Clustering algorithms and introduction to persistent homology

Frédéric Chazal
INRIA Saclay - Ile-de-France
frederic.chazal@inria.fr
Introduction

**Clustering:** A partition of data into groups of similar observations. The observations in each group (cluster) are similar to each other and dissimilar to observations from other groups.

**Input:** a finite set of observations: point cloud embedded in an Euclidean space (with coordinates) or a more general metric space (pairwise distance/similarity) matrix.

**Goal:** partition the data into a relevant family of subsets (clusters).

![Clustered data examples](image)
Introduction

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Not a single/universal notion of cluster.

A wealth of approaches:

- Variational
- Spectral
- Density based
- Hierarchical
- etc...
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In this lecture:
- a few basic classical “algorithms” motivating and bringing us to the introduction of persistent homology.
The k-means algorithm

**Input:** A (large) set of $N$ points $X$ and an integer $k < N$.

**Goal:** Find a set of $k$ points $L = \{y_1, \ldots, y_k\}$ that minimizes

$$E = \sum_{i=1}^{N} d(x_i, L)^2$$
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This is a NP hard problem!

The Lloyd’s algorithm: a very simple local search algorithm $\rightarrow$ local minimum.
The k-means algorithm

The Lloyd's algorithm

- Select \( L^1 = \{y^1_1, \cdots y^1_k\} \) initial "seeds";
- \( i = 1; \)
- Repeat
  - For \((j = 1; j \leq k; j + +)\) \( S^i_j = \{x \in X : d(x, y^i_j) = d(x, L^i)\}; \)
  - For \((j = 1; j \leq k; j + +)\)
    \[
    y^i_{j+1} = \frac{1}{|S^i_j|} \sum_{x \in S^i_j} x
    \]
  - \( i + +; \)
- Until convergence
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Warning:

- Lloyd’s algorithm does not ensure convergence to a global minimum!
- The speed of convergence is not guaranteed.
- The choice of the initial seeds may be critical (but there exists some strategies → k-means++).
Hierarchical clustering algorithms

Build a hierarchy of clusters (nested family of clustering partitions)
Hierarchical clustering algorithms

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**Agglomerative (bottom-up)**

Start with single point cluster and recursively merge the most similar clusters to one parent cluster until reaching a stopping criterion (e.g. number of clusters).
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Dendogram, i.e. a tree such that:
- each leaf node is a singleton,
- each node represent a cluster,
- the root node contains the whole data,
- each internal node has two daughters, corresponding to the clusters that were merged to obtain it.
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```
    p3
     
    p4  p5
     
    p1  p2
```

**Dividing (top-down)**
Start with a single global cluster and recursively split each cluster until reaching a stopping criterion.

```
    p1  p2  p3  p4  p5  p6
     
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```
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Single linkage clustering

Input: A set $X_n = \{x_1, \cdots, x_n\}$ in a metric space $(X, d)$ (or just a matrix of pairwise dissimilarities $(d_{i,j})$).

Given two clusters $C, C' \subseteq X_n$ let

$$d(C, C') = \inf_{x \in C, x' \in C'} d(x, x')$$

1. Start with a clustering where each $x_i$ is a cluster.

2. At each step, merge the two closest clusters until it remains a single cluster (containing all data points).

Output: the resulting dendogram
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- However, the “merging times” remain stable.

- (For Euclidean data), the single linkage clustering keeps track of the evolution of the connected components of the distance function to the data.
The unstability of dendograms

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- However, the “merging times” remain stable.
- (For Euclidean data), the single linkage clustering keeps track of the evolution of the connected components of the distance function to the data.

Persistent homology!
Mode seeking clustering

- Data points are sampled according to some (unknown) probability density.
- Clusters = the basins of attractions of the density

Two approaches:

- Iterative, such as, e.g., Mean Shift [Comaniciu et al, IEEE Trans. on Pattern Analysis and Machine Intelligence, 2002].
- Graph-based, such as, e.g., [Koontz et al, IEEE Trans. on Computers 1976].
The Koonz, Narendra and Fukunaga algorithm (1976)
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Density estimation
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Density estimation

Neighborhood graph
The Koonz, Narendra and Fukunaga algorithm (1976)

Density estimation

Discrete approximation of the gradient; for each vertex $v$, a gradient edge is selected among the edges adjacent to $v$. 
The Koonz, Narendra and Fukunaga algorithm (1976)

The algorithm:

**Input:** neighborhood graph $G$ with $n$ vertices (the data points) and a $n$-dimensional vector $\hat{f}$ (density estimate)

Sort the vertex indices $\{1, 2, \cdots, n\}$ in decreasing order: $\hat{f}(1) \geq \hat{f}(2) \geq \cdots \geq \hat{f}(n)$;

Initialize a union-find data structure (disjoint-set forest) $U$ and two vectors $g, r$ of size $n$;

**for** $i = 1$ **to** $n$ **do**

Let $N$ be the set of neighbors of $i$ in $G$ that have indices higher than $i$;

**if** $N = \emptyset$

Create a new entry $e$ in $U$ and attach vertex $i$ to it;

$r(e) \leftarrow i$ // $r(e)$ stores the root vertex associated with the entry $e$

**else**

$g(i) \leftarrow \text{argmax}_{j \in N} \hat{f}(j)$ // $g(i)$ stores the approximate gradient at vertex $i$

$e_i \leftarrow U.\text{find}(g(i))$;

Attach vertex $i$ to the entry $e_i$;

**Output:** the collection of entries $e$ in $U$
The Koonz, Narendra and Fukunaga algorithm (1976)

Drawbacks:

- As many clusters as local maxima of the density estimate $\rightarrow$ sensitivity to noise!
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Approaches to overcome these issues:

- Smooth out the density estimate (e.g. mean-shift)... But pb of choice of a smoothing param.
- Merge clusters: various way to do that. In the following: use persistent homology!
Persistent homology

- A general mathematical framework to encode the evolution of the topology (homology) of families of nested spaces (filtered complex, sublevel sets,...).
- Multiscale topological information.
- Barcodes/persistence diagrams can be efficiently computed.
- Stability properties
(0-dimensional) persistent homology for functions

- Nested family (filtration) of sublevel-sets $f^{-1}((-\infty, \alpha])$ for $\alpha = -\infty$ to $+\infty$.
- Track evolution of connectedness throughout the family.
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(0-dimensional) persistent homology for functions

- Nested family (filtration) of sublevel-sets $f^{-1}((\alpha, \infty]]$ for $\alpha = -\infty$ to $+\infty$.
- Track evolution of connectedness throughout the family.
- Finite set of intervals (barcode) encodes births/deaths of topological features.
(0-dimensional) persistent homology for functions

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Persistence barcode

Persistence diagram
What if $f$ is slightly perturbed?

**Theorem (Stability):**
For any tame functions $f, g : X \to \mathbb{R}$, $d(Df, Dg) \leq \|f - g\|_{\infty}$.

[Cohen-Steiner, Edelsbrunner, Harer 05], [C., Cohen-Steiner, Glisse, Guibas, Oudot 09], [C., de Silva, Glisse, Oudot 12]
The bottleneck distance between two diagrams \(D_1\) and \(D_2\) is

\[
d_B(D_1, D_2) = \inf_{\gamma \in \Gamma} \sup_{p \in D_1} \|p - \gamma(p)\|_{\infty}
\]

where \(\Gamma\) is the set of all the bijections between \(D_1\) and \(D_2\) and \(\|p - q\|_{\infty} = \max(|x_p - x_q|, |y_p - y_q|)\).
The example of distance functions
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\[ f_P : \mathbb{R}^2 \to \mathbb{R} \]
\[ x \mapsto \min_{p \in P} \|x - p\|_2 \]

Link with single linkage clustering
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Link with single linkage clustering
The case of density and back to mode seeking

Given a probability density \( f \):

- Consider the superlevel-sets filtration \( f^{-1}([t, +\infty)) \) for \( t \) from \( +\infty \) to \( -\infty \), instead of the sublevel-sets filtration.

- Persistence is defined in the same way.
The case of density and back to mode seeking

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The case of density and back to mode seeking

Given an estimator $\hat{f}$:

Stability Theorem $\implies d_B(Df, D\hat{f}) \leq \|f - \hat{f}\|_{\infty}$.
Persistence-based clustering

Combine a mode seeking approach with (0-dim) persistence computation.

Input:
1. A finite set $X$ of observations (point cloud with coordinates or pairwise distance matrix),
2. A real valued function $f$ defined on the observations (e.g. density estimate).

Goal: Partition the data according to the basins of attraction of the peaks of $f$
Persistence-based clustering

Combine a mode seeking approach with (0-dim) persistence computation.

[C., Guibas, Oudot, Skraba - J. ACM 2013]

1. Build a neighboring graph $G$ on top of $X$.
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1. Build a neighboring graph $G$ on top of $X$.
2. Compute the (0-dim) persistence of $f$ to identify prominent peaks $\rightarrow$ number of clusters (union-find algorithm).
3. Chose a threshold $\tau > 0$ and use the persistence algorithm to merge components with prominence less than $\tau$. 
Persistence-based clustering

Combine a mode seeking approach with (0-dim) persistence computation.

\[ \tau = 0 \]

Complexity of the algorithm: \( O(n \log n) \)

Theoretical guarantees:
- Stability of the number of clusters (w.r.t. perturbations of \( X \) and \( f \)).
- Partial stability of clusters: well identified stable parts in each cluster.

“soft” clustering
Application to non-rigid shape segmentation

[Skraba, Ovsjanikov, C., Guibas, NORDIA 10]

$X$: a 3D shape

$f = \text{HKS function on } X$

**Problem:** some part of clusters are unstable $\rightarrow$ dirty segments
Application to non-rigid shape segmentation

Problem: some part of clusters are unstable \(\rightarrow\) dirty segments

Idea:
- Run the persistence based algorithm several times on random perturbations of \(f\) (size bounded by the “persistence” gap).
- Partial stability of clusters allows to establish correspondences between clusters across the different runs \(\rightarrow\) for any \(x \in X\), a vector giving the probability for \(x\) to belong to each cluster.
Application to non-rigid shape segmentation

[Skraba, Ovsjanikov, C., Guibas, NORDIA 10]
Other applications: classification, object recognition

Examples:
- Hand gesture recognition [Li, Ovsjanikov, C. - CVPR'14]
- Persistence-based pooling for shape recognition [Bonis, Ovsjanikov, Oudot, C. 2015]
Filtrations of simplicial complexes

A filtration of a (finite) simplicial complex $K$ is a sequence of subcomplexes such that

i) $\emptyset = K^0 \subset K^1 \subset \cdots \subset K^m = K$,

ii) $K^{i+1} = K^i \cup \sigma^{i+1}$ where $\sigma^{i+1}$ is a simplex of $K$.

There are many ways to build filtrations - see the following of the course.
Sublevel set filtration associated to a function

- $f$ a real valued function defined on the vertices of $K$
- For $\sigma = [v_0, \cdots, v_k] \in K$, $f(\sigma) = \max_{i=0,\cdots,k} f(v_i)$
- The simplices of $K$ are ordered according increasing $f$ values (and dimension in case of equal values on different simplices).

**Exercise:** show that this is a filtration

General case: if $f : X \to \mathbb{R}$, $X$ a topological space, $\forall t \leq t' \in \mathbb{R}$, $f^{-1}((-\infty,t]) \subseteq f^{-1}((-\infty,t']) \to$ filtration of $X$ by the sublevel sets of $f$. 
Sublevel set filtration associated to a function

- $f$ a real valued function defined on the vertices of $K$
- For $\sigma = [v_0, \cdots, v_k] \in K$, $f(\sigma) = \max_{i=0,\cdots,k} f(v_i)$
- The simplices of $K$ are ordered according increasing $f$ values (and dimension in case of equal values on different simplices).

Exercise: show that this is a filtration

General case: if $f : X \to \mathbb{R}$, $X$ a topological space, $\forall t \leq t' \in \mathbb{R}$, $f^{-1}((-\infty, t]) \subseteq f^{-1}((-\infty, t']) \to$ filtration of $X$ by the sublevel sets of $f$. 

Note: the upper level set filtration is defined similarly.