Clustering

Part 2

Cluster Evaluation

GOALs:

- Clustering tendency: assessment whether the data contain meaningful clusters (e.g., clusters that are unlikely to occur in random data)
- Unsupervised evaluation: assessment of the quality of a custering (resp., the relative quality of two clusterings) *without* reference to external information
- Supervised evaluation: assessment of the quality of a custering (resp., the relative quality of two clusterings) *with* reference to external information (e.g., class labels)

Cluster Evaluation: clustering tendency

Let P be a dataset of N points in some metric space (M, d).

The Hopkins statistic measures to what extent the points of P can be regarded as taken randomly from M. For some fixed $t < N$:

- $X = \{x_1, x_2, \ldots, x_t\}$ random sample from P
- $Y = \{y_1, y_2, \ldots, y_t\}$ random set of points from M
- $w_i =$ distance between x_i and the closest point in P
- $u_i =$ distance between y_i and the closest point in P
- The Hopkins Statistic is

$$H = \frac{\sum_{i=1}^{t} w_i}{\sum_{i=1}^{t} u_i + \sum_{i=1}^{t} w_i}$$

If H is close to 0, then P is likely to have a clustering structure, while if H is close to 1, then the points of P are likely to be well (i.e., regularly) spaced. If H is close to 0.5, then P is likely to be a random set.

Cluster Evaluation: unsupervised evaluation

- In the case of k-center, k-means, and k-median, the value of the objective function can be employed to assess the quality a clustering or the relative quality of two clusterings.
- In general, one could measure the cohesion of an individual cluster C as the average distance between two points in C (over all such pairs of points), or the separation between two clusters C_1 and C_2 as the average distance between a point ot C_1 and a point of C_2 (over all such pairs of points). The values of cohesion (resp., separation) can be ranked or averaged over all clusters (resp., pairs of clusters)

Cluster Evaluation: unsupervised evaluation (cont'd)

- Silhouette coefficient. Consider a clustering $\mathcal{C}$ of a pointset P. For a point $p \in P$ belonging to some cluster $C \in \mathcal{C}$
  - $a_p =$ average distance between p and the other points in C
  - $b_p =$ mininum, over all clusters $C' \neq C$ of the average distance between p and the other points in C'
  - The silhouette coefficient for p is

$$s_p = \frac{b_p - a_p}{\max\{a_p, b_p\}}$$

The value of s_p varies between -1 and 1. The closer s_p to 1 the better.

As a quality measure of the clustering one could take the average silhouette coefficient over all points of P.

Cluster Evaluation: supervised evaluation

Consider a clustering $\mathcal{C}$ of a pointset P. Suppose that each point $p \in P$ is associated with a class label out of a domain of L class labels.

For each cluster $C \in \mathcal{C}$ and class i, let

$$\begin{aligned} m_C &= \#\text{points in cluster } C \\ m_i &= \#\text{points of class } i \\ m_{C,i} &= \#\text{points of class } i \text{ in cluster } C \end{aligned}$$

Entropy of a cluster C:

$$-\sum_{i=1}^{L} \frac{m_{C,i}}{m_C} \log_2 \frac{m_{C,i}}{m_C} \quad (\text{N.B. } 0 \log_2 0 = 0)$$

It measures the *impurity* of C, ranging from 0 (i.e., min impurity when all points of C belong to the same class), to $\log_2 L$ (i.e., max impurity when all classes are equally represented in C).

Cluster Evaluation: supervised evaluation (cont'd)

Entropy of a class i:

$$-\sum_{C \in \mathcal{C}} \frac{m_{C,i}}{m_i} \log_2 \frac{m_{C,i}}{m_i}$$

It measures how evenly the points of class i are spread among clusters, ranging from 0 (i.e., all points of class i concentrated in the same cluster), to $\log_2 K$ (i.e., the points of class i are evenly spread among all clusters), where K is the number of clusters.

It is defined also when points belong to multiple classes (e.g., categories of wikipedia pages)

Cluster Evaluation: supervised evaluation (cont'd)

Let

$$\begin{aligned} f_{00} &= \#\text{pairs of points of distinct classes in distinct clusters} \\ f_{01} &= \#\text{pairs of points of distinct classes in the same cluster} \\ f_{10} &= \#\text{pairs of points of the same class in distinct clusters} \\ f_{11} &= \#\text{pairs of points of the same class in the same cluster} \end{aligned}$$

Rand statistic:

$$\frac{f_{00} + f_{11}}{f_{00} + f_{01} + f_{10} + f_{11}}$$

It measures whether the clustering is in accordance with the partition induced by the classes, ranging from 0 (no accordance) to 1 (maximum accordance)

Cluster Evaluation: supervised evaluation (cont'd)

Jaccard coefficient:

$$\frac{f_{11}}{f_{01} + f_{10} + f_{11}}$$

that is, the proportion of pairs of the same class in the same cluster relatively to the total number of pairs that are of the same class or in the same cluster. It is an alternative measure of the accordance of the clustering with the classes.

Case Study

Analysis of votes in the Italian Chamber of Deputies

Goal: Cluster Italian deputies based on their votes in Parliament

- Data source: Openparlamento (from Openpolis) `https://parlamento17.openpolis.it/`
- 630 deputies
- Restriction to key votes, i.e., high political relevance. Overall 149 votes, from beginning of term until end of 2015
- Dataset: one row (”point” for each deputy) containing
  - ID of the deputy
  - Group: 24 = Mixed Group; 71 = PD; 90 = FI; 115 = Fratelli d’Italia; 117 = M5S; 119 = Sinistra Italiana; 120 = Lega Nord; 121 = Scelta Civica; 124 = Area Popolare; 125 = Democrazia Solidale;
  - For each vote: -2 = against; -1 = abstention; 0 = missing; 2 = in favor.
- Distance: Manhattan distance

Case Study (cont'd)

- All deputies except for Mixed Group (630-62=568 deputies)
- Algorithm: k-means with $k = 12$
- Results:

	Cluster											
Group	0	1	2	3	4	5	6	7	8	9	10	11
71	174	26	2	2	12	26	13	32	10	3	0	0
90	1	1	0	17	0	0	0	0	0	0	36	0
115	0	0	0	7	0	0	0	0	0	1	0	0
117	0	0	0	2	0	0	0	0	0	89	0	0
119	0	0	0	1	4	0	1	0	0	0	0	25
120	0	0	0	2	1	0	0	0	0	10	3	0
121	4	2	10	1	0	1	0	0	3	1	0	1
124	3	11	1	4	0	0	0	4	7	0	1	0
125	1	3	1	1	1	0	1	4	1	0	0	0
Entropy	0.37	1.54	1.29	2.42	1.34	0.23	..	..	..	..	..	0.24

- Entropy of PD (G.71): 2.12; Entropy of M5S (G.117): 0.15

Case Study (cont'd)

- Deputies from PD (G.71), FI (G.90), M5S (G.117) who never changed group (422 deputies out of 446)
- Algorithm: k-means with $k = 5$
- Results:

	Cluster				
Group	0	1	2	3	4
71	186	43	0	0	51
90	0	3	48	0	0
117	0	0	0	91	0
Entropy	0	0.35	0	0	0

- Unlike FI and M5S, the PD group is split into 3 subgroups probably reflecting a political subdivision (e.g., Orfini and Guerini in Cluster 0; Bersani in Cluster 1; Cuperlo in Cluster 4)

Hierarchical clustering

- Produces a hierarchy of nested clusterings of decreasing cardinalities
- Two alternative high-level strategies:
    - Agglomerative: Starts with each input point in a separate cluster and progressively merges suitably selected pairs of clusters. It is the most common strategy and we focus on it.
    - Divisive: Starts with one cluster containing all points and progressively splits a cluster into two.
- Features:
    - Flexibility with respect to number of clusters
    - No cluster centers are required
    - May capture clusters of arbitrary shapes

General Agglomerative Strategy

Let P be a set of N points in a metric space (M, d).

```
Make each point as a distinct singleton cluster
while (!stopping-condition) do
  merge the two closest clusters
return the current set of clusters
```

Observations:

- In order to instantiate the algorithm one needs to decide when to stop (*stopping condition*) and which pair of clusters to merge at each iteration (*closest clusters*)
- The number of clusters decreases by 1 at each iteration
- Instead of returning the clustering resulting after the last iteration, one may return the dendogram, i.e., the tree/forest defined by all clusters created at the various iterations.

Merging criterion

How do we measure the distance between two clusters C_1, C_2 so to be able to identify the "two closest clusters" at each iteration?

- Single linkage: $\text{dist}(C_1, C_2) = \min_{x \in C_1, y \in C_2} d(x, y)$
- Complete linkage: $\text{dist}(C_1, C_2) = \max_{x \in C_1, y \in C_2} d(x, y)$
- Average linkage: (average distance between C_1 and C_2)

$$\text{dist}(C_1, C_2) = \frac{1}{|\{(x, y) \ : \ x \in C_1, y \in C_2\}|} \sum_{x \in C_1, y \in C_2} d(x, y)$$

- Ward's method (in Euclidean space):

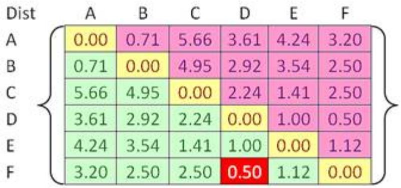
$$\text{dist}(C_1, C_2) = \text{cost}(C_1 \cup C_2) - \text{cost}(C_1) - \text{cost}(C_2),$$

where, for a cluster C with centroid c, $\text{cost}(C) = \sum_{x \in C} (d(x, c))^2$.

Remark about Ward's method: at each iteration we merge the two clusters that yield the smallest increase to the k-means objective.

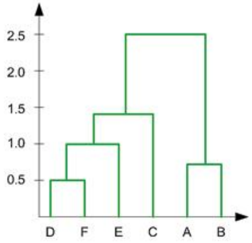
Example (single linkage)

- Distance matrix (6 points: A,B,C,D,E,F):



Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

- Dendogram (stopping condition: 1 cluster left):



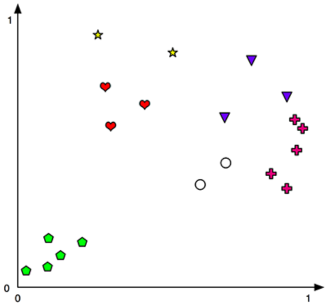
  - It shows sequence of mergings: D-F; A-B; DF-E; DFE-C; DFEC-AB
  - y-axis: inter-cluster distances. E.g., root of subtree for DFEC has $y = 1.41$, which is the distance between cluster DFE and cluster C

Stopping condition

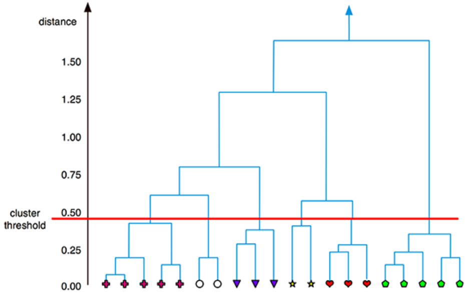
Depending on the application, the merging process can be stopped using one of the following conditions

- A desired number K of clusters is obtained (i.e., after $N - K$ iterations)
- The distance between the next pair of clusters to be merged exceeds a fixed cluster threshold t
- The clustering resulting after the next merge would violate some specific condition on the density or cohesion of the clusters (e.g., threshold on maximum distance of a point from the centroid of its cluster in Euclidean space)

Example (single linkage)



sample dataset



hierachical clustering of the sample dataset

Time Complexity

Consider the execution of the hierarchical clustering strategy for a set P of N points.

At each iteration, maintain with each point the ID of the cluster it belongs to ($\Theta(N)$ space).

Straightforward implementation:

- In each iteration, search for the pair of closest clusters by computing (or reading, if precomputed) the distances between all pairs of points
- $\Theta\left(N^2\right)$ time per iteration, hence $\Theta\left(N^3\right)$ overall time, if full hierarchy is sought.
- $\Theta(N)$ space, if distances are computed on-the-fly, while $\Theta\left(N^2\right)$ space if all distances are precomputed (may be advisable in high dimensions)

Time Complexity (cont'd)

Improved implementation (for single linkage):

- Precompute all $\Theta\left(N^2\right)$ distances and store each pair of points (x, y) into a min-heap H, using $d(x, y)$ as a key.
- Extract, one after the other, the pairs of points from H in increasing order of distance. After extracting pair (x, y), if the two points belong to different clusters, then merge the two clusters.
- The initialization requires $\Theta\left(N^2\right)$ time and space. Each extraction from H takes $O(\log N)$ time, while each merge takes $O(N)$ time. Thus, the implementation requires
  $O\left(N^2 \log N\right)$ overall running time and $\Theta\left(N^2\right)$space.

Remarks

- More efficient implementations for both single and complete linkage ($O\left(N^2\right)$ time and $O(N)$ space) exist: see [MC12] for details.
- For a Spark implementation (single linkage), see [J+15]

Observations on Hierarchical Clustering

Pros

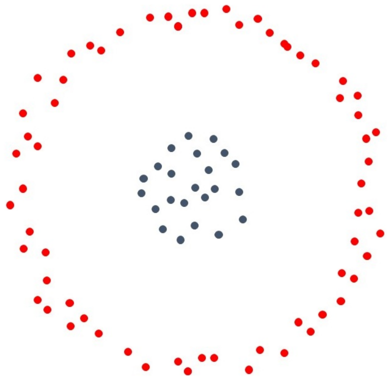
- Useful when some sort of *hierarchical taxonomy* is sought and/or a precise number of clusters cannot be established apriori
- Can capture clusters of non-elliptical shapes (especially single linkage): see example in the next slide.

Cons

- Does not optimize any specific objective function
- Sensitive to noise (especially single linkage), since each merge is final
- Computationally expensive

Example

The pointset in the following example exhibits two natural clusters



A hierarchical clustering run with single linkage and a suitable cluster threshold would capture the two clusters accurately, while a center-based clustering would not.

The following theorem generalizes this special case

Accuracy

Let P be a set of N points in some metric space (M, d).

For a given distance threshold $\sigma > 0$ define the graph $G_{P,\sigma} = (V; E)$ as follows:

$$\begin{aligned} V &= P \\ E &= \{(x, y) \; : \; x, y \in P \wedge d(x, y) \leq \sigma\} \end{aligned}$$

Suppose that $G_{P,\sigma}$ has K connected components. (Note that the pointset of the previous example has $K = 2$, for small enough σ.)

The following two properties are immediately proved

- The distance between any two points in distinct connected components is $> \sigma$
- For any non-trivial bipartition of a connected component, there are two points x, y in different subsets of the bipartition such that $d(x, y) \leq \sigma$

Accuracy (cont'd)

Theorem (Thm. 8.9 in BHK16)

Using cluster threshold σ as a stopping condition (i.e., only clusters at distance at most σ can be merged), the hierarchical clustering with single linkage applied to the above pointset P returns the set of K connected components as clusters.

Proof

Let $\mathcal{C}^{(i)}$ be the current clustering at the end of Iteration i of the clustering algorithm. Note that $\mathcal{C}^{(i)}$ consists of $N - i$ clusters. In particular, $\mathcal{C}^{(0)}$ is the initial clustering comprising N singleton clusters.

In order to prove the theorem, it is sufficient to show that the following property holds: *for every $i \leq N - K$, and every cluster $C \in \mathcal{C}^{(i)}$, C is a subset of one of the connected components of $G_{P,\sigma}$*. This immediately implies that at the end of Iteration $N - K$ the current clustering coincides with the partition into connected components of $G_{P,\sigma}$.

Accuracy (cont'd)

Proof of Theorem (cont'd).

We show the above property by induction on $i \leq N - K$.

BASIS: the property trivially holds for $i = 0$

INDUCTIVE STEP: Suppose that the property holds up to some Iteration i, with $0 \leq i < N - K$, and consider Iteration $i + 1$. Note that at the end of Iteration i there are $N - i > K$ clusters and, by the inductive hypothesis, each of them is fully contained in a connected component of $G_{P,\sigma}$. This implies that there exists two current clusters C_1, C_2 such that $\text{dist}(C_1, C_2) \leq \sigma$ and that any two such clusters must be subsets of the same connected component. Therefore, in the $i + 1$-st iteration, two clusters, subsets of the same connected component, are merged, hence the property is maintained. $\square$

Case Study

Battere Calderoli usando Python

Dal blog di Jacopo Notarstefano (02/2016)

`http://www.jacquerie.it/battere-calderoli-usando-python`

Theory questions

- Define the Manhattan distance for points in $\Re^d$, and show that it satisfies the triangle inequality
- Rigorously define the objective of k-center clustering
- Suppose that you want to open some hospitals to serve N cities so that each city is at distance at most t from a hospital and the costs (proportional to the number of opened hospitals) are minimized. What would you do?
- Show that the k-means algorithm always terminates.
- Describe what the *unsupervised evaluation* of a clustering is, and define a measure that can be used to this aim.

References

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