— INF4820 —
Algorithms for AI and NLP

Evaluating Classifiers
Clustering

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Language Technology Group (LTG)

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Today

- Recap
- Evaluation of classifiers
- Unsupervised machine learning for class discovery: Clustering
- Flat clustering.
- k-means clustering

Recap – Classification

- Supervised vs unsupervised learning.

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- Linear vs non-linear decision boundaries.

Testing a classifier

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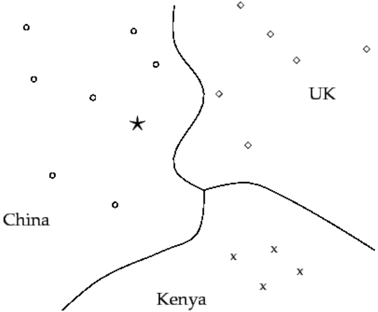
- To evaluate the boundary, we measure the number of correct classification predictions on unseeen test items.
- Many ways to do this...



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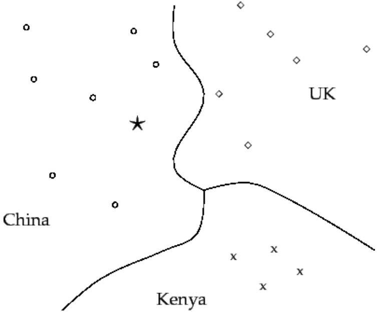
- Many ways to do this. . .
- We want to test how well a model *generalizes* on a held-out test set.
- Labeled test data is sometimes refered to as the gold standard.
- Why can't we test on the training data?



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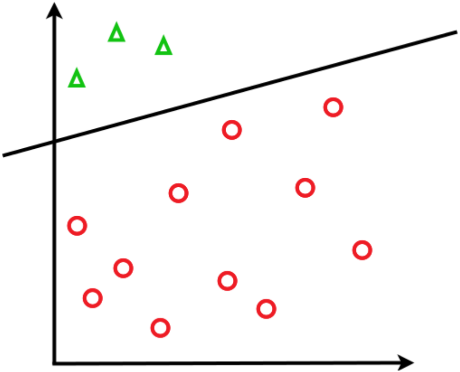

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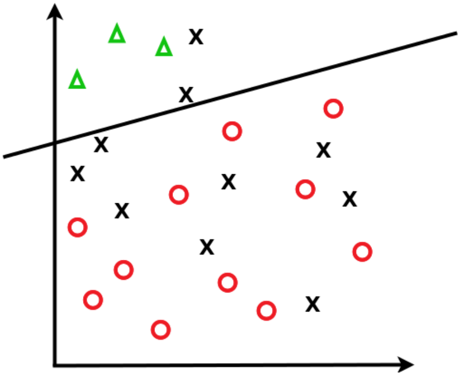

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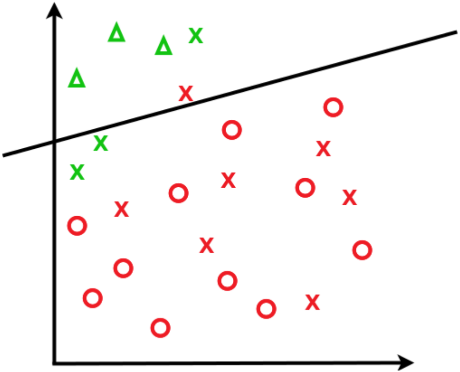

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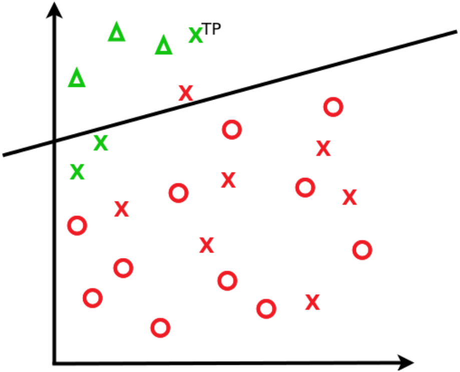

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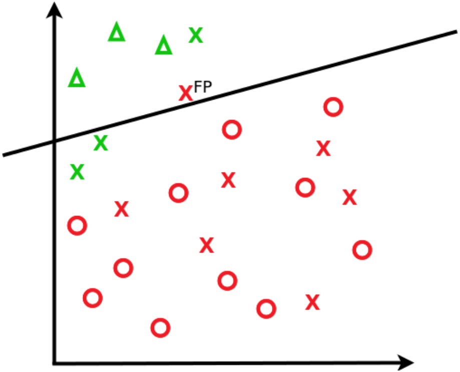

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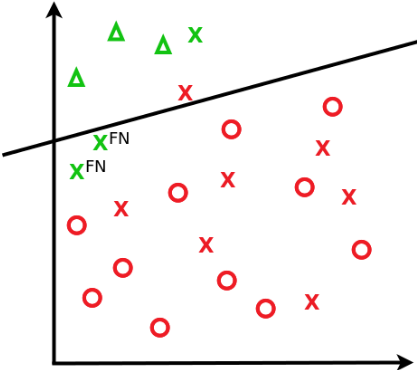

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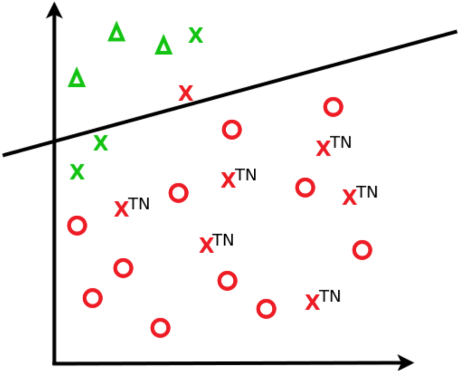

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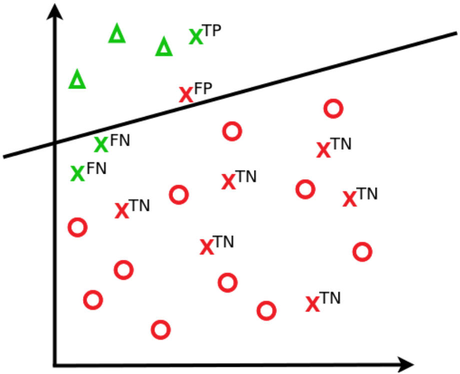

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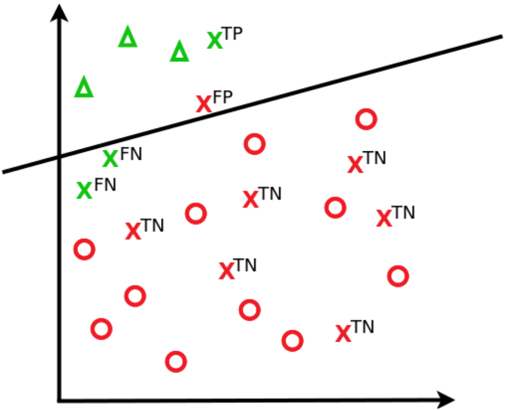

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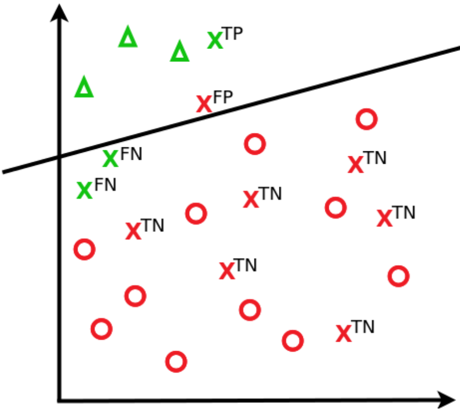

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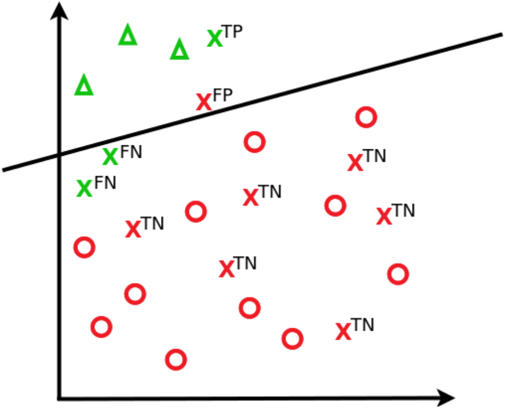

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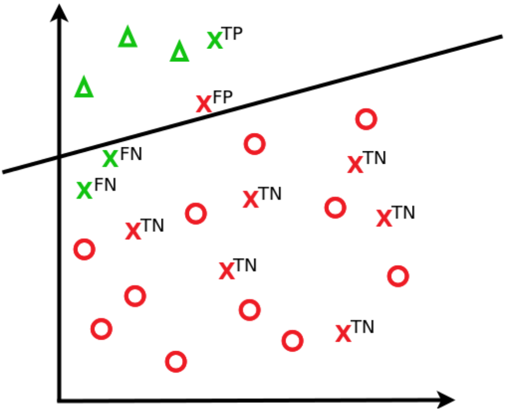

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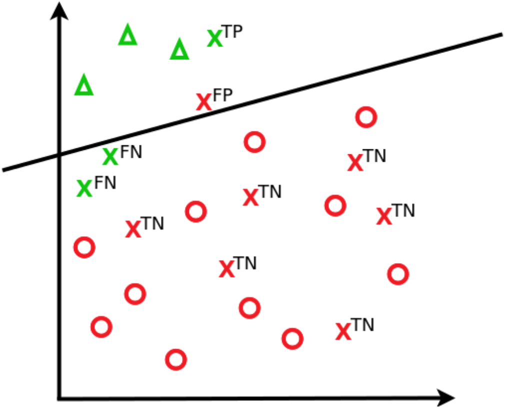

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$$\textit{F-score} = 2 \times \frac{\textit{precision} \times \textit{recall}}{\textit{precision} + \textit{recall}} = 0.4$$

Evaluation measures

- $accuracy = \frac{TP+TN}{N} = \frac{TP+TN}{TP+TN+FP+FN}$
  - The ratio of correct predictions.
  - Not suitable for unbalanced numbers of positive / negative examples.
- $precision = \frac{TP}{TP+FP}$
  - The number of detected class members that were correct.
- $recall = \frac{TP}{TP+FN}$
  - The number of actual class members that were detected.
  - Trade-off: Positive predictions for all examples would give 100% recall but (typically) terrible precision.
- $F\text{-}score = 2 \times \frac{precision \times recall}{precision + recall}$
  - Balanced measure of precision and recall (harmonic mean).

Evaluating multi-class predictions

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Micro-averaging

- Sum TPs, FPs, and FNs for all points/objects across all classes, and then compute global precision and recall.
- The micro average will be highly influenced by the large classes.

Clustering or cluster analysis

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- Cluster: "A group of similar things or people positioned or occurring closely together." *Oxford Dictionaries Online*
- Clustering: A set of clusters.
- Originates in anthropology and psychology: empirically based typologies of cultures and of individuals.
- A clustering algorithm groups objects based on a set of features describing each object.

Two categorization tasks in machine learning

Classification

- Supervised learning, requiring labeled training data.
- Given some training set of examples with class labels, train a classifier to predict the class labels of new objects.

Clustering

- Unsupervised learning from unlabeled data.
- Automatically group similar objects together.
- No pre-defined classes: we only specify the similarity measure.
- 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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  - Presenting the search results: Instead of ranked lists, organize the results as clusters.
- Dimensionality reduction: class-based features.
- News aggregation, topic directories.
- Social network analysis; identify sub-communities and user segments.
- Product recommendations, demographic analysis, ...

Main types of clustering methods

Flat

- Tries to directly decompose the data into a set of clusters.
- Membership:
  - Partitional clustering.
  - Hard clustering.
  - Soft clustering.

Hierarchical

- Creates a tree structure of hierarchically nested clusters.
- Not part of the curriculum this year!

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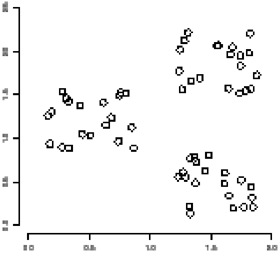
- Essentially the same as the contiguity hypothesis in classification



Flat clustering

- Given a set of objects $O = \{o_1, \ldots, o_n\}$, construct a set of clusters $C = \{c_1, \ldots, c_k\}$, where each object o_i is assigned to a cluster c_j.
- Parameters:
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- Parameters:
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- More formally, we want to define an assignment $\gamma : O \to C$ that optimizes some objective function $F_s(\gamma)$.
- In general terms, 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 partitionings of O.
- Naive solution: enumerate all possible assignments $\Gamma = \{\gamma_1, \ldots, \gamma_m\}$ and choose the best one,

$$\hat{\gamma} = \arg\min_{\gamma \in \Gamma} F_s(\gamma)$$

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

k-means

- Unsupervised variant of the Rocchio classifier.
- Goal: Partition the n observed objects into k clusters C so that each point $\vec{x}_j$ belongs to the cluster c_i with the nearest centroid $\vec{\mu}_i$.
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- The optimization problem: For each cluster, minimize the *within-cluster sum of squares*, $F_s = \mathrm{WCSS}$:

$$\mathrm{WCSS} = \sum_{c_i \in C} \sum_{\vec{x}_j \in c_i} \|\vec{x}_j - \vec{\mu}_i\|^2$$

- Equivalent to minimizing the average squared distance between objects and their cluster centroids (since n is fixed) – a measure of how well each centroid represents the members assigned to the cluster.

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Algorithm

Initialize: Randomly select k centroid seeds.

Iterate:

- Assign each object to the cluster with the nearest centroid.
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Terminate: When stopping criterion is satisfied.

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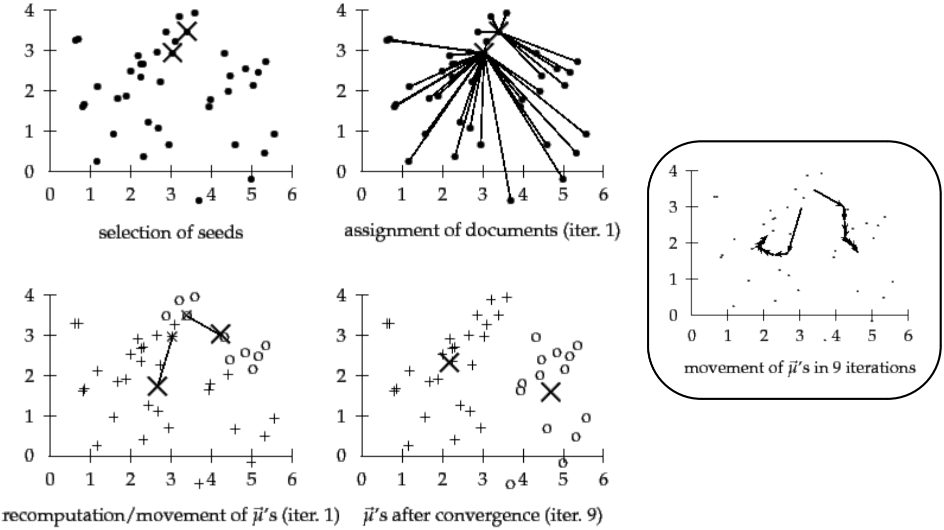
- In short, we iteratively reassign memberships and recompute centroids until the configuration stabilizes.

k-means example for $k = 2$ in R^2 (Manning, Raghavan & Schütze 2008)



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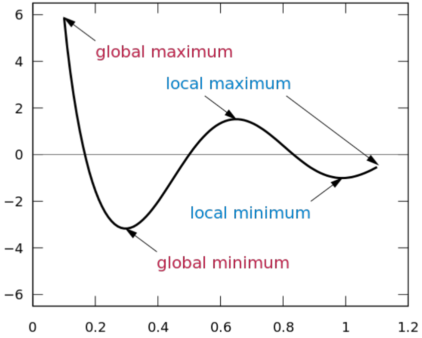
- Guaranteed to converge but not to find the global minimum.
- Possible solution: multiple random initializations



Comments on k-means

"Seeding"

- We initialize the algorithm by choosing random *seeds* that we use to compute the first set of centroids.
- Many possible heuristics for selecting seeds:
  - pick k random objects from the collection;
  - pick k random points in the space;
  - pick k sets of m random points and compute centroids for each set;
  - compute a hierarchical clustering on a subset of the data to find k initial clusters; etc..

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  - compute a hierarchical clustering on a subset of the data to find k initial clusters; etc..
- The initial seeds can have a large impact on the resulting clustering (because we typically end up only finding a local minimum of the objective function).
- Outliers are troublemakers.

Comments on k-means

Possible termination criteria

- Fixed number of iterations
- Clusters or centroids are unchanged between iterations.
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Some close relatives of k-means

- k-medoids: Like k-means but uses medoids instead of centroids to represent the cluster centers.
- Fuzzy c-means (FCM): Like k-means but assigns soft memberships in $[0, 1]$, where membership is a function of the centroid distance.
  - The computations of both WCSS and centroids are weighted by the membership function.

Flat Clustering: The good and the bad

Pros

- Conceptually simple, and easy to implement.
- Efficient. Typically linear in the number of objects.

Cons

- The dependence on random seeds as in k-means makes the clustering non-deterministic.
- The number of clusters k must be pre-specified. Often no principled means of *a priori* specifying k.
- The clustering quality often considered inferior to that of the less efficient hierarchical methods.
- Not as informative as the more structured clusterings produced by hierarchical methods.

Connecting the dots

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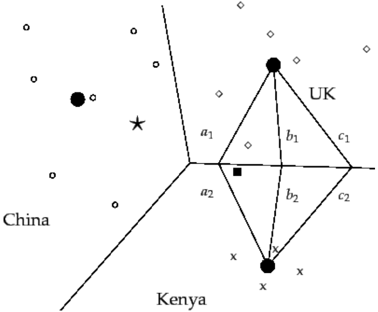
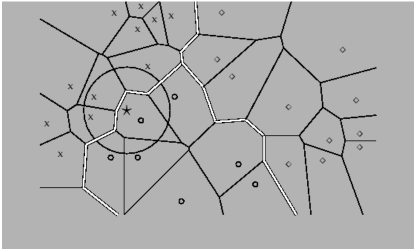
- Note how k-means clustering can be thought of as performing Rocchio classification in each iteration.
- Moreover, Rocchio can be thought of as a 1 Nearest Neighbor classifier with respect to the centroids.
- How can this be? Isn't kNN non-linear and Rocchio linear?

Connecting the dots

- Recall that the kNN decision boundary is locally linear for each cell in the Voronoi diagram.
- For both Rocchio and k-means, we're partitioning the observations according to the Voronoi diagram generated by the centroids.





► **Figure 14.3** Voronoi tessellation and decision boundaries (double lines) in 1NN classification. The three classes are: X, circle and diamond.

A note on obligatory assignment 2b

- Builds on oblig 2a: Vector space representation of a set of words based on BoW features extracted from a sample of the Brown corpus.
- For 2b we provide class labels for most of the words.
- Train a Rocchio classifier to predict labels for a set of unlabeled words.

Label	**Examples**
FOOD	*potato, food, bread, fish, eggs . . .*
INSTITUTION	*embassy, institute, college, government, school . . .*
TITLE	*president, professor, dr, governor, doctor . . .*
PLACE_NAME	*italy, dallas, france, america, england . . .*
PERSON_NAME	*lizzie, david, bill, howard, john . . .*
UNKNOWN	*department, egypt, robert, butter, senator . . .*

A note on obligatory assignment 2b

- For a given set of objects $\{o_1, \ldots, o_m\}$ the proximity matrix R is a square $m \times m$ matrix where R_{ij} stores the proximity of o_i and o_j.
- For our word space, R_{ij} would give the dot-product of the normalized feature vectors $\vec{x}_i$ and $\vec{x}_j$, representing the words o_i and o_j.

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- Computing all the pairwise similarities *once* and then storing them in R can help save time in many applications.
  - R will provide the input to many clustering methods.
  - By sorting the row elements of R, we get access to an important type of similarity relation; nearest neighbors.
- For 2b we will implement a proximity matrix for retrieving knn relations.

Quiz!

kahoot.it