Foundations of AI

17. Machine Learning Revisted

Supervised and Unsupervised Learning

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Machine Learning

- Can be roughly divided into:
  - Supervised Learning: Trying to learn in order to predict an class or a value
  - Unsupervised Learning: Trying to group similar examples together or to find interesting patterns in the data

Supervised Learning

- Algorithms (small example set)
  - Decision Tree Learning
  - Rule Induction
  - Neural Networks
  - SVM
  - ...

Unsupervised Learning

- Algorithms (small example set)
  - Clustering
    - K-Means, Spectral Clustering, ...
  - Local Pattern Mining
    - Item set mining, sub-sequence mining, subgraph mining
    - Association Rules
  - ...

Supervised Learning: Rule Induction

- Method 1:
  - Learn decision tree, convert to rules
- Method 2:
  - Sequential covering algorithm:
    - Learn one rule with high accuracy, any coverage
    - Remove positive examples covered by this rule
    - Repeat

Sequential Covering Algorithm

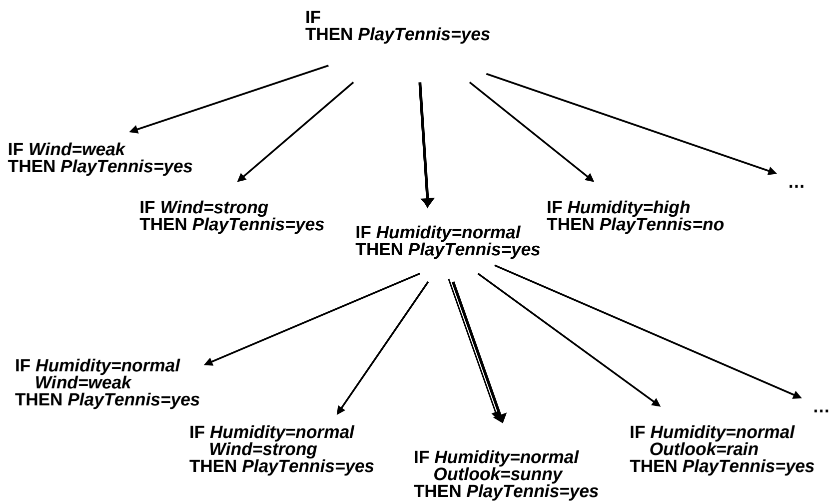
Sequential-Covering(*Target_attribute*, *Attributes*, *Examples*, *Threshold)*
Output: *Set of Rules*

- *Learned_rules* ← { }
- *Rule* ← Learn-one-rule(*Target_attribute*, *Attributes*, *Examples*)
- While Performance(*Rule, Examples*) > *Threshold*, do
  - *Learned_rules* ← *Learned_rules* ∪ {*Rule*}
  - *Examples* ← *Examples* / {examples correctly classified by *Rule*}
  - *Rule* ← Learn-one-rule(*Target_attribute*, *Attributes*, *Examples*)
- *Learned_rules* ← sort *Learned_rules* according to Performance over *Examples*
- return *Learned_rules*

EnjoySports

Sky	Temperature	Humidity	Wind	Water	Forecast	**PlayTennis**
sunny	warm	normal	strong	warm	same	**yes**
sunny	sunny	high	strong	warm	same	**yes**
rainy	cold	high	strong	warm	change	**no**
sunny	sunny	high	strong	cool	change	**yes**

Learn-One-Rule



Learn One Rule

General-to-Specific Search:

- Consider the most general rule (hypothesis) which matches every instances in the training set.
- Repeat
  - Add the attribute that most improves rule performance measured over the training set.
- Until the hypothesis reaches an acceptable level of performance.

General-to-Specific Beam Search (CN2):

- Rather than considering a single candidate at each search step, keep track of the ***k*** best candidates.

Learn One Rule

While *Pos*, do

Learn a NewRule

- *NewRule :=* most general rule possible
- *NewRuleNeg := Neg*
- while *NewRuleNeg,* do
  1. *Candidate_literals :=* generate candidates
  2. *Best_literal := argmax*$_{L \in Candidate\_literals}$ *Performance(SpecializeRule(NewRule, L))*
  3. add *Best_literal* to *NewRule* preconditions
  4. *NewRuleNeg :=* subset of *NewRuleNeg* that satisfies *NewRule* preconditions
- *Learned_rules := Learned_rules + NewRule*
- *Pos := Pos – {*members of *Pos* covered by *NewRule}*

Return *Learned_rules*

Subtleties: Learn One Rule

- Easily generalizes to multi-valued target functions
- Choose evaluation function to guide search:
  - Entropy (i.e., information gain)
  - Sample accuracy: $\frac{n_c}{n}$
  - m-estimate $\frac{n_c + mp}{n + m}$
    - Where n_c correct rule predictions (support)
    - and n all predictions (coverage)

Variants of Rule Learning Programs

- *Sequential* or *simultaneous* covering of data?
- General to specific, or specific to general?
- Generate-and-test, or example-driven?
- Whether and how to post-prune?
- What statistical evaluation function?
- How to combine predictions for multiple classes ?

Ripper

- A state of the art rule-learner (Cohen)
- Key idea:
  - apply reduced error pruning on rule set (IREP)
    - rule IF c_1 and c_2 and … and c_n THEN class
    - post prune by consider deleting “c_i and … and c_n”
  - once all rules have been learned optimize rule set R_1, …, R_k
    - try to improve rules R_i by
      - growing and pruning
      - deleting
- Standard approach by now

Unsupervised Methods: Clustering

Sky	Temperature	Humidity	Wind	Water	Forecast	**PlayTennis**
sunny	warm	normal	strong	warm	same	**yes**
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Clustering (1)

- Common technique for statistical data analysis (machine learning, data mining, pattern recognition, …)
- Classification of a data set into subsets (clusters)
- Ideally, data in each subset have a similar characteristics (proximity according to distance function)

Clustering (2)

- Needed: distance (similarity / dissimilarity) function, e.g., Euclidian distance
- Clustering quality
  - Inter-clusters distance maximized
  - Intra-clusters distance minimized
- The quality depends on
  - Clustering algorithm
  - Distance function
  - The application (data)

Types of Clustering

- Hierarchical Clustering
  - Agglomerative Clustering (buttom up)
  - Divisive Clustering (top-down)
- Partitional Clustering
  - K-Means Clustering (hard & soft)
  - Gaussian Mixture Models (EM-based)

K-Means Clustering

- Partitions the data into *k* clusters (k is to be specified by the user)
- Find *k* reference vectors $\boldsymbol{m}_j$, $j = 1,\ldots,k$ which best explain the data $\boldsymbol{X}$
- Assign data vectors to nearest (most similar) reference $\boldsymbol{m}_i$

$$\|\mathbf{x}^t - \mathbf{m}_i\| = \min_j \|\mathbf{x}^t - \mathbf{m}_j\|$$

r-dimensional data vector in a real-valued space

reference vector (center of cluster = mean)

Reconstruction Error

(K-Means as Compression Alg.)

- The total reconstruction error is defined as

$$E\left(\{\mathbf{m}_i\}_{i=1}^k \,\middle|\, \mathrm{X}\right) = \sum_t \sum_i b_i^t \|\mathbf{x}^t - \mathbf{m}_i\|^2$$

with

$$b_i^t = \begin{cases} 1 & \text{if } \|\mathbf{x}^t - \mathbf{m}_i\| = \min_j \|\mathbf{x}^t - \mathbf{m}_j\| \\ 0 & \text{otherwise} \end{cases}$$

- Find reference vectors which minimize the error
- Taking its derivative with respect to m_i and setting it to 0 leads to

$$\mathbf{m}_i = \frac{\sum_t b_i^t \mathbf{x}^t}{\sum_t b_i^t}$$

K-Means Algorithm

Initialize $\boldsymbol{m}_i, i = 1, \ldots, k$, for example, to k random $\boldsymbol{x}^t$
Repeat
  For all $\boldsymbol{x}^t \in \mathcal{X}$
  $$b_i^t \leftarrow \begin{cases} 1 & \text{if } \|\boldsymbol{x}^t - \boldsymbol{m}_i\| = \min_j \|\boldsymbol{x}^t - \boldsymbol{m}_j\| \\ 0 & \text{otherwise} \end{cases}$$
  For all $\boldsymbol{m}_i, i = 1, \ldots, k$
  $$\boldsymbol{m}_i \leftarrow \sum_t b_i^t \boldsymbol{x}^t / \sum_t b_i^t$$
Until $\boldsymbol{m}_i$ converge

Recompute the cluster centers $\boldsymbol{m}_i$ using current cluster membership

Assign each $\boldsymbol{x}^t$ to the closest cluster

K-Means Example

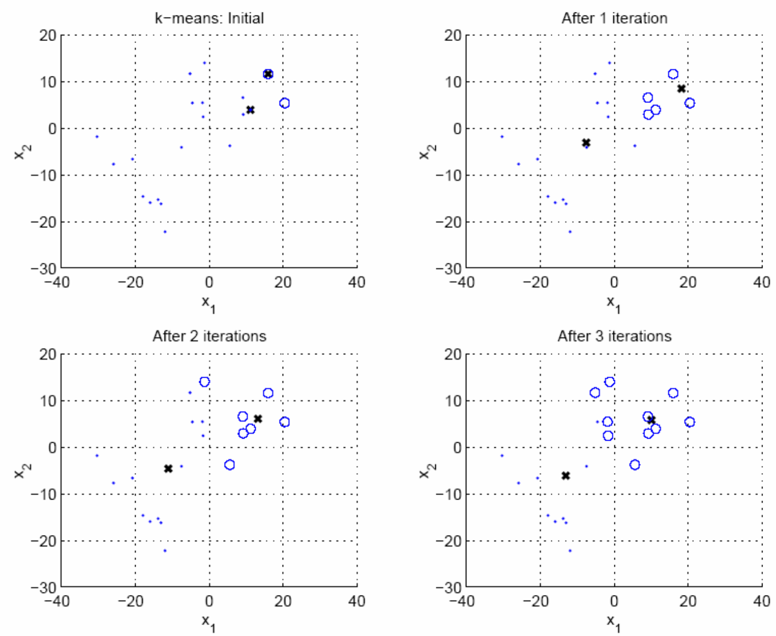


Image source: Alpaydin, Introduction to Machine Learning

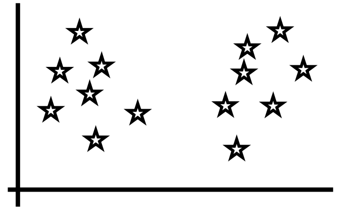
Strength of K-Means

- Easy to understand and to implement
- Efficient O(nkt)
  n = #iterations, *k* = #clusters, *t* = #data points
- Converges to a local optimum (global optimum is hard to find)
- Most popular clustering algorithm

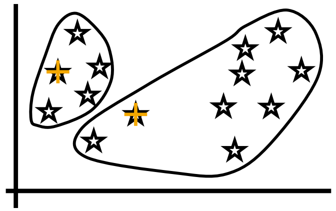
Weaknesses of K-Means

- User needs to specify #clusters (*k*)
- Sensitive to initialization (strategy: use different seeds)
- Sensitive to outliers since all data points contribute equally to the mean (strategy: try to eliminate outliers)

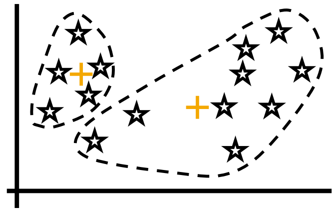
An example



(A). Random selection of *k* centers

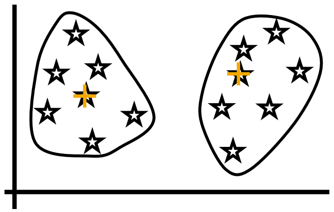


***Iteration* 1: (B). Cluster assignment**

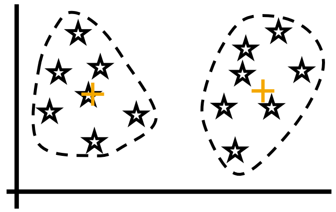


(C). Re-compute centroids

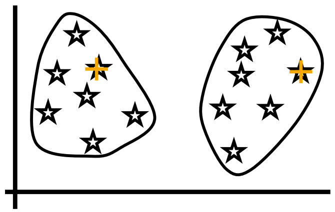
An example (cont ...)



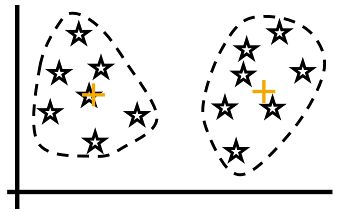
Iteration **2: (D). Cluster assignment**



(E). Re-Compute centeroids

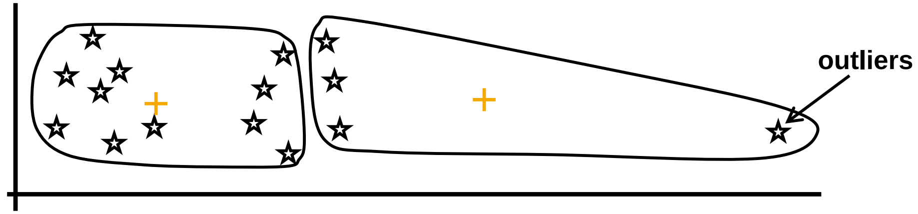


Iteration **3: (F). Cluster assignment**

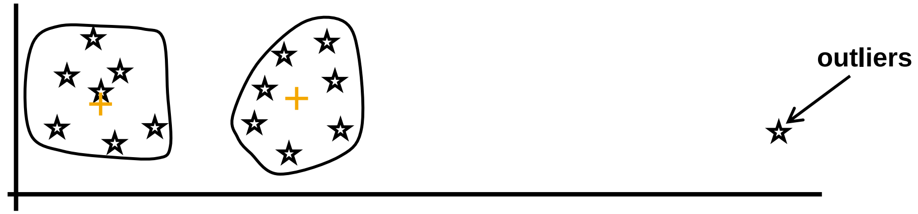


(G). Re-Compute centeroids

Weaknesses of k-means: Problems with outliers



(A): Undesirable clusters



(B): Ideal clusters

Soft Assignments

- So far, each data point was assigned to exactly one cluster
- A variant called soft k-means allows for making fuzzy assignments
- Data points are assigned to clusters with certain probabilities

Soft K-Means Clustering

- Each data point is given a soft assignment to all means

$$c_{tk} = \frac{\exp(-\beta\, ||x^t - m_k||^2)}{\sum_i \exp(-\beta\, ||x^t - m_i||^2)}, \; \sum_k c_{tk} = 1$$

- β is a “stiffness” parameter and plays a crucial role
- Means are updated

$$m_k = \frac{\sum_t c_{tk} x^t}{\sum_t c_{tk}}$$

- Repeat assignment and update step until assignments do not change anymore

Soft K-Means Clustering

- Points between clusters get assigned to both of them
- Points near the cluster boundaries play a partial role in several clusters
- Additional parameter β
- Clusters with varying shapes can be treated in a probabilistic framework (mixtures of Gaussians)

After Clustering

- Dimensionality reduction methods find correlations between features and group features
- Clustering methods find similarities between instances and group instances
- Allows knowledge extraction through

  number of clusters,

  prior probabilities,

  cluster parameters, i.e., center, range of features.

Example: CRM, customer segmentation

Clustering as Preprocessing

- Estimated group labels h_j (soft) or b_j (hard) may be seen as the dimensions of a new k dimensional space, where we can then learn our discriminant or regressor.
- Local representation (only one b_j is 1, all others are 0; only few h_j are nonzero) vs

  Distributed representation (After PCA; all z_j are nonzero)

Summary

- K-Means is the most popular clustering algorithm
- It is efficient and easy to implement
- Converges to a local optimum
- A variant of hard k-means exists allowing soft assignments
- Soft k-means corresponds to the EM algorithm which is a general optimization procedure