Advanced Machine Learning

Lecture 3: Hierarchical Clustering

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CentraleSupélec

Content

Today's Lecture

1. Introduction

2. Reminders on Clustering
   1. Types of methods and clusters
   2. Distance and Dissimilarity
   3. Clustering Quality

3. From Partitional to Hierarchical Clustering
   1. K-means
   2. Hierarchical Clustering
   3. DBSCAN
   4. HDBSCAN

Key references

- Tan, P. N., Steinbach, M., Kumar V., *Data mining cluster analysis: basic concepts and algorithms. Introduction to data mining*. 2013.
- Bishop, C. M. *Pattern Recognition and Machine Learning.* Springer, 2006.
- Hastie, T., Tibshirani, R. and Friedman, J. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction.* Second edition. Springer, 2009.
- James, G., Witten, D., Hastie, T. and Tibshirani, R. *An Introduction to Statistical Learning, with Applications in R.* Springer, 2013

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Clustering: An Unsupervised Approach

- Extract homogeneous meaningful or useful categories from the data
- Discover/learn how the data is organized, natural structure
- No ground-truth outputs for training : unsupervised

Objectives

1. Understanding: Biology and medicine, finance, text mining, web, ...
2. Utility: Use cluster characteristics instead of the original data (dimension reduction, regression of high-dimensional data, ...)

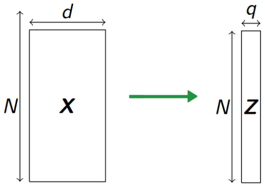
The labels are unknown!

Dimension reduction vs Clustering

Let $\boldsymbol{X} = (x_1, \dots, x_N)$ be a set of N training samples

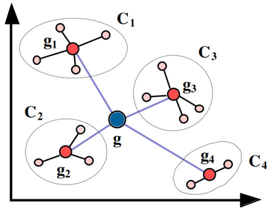
Dimension reduction

- Project $\boldsymbol{X} \in \mathbb{R}^{N,d}$ onto $\boldsymbol{Z} \in \mathbb{R}^{N,q}$ with $q < d$
- Visualize, denoise, reduce computational cost, ...



Clustering

- Groupe similar samples $\boldsymbol{x}_i$ into clusters C_k
- Based on a dissimilarity metric $\mathcal{D}(C_1, C_2)$



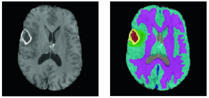
Clustering Applications

Market segmentation

- x: purchase history
- C_k: market segments

Medical image segmentation

- x: image pixels, voxels
- C_k: blood, muscle, tumor, ...



Text mining

- x: text, e-mails, ...
- C_k: folders, themes, ...

Key Questions on Clustering

- Types of clustering ?
- How to characterize a cluster ?
- How to define similarity or dissimilarity between samples ?
- The real/optimal number of clusters ?
- What algorithms can we use and when ?
- How to evaluate a clustering result ? (subjectivity)

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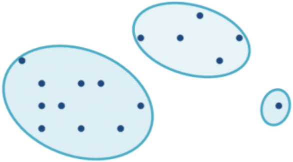
Types of clustering: Partitional vs Hierarchical

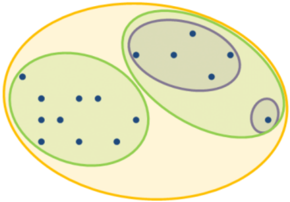
Partitional

- Division into non-overlapping subsets
- Each data point is in exactly one subset



Hierarchical

- Clusters can have sub-clusters
- Set of nested clusters, organized as a tree



Types of Clusters

- Well-separated: Any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.
- Prototype-Based: an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster → Assumptions about shape
  - Center = centroid (average) or medoid (most representative)
- Density-based: dense region of points, which is separated by low-density regions, from other regions of high density. Used when the clusters are irregular or intertwined, and when noise and outliers are present → Is data driven
- Others... graph-based...

Distinctions between sets of clusters

- Exclusive vs non-exclusive (overlapping): separate clusters vs points may belong to more than one cluster
- Fuzzy vs non-fuzzy: each observation $\mathbf{x}_i$ belongs to every cluster $\mathcal{C}_k$ with a given weight $w_k \in [0, 1]$ and $\sum_{k=1}^{K} w_k = 1$ (Similar to probabilistic clustering).
- Partial vs Complete: all data are clustered vs there may be non-clustered data, e.g., outliers, noise, "uninteresting background"...
- Homogeneous vs Heterogeneous: Clusters with $\neq$ size, shape, density...

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Dissimilarity Measures

Dissimilarity is a function of the pair (x, y): $\mathcal{D} : \mathbb{E} \times \mathbb{E} \to \mathbb{R}^+$ s.t

$$\mathcal{D}(x, y) = \mathcal{D}(y, x) \geq 0 \quad \text{and} \quad \mathcal{D}(x, x) = 0 \ \forall x \in \mathbb{E}$$

Distance is a dissimilarity measure that satisfies also

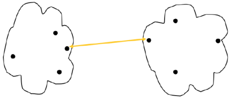
1. $\mathcal{D}(x, y) = 0 \iff x = y$
2. $\mathcal{D}(x, y) \leq \mathcal{D}(x, z) + \mathcal{D}(z, y)$ (metric)

Common distances

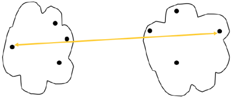
- Minkowski: $\mathcal{D}(x, y) = \left(\sum_{j=1}^{d} |x_j - y_j|^q\right)^{\frac{1}{q}}$
  ($q = 2 \ \to$ Euclidian distance, $q = 1 \ \to$: Manhattan distance)
- Mahalanobis: $\mathcal{D}(x, y) = \left[(x - y)^T \Sigma^{-1} (x - y)\right]^{\frac{1}{2}}$
- Hamming: number of indexes where the 2 vectors differ

Dissimilarity Between Clusters (1/2)

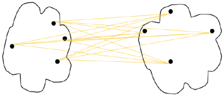
Minimum : $\mathcal{D}(\mathcal{C}_i, \mathcal{C}_j) = \min_{\mathbf{x}\in\mathcal{C}_i, \mathbf{y}\in\mathcal{C}_j} \mathcal{D}(\mathbf{x}, \mathbf{y})$



Maximum : $\mathcal{D}(\mathcal{C}_i, \mathcal{C}_j) = \max_{\mathbf{x}\in\mathcal{C}_i, \mathbf{y}\in\mathcal{C}_j} \mathcal{D}(\mathbf{x}, \mathbf{y})$

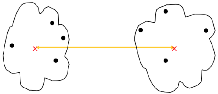


Group Average : $\mathcal{D}(\mathcal{C}_i, \mathcal{C}_j) = \dfrac{1}{n_i\, n_j} \sum_{\mathbf{x}\in\mathcal{C}_i} \sum_{\mathbf{y}\in\mathcal{C}_j} \mathcal{D}(\mathbf{x}, \mathbf{y})$



Between Centroids : $\mathcal{D}(\mathcal{C}_i, \mathcal{C}_j) = \mathcal{D}(m_i, m_j)$,

with $m_i = \dfrac{1}{n_i} \sum_{\mathbf{x}\in\mathcal{C}_i} \mathbf{x}$



Dissimilarity Between Clusters (2/2)

Objective function distances

- Ward distance: $\mathcal{D}(\mathcal{C}_i, \mathcal{C}_j) = \sqrt{\frac{2\, n_i\, n_j}{n_i + n_j}}\mathcal{D}(m_i, m_j)$
- WPGMA (Weighted Pair Group Method with Arithmetic Mean) recursive distance

$$\mathcal{D}(\mathcal{C}_i, \mathcal{C}_j) == \frac{\mathcal{D}(\mathcal{C}_i^1, \mathcal{C}_j) + \mathcal{D}(\mathcal{C}_i^2, \mathcal{C}_j)}{2}$$

where $\mathcal{C}_i^1, \mathcal{C}_i^2$ are the child clusters of $\mathcal{C}_i$

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What makes a good clustering ?

- Centroid: $\boldsymbol{m}_i = \dfrac{1}{n_i} \sum_{\mathbf{x} \in \mathcal{C}_i} \mathbf{x}$
- Inertia: $J_i = \sum_{\mathbf{x} \in \mathcal{C}_i} \mathcal{D}^2(xg, \boldsymbol{m}_i)$
  (low J_i corresponds to a smaller dispersion of points around $\boldsymbol{m}_i$.)
- Within distance: $J_w = \sum_i \sum_{\mathbf{x} \in \mathcal{C}_i} \mathcal{D}^2(xg, \boldsymbol{m}_i) = \sum_i J_i$
- Between distance: $J_b = \sum_i n_i \mathcal{D}^2(\boldsymbol{m}_i, \boldsymbol{m})$
  where $\boldsymbol{m}$ is the sample mean $\boldsymbol{m} = \dfrac{1}{n} \sum \mathbf{x}$

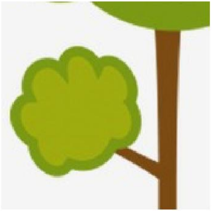
A good clustering...

Minimizes the within distance J_w and maximizes the between distance J_b

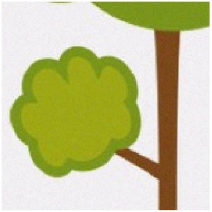
Illustrative Example

Objective

Cluster noisy data for a segmentation application in image processing



(a) Tree data



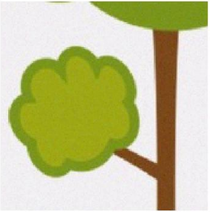
(b) Noisy tree data

Illustrative Example

Objective

Cluster noisy data for a segmentation application in image processing

(c) Tree data



(d) Noisy tree data

Looks easy! But...

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K-means

- Partition the data into K clusters
- Find K clusters and their center μ_k that minimize the cluster within distance J_w
- J_w can be defined as

$$J_w = \Sigma_{k=1}^{K} \Sigma_{x^i \in C_k}^{K} \|\boldsymbol{x}^i - \mu_k\|^2$$

How can we solve this problem?

- NP-hard problem: number of partitions of $\mathbf{x}$ into K subsets

$$P(n, K) = \frac{1}{K!} \sum_{k=0}^{K} k^n \, (-1)^{K-k} \, \frac{K!}{k! \, (K-k)!} \text{ for } K < n$$

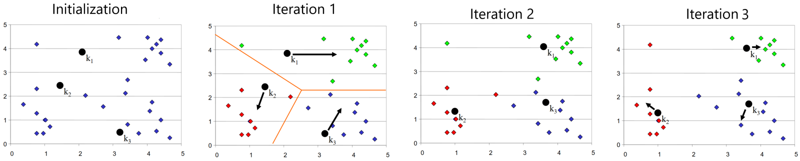
Example: $P(100, 5) \approx 10^{68}$!!!!

- Local solution is obtained with k-means ($O(tKN)$)

K-means algorithm

Iterative minimization

1. Initialize K cluster centers μ_k
2. Assign each $\boldsymbol{x}^i$ to the nearest cluster (nearest center)
   e.g., $\boldsymbol{s}_i \leftarrow \arg\min_k \|\boldsymbol{x}^i - \mu_k\|^2$
3. Re-estimate K cluster centers
   e.g., $\mu_k = \frac{1}{K} \sum_{x^i \in C_k} \boldsymbol{x}^i$
4. Repeat until stopping criterion is reached



K-means Drawbacks and Alternatives

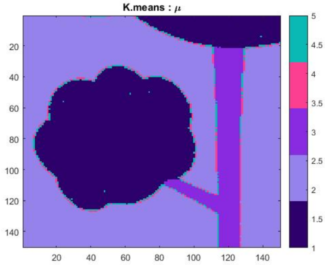
K-means is simple but ...

- Solution depends on initialization
- Need to know K in advance
- Can't handle noise or outliers : *non-robust*
- Fails with clusters of *non-convex* shapes

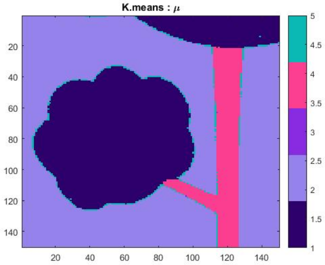
Several alternatives

- K-means++: seeding algorithm $\rightarrow$ initialize clusters with centroids "spread-out" throughout the data
- K-medoids $\rightarrow$ address the robustness aspects
- Kernel K-means $\rightarrow$ overcoming the convex shape limitation
- Many others ...

Results on the tree example



(e) K-means++



(f) “Clusters”

Figure: Clustering obtained with two different initializations

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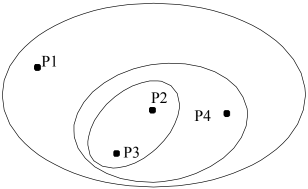
Hierarchical clustering Principles

- Produces a set of nested clusters organized as a hierarchical tree $\rightarrow$ bypass choice of K
- Can be visualized as a dendrogram: a tree like diagram that records the sequences of merges or splits with branch length corresponding to cluster distance

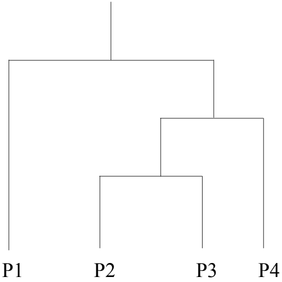
Two approaches

1. Agglomerative: *Bottom-up* - Start with as much clusters as observations and iteratively *aggregate* observations using a given *distance*
2. Divise: *Top-down* - Start with one cluster containing all observations and iteratively *split* into smaller clusters

Hierarchical Clustering: The tree



(a) Hierarchical Clusters



(b) Dendrogram

We can see that ...

- Each node (cluster) in the tree (except the leaf nodes) is the union of its children (subclusters)
- The root of the tree is the cluster containing all objects.

Hierarchical Clustering: Example

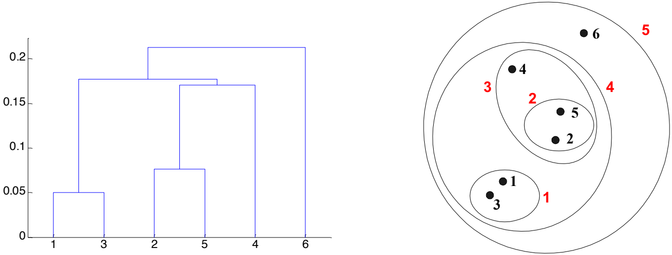


Figure: General principles

Agglomerative Hierarchical Clustering

Algorithm 1 : Agglomerative Hierarchical Clustering

- **Input** : **x** observation vectors and "cutting" threshold λ
- **Output** : all merged clusters set (at each iteration) and "inter-cluster" distances (between clusters)
- **Initialization** : n = sample size = number of clusters.

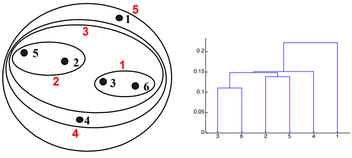
While Number of clusters > 1

1. Compute distances between clusters
2. Merged the two nearest clusters

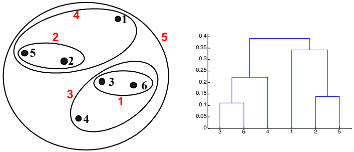
Recall: Inter-Cluster distances

- MIN $\rightarrow$ Single Linkage: $d(\mathcal{C}_i, \mathcal{C}_j) = \min_{\mathbf{x} \in \mathcal{C}_i, \mathbf{y} \in \mathcal{C}_j} d(\mathbf{x}, \mathbf{y})$
- MAX $\rightarrow$ Complete Linkage: $d(\mathcal{C}_i, \mathcal{C}_j) = \max_{\mathbf{x} \in \mathcal{C}_i, \mathbf{y} \in \mathcal{C}_j} d(\mathbf{x}, \mathbf{y})$
- Group Average $\rightarrow$ Average Linkage: $d(\mathcal{C}_i, \mathcal{C}_j) = \frac{1}{n_i n_j} \sum_{\mathbf{x} \in \mathcal{C}_i} \sum_{\mathbf{y} \in \mathcal{C}_j} d(\mathbf{x}, \mathbf{y})$
- Between centroids $\rightarrow$ Centroid Linkage: $d(\mathcal{C}_i, \mathcal{C}_j) = d(m_i, m_j)$
- Objective function $\rightarrow$ Objective Linkage:
  - Ward distance $d(\mathcal{C}_i, \mathcal{C}_j) = \sqrt{\frac{2\, n_i\, n_j}{n_i + n_j}} d(m_i, m_j)$
  - WPGMA recursive distance $d(\mathcal{C}_i, \mathcal{C}_j) == \frac{d(\mathcal{C}_i^1, \mathcal{C}_j) + d(\mathcal{C}_i^2, \mathcal{C}_j)}{2}$ where $\mathcal{C}_i^1, \mathcal{C}_i^2$ are the child clusters of $\mathcal{C}_i$

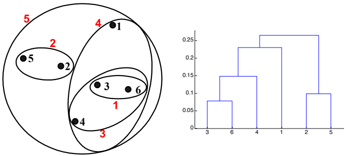
Different distances $\Rightarrow$ Different results



(a) MIN



(b) MAX



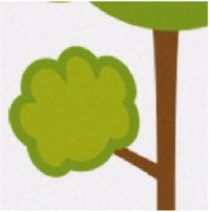
(c) Group average
(Ward provides very similar results)

Different distances $\Rightarrow$ Different results

Pros and cons of different distances

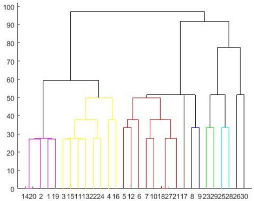
- MIN: can handle non-elliptical shape BUT sensitive to outliers, noise...
- MAX: less sensitive to outliers BUT can break large clusters and biased towards globular clusters
- Average: don't break large clusters BUT biased towards globular clusters
- Ward: Hierarchical analogue of K-means

The Tree Example : Single Linkage

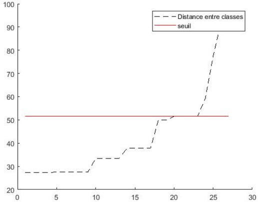


(c) Noisy Tree

(d) Single Linkage

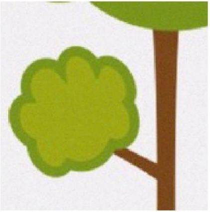


(e) Dendrogram

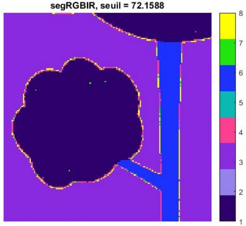


(f) Cutting Threshold

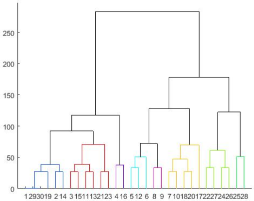
The Tree Example : Complete Linkage



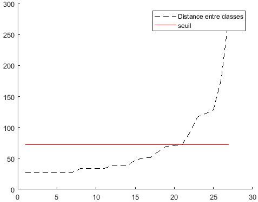
(g) Noisy Tree



(h) Complete Linkage

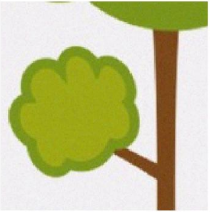


(i) Dendrogram

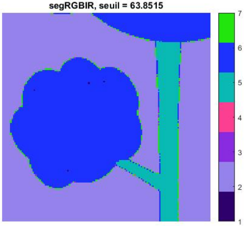


(j) Cutting Threshold

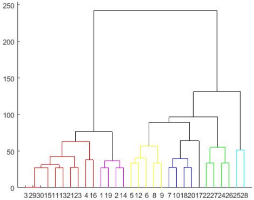
The Tree Example : Average Linkage



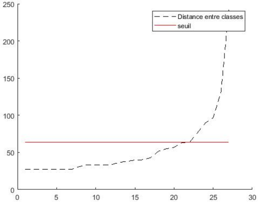
(k) Noisy Tree



(l) Average Linkage

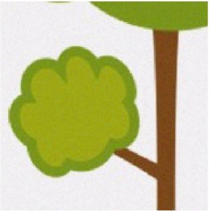


(m) Dendrogram

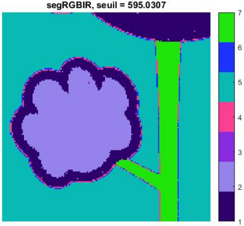


(n) Cutting Threshold

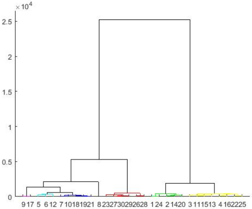
The Tree Example : Ward Linkage



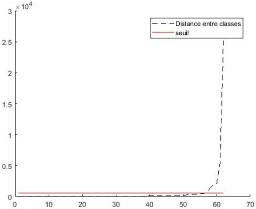
(o) Noisy Tree



(p) Average Linkage

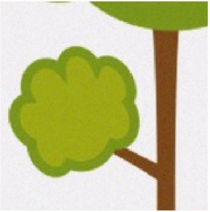


(q) Dendrogram

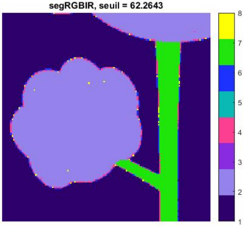


(r) Cutting Threshold

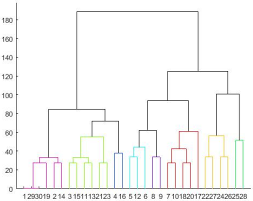
The Tree Example : WPGMA Linkage



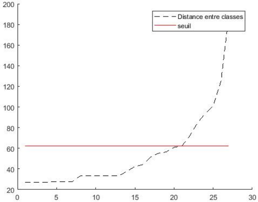
(s) Noisy Tree



(t) Average Linkage



(u) Dendrogram



(v) Cutting Threshold

Hierarchical clustering : Pros and cons

Pros

- Simple and intuitive
- Unsupervised: no *a priori* assumptions
- Interpretable: number of clusters, used distance...

Cons

- Computational cost: single linkage (O(n^3),O(n^2) or O(n)), complete linkage (O(n^3) or O(n^2)), average (O(n^3)), Ward's method (O(n^3)), ...
- Cutting threshold: challenging choice!
- Lack of robustness: sensitivity to outliers and noise
- No global objective function to optimize
- Handle heterogeneous data (clusters of $\neq$ size, non-globular shapes...)

Today's Lecture

1. Introduction

2. Reminders on Clustering
   1. Types of methods and clusters
   2. Distance and Dissimilarity
   3. Clustering Quality

3. From Partitional to Hierarchical Clustering
   1. K-means
   2. Hierarchical Clustering
   3. DBSCAN
   4. HDBSCAN

DBSCAN : A Density-based Algorithm

For an observation $\mathbf{x}_i$, find a sufficiently (MinPts) large neighborhood (ε), then

- aggregate the new observations (neighbors) to the cluster $\mathcal{C}_k$ of $\mathbf{x}_i$,
- else $\mathbf{x}_i$ is an isolated observation (outlier).

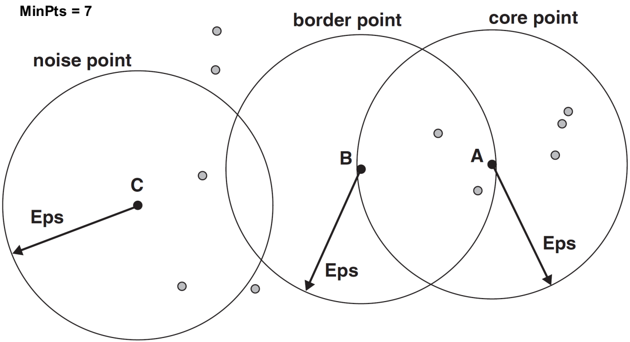
This results in three types of points called core, border, or noise points.

Key parameters

- ε and ε-neighborhood: $\mathcal{N}_\varepsilon(\mathbf{x}_i) = \{\mathbf{z} | d(\mathbf{x}_i, \mathbf{z}) < \varepsilon\}$
- MinPts: n_{min} for defining core points $\mathbf{x}_i$ s.t. $\mathrm{card}(\mathcal{N}_\varepsilon(\mathbf{x}_i)) \geq n_{min}$

DBSCAN: Three Types of Points

1. Core point: is near the center of a cluster/has MinPts neighbors
2. Border point: is not a core point, but is in the neighborhood of a core point
3. Noise point: is any point that is neither a core nor a border point

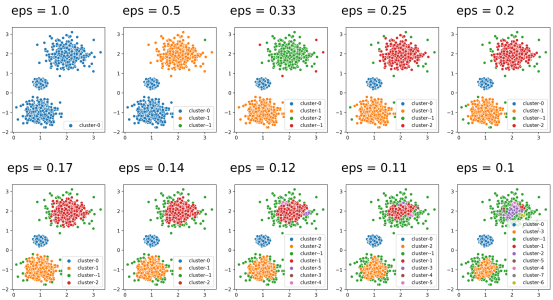


DBSCAN: Influence of ϵ

The parameter ϵ represents the minimum distance between two non-neighboring points:

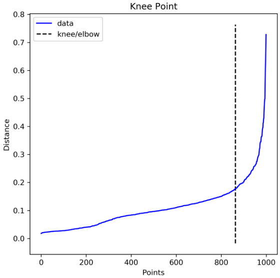
→ A very large ϵ causes all possible clusters to merge into one cluster

→ A very small ϵ leads to a lot of noise, points are not assigned to clusters



DBSCAN: So how do we choose ϵ ?

- Depends on the distance between the data points
- The Elbow trick on the k-NN plot is commonly used in practice (***k*** is MinPts!):
  - $\rightarrow$ x-axis all the points
  - $\rightarrow$ y-axis the average distance of each point to their its k-NN
- Remains a difficult choice!



DBSCAN Algorithm

Algorithm 2-a: DBSCAN

- **Input**: $\mathbf{x}$ observations, ε, MinPts
- **Output**: $\mathcal{Z}$, labels of $\mathbf{x}$

For all $\mathbf{x}_i$

1. Verify that $\mathbf{x}_i$ has not been visited by the algo, else $\mathbf{x}_i$ is marked "as visited"
2. Identify the ε-neighborhood of $\mathbf{x}_i$, $\mathcal{N}_\varepsilon(\mathbf{x}_i)$.
3. **If** $\mathrm{card}(\mathcal{N}_\varepsilon(\mathbf{x}_i)) \leq n_{min}$, then mark P as an isolated point.
   Else Create a cluster $\mathcal{C}_k$ containing $\mathbf{x}_i$ and run class_extension$(\mathcal{C}_k, \mathbf{x}_i, \varepsilon, n_{min})$

DBSCAN Algorithm : Cluster Extension

Algorithm 2-b: DBSCAN Class extension

- **Input**: Cluster $\mathcal{C}_k$ to increase, observation $\mathbf{x}_i$ of $\mathcal{C}_k$, n_{min}, ε.
- **Output** : $\mathcal{Z}$ labels of observations in $\mathcal{N}_\varepsilon(\mathbf{x}_i)$

For all $\mathbf{x}_j, i \neq j$ of $\mathcal{N}_\varepsilon(\mathbf{x}_i)$

1. Verify that $\mathbf{x}_j$ has not been visited by the algo, else $\mathbf{x}_j$ is marked “as visited”
2. Identify the ε-neighborhood of $\mathbf{x}_j$, $\mathcal{N}_\varepsilon(\mathbf{x}_j)$.
3. **If** $\mathrm{card}(\mathcal{N}_\varepsilon(\mathbf{x}_j)) \geq n_{min}$
   $\mathcal{N}_\varepsilon(\mathbf{x}_i) = \mathcal{N}_\varepsilon(\mathbf{x}_i) + \mathcal{N}_\varepsilon(\mathbf{x}_j)$
4. **If** $\mathbf{x}_j$ is not clustered, add to $\mathcal{C}_k$.

Illustration of DBSCAN Principles

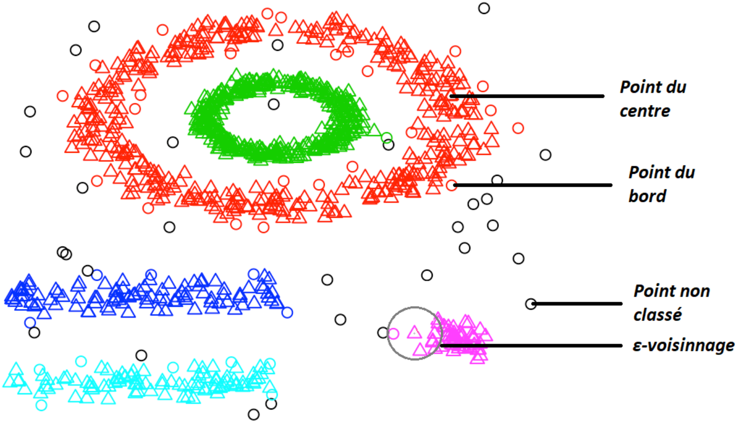


Figure: Clustering results obtained with DBSCAN algorithm.

Algorithms comparison

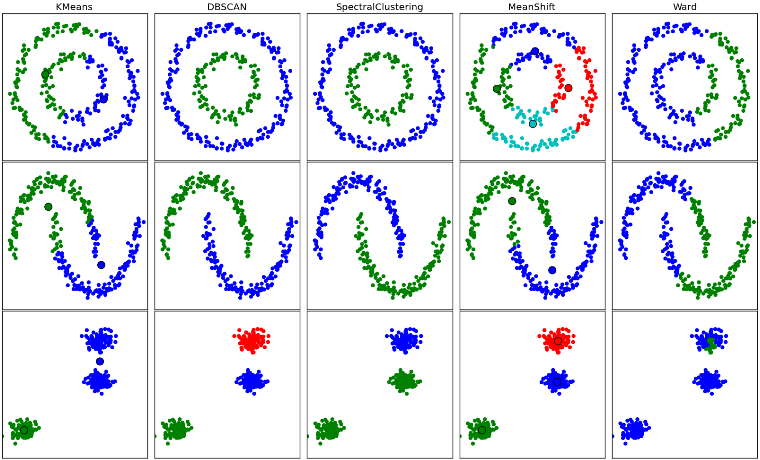
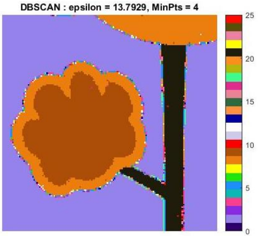
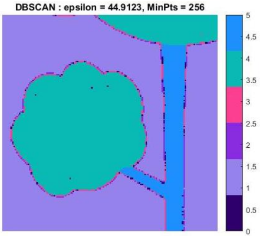


Figure: From Scikits learn: `https://ogrisel.github.io/scikit-learn.org/sklearn-tutorial/modules/clustering.html`

The Tree Data - DBSCAN



(a) MinPts = 4



(b) MinPts = 256

- Pros: Resistant to Noise, can handle clusters of different shapes and sizes
- Cons: Lack of interpretable parameters (estimation), Varying densities, High-dimensional data

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HDBSCAN

Key Idea: Convert DBSCAN into a hierarchical clustering algorithm and

→ bypass the choice of the ϵ-parameter!

→ scan all possible solutions with all values of ϵ

Five main steps

1. Transform the space according to the density/sparsity
2. Build the minimum spanning tree of the distance weighted graph
3. Construct a cluster hierarchy of connected components
4. Condense the cluster hierarchy based on minimum cluster size
5. Extract the stable clusters from the condensed tree

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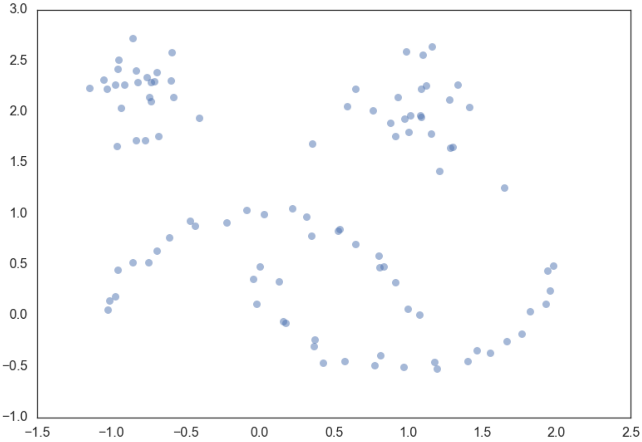
Easier to understand with an example!

HDBSCAN : Illustrative Example



©https://hdbscan.readthedocs.io/en/latest/how$_h$*dbscan$_w$orks.html*

Step 1: Transform The Space

- Goal: Prepare the data for a single linkage clustering (real data is noisy and single linkage is not robust!)
- Key idea: Push sparse points away from the rest of the data before clustering
- The *islands/sea* analogy $\rightarrow$ Make *sea* points more distant from each other and from the *land*

How do we evaluate density ?

- Need an inexpensive density estimate $\Rightarrow$ k-NN is the simplest
- Call it the core distance for parameters k and point $\mathbf{x}_i$, $\mathrm{core}_k(\mathbf{x}_i)$

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And how do we connect points now ?

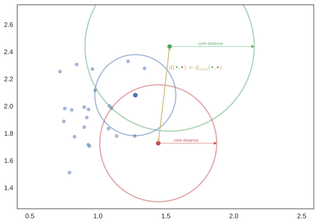
Step 1 : Mutual Reachability Distance

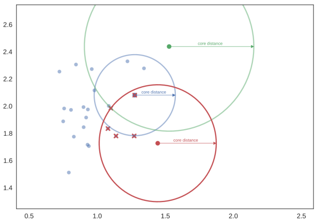
A new distance metric is defined as

$$d_{mreach-k}(\mathbf{x}_i, \mathbf{x}_j) = \max(\mathrm{core}_k(\mathbf{x}_i), \mathrm{core}_k(\mathbf{x}_j), d(\mathbf{x}_i, \mathbf{x}_j)),$$

Meaning that we want to connect points that are

1. Close enough to each other : $d(\mathbf{x}_i, \mathbf{x}_j)$
2. In a dense enough region : $\mathrm{core}_k(\mathbf{x}_i)$



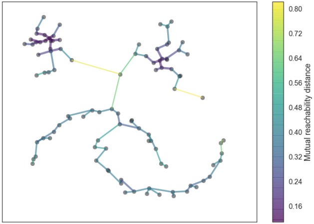


Step 2 : The Minimum Spanning Tree

- Goal: Prepare the data for clustering using d_{mreach}
- Key ideas:
  - Construct a graph that connects all points
  - Start disconnecting them by lowering a threshold (sea level drops)
  - Points are the vertices and the *edges* are weighted by d_{mreach}
  - n^2 possible edges $\rightarrow$ the minimum spanning tree

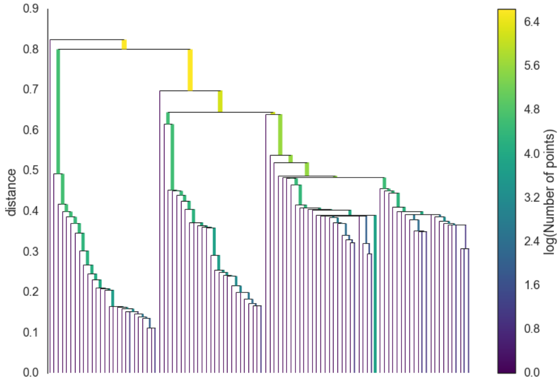
Algorithms from graph theory

- Prim's algorithm
- Dual Tree Boruvka



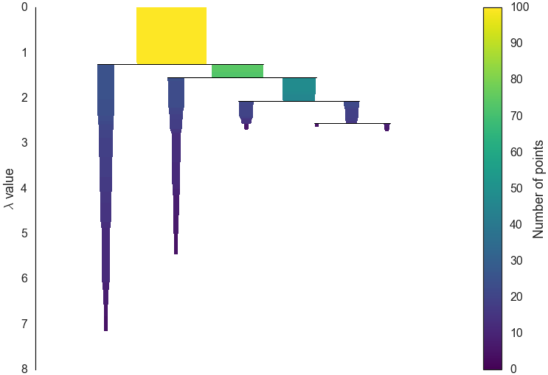
Step 3: Build the cluster hierarchy

Clusters emerge progressively as we lower the d_{mreach} threshold ($\rightarrow$ sort the edges and start single linkage)



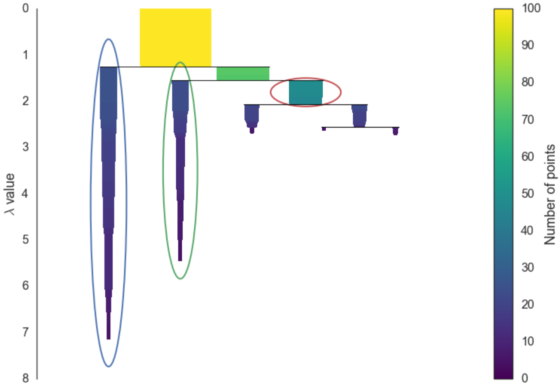
Step 4 : Condense the cluster tree

Get rid of levels that resulted in noise : nbr of points $\leq C_{\min}$
(clusters are shrinking $\neq$ splitting)

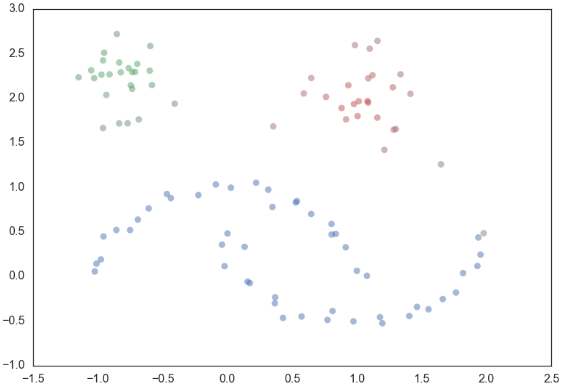


Extract the clusters

Key idea: Choose clusters that persist (live for a long time) and that are large → maximize a stability criterion
(flat clustering: can't select descendance of a selected cluster!)



Results



HDBSCAN: Summary

Implementation: The 5 main steps

1. Compute $\mathrm{core}_k(\mathbf{x}_i)$ using *MinPts* $\rightarrow$ Measure density
2. Transform the space: use new metric d_{mreach}
3. Construct a minimum spanning tree
4. Simplify/condense the tree using $C_{\min}$
5. Extract final clustering results

In conclusion: Two parameters (*MinPts* and $C_{\min}$), varying densities, robust to outliers, interpretability...

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   $\rightarrow$ Maximize cluster stability

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