Clustering

Supervised Learning vs. Unsupervised Learning

- **Supervised Learning**
  - Classification: partition examples into groups according to pre-defined categories
  - Regression: assign value to feature vectors
  - Requires labeled data for training
- **Unsupervised Learning**
  - Clustering: partition examples into groups when no pre-defined categories/classes are available
  - Signal separation: recover components of a mixed signal
  - Embeddings: find low dimensional representation of high dimensional data
  - Outlier detection: find unusual events (e.g. hackers)
  - Novelty detection: find changes in data
  - Only instances required, but no labels

Clustering

- Partition unlabeled examples into disjoint subsets of *clusters*, such that:
  - Examples within a cluster are similar
  - Examples in different clusters are different
- Discover new categories in an *unsupervised* manner (no sample category labels provided).

Applications of Clustering

- Exploratory data analysis
- Cluster retrieved documents in search engine
- Detecting near duplicates
  - Entity resolution
    - E.g. “Thorsten Joachims” == “Thorsten B Joachims”
  - Cheating detection
- Automated (or semi-automated) creation of taxonomies
  - E.g. phylogenetic tree
- Compression

Clustering Example
Clustering Example

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Clustering Example

Clustering Example

Similarity (Distance) Measures

- Euclidian distance ($L_2$ norm):
  \[ L_2(\mathbf{x}, \mathbf{x}') = \sqrt{\sum_{i=1}^{N} (x_i - x_i')^2} \]
- $L_1$ norm:
  \[ L_1(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^{N} |x_i - x_i'| \]
- Cosine similarity:
  \[ \cos(\mathbf{x}, \mathbf{x}') = \frac{\mathbf{x} \cdot \mathbf{x}'}{\|\mathbf{x}\| \|\mathbf{x}'\|} \]
- Kernels

Hierarchical Clustering

- Build a tree-based hierarchical taxonomy from a set of unlabeled examples.
- Recursive application of a standard clustering algorithm can produce a hierarchical clustering.

Agglomerative vs. Divisive Clustering

- **Agglomerative** (bottom-up) methods start with each example in its own cluster and iteratively combine them to form larger and larger clusters.
- **Divisive** (top-down) separate all examples immediately into clusters.
Hierarchical Agglomerative Clustering (HAC)

- Assumes a similarity function for determining the similarity of two clusters.

- Basic algorithm:
  - Start with all instances in their own cluster.
  - Until there is only one cluster:
    - Among the current clusters, determine the two clusters, \( c_i \) and \( c_j \), that are most similar.
    - Replace \( c_i \) and \( c_j \) with a single cluster \( c_i \cup c_j \)

- The history of merging forms a binary tree or hierarchy.

Cluster Similarity

- How to compute similarity of two clusters each possibly containing multiple instances?
  - Single link: Similarity of two most similar members.
  - Complete link: Similarity of two least similar members.
  - Group average: Average similarity between members.

Single-Link HAC

- When computing cluster similarity, use maximum similarity of pairs:

\[
sim(c_i, c_j) = \max \sim(x, y)_{x \in c_i, y \in c_j}
\]

- Can result in “straggly” (long and thin) clusters due to chaining effect.

Complete-Link HAC

- When computing cluster similarity, use minimum similarity of pairs:

\[
sim(c_i, c_j) = \min \sim(x, y)_{x \in c_i, y \in c_j}
\]

- Makes more “tight,” spherical clusters.

Computational Complexity of HAC

- In the first iteration, all HAC methods need to compute similarity of all pairs of \( n \) individual instances which is \( O(n^2) \).
- In each of the subsequent \( O(n) \) merging iterations,
  - must find smallest distance pair of clusters \( \rightarrow \) Maintain heap \( O(n \log n) \)
  - it must compute the distance between the most recently created cluster and each other existing cluster. Can this be done in constant time? \( \rightarrow O(n^2 \log n) \) overall.

Computing Cluster Similarity

- After merging \( c_i \) and \( c_j \), the similarity of the resulting cluster to any other cluster, \( c_k \), can be computed by:
  - Single Link:
    \[
    \sim((c_i \cup c_j), c_k) = \max(\sim(c_i, c_k), \sim(c_j, c_k))
    \]
  - Complete Link:
    \[
    \sim((c_i \cup c_j), c_k) = \min(\sim(c_i, c_k), \sim(c_j, c_k))
    \]
Single-Link Example

<table>
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<tr>
<th></th>
<th>c2</th>
<th>c1</th>
<th>x5</th>
</tr>
</thead>
<tbody>
<tr>
<td>x1</td>
<td>1</td>
<td>0.8</td>
<td>0.9</td>
</tr>
<tr>
<td>x2</td>
<td>0.8</td>
<td>1</td>
<td>0.5</td>
</tr>
<tr>
<td>x3</td>
<td>0.7</td>
<td>0.5</td>
<td>1</td>
</tr>
<tr>
<td>x4</td>
<td>0.6</td>
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<tr>
<td>x5</td>
<td>0.3</td>
<td>0.5</td>
<td>1</td>
</tr>
</tbody>
</table>

Merge x3, x4 replace with max

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Merge x1, x2 replace with max

Group Average Agglomerative Clustering
- Use average similarity across all pairs within the merged cluster to measure the similarity of two clusters.

\[
sim(c_i, c_j) = \frac{1}{|c_i \cup c_j|} \sum_{x \in c_i \cup c_j} \sum_{y \in c_i \cup c_j} \text{sim}(x, y)
\]

- Compromise between single and complete link.

Computing Group Average Similarity
- Assume cosine similarity and normalized vectors with unit length.
- Always maintain sum of vectors in each cluster.

\[
sim(c_i) = \sum_{x \in c_i} \frac{x}{\|x\|}
\]

- Compute similarity of clusters in constant time:

\[
sim(c_i, c_j) = \frac{(\bar{s}(c_i) + \bar{s}(c_j)) \cdot (\bar{s}(c_i) + \bar{s}(c_j)) - (|c_i| + |c_j|)}{|c_i| + |c_j| + |c_i| \cdot |c_j| - |c_i| \cdot |c_j| - 1)}
\]

Non-Hierarchical Clustering
- K-means clustering (“hard”)
- Mixtures of Gaussians and training via Expectation maximization Algorithm (“soft”)

Clustering Criterion
- Evaluation function that assigns a (usually real-valued) value to a clustering
  - Clustering criterion typically function of
    - within-cluster similarity and
    - between-cluster dissimilarity
- Optimization
  - Find clustering that maximizes the criterion
    - Global optimization (often intractable)
    - Greedy search
    - Approximation algorithms

K-Means Algorithm
- Input: \( k \) = number of clusters, Euclidian distance \( d \)
- Select \( k \) random instances \( \{s_1, s_2, \ldots, s_k\} \) as seeds.
- Until clustering converges or other stopping criterion:
  - For each instance \( x_i \):
    - Assign \( x_i \) to the cluster \( c_j \) such that \( d(x_i, s_j) \) is min.
  - For each cluster \( c_j \), update the centroid of each cluster
    - \( s_j = \bar{\mu}(c_j) \)

Note: Clusters represented via centroids

\[
\bar{\mu}(c) = \frac{1}{|c|} \sum_{x \in c} x
\]
**K-means Example**
(k=2)

- Pick seeds
- Reassign clusters
- Compute centroids
- Reassign clusters
- Compute centroids
- Reassign clusters
- Converged!

**Time Complexity**

- Assume computing distance between two instances is $O(N)$ where $N$ is the dimensionality of the vectors.
- Reassigning clusters for $n$ points: $O(kn)$ distance computations, or $O(knN)$.
- Computing centroids: Each instance gets added once to some centroid: $O(nN)$.
- Assume these two steps are each done once for $i$ iterations: $O(iknN)$.
- Linear in all relevant factors, assuming a fixed number of iterations.

**Buckshot Algorithm**

**Problem**
- Results can vary based on random seed selection, especially for high-dimensional data.
- Some seeds can result in poor convergence rate, or convergence to sub-optimal clusterings.

**Idea:** Combine HAC and K-means clustering.

- First randomly take a sample of instances of size $n^{1/2}$
- Run group-average HAC on this sample
- Use the results of HAC as initial seeds for K-means.
- Overall algorithm is efficient and avoids problems of bad seed selection.

**Non-Hierarchical Clustering**

- K-means clustering (“hard”)
- Mixtures of Gaussians and training via Expectation maximization Algorithm (“soft”)