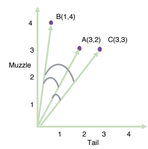
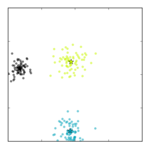
Clustering: k-means, Expectation-Maximization Ethics: Ethical Questions in AI



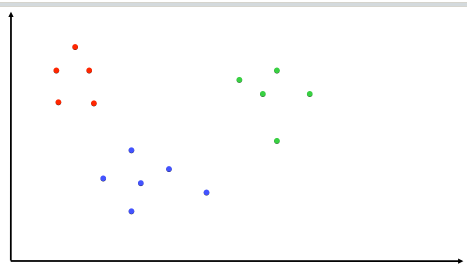


Based partly on: M desJardins, T Oates, P Matuszek, RJ Mooney: www.cs.utexas.edu/~mooney/cs388/slides/TextClustering.ppt, and other sources as noted

What is Clustering?

- Given some instances of data: group them such that
  - Examples within a group are similar
  - Examples in different groups are different
- These groups are **clusters**
- A kind of unsupervised learning – the instances do not include a class attribute.

Clustering Example



A Different Example

- How would you group
  - 'The price of crude oil has increased significantly'
  - 'Demand for crude oil outstrips supply'
  - 'Some people do not like the flavor of olive oil'
  - 'The food was very oily'
  - 'Crude oil is in short supply'
  - 'Oil platforms extract oil'
  - 'Canola oil is supposed to be healthy'
  - 'Iraq has significant oil reserves'
  - 'There are different types of cooking oil'

A note: you might or might not know how many clusters to look for.

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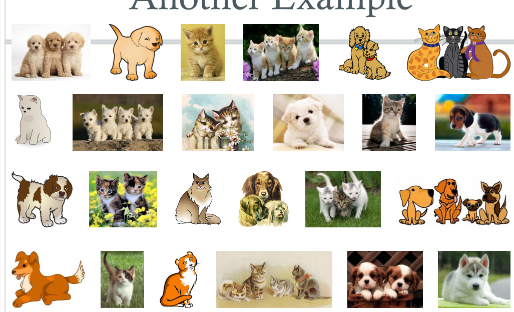
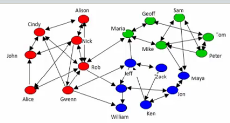
Another Example

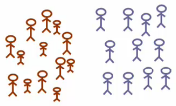


Some Example Uses

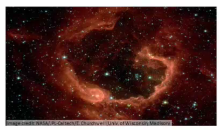
Organize computing clusters



Social network analysis



Market segmentation



Astronomical data analysis

Clustering Basics

- Collect examples
- Compute **similarity** among examples according to some metric
- Group examples together such that:
  1. Examples within a cluster are similar
  2. Examples in different clusters are different
- Summarize each cluster
- **Sometimes**: assign new instances to the cluster it I most similar to

Measures of Similarity

- To do clustering we need some measure of similarity.
- This is basically our "critic"
- Computed over a vector of values representing instances
- Types of values depend on domain:
  - Documents: bag of words, linguistic features
  - Purchases: cost, purchaser data, item data
  - Census data: most of what is collected
- Multiple different measures exist

Measures of Similarity

- Semantic similarity (but that's hard)
  - For example, olive oil/crude oil
- Similar attribute counts
  - Number of attributes with the same value
  - Appropriate for large, sparse vectors
  - Bag-of-Words: BoW
- More complex vector comparisons:
  - Euclidean Distance
  - Cosine Similarity

Euclidean Distance

- Euclidean distance: distance between two measures summed across each feature

$$\text{dist}(x_i, x_j) = \text{sqrt}((x_{i1}-x_{j1})^2+(x_{i2}-x_{j2})^2+..+(x_{in}-x_{jn})^2)$$

- Squared differences give more weight to larger differences
  - $\text{dist}([1,2],[3,8]) = \text{sqrt}((1-3)^2+(2-8)^2) = \text{sqrt}((-2)^2+(-6)^2) = \text{sqrt}(4+36) = \text{sqrt}(40) = \sim 6.3$

Euclidean

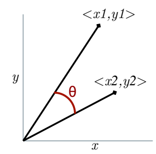
- Calculate differences
  - Ears: pointy?
  - Muzzle: how many inches long?
  - Tail: how many inches long?

$$\text{dist}(x_1, x_2) = \text{sqrt}((0-1)^2+(3-1)^2+..+(2-4)^2)=\text{sqrt}(9)=3$$

$$\text{dist}(x_1, x_3) = \text{sqrt}((0-0)^2+(3-3)^2+..+(2-3)^2)=\text{sqrt}(1)=1$$

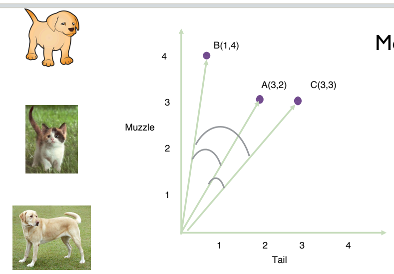
Cosine Similarity

- A measure of similarity between vectors
  - Find **cosine of the angle** between them
  - Cosine = 1 when angle = 0
  - Cosine < 1 otherwise
- As angle between vectors shrinks, θ approaches 1
  - Meaning: the two vectors are getting closer
  - Meaning: the **similarity** of whatever is represented by the vectors **increases**
- Vectors can have any number of dimensions



Based on home.iitk.ac.in/~mfelixor/Files/non-numeric-Clustering-seminar.ppt, with thanks

Cosine Similarity



Euclidean Distance *vs* Cosine Similarity *vs* Other

- Cosine Similarity:
  - Measures **relative** proportions of various features
  - Ignores magnitude
  - When all the correlated dimensions between two vectors are in proportion, you get maximum similarity
- Euclidean Distance:
  - Measures **actual** distance between two points
  - More concerned with absolutes
- Often similar in practice, especially on high dimensional data
- Consider meaning of features/feature vectors **for your domain**

Justin Washtell @ semanticvoid.com/blog/2007/02/23/similarity-measure-cosine-similarity-or-euclidean-distance-or-both/

Clustering Algorithms

- Flat:
  - K means
- Hierarchical:
  - Bottom up
  - Top down (not common)
- Probabilistic:
  - Expectation Maximization (E-M)

Partitioning (Flat) Algorithms

- Partitioning method
  - Construct a **partition** of n instances into a set of k clusters
- Given: a set of documents and the number k
- Find: a partition of k clusters that optimizes the chosen partitioning criterion
  - Globally optimal: exhaustively enumerate all partitions.
  - Usually too expensive.
  - Effective heuristic methods: k-means algorithm.

www.csee.umbc.edu/~nicholas/676/MRSslides/lecture17-clustering.ppt

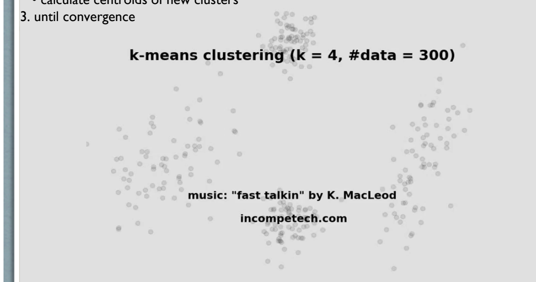
k-means Clustering

- Simplest hierarchical method, widely used
- Create clusters based on a centroid; each instance is assigned to the closest centroid
- K is given as a parameter
- Heuristic and iterative

k-means Algorithm

1. Choose k (the number of clusters)
2. Randomly choose k instances to center clusters on
3. Assign each point to the centroid it's closest to, forming clusters
4. Recalculate centroids of new clusters
5. Reassign points based on new centroids
6. Iterate until…
7. Convergence (no point is reassigned) or after a fixed number of iterations.

1. randomly place centroids
2. iteratively:
   - assign points to closest centroid, forming clusters
   - calculate centroids of new clusters
3. until convergence



This (happens to be) a pretty good random initialization!

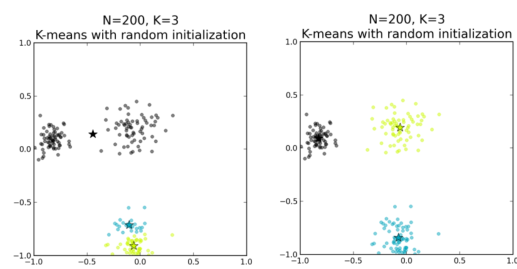
www.youtube.com/watch?v=5I3Ei69I40s

k-means

- Tradeoff between having more clusters (better focus within each cluster) and having too many clusters.
  - Overfitting is a possibility with too many!
- Results depend on random seed selection.
  - Some seeds can result in slow convergence or convergence to poor clusters
- Algorithm is sensitive to outliers
  - Data points that are very far from other data points
  - Could be errors, special cases, …

www.csee.umbc.edu/~nicholas/676/MRSslides/lecture17-clustering.ppt

Problem: Bad Initial Seeds



datasciencelab.wordpress.com/2014/01/15/improved-seeding-for-clustering-with-k-means/

Evaluation of k-means

Advantages

- Easy to understand, implement
- Most popular clustering algorithm
- Efficient, almost linear
  - Time complexity: O(tkn)
    - n = number of data points
    - k = number of clusters
    - t = number of iterations.
- In practice, **performs well** (especially on text)

Disadvantages

- Must choose k beforehand
  - Bad k → bad clusters
  - Sometimes we don't know
- Sensitive to initialization
  - One fix: run several times with different random centers and look for agreement
- Sensitive to outliers, irrelevant features

Expectation Maximization Clustering

- Expectation-Maximization is a core ML algorithm
  - Not just for clustering!
- Basic idea: assign instances to clusters **probabilistically** rather than **absolutely**
  - Instead of assigning membership in a group, learn a probability function for each group
- Instead of absolute assignments, output is probability of each instance being in each cluster

EM Clustering Algorithm

- **Goal:** maximize overall probability of data
- Iterate between:
  - Expectation: **estimate probability** that each instance belongs to each cluster
  - Maximization: **recalculate parameters** of probability distribution for each cluster
- Until convergence or iteration limit.

Expectation Maximization (EM)

- **Probabilistic method for soft clustering**
- Idea: learn k classifications from **unlabeled** data
- Assumes k clusters: $\{c_1, c_2, \ldots c_k\}$
- "Soft" version of k-means
- Assumes a probabilistic model of categories (such as Naive Bayes)
- Allows computing $P(c_i \mid I)$ for each category, c_i, for a given instance I

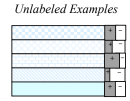
(Slightly) More Formally

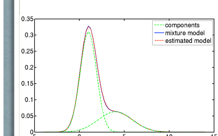
- Iteratively learn **probabilistic categorization model** from **unsupervised data**
- Initially assume random assignment of examples to categories
  - "Randomly label" data
- Learn initial probabilistic model by estimating **model parameters** θ from randomly labeled data
- Iterate until convergence:
  - **Expectation (E-step):**
    - Compute $P(c_i \mid I)$ for each instance (example) given the current model
    - Probabilistically re-label the examples based on these posterior probability estimates
  - **Maximization (M-step):** Re-estimate model parameters, θ, from re-labeled data

EM

Initialize:
Assign random probabilistic labels to unlabeled data

Unlabeled Examples

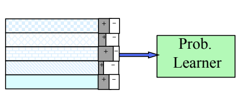




https://www.mathworks.com/matlabcentral/fileexchange/24867-gaussian-mixture-model-m

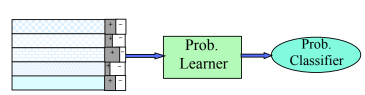
EM

Initialize:
Give soft-labeled training data to a probabilistic learner



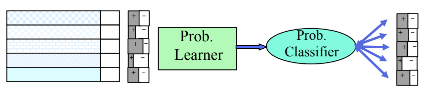
EM

Initialize:
Produce a probabilistic classifier



EM

E Step:
Relabel unlabled data using the trained classifier



EM

M step:
Retrain classifier on relabeled data

Continue EM iterations until probabilistic labels on unlabeled data converge.

EM Summary

- Basically a probabilistic k-means.
- Has many of same advantages and disadvantages
  - Results are easy to understand
  - Have to choose k ahead of time
- Useful in domains when we want likelihood that an instance belongs to more than one cluster
  - Natural language processing for instance