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
Clustering Example
Similarity (Distance) Measures

• Euclidian distance ($L_2$ norm):

$$L_2(\hat{x}, \hat{x}') = \sqrt{\sum_{i=1}^{N} (x_i - x'_i)^2}$$

• $L_1$ norm:

$$L_1(\hat{x}, \hat{x}') = \sum_{i=1}^{N} |x_i - x'_i|$$

• Cosine similarity:

$$\cos(\hat{x}, \hat{x}') = \frac{\hat{x} \ast \hat{x}'}{||\hat{x}|| \ ||\hat{x}'||}$$

• 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.

```
animal
  \--- vertebrate
       \--- fish
       \--- reptile
       \--- amphib.
       \--- mammal
```

```
invertebrate
  \--- worm
  \--- insect
  \--- crustacean
```
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.
When computing cluster similarity, use maximum similarity of pairs:

$$sim(c_i, c_j) = \max_{x \in c_i, y \in c_j} sim(x, y)$$

→ Can result in “straggly” (long and thin) clusters due to chaining effect.
When computing cluster similarity, use minimum similarity of pairs:

$$sim(c_i, c_j) = \min_{x \in c_i, y \in c_j} sim(x, y)$$

→ 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 $O(n^2 \log n)$
  – 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:
    \[
    \text{sim}((c_i \cup c_j), c_k) = \max(\text{sim}(c_i, c_k), \text{sim}(c_j, c_k))
    \]
  - Complete Link:
    \[
    \text{sim}((c_i \cup c_j), c_k) = \min(\text{sim}(c_i, c_k), \text{sim}(c_j, c_k))
    \]
Single-Link Example

```
<table>
<thead>
<tr>
<th></th>
<th>x1</th>
<th>x2</th>
<th>x3</th>
<th>x4</th>
<th>x5</th>
</tr>
</thead>
<tbody>
<tr>
<td>x1</td>
<td>1</td>
<td>0.8</td>
<td>0.2</td>
<td>0.7</td>
<td>0.3</td>
</tr>
<tr>
<td>x2</td>
<td>0.8</td>
<td>1</td>
<td>0.1</td>
<td>0.5</td>
<td>0.2</td>
</tr>
<tr>
<td>x3</td>
<td>0.2</td>
<td>0.1</td>
<td>1</td>
<td>0.9</td>
<td>0.5</td>
</tr>
<tr>
<td>x4</td>
<td>0.7</td>
<td>0.5</td>
<td>0.9</td>
<td>1</td>
<td>0.4</td>
</tr>
<tr>
<td>x5</td>
<td>0.3</td>
<td>0.2</td>
<td>0.5</td>
<td>0.4</td>
<td>1</td>
</tr>
</tbody>
</table>

Merge x3, x4 replace with max
```

```
<table>
<thead>
<tr>
<th></th>
<th>x1</th>
<th>x2</th>
<th>c1</th>
<th>x5</th>
</tr>
</thead>
<tbody>
<tr>
<td>x1</td>
<td>1</td>
<td>0.8</td>
<td>0.7</td>
<td>0.3</td>
</tr>
<tr>
<td>x2</td>
<td>0.8</td>
<td>1</td>
<td>0.5</td>
<td>0.2</td>
</tr>
<tr>
<td>c1</td>
<td>0.7</td>
<td>0.5</td>
<td>1</td>
<td>0.5</td>
</tr>
<tr>
<td>x5</td>
<td>0.3</td>
<td>0.2</td>
<td>0.5</td>
<td>1</td>
</tr>
</tbody>
</table>

Merge x1, x2 replace with max
```

```
<table>
<thead>
<tr>
<th></th>
<th>c2</th>
<th>c1</th>
<th>x5</th>
</tr>
</thead>
<tbody>
<tr>
<td>c2</td>
<td>1</td>
<td>0.7</td>
<td>0.3</td>
</tr>
<tr>
<td>c1</td>
<td>0.7</td>
<td>1</td>
<td>0.5</td>
</tr>
<tr>
<td>x5</td>
<td>0.3</td>
<td>0.5</td>
<td>1</td>
</tr>
</tbody>
</table>

Merge c1, c2 replace with max
```

```
<table>
<thead>
<tr>
<th></th>
<th>c3</th>
<th>x5</th>
</tr>
</thead>
<tbody>
<tr>
<td>c3</td>
<td>1</td>
<td>0.5</td>
</tr>
<tr>
<td>x5</td>
<td>0.5</td>
<td>1</td>
</tr>
</tbody>
</table>
```

Merge c1, c2 replace with max
Group Average Agglomerative Clustering

• Use average similarity across all pairs within the merged cluster to measure the similarity of two clusters.

\[
sim(c_i, c_j) = \frac{1}{\left| c_i \cup c_j \right| \left( \left| c_i \cup c_j \right| - 1 \right)} \sum_{\tilde{x} \in (c_i \cup c_j)} \sum_{\tilde{y} \in (c_i \cup c_j) : \tilde{y} \neq \tilde{x}} \sim(\tilde{x}, \tilde{y})
\]

• 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.

\[
\tilde{s}(c_j) = \sum_{\tilde{x} \in c_j} \tilde{x}
\]

- Compute similarity of clusters in constant time:

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

Note: Clusters represented via **centroids**

\[
\bar{\mu}(c) = \frac{1}{|c|} \sum_{\bar{x} \in c} \bar{x}
\]
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.


• 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")