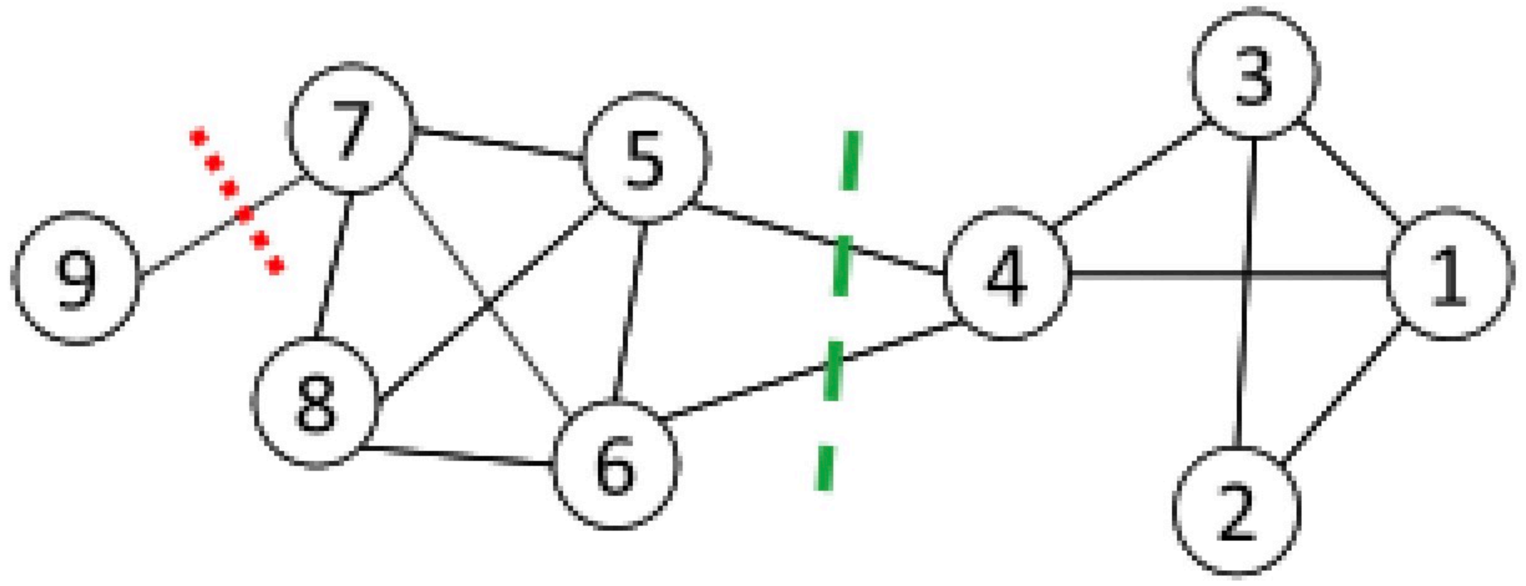
Clustering

Objective function that consider balance

- Ratio-Cut:
- $$\min_{V_1,V_2}\{\frac{\text{cut}(V_1,V_2)}{|V_1|}+\frac{\text{cut}(V_1,V_2)}{|V_2|}\} := RC(V_1,V_2)$$
- Normalized-Cut:
- $$\min_{V_1,V_2}\{\frac{\text{cut}(V_1,V_2)}{\text{deg}(V_1)}+\frac{\text{cut}(V_1,V_2)}{\text{deg}(V_2)}\} := RC(V_1,V_2)$$
- Where $\text{deg}(V_c) := \sum_{v_i \in V_c,(i,j)\in E} W_{i,j} = \text{links}(V_c, V)$

Clustering

Cut example



Cut(Red) = 1

Cut(Green) = 2

Ratio-Cut(Red) = $\frac{1}{1} + \frac{1}{8} = \frac{9}{8}$

Ratio-Cut(Green) = $\frac{2}{5} + \frac{2}{4} = \frac{18}{20}$

Normalized-Cut(Red) = $\frac{1}{1} + \frac{1}{27} = \frac{28}{27}$

Normalized-Cut(Green) = $\frac{2}{12} + \frac{2}{16} = \frac{14}{48}$

Minimizing **Normalized-cut** is even better for Green due to density constraint (volume)

Clustering

Generalize to k clusters

- Ratio-Cut:
  - $$\min_{V_1,\ldots,V_k} \sum_{c=1}^{k} \frac{\mathrm{cut}(V_c, V - V_c)}{|V_c|}$$
- Normalized-Cut:
  - $$\min_{V_1,\ldots,V_k} \sum_{c=1}^{k} \frac{\mathrm{cut}(V_c, V - V_c)}{\mathrm{deg}(V_c)}$$

Clustering
Reformulation

- Recall deg(V_c) = links(V_c, V)
- Define a diagonal matrix
- $$D = \begin{bmatrix} \text{deg}(v_1) & 0 & 0 & \dots \\ 0 & \text{deg}(v_2) & 0 & \dots \\ 0 & 0 & \text{deg}(v_3) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$
- $y_c = \{0,1\}^n$: indicator vector for the c-th cluster

Clustering
Reformulation

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- $y_c = \{0,1\}^n$: indicator vector for the c-th cluster
- We have
- $$y_c^T y_c = |V_c|$$ $$y_c^T D y_c = \text{deg}(V_c)$$ $$y_c^T W y_c = \text{links}(V_c, V_c)$$

Clustering

Ratio Cut

- $$\begin{aligned} RC(V_1, \ldots, V_k) &= \sum_{c=1}^{k} \frac{\text{cut}(V_c, V - V_c)}{|V_C|} \\ &= \sum_{c=1}^{k} \frac{\text{deg}(V_c) - \text{links}(V_c, V_c)}{|V_C|} \\ &= \sum_{c=1}^{k} \frac{y_c^T D y_c - y_c^T W y_c}{y_c^T y_c} \\ &= \sum_{c=1}^{k} \frac{y_c^T (D - W) y_c}{y_c^T y_c} \\ &= \sum_{c=1}^{k} \frac{y_c^T L y_c}{y_c^T y_c} \end{aligned}$$

(L=D-W is "Graph Laplacian")

Clustering

More on graph laplacian

- L is symmetric positive semi-definite

Clustering

Solving Ratio-Cut

- We have shown Ratio-Cut is equivalent to
- $\text{RCut} = \sum_{c=1}^{k} \frac{y_c^T L y_c}{y_c^T y_c} = \sum_{c=1}^{k} (\frac{y_c}{\|y_c\|})^T L (\frac{y_c}{\|y_c\|})$
- Define $\bar{y_c} = y_c / \|y_c\|$ (normalized indicator),
  - $Y = [\bar{y_1}, \bar{y_2}, \ldots, \bar{y_k}] \Rightarrow Y^T Y = I$

Clustering

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- Relaxed to real valued problem
  - $\min_{Y^T Y = I}$ Trace$(Y^T L Y)$

Clustering

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- Relaxed to real valued problem
    - $\min_{Y^T Y = I}$ Trace$(Y^T L Y)$
- Solution: Eigenvectors corresponding to the smallest k eigenvalues of L

Clustering

Solving Ratio-Cut

- Let $Y* \in \mathbb{R}^{n \times k}$ be these eigenvectors. Are we done?

Clustering

Solving Ratio-Cut

- Let $Y^* \in \mathbb{R}^{n \times k}$ be these eigenvectors. Are we done?
- No, Y^* does not have 0/1 values (not indicators)
    - (Since we are solving a **relaxed** problem)
- Solution: Run k-means on the rows of Y^*

Clustering

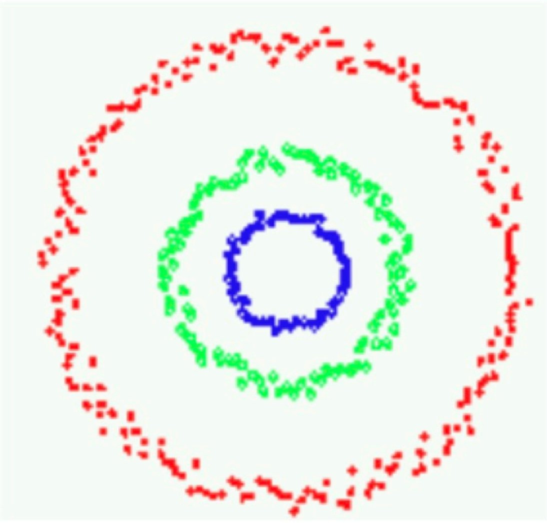
Solving Ratio-Cut

- Let $Y* \in \mathbb{R}^{n \times k}$ be these eigenvectors. Are we done?
- No, $Y*$ does not have 0/1 values (not indicators)
  - (Since we are solving a **relaxed** problem)
- Solution: Run k-means on the rows of $Y*$
- Summary of Spectral clustering algorithms:
  - Compute $Y* \in \mathbb{R}^{n \times k}$: eigenvectors corresponds to k smallest eigenvalues of (normalized) Laplacian matrix
  - Run k-means to cluster rows of $Y*$

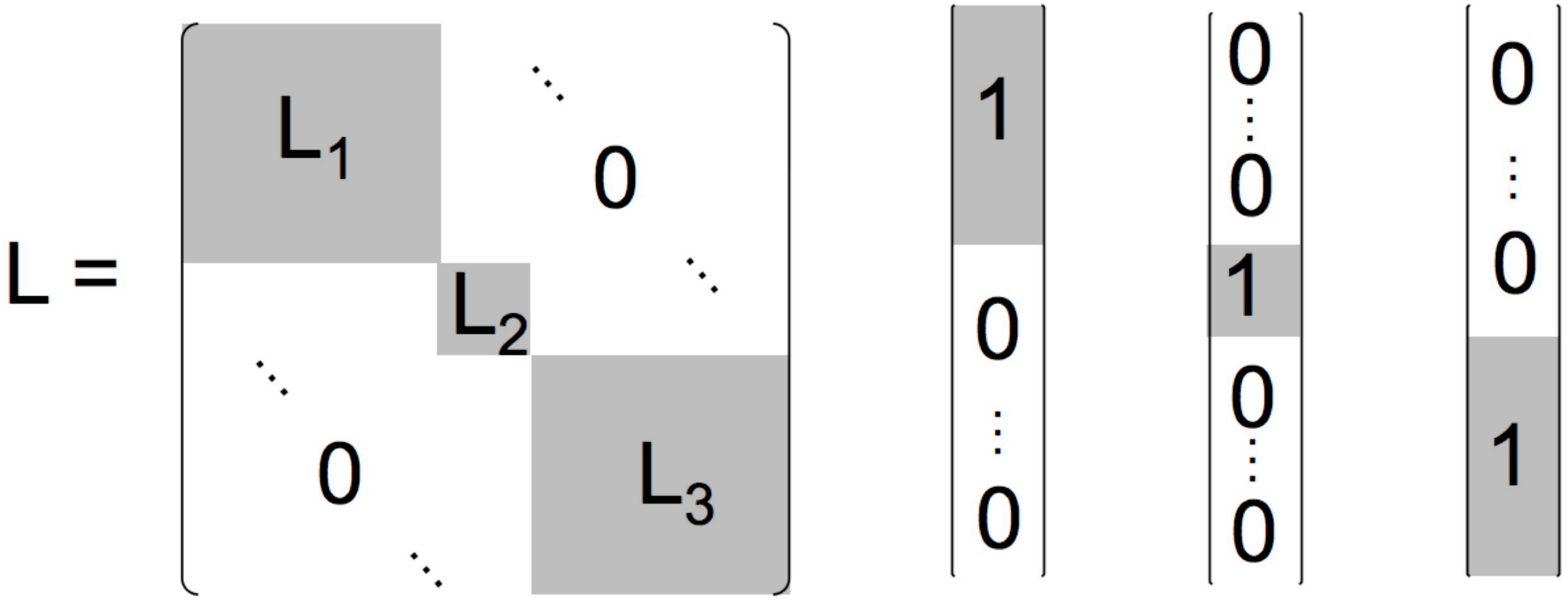
Clustering

Eigenvectors of Laplacian

- If graph is disconnected (k connected components), Laplacian is block diagonal and first k Eigen-vectors are:



OR



First three eigenvectors

Clustering

Eigenvectors of Laplacian

- What if the graph is connected?

Clustering

Eigenvectors of Laplacian

- What if the graph is connected?
- There will be only one smallest eigenvalue/eigenvector:
  - $L\mathbf{1} = (D - A)\mathbf{1} = 0$
  - ($\mathbf{1} = [1,1,\ldots,1]^T$ is the eigenvector with eigenvalue 0)

Clustering

Eigenvectors of Laplacian

- What if the graph is connected?
- There will be only one smallest eigenvalue/eigenvector:
  - $L\mathbf{1} = (D - A)\mathbf{1} = 0$ ($\mathbf{1} = [1,1,\ldots,1]^T$ is the eigenvector with eigenvalue 0)
- However, the 2nd to k-th smallest eigenvectors are still useful for clustering

1st evec is constant since graph is connected

Sign of 2nd evec indicates blocks

Clustering

Normalized Cut

- Rewirte Normalized Cut:

$$NCut = \sum_{c=1}^{k} \frac{\text{cut}(V_c, V - V_c)}{\text{deg}(V_c)}$$

  - $$= \sum_{c=1}^{k} \frac{y_c^T (D - A) y_c}{y_c^T D y_c}$$

- Let $\tilde{y}_c = \dfrac{D^{1/2} y_c}{\|D^{1/2} y_c\|}$,then

  - $$NCut = \sum_{c=1}^{k} \frac{\tilde{y}_c{}^T D^{-1/2} (D - A) D^{-1/2} \tilde{y}_c}{\tilde{y}_c{}^T \tilde{y}_c}$$

- Normalized Laplacian:

  - $\tilde{L} = D^{-1/2}(D - A)D^{-1/2} = I - D^{-1/2} A D^{-1/2}$

- Normalized Cut → eigenvectors correspond to the smallest eigenvalues

Clustering

Kmeans vs Spectral Clustering

- Kmeans: decision boundary is linear
- Spectral clustering: boundary can be non-convex curves
    - σ in $W_{ij} = e^{\frac{-\|x_i - x_j\|^2}{\sigma^2}}$ controls the clustering results (focus on local or global structure)

Clustering

Kmeans vs Spectral Clustering