—INF4820—

Classification
Clustering

Erik Velldal

University of Oslo

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Topics for Today

- Quick recap from last lecture:
  - Neighbor relations; kNN and RNN
  - Ways to represent classes (exemplar-based vs. centroid-based).
  - Ways to represent class membership (hard vs. soft).
  - The classification problem in vector space models.
- More on Rocchio classifiers and kNN classifiers
- Linear vs. non-linear classifiers
- Voronoi Tessellations
- Unsupervised machine learning for class discovery: Clustering
- Flat vs. hierarchical clustering
- k-Means Clustering
- Reading: Chapter 16 in Manning, Raghavan & Schütze (2008), *Introduction to Information Retrieval*; `http://informationretrieval.org/`.

The Classification Task

- The task of automatically assigning objects to pre-defined classes.
- A core problem in machine learning (ML).
- Example of a supervised learning task (the training data contains labeled data, indicating what we want to learn).
- Vector space classification relies on the assumption that objects (i.e. points) in the same class form contiguous and non-overlapping regions in the space. ("The contiguity hypothesis")
- Classification amounts to defining boundaries in the space that separate objects in different classes: *The decision boundaries*.
- The goal is to find boundaries that gives high classification accuracy on unseen test items.

Rocchio Classification

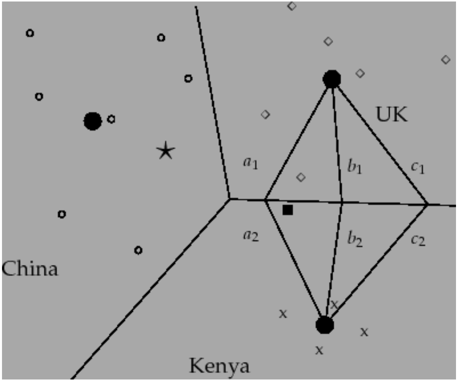
- Uses centroids to represent classes and define the boundaries of the class regions.
- Each class c_i represented by its centroid $\vec{\mu}_i$, computed as the average of the normalized vectors $\vec{x}_j$ of its members;

$$\vec{\mu}_i = \frac{1}{|c_i|} \sum_{\vec{x}_j \in c_i} \vec{x}_j$$

- To classify a new object o_j, represented by a feature vector $\vec{x_j}$, determine which centroid $\vec{\mu}_i$ that $\vec{x_j}$ is closest to, and assign it to the corresponding class c_i.

The Decision Boundary of the Rocchio Classifier

- Defines the boundary between two classes by the set of points that are equidistant from the centroids.
- In two dimensions: This set of points always corresponds to a *line*.
- In multiple dimensions: A line in 2D corresponds to a *hyperplane* in a higher-dimensional space.



Problems with the Rocchio Classifier

- Implicitly assumes that classes are *spheres with similar radii*.
- Ignores details of the distribution of points within a class, only based on the centroid distance.
- Does not work well for classes than cannot be accurately represented by a single prototype or "center" (e.g. classes covering disconnected or elongated regions).

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- Does not work well for classes than cannot be accurately represented by a single prototype or "center" (e.g. classes covering disconnected or elongated regions).
- Because the Rocchio classifier defines a linear decision boundary, it is only suitable for problems involving *linearly separable* classes.

KNN-classification

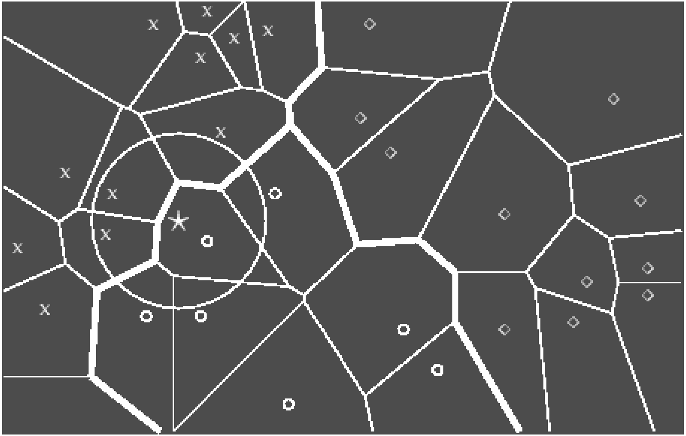
- k Nearest Neighbor classification.
- An example of a non-linear classifier.
- For $k = 1$: Assign each object to the class of its closest neighbor.
- For $k > 1$: Assign each object to the majority class among its k closest neighbors.
- Rationale: given *the contiguity hypothesis*, we expect a test object o_i to have the same label as the training objects located in the local region surrounding $\vec{x_i}$.
- The parameter k must be specified in advance, either by manually or by optimizing on held-out data.

KNN-classification (cont'd)

The Voronoi Tessellation

- Defines the decision boundaries of the kNN classifier.
- Assuming $k = 1$: For a given set of objects in the space, let each object define a cell consisting of all points that are closer to that object than to other objects.
- Each such *Voronoi cell* will be a convex polygon.
- Decomposing a space into such Voronoi cells gives us the so-called Voronoi tessellation.
- In the general case of $k \geq 1$, the Voronoi cells will be given by the regions in the space for which the set of k nearest neighbors is the same. Partitions the space into convex polygons.

Voronoi Tessellation for 1NN (Manning, Raghavan & Schütze 2008)



The decision boundary for the 1NN classifier is defined along the regions of Voronoi cells for the objects in each class. Shows the non-linearity of kNN.

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A Probabilistic Version

- Estimate the probability of membership in class c as the proportion of the k nearest neighbors in c.

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A Distance Weighted Version

- The score for a given class c_i can be computed as

$$\text{score}(c_i, o_j) = \sum_{\vec{x_n} \in \text{knn}(\vec{x}_j)} \text{I}(c_i, \vec{x}_n)\, \text{sim}(\vec{x_n}, \vec{x_j})$$

  where $\text{knn}(\vec{x}_j)$ is the set of k nearest neighbors of $\vec{x}_j$, sim is whatever similarity measure we're using, e.g. the cosine function, and $\text{I}(c_i, \vec{x}_n)$ is simply a membership function returning 1 if $\vec{x}_n \in c_i$ and 0 otherwise.
- Such distance weighted votes can often give more accurate results, e.g. in the case of ties.

Two Categorization Tasks in Machine Learning

Classification

- Supervised learning, requiring labeled training data.
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Clustering

- Unsupervised learning from unlabeled data.
- Automatically group similar objects together.
- No predefined classes or structure, we only specify the similarity measure. Relies on "self-organization".
- General objective: partition the data into subsets, so that the similarity among members of the same group is high (homogeneity) while the similarity between the groups themselves is low (heterogeneity).

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  - Helps alleviating the sparse data problem.

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- Many applications within IR. Examples:
  - Speed up search: For a clustered document collection, first retrieve the most relevant cluster, then retrieve documents from within the cluster.
  - Presenting the search results: Instead of ranked lists, organize the results as clusters (see e.g. Clusty.com or Google's *wonder wheel*).

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- News aggregation / topic directories.
- Social network analysis; identify sub-communities and user segments.

Types of Clustering Methods

Different methods can be divided according to the *memberships* they create and the procedure by which the *clusters* are formed:

$$\text{Procedure}\begin{cases}\text{Flat}\\ \text{Hierarchical}\begin{cases}\text{Agglomerative}\\ \text{Divisive}\end{cases}\\ \text{Hybrid}\end{cases}$$

$$\text{Memberships}\begin{cases}\text{Hard}\\ \text{Soft}\\ \text{Disjunctive}\end{cases}$$

Types of Clustering Methods (cont'd)

Hierarchical

- Creates a tree structure of hierarchically nested clusters
- Divisive (top-down): Let all objects be members of the same cluster; then successively split the group into smaller and maximally dissimilar clusters until all objects is its own singleton cluster.
- Agglomerative (bottom-up): Let each object define its own cluster; then successively merge most similar clusters until only one remains.

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Flat

- Often referred to as partitional clustering when assuming hard and disjoint clusters. (But can also be soft.)
- Tries to directly decompose the data into a set of clusters.

Flat Clustering

- Given a set of objects $O = \{o_1, \ldots, o_n\}$, a hard flat clustering algorithm seeks to construct a set of clusters $C = \{c_1, \ldots, c_k\}$, where each object o_i is assigned to a single cluster c_i.
- More formally, we want to define an assignment $\gamma : O \rightarrow C$ that optimizes some objective function $F_s(\gamma)$.
- The cardinality k (= the number of clusters) must typically be manually specified as a parameter to the algorithm.
- But the most important parameter is the similarity function s.
- The objective function is defined in terms of the similarity function, and generally we want to optimize for:
  - High intra-cluster similarity
  - Low inter-cluster similarity

Flat Clustering (cont'd)

- Optimization problems are search problems:
  - There's a finite number of possible of partitionings of O.
  - Naive solution: enumerate all possible assignments $\Gamma = \{\gamma_1, \ldots, \gamma_m\}$ and choose

$$\hat{\gamma} = \underset{\gamma \in \Gamma}{\arg\min}\, F_s(\gamma)$$

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  - Problem: Exponentially many possible partitions
  - Instead, approximate the solution by iteratively improving on an initial (possibly random) partition until some stopping criterion is met.

Next Week

- More on flat clustering: k-Means
- Different ways of measuring the distance between classes or clusters.
- Flat vs. hierarchical clustering
- Agglomerative vs. divisive hierarchical clustering
- Reading: Chapter 17 in Manning, Raghavan & Schütze (2008), *Introduction to Information Retrieval*; `http://informationretrieval.org/` (see course web-page for the relevant sections).