Machine Learning

Lecture 10
Clustering

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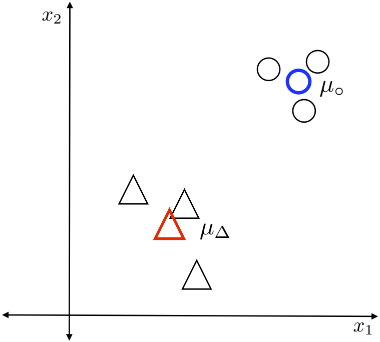
Clustering

Psychological Models of Categorization: Prototypes



Prototypes $\boldsymbol{\mu}_\Delta$ and $\boldsymbol{\mu}_o$:

$$\boldsymbol{\mu}_\Delta = 1/N_\Delta \sum_n^{N_\Delta} \mathbf{x}_{\Delta,n}$$

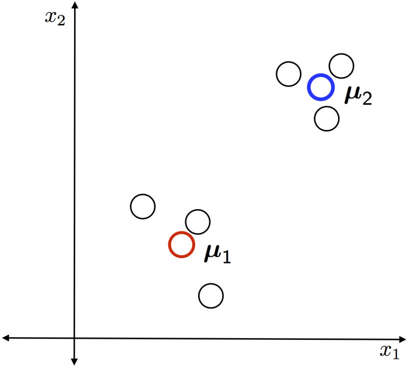
$$\boldsymbol{\mu}_o = 1/N_o \sum_n^{N_o} \mathbf{x}_{o,n}$$

New data points x are assigned to their closest cluster center μ^*

$$\boldsymbol{\mu}^* = \underset{i}{\operatorname{argmin}}(\|\boldsymbol{\mu}_i - \mathbf{x}\|_2) \tag{1}$$

Clustering

Psychological Models of Categorization: Prototypes



The only difference for clustering is:
We do not have labels.

K-means Clustering

Goal: Given data $\mathbf{x}_1, \ldots, \mathbf{x}_N$ find cluster centers $\boldsymbol{\mu}_1, \ldots \boldsymbol{\mu}_K$ such that the distances of data points to their respective cluster centre are minimized

$$\mathcal{J} = \sum_{n=1}^{N} \sum_{k=1}^{K} \mathbf{c}_{n,k} \|\mathbf{x}_n - \boldsymbol{\mu}_{\mathbf{c}_k}\| \tag{2}$$

$$\text{where } \mathbf{c}_{n,k} \begin{cases} 1 & \text{if } \mathbf{x}_n \text{ belongs to cluster } k \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

K-means Clustering

K-Means Algorithm

Re-iterating two steps:

1. Assign each data point $\mathbf{x}_i$ to their closest cluster $\boldsymbol{\mu}_k$
2. Update $\boldsymbol{\mu}_k$ to the mean of the members in that cluster

K-means Clustering Algorithm

Algorithm 1 K-means clustering

Require: data $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^D$, number of clusters k, iterations m.

Choose random data points as initial cluster centres $\boldsymbol{\mu}_1 \leftarrow \mathbf{x}_{i_1}, \dots, \boldsymbol{\mu}_k \leftarrow \mathbf{x}_{i_k}$ where $i_j \neq i_l$ for all $j \neq l$.

$\mathbf{c} \leftarrow \mathbf{0}_N$

$\mathbf{c}^{\text{old}} \leftarrow \mathbf{0}_N$

$i \leftarrow 0$

while $i < m$ **do**

  for $j = 1$ to N **do**

    Find nearest cluster centre $\mathbf{c}_j \leftarrow \text{argmin}_{1 \leq l \leq k} \|\mathbf{x}_j - \boldsymbol{\mu}_l\|_2$

  end for

  for $j \leftarrow 1$ to k **do**

    Compute new cluster centre $\boldsymbol{\mu}_j \leftarrow \frac{1}{|\{l : \mathbf{c}_l = j\}|} \sum_{l : \mathbf{c}_l = j} \mathbf{x}_l$

  end for

  if $\mathbf{c}^{\text{old}} = \mathbf{c}$ **then**

    break

  end if

  $\mathbf{c}^{\text{old}} \leftarrow \mathbf{c}$

  $i \leftarrow i + 1$

end while

return cluster centres $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_k \in \mathbb{R}^D$, assignment vector $\mathbf{c}^{\text{old}} \in \mathbb{R}^n$

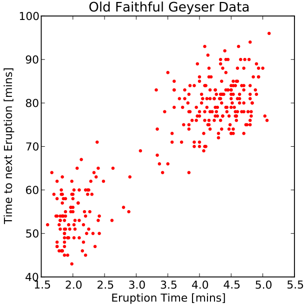
Application Example: Geyser Eruptions

Old Faithful Geyser
Yellowstone National Park,
USA

Famous data set for clustering

- Old Faithful Eruptions
- Two dimensions
  1. Time of Eruption [mins]
  2. Time until next Eruption [mins]

Application Example: Geyser Eruptions



Famous data set for clustering

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    1. Time of Eruption [mins]
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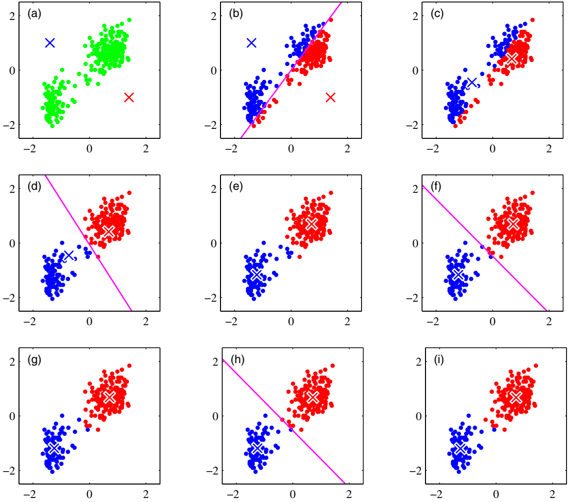
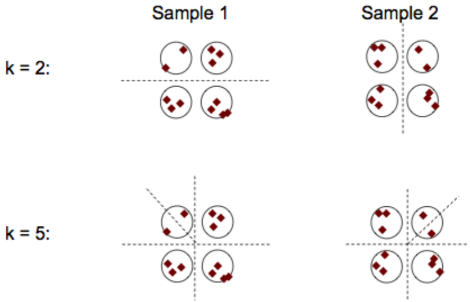
K-means Clustering Step-by-Step



Clustering Instability

Number of Clusters is a critical parameter



Clusterings are instable if number of clusters is too small or too large

Clustering Instability

- Number of clusters is critical hyper parameter
- In supervised settings we use cross-validation to optimize hyper-parameters for accuracy on test data
- How can we optimize the number of clusters?

→ Choose that k that results in most **stable** clusterings
For a review see e.g. [von Luxburg, 2009]

Clustering Instability Algorithm

Algorithm 2 Clustering Instability

Require: data points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$, clustering algorithm $\mathcal{A}$, maximal number of clusters K, iterations i.

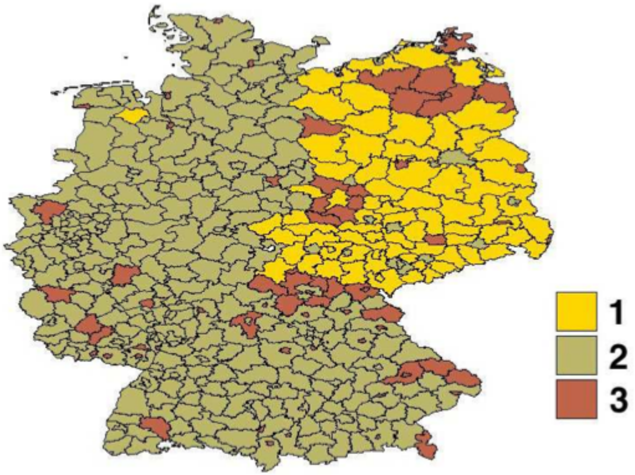
Ensure: optimal number of clusters k^*

1: **for** $k = 2$ to K **do**
2: Resample data set (e.g. random draws with replacement)
3: **for** $it = 1$ to i **do**
4: Cluster data using algorithm $\mathcal{A}$ into k clusters
5: **end for**
6: Compute minimal (across all label permutations) distance between clusterings
7: **end for**
8: Chose that k that has the minimal instability over resamplings

Application: Clustering 'Mentality' of German Population

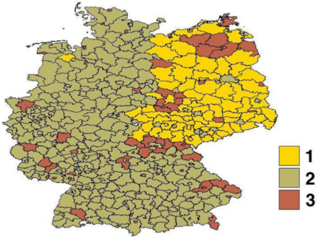
- Until 1989 Germany was divided into
  - a free capitalistic western part
  - a communist eastern part
- Political systems influence mentality of people
- The survey "Perspektive Deutschland" investigated this
  Survey asked questions about:
  - what people desire
  - what people are afraid of

German Regions clustered by 'Mentality' of Population



...based on questionnaires, 'Perspektive Deutschland' poll 2005.

German Regions clustered by 'Mentality' of Population



People in cluster 1 say:
Helping others is important
I am afraid of loosing my job

People in cluster 2 say:
Reaching my own goals is important
I am afraid of loosing my health

Online K-Means

$$\begin{aligned}
\mathcal{E}(\boldsymbol{\mu}_k) =& \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_k)^2 \quad (4)\\
=& \frac{1}{2}\mathbf{x}^\top \mathbf{x} - \frac{1}{2} 2\mathbf{x}^\top \boldsymbol{\mu}_k - \frac{1}{2}\boldsymbol{\mu}_k^\top \boldsymbol{\mu}_k\\
\frac{\partial \mathcal{E}(\boldsymbol{\mu}_k)}{\partial \boldsymbol{\mu}_k} =& \boldsymbol{\mu}_k - \mathbf{x}\\
\text{Learning rate } \eta =& \frac{1}{n_k} \; (n_k = \text{number of samples in cluster } k)\\
\text{Gradient Step } \boldsymbol{\mu}_k \leftarrow & \boldsymbol{\mu}_k - \eta \frac{\partial \mathcal{E}(\boldsymbol{\mu}_k)}{\partial \boldsymbol{\mu}_k} = \boldsymbol{\mu}_k - \frac{1}{n_k}(\mathbf{x} - \boldsymbol{\mu}_k)
\end{aligned}$$

Online K-Means Algorithm

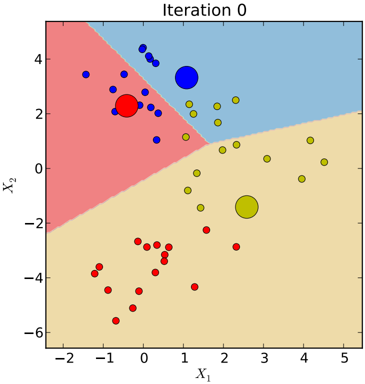
Algorithm 3 Online K-means clustering

Require: data points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$, number of clusters k, iterations m.
Ensure: cluster centres $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k \in \mathbb{R}^d$

```
Choose random data points as initial cluster centres
  μ_k ← x_i, ..., μ_k ← x_{i_k} where i_j ≠ i_l for all j ≠ l.
Initialize cluster assignment counts n_1, ..., n_k ← 0
for i = 1, ..., m do
    Draw a new data point randomly x_i
    Find nearest cluster centre k* ← argmin_k ||x_i − μ_k||_2
    Update cluster counts n_{k*} ← n_{k*} + 1
    Update cluster centers μ_{k*} ← μ_{k*} + (1/n_{k*})(x_i − μ_{k*})
end for
```

$$\boldsymbol{\mu}_k \leftarrow \mathbf{x}_i, \ldots, \boldsymbol{\mu}_k \leftarrow \mathbf{x}_{i_k}, \quad k^* \leftarrow \operatorname{argmin}_k \|\mathbf{x}_i - \boldsymbol{\mu}_k\|_2, \quad \boldsymbol{\mu}_{k^*} \leftarrow \boldsymbol{\mu}_{k^*} + \frac{1}{n_{k^*}}(\mathbf{x}_i - \boldsymbol{\mu}_{k^*})$$

Online K-Means Algorithm - Example



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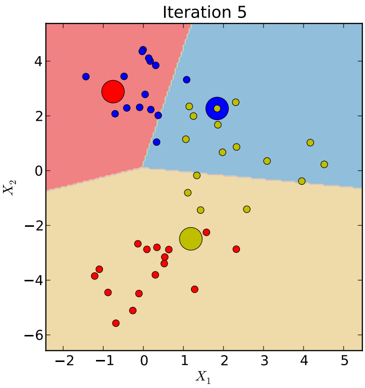

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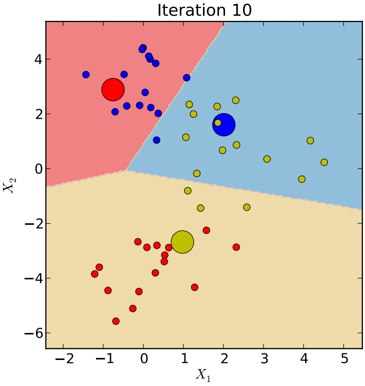

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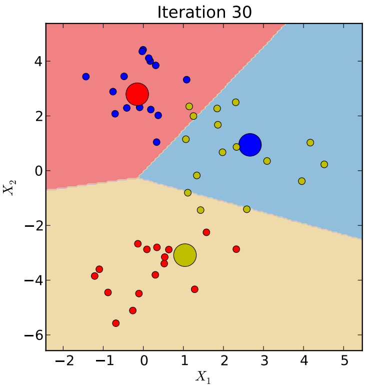

Distance Measures for Real-Valued Data $\mathbf{x} \in \mathbb{R}^D$

Clustering Algorithms need a **distance function** $d(\mathbf{x}_i, \mathbf{x}_j)$

- For real valued data $\mathbf{x} \in \mathbb{R}^D$ we can use the Euclidean distance

$$d(\mathbf{x}_i, \mathbf{x}_j) = \|\mathbf{x}_i - \mathbf{x}_j\|_2^2 \tag{5}$$

- More robust (less sensitive to outliers) is the **city block distance** or $\mathcal{L}_1$ norm

$$d(\mathbf{x}_i, \mathbf{x}_j) = \|\mathbf{x}_i - \mathbf{x}_j\|_1 \tag{6}$$

- Another alternative is the correlation coefficient (also called cosine similarity)

$$d(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{x}_1^\top \mathbf{x}_2}{\|\mathbf{x}_1\|_2 \|\mathbf{x}_2\|_2} \tag{7}$$

For standardized data $\sum_i \mathbf{x}_i = 0,\ \sum_i \mathbf{x}_i^2 = 1$ maximizing correlation is the same as minimizing euclidean distance.

Distance Measures for Non-Real-Valued Data

- For ordinal variables $\mathbf{x} \in \{\text{low}, \text{medium}, \text{high}\}^D$ we can transform the values into real-valued numbers (for three possible values e.g. $1/3, 2/3, 3/3$) and then apply distance functions for real-valued data
- For categorial variables $\mathbf{x} \in \{\text{red}, \text{green}, \text{blue}\}^D$ we can use a binary coding for the differences

$$d(\mathbf{x}_i, \mathbf{x}_j) = \sum_{d}^{D} \mathbf{x}_{id} \neq \mathbf{x}_{jd} \tag{8}$$

This metric is called **Hamming Distance**

For the sake of simplicity we only consider the euclidean distance

Hierarchical Clustering

- K-Means produces **flat** clusterings
- Often we are interested in a **hierarchy** of clusterings
- Examples:
  - Biological Species
  - Topics in Text Documents

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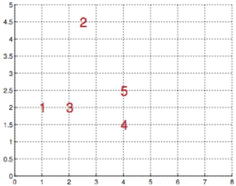

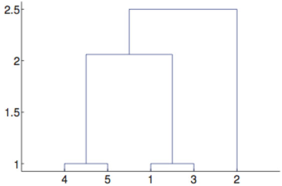

Hierarchical Clustering

- A popular approach to hierarchical clustering is
  1. Start with each data point as one cluster
  2. Successively merge (*agglomerate*) similar clusters

$\rightarrow$ **Agglomerative Clustering**

As most clustering algorithms, these procedures are not defined via objective functions but via algorithms

$\rightarrow$ Difficult to establish convergence criteria

Agglomerative Clustering

Merging requires distance function $d(C_i, C_j)$ for clusters $C_i,\ C_j$

Agglomerative Clustering

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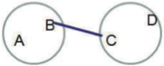
Single Linkage
Distance between two closest points in $C_i,\ C_j$

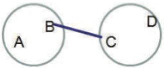


$$d(C_i, C_j) = \min_{\mathbf{x}_i \in C_i, \mathbf{x}_j \in C_j} d(\mathbf{x}_i, \mathbf{x}_j)$$

Agglomerative Clustering

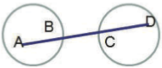
Merging requires distance function $d(C_i, C_j)$ for clusters $C_i,\ C_j$

Single Linkage
Distance between two closest points in $C_i,\ C_j$



$d(C_i, C_j) = \min_{\mathbf{x}_i \in C_i, \mathbf{x}_j \in C_j} d(\mathbf{x}_i, \mathbf{x}_j)$

Complete Linkage
Distance between two most distant points

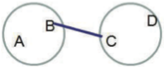


$d(C_i, C_j) = \max_{\mathbf{x}_i \in C_i, \mathbf{x}_j \in C_j} d(\mathbf{x}_i, \mathbf{x}_j)$

Agglomerative Clustering

Merging requires distance function $d(C_i, C_j)$ for clusters $C_i,\ C_j$

Single Linkage
Distance between two closest points in $C_i,\ C_j$



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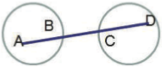
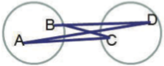


$d(C_i, C_j) = \max_{\mathbf{x}_i \in C_i, \mathbf{x}_j \in C_j} d(\mathbf{x}_i, \mathbf{x}_j)$

Average Linkage
Average distance between all $N_i N_j$ pairs



$d(C_i, C_j) = \frac{1}{N_i N_j} \sum_{\mathbf{x}_i \in C_i, \mathbf{x}_j \in C_j} d(\mathbf{x}_i, \mathbf{x}_j)$

Agglomerative Clustering Algorithm

Algorithm 4 Agglomerative Clustering

Require: Data points $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^D$, number of clusters k, distance function $d(.,.)$

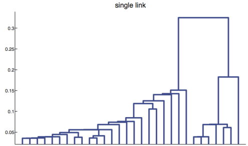
Ensure: Binary tree of clusters

Initialize each data point as cluster
for $i = 1$ to N **do**
  $C_i \leftarrow i$
end for
Initialize each cluster as available for merging
$\mathcal{S} \leftarrow \{1, \ldots, N\}$
while There are clusters to merge **do**
  Pick 2 most similar clusters to merge
  $j, k \leftarrow \mathrm{argmin}_{j,k}\, d(j,k)$
  Merge clusters to new cluster $C_l \leftarrow C_j \cup C_k$
  Mark j, k as unavailable for merging
  $\mathcal{S} \leftarrow \mathcal{S} \setminus \{j, k\}$
  if $C_l \notin \mathcal{S}$ **then**
    $\mathcal{S} \leftarrow \mathcal{S} \cup \{l\}$
  end if
end while

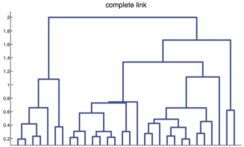
Examples Hierarchical Clustering

Dendrograms (binary clustering trees) of yeast gene expression data

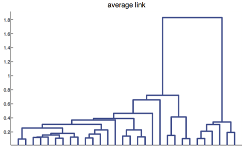
Single Linkage



Complete Linkage



Average Linkage



Taken from [Murphy, 2012]

Summary

- Clustering Algorithms find clusters in data
- Clustering Performance depends on distance function used
- K-Means is one of the most popular clustering algorithms
- For large data sets use Online K-Means
- Wrong number of clusters leads to unstable results
- Hierarchical clustering

References

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