Introduction to Machine Learning

Clustering

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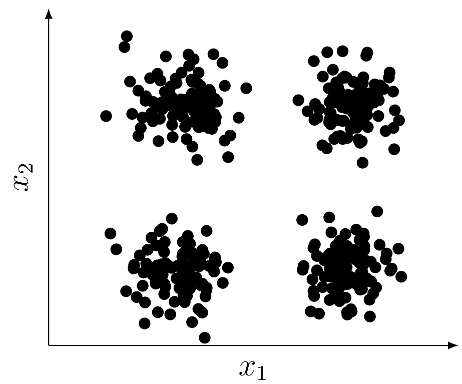
Outline

Contents

1 Clustering

Publishing a Magazine

- Imagine your are a magazine editor
- Need to produce the next issue
- What do you do?
  - Call your four assistant editors
    1. Politics
    2. Health
    3. Technology
    4. Sports
  - Ask each to send in k articles
  - Join all to create an issue



Treating a Magazine Issue as a Data Set

- Each article is a data point consisting of words, etc.
- **Each article has a (hidden) *type* - sports, health, politics, and technology**

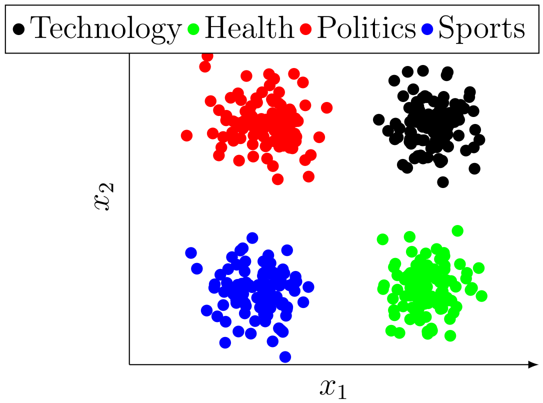
Now imagine your are the reader

- Can you assign the type to each article?
- Simpler problem: **Can you group articles by type?**
- Clustering

1.1 Clustering Definition

- Grouping similar things together
- A notion of a similarity or distance metric
- A type of **unsupervised learning**
  - Learning without any labels or target

Expected Outcome of Clustering



1.2 K-Means Clustering

- **Objective**: Group a set of N points ($\in \Re^D$) into K clusters.

1. **Start** with k *randomly initialized* points in D dimensional space
   - Denoted as $\{\mathbf{c}_k\}_{k=1}^{K}$
   - Also called *cluster centers*
2. **Assign** each input point $\mathbf{x}_n$ ($\forall n \in [1, N]$) to cluster k, such that:

$$\min_k \text{dist}(\mathbf{x}_n, \mathbf{c}_k)$$

3. **Revise** each cluster center $\mathbf{c}_k$ using all points assigned to cluster k
4. **Repeat** 2

1.3 Instantations and Variants of K-Means

- Finding distance
  - Euclidean distance is popular
- Finding cluster centers
  - Mean for K-Means
  - Median for k-medoids

1.4 Choosing Parameters

1. Similarity/distance metric
   - Can use non-linear transformations
   - K-Means with Euclidean distance produces "circular" clusters
2. How to set k?
   - Trial and error
   - How to evaluate clustering?
   - K-Means objective function

$$J(\mathbf{c}, \mathbf{R}) = \sum_{n=1}^{N} \sum_{k=1}^{K} R_{nk} \|\mathbf{x}_n - \mathbf{c}_k\|^2$$

   - $\mathbf{R}$ is the cluster assignment matrix

$$R_{nk} = \begin{cases} 1 & \text{If } \mathbf{x}_n \in \text{ cluster } k \\ 0 & \text{Otherwise} \end{cases}$$

1.5 Initialization Issues

- Can lead to wrong clustering
- Better strategies
  1. Choose first centroid randomly, choose second farthest away from first, third farthest away from first and second, and so on.
  2. Make multiple runs and choose the best

1.6 K-Means Limitations

Strengths

- Simple
- Can be extended to other types of data
- Easy to parallelize

Weaknesses

- Circular clusters (not with kernelized versions)
- Choosing K is always an issue
- Not guaranteed to be optimal
- Works well if natural clusters are round and of equal densities
- **Hard Clustering**

Issues with K-Means

- "Hard clustering"
- Assign every data point to exactly one cluster
- **Probabilistic Clustering**
  - Each data point can belong to multiple clusters with varying probabilities
  - In general
    $$P(\mathbf{x}_i \in C_j) > 0 \quad \forall j = 1 \dots K$$
  - For hard clustering probability will be 1 for one cluster and 0 for all others

References

Murphy book Chapter 21.3

References