# Cluster Analysis (b)

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# Outline

- **Grid-Based and Density-Based Algorithms**
- Graph-Based Algorithms
- Non-negative Matrix Factorization
- Cluster Validation
- Summary

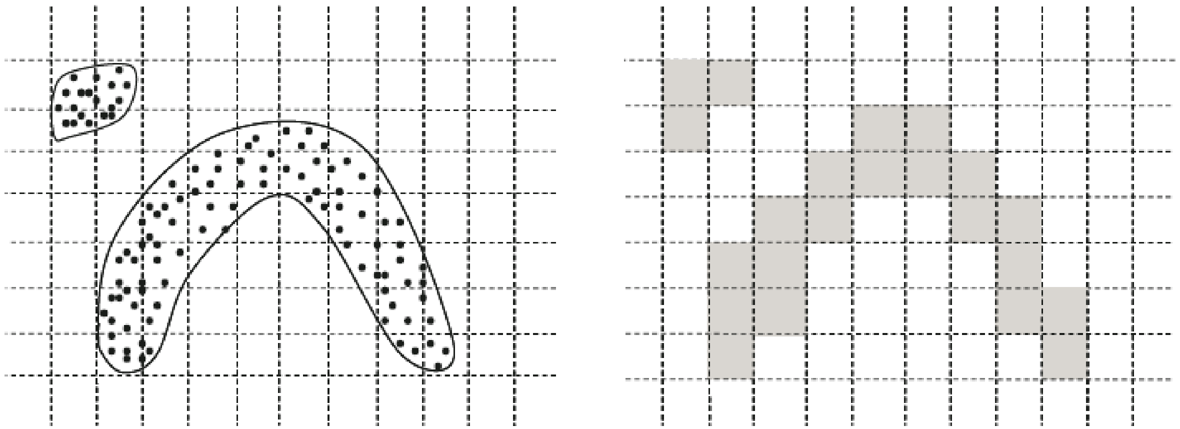
# Density-Based Algorithms

- One Motivation
  - Find clusters with arbitrary shape
- The Key Idea
  - Identify fine-grained dense regions
  - Merge regions into clusters
- Representative Algorithms
  - Grid-Based Methods
  - DBSCAN
  - DENCLUE

# Grid-Based Methods

## The Algorithm

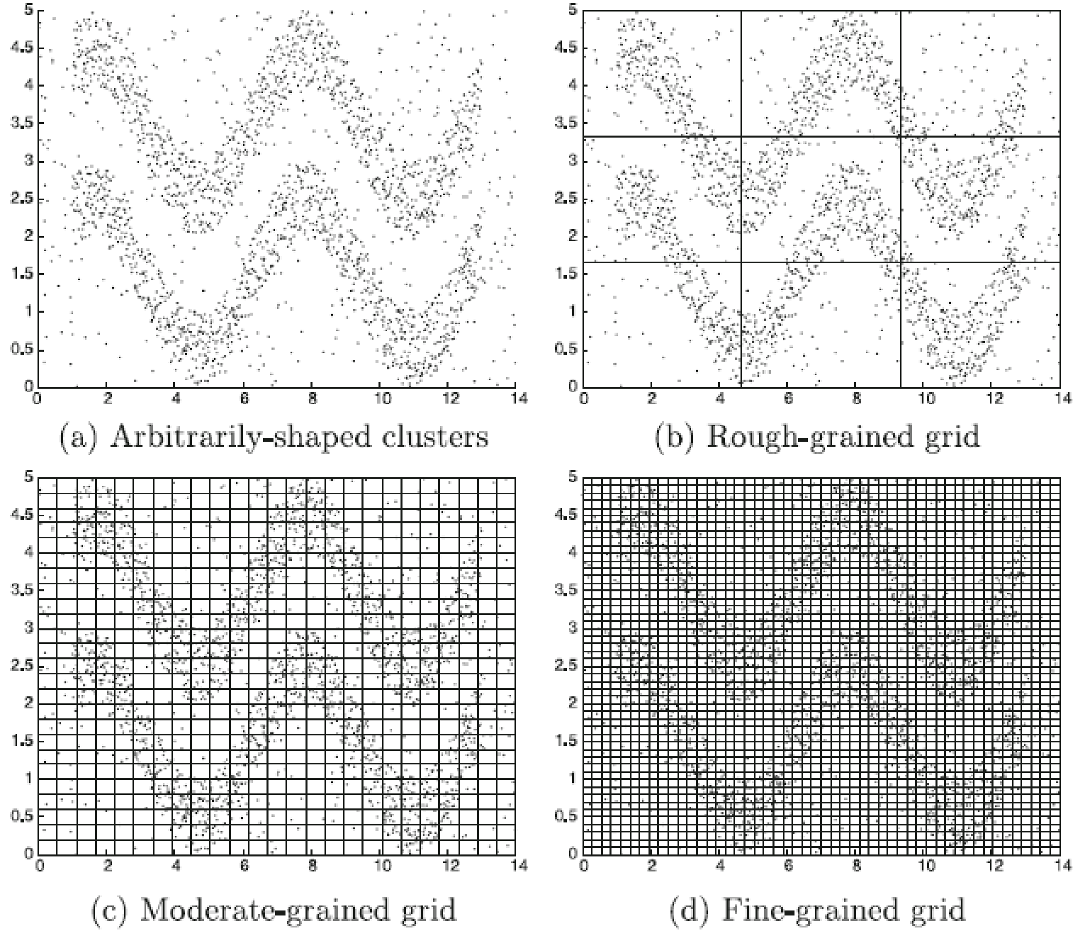
**Algorithm** *GenericGrid*(Data: $\mathcal{D}$, Ranges: $p$, Density: $\tau$ )
**begin**
  Discretize each dimension of data $\mathcal{D}$ into $p$ ranges;
  Determine dense grid cells at density level $\tau$;
  Create graph in which dense grids are connected if they are adjacent;
  Determine connected components of graph;
  **return** points in each connected component as a cluster;
**end**



(a) Data points and grid　　(b) Agglomerating adjacent grids

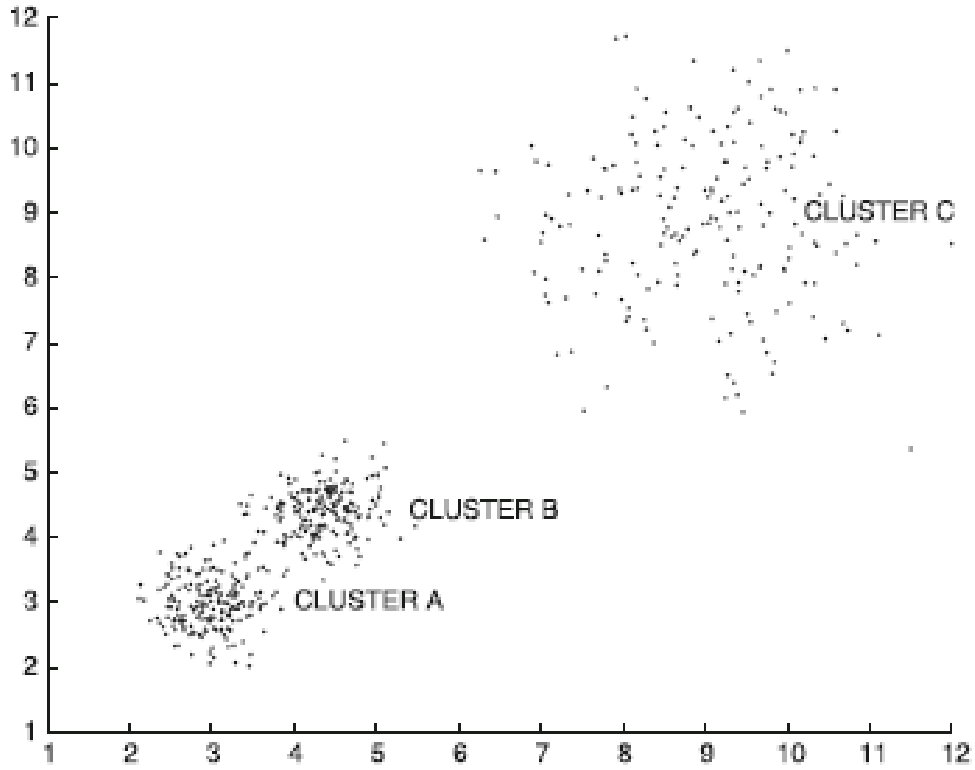
# Limitations-2 Parameters (1)

- The number of Grids



# Limitations-2 Parameters (2)

- The Level of Density

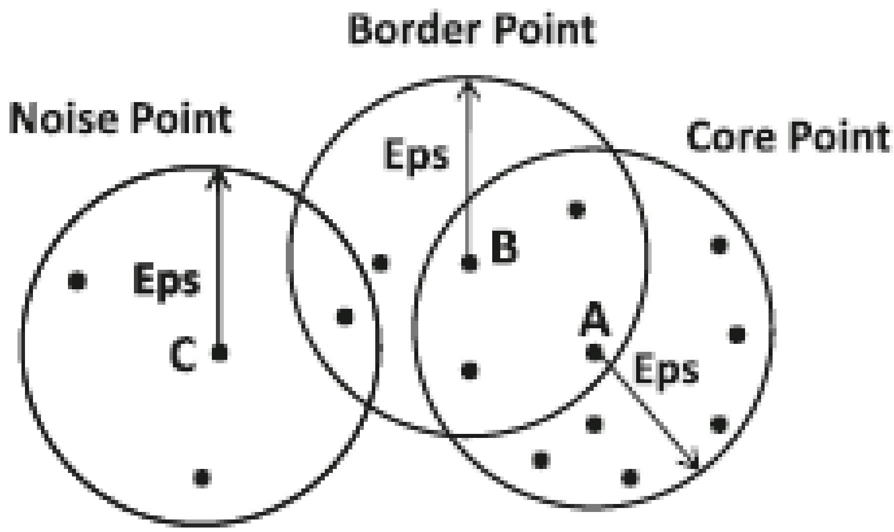


# DBSCAN (1)

1. Classify data points into
   - Core point: A data point is defined as a core point, if it contains at least $\tau$ data points within a radius $Eps$.
   - Border point: A data point is defined as a border point, if it contains less than $\tau$ points, but it also contains at least one core point within a radius $Eps$.
   - Noise point: A data point that is neither a core point nor a border point is defined as a noise point.

# DBSCAN (2)

1. Classify data points into Core point, Border point, and Noise points.

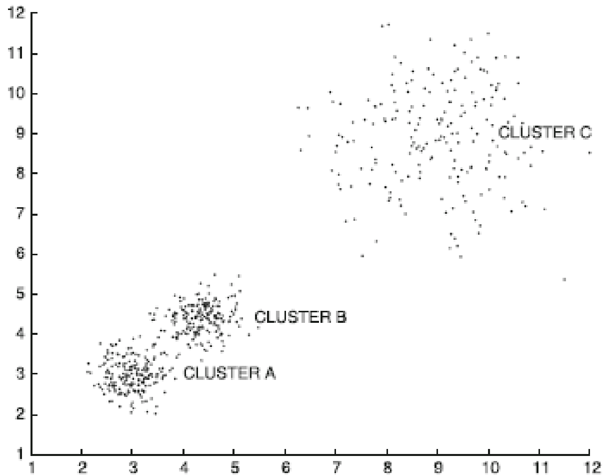


# DBSCAN (3)

1. Classify data points into Core point, Border point, and Noise points.
2. A connectivity graph is constructed with respect to the core points
   - Core points are connected if they are within $Eps$ of one another
3. Determine connected components
4. Assign each border point to connected component
   - with which it is best connected

# Limitations of DBSCAN

- Two Parameters
  - Radius $Eps$ and Level of Density $\tau$




  - They are related to each other
- High Computational Cost
  - Identifying neighbors $O(n^2)$

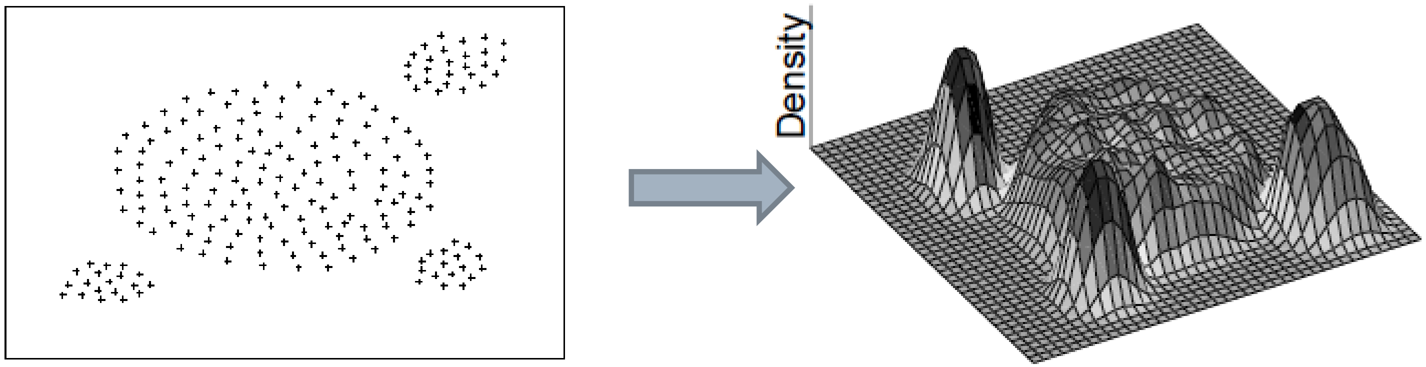
# DENCLUE—Preliminary

- Kernel-density Estimation
  - Given $n$ data points $\overline{X_1}, \ldots, \overline{X_n}$

$$f(\overline{X}) = \frac{1}{n} \sum_{i=1}^{n} K(\overline{X} - \overline{X_i}).$$

  - $K(\cdot)$ is a kernel function

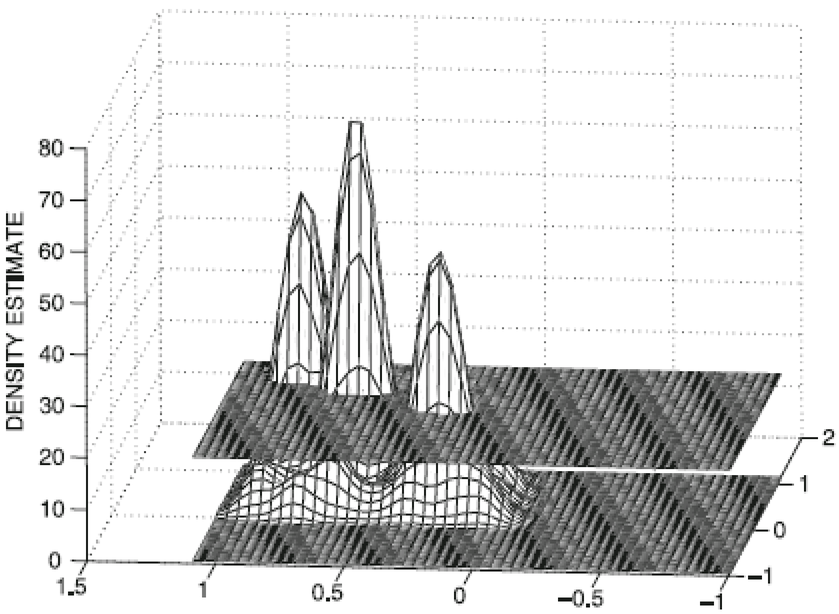
$$K(\overline{X} - \overline{X_i}) = \left(\frac{1}{h\sqrt{2\pi}}\right)^d e^{-\frac{||\overline{X} - \overline{X_i}||^2}{2 \cdot h^2}}.$$



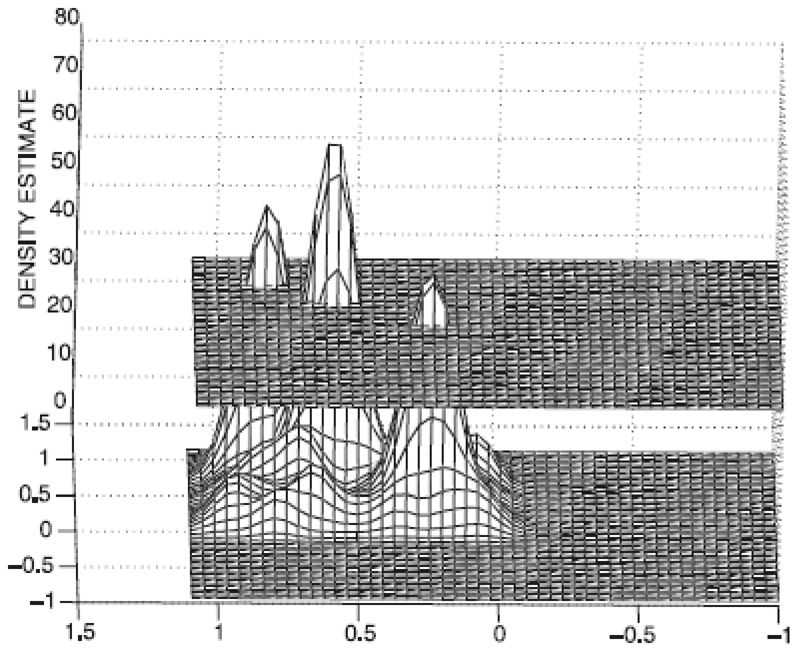

[Hinneburg and Keim, 1998]

# DENCLUE—The Key Idea

- Determine clusters by using a density threshold $\tau$



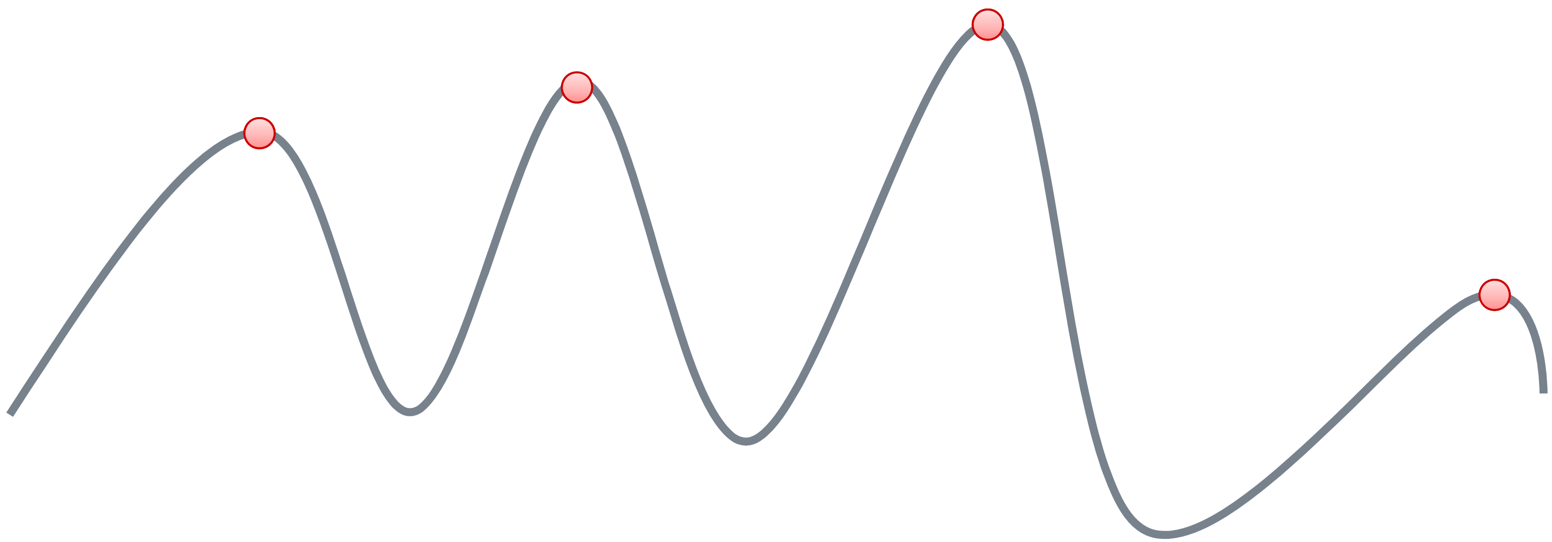

2 clusters




3 clusters

# DENCLUE—Procedure

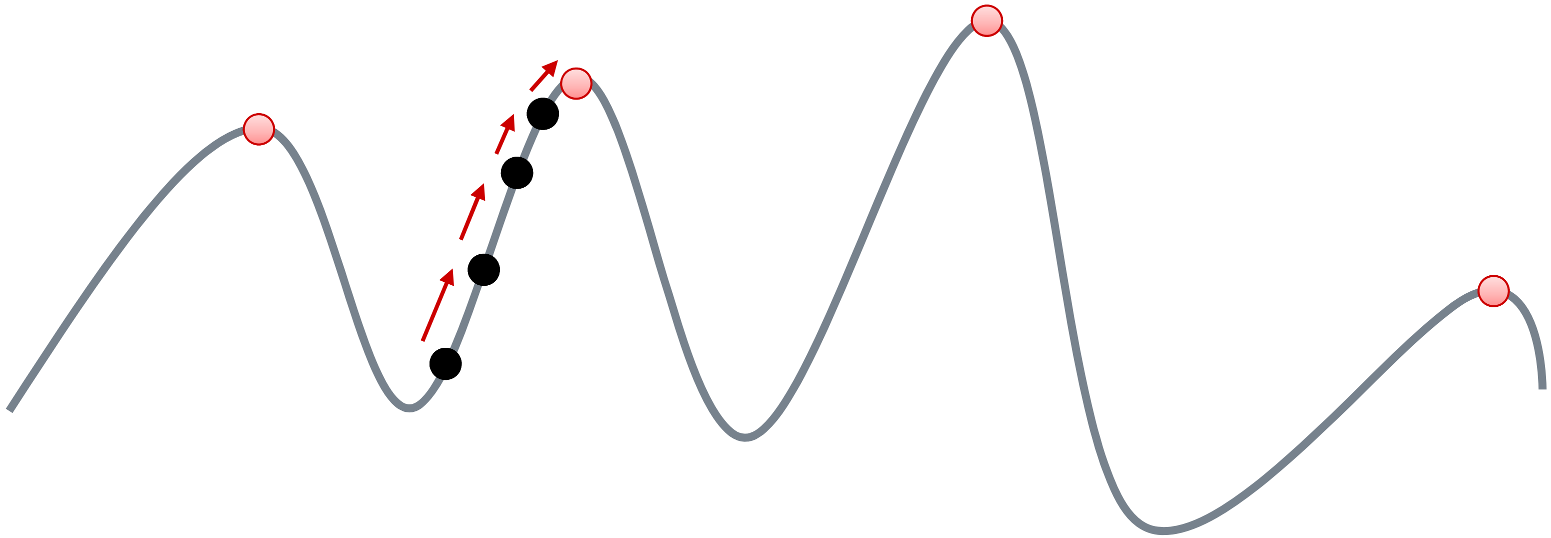
- Density Attractors
  - Local Maximum/Peak



# DENCLUE—Procedure

- Density Attractors
  - Local Maximum/Peak
- Identify a Peak for Each Data Point
  - An iterative gradient ascent

$$\overline{X^{(t+1)}} = \overline{X^{(t)}} + \alpha \nabla f(\overline{X^{(t)}})$$



# DENCLUE—Procedure

- Density Attractors
  - Local Maximum/Peak
- Identify a Peak for Each Data Point
  - An iterative gradient ascent

$$\overline{X^{(t+1)}} = \overline{X^{(t)}} + \alpha \nabla f(\overline{X^{(t)}})$$

- Post-Processing
  - Attractors whose density is smaller than $\tau$ are excluded
  - Density attractors are connected to each other by a path of density at least $\tau$ will be merged

# DENCLUE—Implementation

## Gradient Ascent

- Gradient

$$\nabla f(\overline{X}) = \frac{1}{n}\sum_{i=1}^{n} \nabla K(\overline{X} - \overline{X_i}).$$

- Gaussian Kernel

$$\nabla K(\overline{X} - \overline{X_i}) \propto (\overline{X_i} - \overline{X})K(\overline{X} - \overline{X_i})$$

## Mean-shift Method

$$\overline{X^{(t+1)}} = \frac{\sum_{i=1}^{n} \overline{X_i} K(\overline{X^{(t)}} - \overline{X_i})}{\sum_{i=1}^{n} K(\overline{X^{(t)}} - \overline{X_i})}$$

- Converges much faster

# Outline

- Grid-Based and Density-Based Algorithms
- **Graph-Based Algorithms**
- Non-negative Matrix Factorization
- Cluster Validation
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# Graph Construction for a Set of $n$ Points $\mathcal{O} = \{O_1, \ldots, O_n\}$

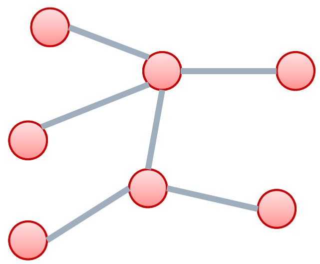
- A node is defined for each $O_i \in \mathcal{O}$
- An edge exists between $O_i$ and $O_j$
  - If the distance $d(O_i, O_j) \leq \epsilon$
  - If either one is a $m$-nearest neighbor of the other (A better approach)
- If there is an edge, then its weight is
  - 1
  - Heat Kernel: $e^{-d(O_i,O_j)^2/t^2}$

# Spectral Clustering

## Dimensionality Reduction

- Find a low-dimensional representation for each node in the graph

$$O_1, O_2, \vdots, O_n \Rightarrow$$



$$\Rightarrow \mathbf{y}_1 \in \mathbb{R}^k, \mathbf{y}_2 \in \mathbb{R}^k, \vdots, \mathbf{y}_n \in \mathbb{R}^k$$

$$W = [w_{ij}] \in \mathbb{R}^{n \times n}$$

- Laplacian Eigenmap [Belkin and Niyogi, 2002]

## $k$-means

- Apply $k$-means to new representations of the data

# Laplacian Eigenmap (1)

- The Objective Function ($k = 1$)
  - $y_i \in \mathbb{R}$ is a 1-dimensional representation of $O_i$
  - $w_{ij}$ is the similarity between $O_i$ and $O_j$

$$O = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} \left( y_i - y_j \right)^2$$

  - Similar points will be mapped closer
    - ✓ Similar points have larger weights

# Laplacian Eigenmap (2)

- The Objective Function ($k = 1$)
  - Vector Form

$$O = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (y_i - y_j)^2 = 2\mathbf{y}^\top L \mathbf{y}$$

  - $\mathbf{y} = [y_1, \dots, y_n]^\top \in \mathbb{R}^n$
  - $L = D - W \in \mathbb{R}^{n \times n}$ is the graph Laplacian
    - ✓ Positive Semidefinite (PSD)
  - $W = [w_{ij}] \in \mathbb{R}^{n \times n}$ is the similarity matrix
  - $D \in \mathbb{R}^{n \times n}$ is a diagonal matrix with $D_{ii} = \sum_{j=1}^{n} w_{ij}$

# Laplacian Eigenmap (3)

- The Optimization Problem ($k = 1$)

$$\min_{\mathbf{y}\in\mathbb{R}^n} \quad \mathbf{y}^\top L\mathbf{y}$$
$$\text{s.t.} \quad \mathbf{y}^\top D\mathbf{y} = 1$$

  - Add a Constraint to Remove Scaling Factor
    - ✓ $D$ is introduced for normalization [Luxburg, 2007]

- The Solution $L\mathbf{y} = \lambda D\mathbf{y}$

  - Generalized Eigenproblem [Luxburg 2007]
  - The smallest eigenvector is $\mathbf{y}^1 = \mathbf{1}$
    - ✓ Useless since $y_1^1 = y_2^1 = \cdots = y_n^1$

# Laplacian Eigenmap (3)

- The Optimization Problem ($k = 1$)

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  - Add a Constraint to Remove Scaling Factor
    - ✓ $D$ is introduced for normalization [Luxburg, 2007]

- The Solution $L\mathbf{y} = \lambda D \mathbf{y}$
  - Generalized Eigenproblem [Luxburg 2007]
  - The smallest eigenvector is $\mathbf{y}^1 = \mathbf{1}$
  - Use the second smallest eigenvector $\mathbf{y}^2$
    - ✓ The new representation for $o_i$ is $y_i^2$

# Laplacian Eigenmap (4)

## The Objective Function ($k > 1$)

- Vector Form

$$O = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} \left\| \mathbf{y}_i - \mathbf{y}_j \right\|_2^2 = 2\mathrm{trace}(Y^T L Y)$$

- $Y = [\mathbf{y}_1, \dots, \mathbf{y}_n]^\mathrm{T} \in \mathbb{R}^{n \times k}$
- $L = D - W \in \mathbb{R}^{n \times n}$ is the graph Laplacian
- $W = [w_{ij}] \in \mathbb{R}^{n \times n}$ is the similarity matrix
- $D \in \mathbb{R}^{n \times n}$ is a diagonal matrix with $D_{ii} = \sum_{j=1}^{n} w_{ij}$

# Laplacian Eigenmap (4)

- The Optimization Problem ($k > 1$)

$$\min_{Y \in \mathbb{R}^{n \times k}} \quad \text{trace}(Y^\top L Y)$$
$$\text{s.t.} \quad Y^\top D Y = I$$

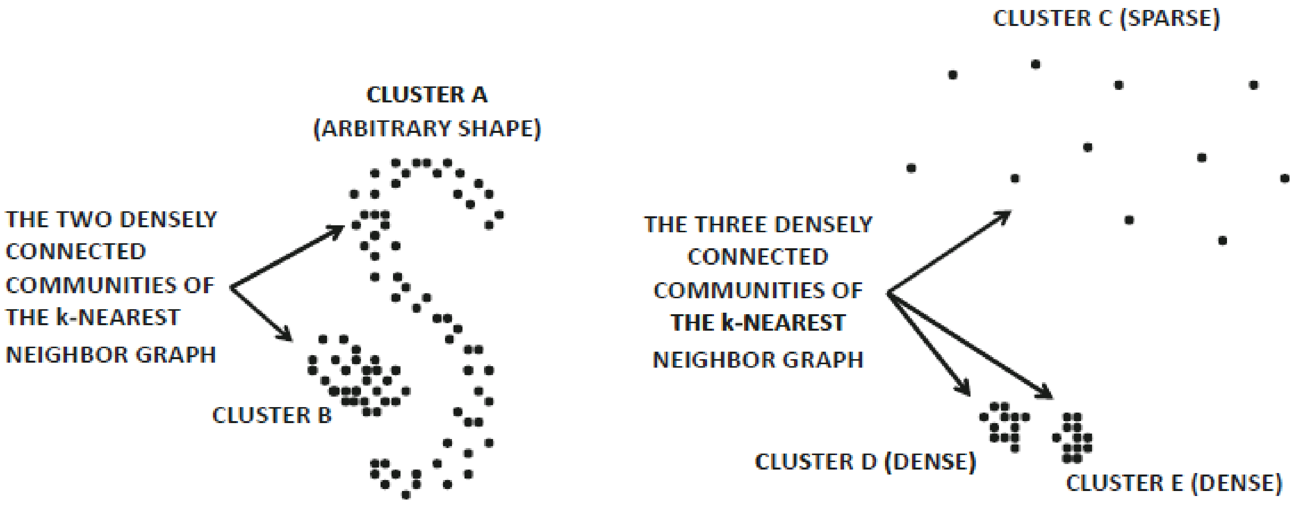
- The Solution

$$L\mathbf{y} = \lambda D \mathbf{y}$$

  - Generalized Eigenproblem [Luxburg 2007]
  - Use $Y = [\mathbf{y}^2, \ldots, \mathbf{y}^{k+1}] \in \mathbb{R}^{n \times k}$ as the optimal solution
    - ✓ $\mathbf{y}^i$ is the $i$-th generalized eigenvector
    - ✓ The new representation $\mathbf{y}_i \in \mathbb{R}^k$ for $O_i$ is the $i$-th row of $Y$
  - Don't forget the normalization $Y^\top D Y = I$

# Properties of Spectral Clustering

- Varying Cluster Shape and Density



(a) Varying cluster shape (b) Varying cluster density

  - Due to the nearest neighbor graph
- High Computational Cost

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# Non-negative Matrix Factorization (NMF)

- Let $X = [\mathbf{x}_1, \ldots, \mathbf{x}_n] = \mathbb{R}^{d \times n}$ be a non-negative data matrix
- NMF aims to factor $X$ as $U \times V^\top$
  - $U \in \mathbb{R}^{d \times k}$ and $V \in \mathbb{R}^{n \times k}$ are non-negative
- The Optimization Problem

$$\min_{U \in \mathbb{R}^{d \times k}, V \in \mathbb{R}^{n \times k}} \quad \|X - UV^\top\|_F^2$$
$$\text{s.t.} \quad U \geq 0, V \geq 0$$

  - Non-convex

# Interpretation of NMF (1)

- Matrix Appromation

$$X \approx UV^\top$$

- Element-wise
  - $X = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$, where $\mathbf{x}_i \in \mathbb{R}^d$
  - $U = [\mathbf{u}_1, \ldots, \mathbf{u}_k] \in \mathbb{R}^{d \times k}$, where $\mathbf{u}_i \in \mathbb{R}^d$
  - $V^\top = [\mathbf{v}_1, \ldots, \mathbf{v}_n] \in \mathbb{R}^{k \times n}$, where $\mathbf{v}_i \in \mathbb{R}^k$
    - ✓ $\mathbf{v}_i$ is the $i$-th column of $V^\top$
    - ✓ $\mathbf{v}_i^\top$ is the $i$-th row of $V$
  - Then,

$$\mathbf{x}_i \approx U\mathbf{v}_i = \sum_{j=1}^{k} \mathbf{u}_j v_{ij}$$

    - ✓ $v_{ij}$ is the $j$-th element of vector $\mathbf{v}_i$

# Interpretation of NMF (2)

## Vector Approximation

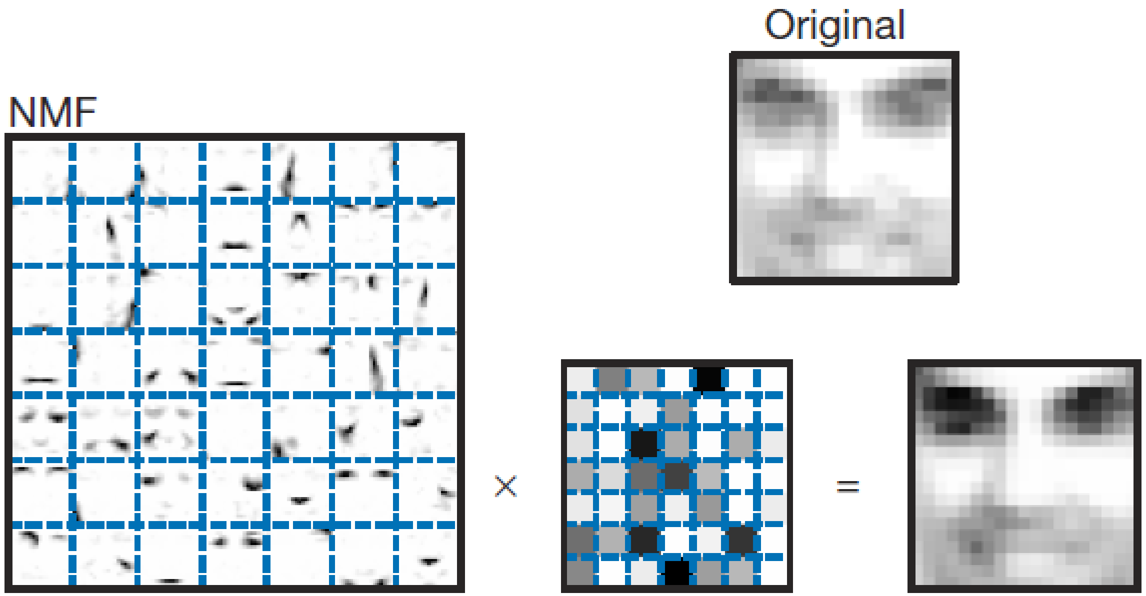
$$\mathbf{x}_i \approx U\mathbf{v}_i = \sum_{j=1}^{k} \mathbf{u}_j v_{ij}$$

- $\mathbf{u}_1, \ldots, \mathbf{u}_k \in \mathbb{R}^d$ can be treated as basis vectors
  - ✓ They may be not orthonormal
  - ✓ They are non-negative

- $\mathbf{v}_i = [v_{i1}, \ldots, v_{ik}]^\top \in \mathbb{R}^k$ can be treated as a new $k$-dimensional representation of $\mathbf{x}_i$

# Parts-Based Representations

- When each $\mathbf{x}_i$ is a face image




  - [Lee and Seung, 1999]

# Clustering by NMF

- Vector Approximation

$$\mathbf{x}_i \approx U\mathbf{v}_i = \sum_{j=1}^{k} \mathbf{u}_j v_{ij}$$

  - $\mathbf{u}_j$ can be treated as an representative of the $j$-th cluster
  - $v_{ij}$ can be treated as the association between $\mathbf{x}_i$ and $\mathbf{u}_j$

- The cluster label $l_i$ for $\mathbf{x}_i$

$$l_i = \mathrm{argmax}_j v_{ij}$$

  - [Xu et al., 2003]

# An Example

- Discover both Row and Column Clusters

| | | | | | |
|---|---|---|---|---|---|
| 2 | 2 | 1 | 2 | 0 | 0 |
| 2 | 3 | 3 | 3 | 0 | 0 |
| 1 | 1 | 1 | 1 | 0 | 0 |
| 2 | 2 | 2 | 3 | 1 | 1 |
| 0 | 0 | 0 | 1 | 1 | 1 |
| 0 | 0 | 0 | 2 | 1 | 2 |

$\approx$

| | |
|---|---|
| 2 | 0 |
| 3 | 0 |
| 1 | 0 |
| 2 | 1 |
| 0 | 1 |
| 0 | 2 |

$\times$

| | | | | | |
|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 0 | 0 |
| 0 | 0 | 0 | 1 | 1 | 1 |

# Optimization in NMF

- Alternating between $U$ and $V$

$$u_{ij} \leftarrow u_{ij} \frac{(\mathbf{XV})_{ij}}{(\mathbf{UV}^T\mathbf{V})_{ij}}$$

$$v_{ij} \leftarrow v_{ij} \frac{(\mathbf{X}^T\mathbf{U})_{ij}}{(\mathbf{VU}^T\mathbf{U})_{ij}}$$

  - Local Optimal Solutions
    - ✓ Run multiple times and choose the best one

- Other Optimization Algorithms are also Possible

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# Concepts

- Cluster validation
  - Evaluate the quality of a clustering
- Internal Validation Criteria
  - Do not need additional information
  - Biased toward one algorithm or the other
- External Validation Criteria
  - Ground-truth clusters are known
  - Ground-truth may not reflect the natural clusters in the data

# Internal Validation Criteria

- Sum of square distances to centroids

$$\sum_{j=1}^{k} \sum_{\mathbf{x}_i \in \mathcal{C}_j} \left\| \mathbf{x}_i - \mathbf{c}_j \right\|_2^2$$

- Intracluster to intercluster distance ratio

$$Intra = \sum_{(\overline{X_i}, \overline{X_j}) \in P} dist(\overline{X_i}, \overline{X_j})/|P|$$

$$Inter = \sum_{(\overline{X_i}, \overline{X_j}) \in Q} dist(\overline{X_i}, \overline{X_j})/|Q|.$$

- Silhouette coefficient
- Probabilistic measure

# External Validation Criteria

- Class Labels
  - The Ground-truth
- Confusion Matrix
  - Each row $i$ corresponds to the class label $j$
  - Each column $j$ corresponds to the algorithm-determined cluster $j$

| Cluster Indices | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| 1 | 97 | 0 | 2 | 1 |
| 2 | 5 | 191 | 1 | 3 |
| 3 | 4 | 3 | 87 | 6 |
| 4 | 0 | 0 | 5 | 195 |

| Cluster Indices | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| 1 | 33 | 30 | 17 | 20 |
| 2 | 51 | 101 | 24 | 24 |
| 3 | 24 | 23 | 31 | 22 |
| 4 | 46 | 40 | 44 | 70 |

  - Ideal clustering $\Rightarrow$ a diagonal matrix after permutation

# Notations

- $m_{ij}$: number of data points from class (*ground-truth*) cluster $i$ that are mapped to (*algorithm-determined*) cluster $j$
- $N_i$: number of data points in *true cluster* $i$

$$N_i = \sum_{j=1}^{k_d} m_{ij} \qquad \forall i = 1 \dots k_t$$

- $M_j$: number of data points in *algorithm-determined* cluster $j$

$$M_j = \sum_{i=1}^{k_t} m_{ij} \qquad \forall j = 1 \dots k_d$$

# Purity

- For a given algorithm-determined cluster $j$, define $P_j$ as number of data points in its *dominant* class

$$P_j = \max_i m_{ij}.$$

- The overall purity

$$\text{Purity} = \frac{\sum_{j=1}^{k_d} P_j}{\sum_{j=1}^{k_d} M_j}.$$

  - High values of the purity are desirable

# Gini index

- Limitation of Purity
  - Only accounts for the dominant label in the cluster and ignores the distribution of the remaining points
- Gini index $G_j$ for column (algorithm-determined cluster) $j$

$$G_j = 1 - \sum_{i=1}^{k_t} \left( \frac{m_{ij}}{M_j} \right)^2$$

- The average Gini coefficient
  - Low values

$$G_{average} = \frac{\sum_{j=1}^{k_d} G_j \cdot M_j}{\sum_{j=1}^{k_d} M_j}$$

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# Summary

- Grid-Based and Density-Based Algorithms
  - Grid-Based Methods
  - DBSCAN, DENCLUE
- Graph-Based Algorithms
  - Laplacian Eigenmap
- Non-negative Matrix Factorization
- Cluster Validation
  - Purity, Gini index

# Reference


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