Clustering and PCA Recitation

Nupur Chatterji, Kenny Marino, Colin White

Clustering

Unsupervised Learning - unlabeled data

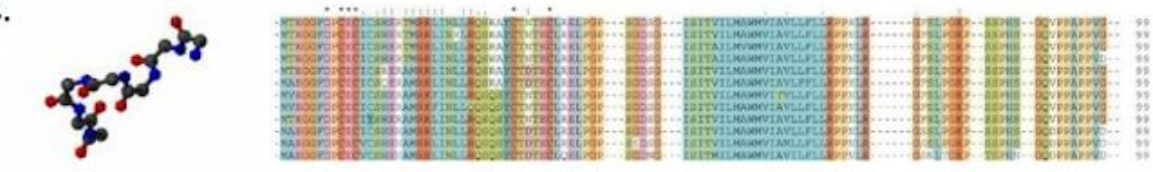
- Automatically organize data
- Understand structure in data
- Preprocessing for further analysis

Applications (Clustering comes up everywhere…)

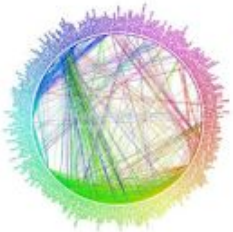
- Cluster news articles or web pages or search results by topic.

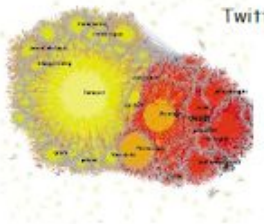


- Cluster protein sequences by function or genes according to expression profile.



- Cluster users of social networks by interest (community detection).


Facebook network


Twitter Network

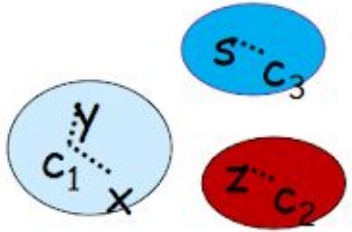
Objective Based Clustering

Input: A set S of n points, also a distance/dissimilarity measure specifying the distance d(x,y) between pairs (x,y).

E.g., # keywords in common, edit distance, wavelets coef., etc.

Goal: output a partition of the data.

- k-means: find center pts $c_1, c_2, \ldots, c_k$ to minimize $\sum_{i=1}^{n} \min_{j\in\{1,\ldots,k\}} d^2(\mathbf{x^i}, \mathbf{c_j})$
- k-median: find center pts $\mathbf{c_1}, \mathbf{c_2}, \ldots, \mathbf{c_k}$ to minimize $\sum_{i=1}^{n} \min_{j\in\{1,\ldots,k\}} d(\mathbf{x^i}, \mathbf{c_j})$



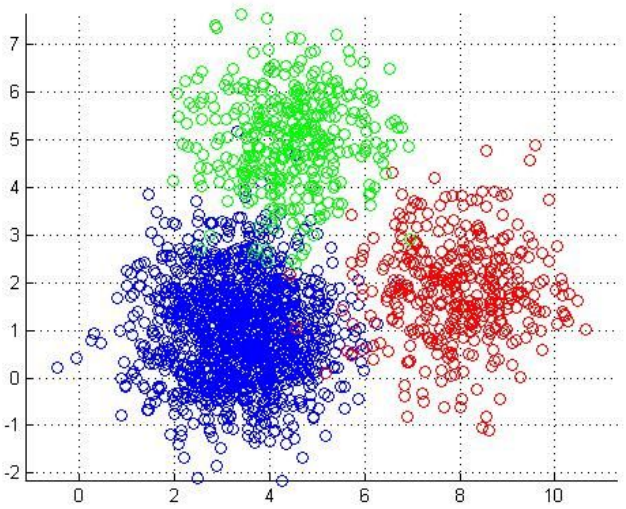
- K-center: find partition to minimize the maximum radius

Euclidean k-means Clustering

- **Input:** a set of n points, $x^1, x^2, \ldots, x^n$, in R^d, an integer k
- **Output:** k "centers" $c_1, c_2, \ldots, c_k$

Try to minimize the distance from each point x^i to its closest center

$$\sum_{i=1}^{n} \min_{j \in \{1,\ldots,k\}} \left|\left|\mathbf{x^i} - \mathbf{c_j}\right|\right|^2$$



K-means complexity

- Hard to solve even when k=2 and d=2
- k=1 is easy to solve
- d=1 is easy to solve (dynamic programming)

Common Heuristic in Practice: The Lloyd's method

[Least squares quantization in PCM, Lloyd, IEEE Transactions on Information Theory, 1982]

Input: A set of n datapoints $\mathbf{x^1}, \mathbf{x^2}, \ldots, \mathbf{x^n}$ in $\mathrm{R^d}$

Initialize centers $\boldsymbol{c_1}, \boldsymbol{c_2}, \ldots, \boldsymbol{c_k} \in \mathrm{R^d}$ and clusters $\mathrm{C_1}, \mathrm{C_2}, \ldots, \mathrm{C_k}$ in any way.

Repeat until there is no further change in the cost.

- For each j: $\mathrm{C_j} \leftarrow \{x \in S$ whose closest center is $\mathbf{c_j}\}$
- For each j: $\mathbf{c_j} \leftarrow$ mean of $\mathrm{C_j}$

Holding $\boldsymbol{c_1}, \boldsymbol{c_2}, \ldots, \boldsymbol{c_k}$ fixed, pick optimal $\mathrm{C_1}, \mathrm{C_2}, \ldots, \mathrm{C_k}$

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Lloyd's initialization

Initialization is very important for Lloyd's method

- Random initialization
- Farthest-first traversal: iteratively choose farthest point from current set
- d^2-sampling (k-means++) iteratively choose a point v with probability $d_{min}(v,C)^2$, where C is the list of current centers

Theorem: k-means++ always attains an O(log k) approximation to the optimal k-means solution in expectation.

K-means runtime

- K-means++ initialization O(nkd) time
- Lloyd's method: O(nkd) time

Exponential number of rounds in the worst case

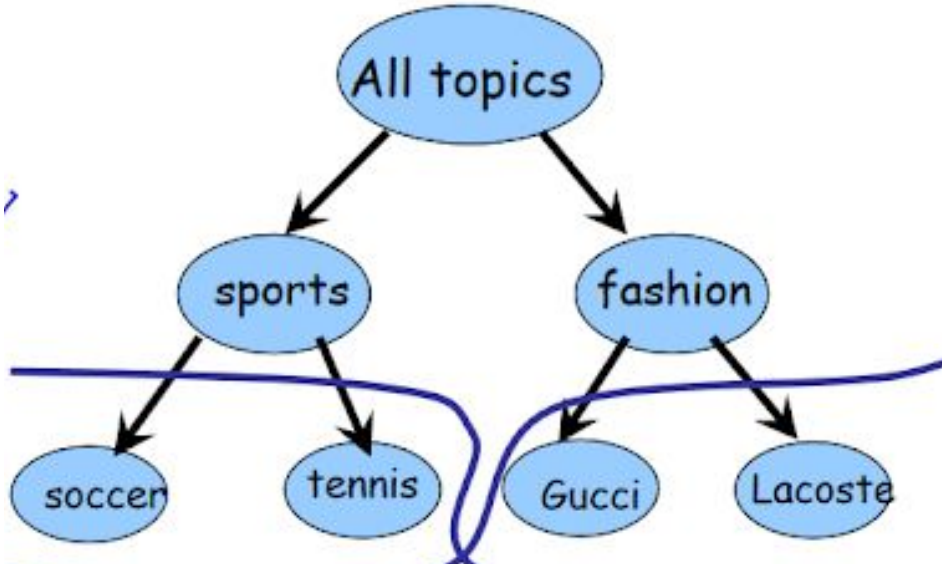
Small number of rounds in practice

Expected number of rounds is polynomial time under *smoothed analysis*

Hierarchical Clustering

- What if we don’t know the right value of k? (often the case)

Often leads to natural solutions

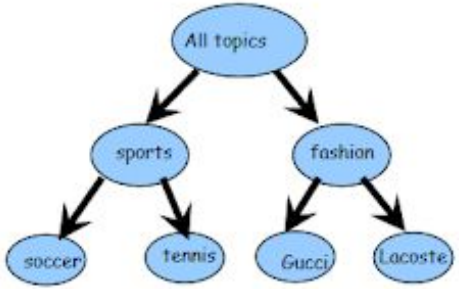


Bottom-Up (agglomerative)

Have a distance measure on pairs of objects.

d(x,y) – distance between x and y

E.g., # keywords in common, edit distance, etc



- Single linkage: $\text{dist}(C, C') = \min_{x \in C, x' \in C'} \text{dist}(x, x')$
- Complete linkage: $\text{dist}(C, C') = \max_{x \in C, x' \in C'} \text{dist}(x, x')$
- Average linkage: $\text{dist}(C, C') = \text{avg}_{x \in C, x' \in C'} \text{dist}(x, x')$

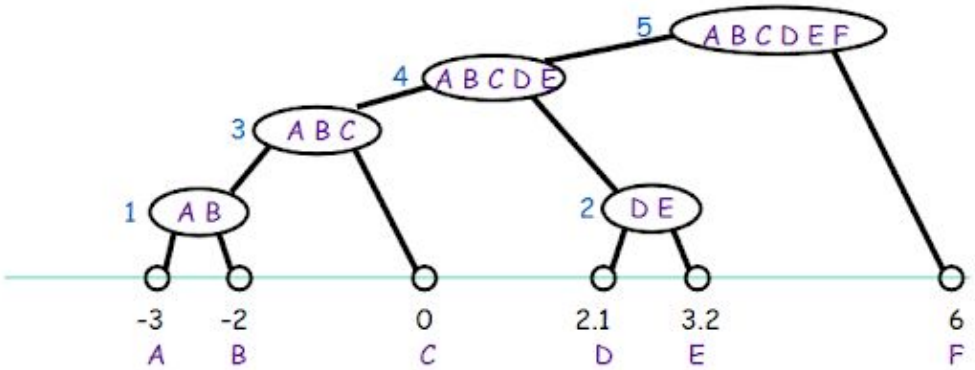
Single Linkage

Bottom-up (agglomerative)

- Start with every point in its own cluster.
- Repeatedly merge the "closest" two clusters.

Single linkage: $\text{dist}(C, C') = \min_{x \in C, x' \in C'} \text{dist}(x, x')$

Dendogram



Runtime:

- $O(n^3)$ is easy
- Can achieve $O(n^2 \log n)$