Artificial Intelligence & Machine Learning and Pattern Recognition — Clustering



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Clustering

- Task: Evolve measures of similarity to cluster a collection of documents/terms into groups within which similarity within a cluster is larger than across clusters.
- Cluster Hypothesis: Given a 'suitable' clustering of a collection, if the user is interested in document/term d/t, he is likely to be interested in other members of the cluster to which d/t belongs.
- Similarity measures
 - Represent documents by vectors
 - Distance between document vectors
 - Cosine of angle between document vectors

Issues

- Large number of noisy dimensions
- Notion of noise is application dependent

Partitional Clustering

- *k*-Means: Repeat...
 - Choose k arbitrary 'centroids'
 - Assign each document to nearest centroid
 - Re-compute centroids

- Example of k-Means (划分法)
 - x1 = (0, 2), x2 = (0, 0), x3 = (1.5, 0), x4 = (5, 0), x5 = (5, 2)
 - $\circ k = 2$

k-Means: Choosing *k*

Mostly problem driven

- Could be 'data driven' only when either
 - Data is not sparse
 - Measurement dimensions are not too noisy

Density-based Clustering

- Density-based clustering locates regions of high density that are separated from one another by regions of low density.
- DBSCAN (Density-Based Spatial Clustering of Applications with Noise) is a simple and effective density-based clustering (基于密度的聚类) algorithm.

- For DBSCAN, we need to estimate the density (密度) for a particular point in the data set.
- This is performed by counting the number of points within or at a specified radius, Eps, of that point.
- The count includes the point itself.

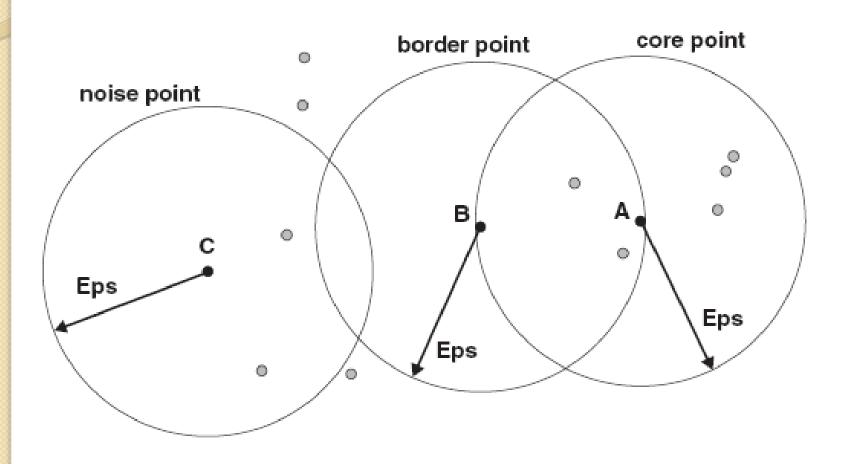
• This technique is illustrated in the following figure.

• The number of points within or at a radius of Eps of point A is 7, including

A itself.

- The density of any point will depend on the specified radius.
- Suppose the number of points in the data set is *m*.
- If the radius is large enough, then all points will have a density of m.
- If the radius is too small, then all points will have a density of 1.

- We need to classify a point as being
 - In the interior of a dense region (a core point, 核心点).
 - At the edge of a dense region (a border point, 边界点)
 - In a sparsely occupied region (a noise or background point, 噪音点).
- The concepts of core, border and noise points are illustrated as follows.



- Core points are in the interior of a density-based cluster.
- A point is a core point if the number of points within or at the boundary of a given neighborhood of the point is greater than or equal to a certain threshold MinPts.
- The size of the neighborhood is determined by the distance function and a user-specified distance parameter, Eps.
- The threshold MinPts is also a user-specified parameter.
- In the above figure, A is a core point for the indicated radius (Eps) if MinPts=7.

- A border point is not a core point, but falls within or at the boundary of the neighborhood of a core point.
- In the above figure, B is a border point.
- A border point can fall within the neighborhoods of several core points.
- A noise point is any point that is neither a core point nor a border point.
- In the above figure, C is a noise point.

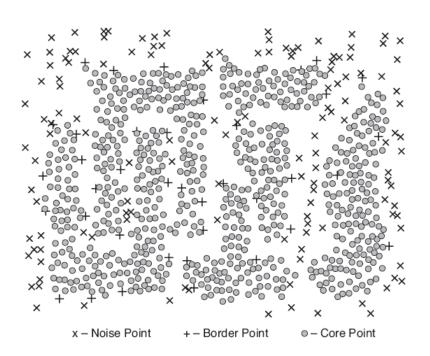
- The DBSCAN can be summarized as follows:
- If all points have been processed, stop.
- For a particular point which has not been previously processed, check whether it is a core point or not.
- If it is not a core point
 - Label it as a noise point (This label may change later).
- If it is a core point, label the point and
 - Form a new cluster C_{new} using this point and include all points within or at the boundary of its Eps-neighborhood in the cluster.
 - Insert all these neighboring points into a queue.
 - While the queue is not empty,
 - Remove the first point from the queue
 - If this point is not a core point, label it as a border point.
 - If this point is a core point, label it and check every point in its neighborhood which was not previously assigned to a cluster. For each of these unassigned neighboring points,
 - Assign the point to the current cluster C_{new}.
 - Insert the point into the queue.

• The left figure on the next slide shows a sample data set with 3000 2-D points.

• The right figure shows the resulting clusters found by DBSCAN.

• The core points, border points and noise points are also displayed.





• DBSCAN is relatively resistant to noise and can handle clusters of arbitrary shapes and sizes.

• As a result, it can find many clusters that cannot be found using *k*-Means.

Unsupervised Learning Reference

- S.J. Rizvi and J.R. Haritsa. Maintaining data privacy in association rule mining. *Proceedings of the 28th VLDB Conference*, 34(6):682-693, 2002.
- A.K. Jain, M.N. Murty, and P.J. Flynn. Data clustering: a review. *ACM Computing Surveys*, 31(2):264-323, 1999.
- A. Rodriguez and A. Laio. Clustering by fast search and find of density peaks. *Science*, 344(6191):1492-1496, 2014.