CS 188: Artificial Intelligence
Spring 2006

Lecture 13: Clustering and Similarity
2/28/2006

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Many slides from either Stuart Russell or Andrew Moore

Today

- Clustering
  - K-means
  - Similarity Measures
  - Agglomerative clustering
- Case-based reasoning
  - K-nearest neighbors
  - Collaborative filtering

Recap: Classification

- Classification systems:
  - Supervised learning
  - Make a rational prediction given evidence
  - We've seen several methods for this
  - Useful when you have labeled data (or can get it)

Clustering

- Clustering systems:
  - Unsupervised learning
  - Detect patterns in unlabeled data
    - E.g. group emails or search results
    - E.g. find categories of customers
    - E.g. detect anomalous program executions
  - Useful when don't know what you're looking for
  - Requires data, but no labels
  - Often get gibberish

Clustering

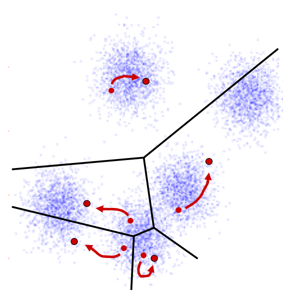
- Basic idea: group together similar instances
- Example: 2D point patterns

- What could "similar" mean?
  - One option: small (squared) Euclidean distance

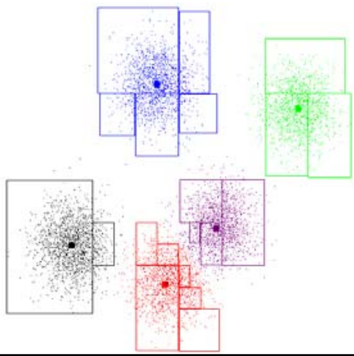
$$\text{dist}(x,y) = (x-y)^{\top}(x-y) = \sum_i (x_i - y_i)^2$$

K-Means

- An iterative clustering algorithm
  - Pick K random points as cluster centers (means)
  - Alternate:
    - Assign data instances to closest mean
    - Assign each mean to the average of its assigned points
  - Stop when no points' assignments change



K-Means Example



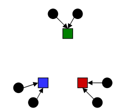
K-Means as Optimization

- Consider the total distance to the means:

$$\phi(\{x_i\},\{a_i\},\{c_k\}) = \sum_i \mathsf{dist}(x_i, c_{a_i})$$

points assignments means

- Each iteration reduces phi
- Two stages each iteration:
  - Update assignments: fix means c, change assignments a
  - Update means: fix assignments a, change means c



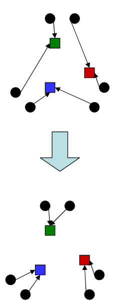
Phase I: Update Assignments

- For each point, re-assign to closest mean:

$$a_i = \underset{k}{\mathsf{argmin}}\ \mathsf{dist}(x_i, c_k)$$

- Can only decrease total distance phi!

$$\phi(\{x_i\},\{a_i\},\{c_k\}) = \sum_i \mathsf{dist}(x_i, c_{a_i})$$

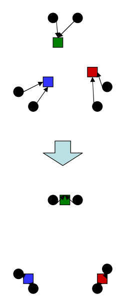


Phase II: Update Means

- Move each mean to the average of its assigned points:

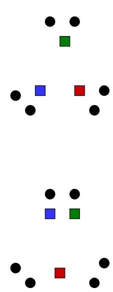
$$c_k = \frac{1}{|\{i : a_i = k\}|} \sum_{i:a_i=k} x_i$$

- Also can only decrease total distance!
- Why?
- Fun fact: the point y with minimum squared Euclidean distance to a set of points {x} is their mean



Initialization

- K-means is non-deterministic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?
  - Various schemes for preventing this kind of thing: variance-based split / merge, initialization heuristics



K-Means Getting Stuck

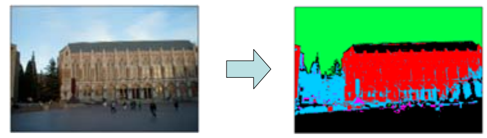
- A local optimum:

K-Means Questions

- Will K-means converge?
  - To a global optimum?
- Will it always find the true patterns in the data?
  - If the patterns are very very clear?
- Will it find something interesting?
- Do people ever use it?
- How many clusters to pick?

Clustering for Segmentation

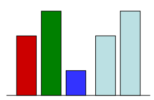
- Quick taste of a simple vision algorithm
- Idea: break images into manageable regions for visual processing (object recognition, activity detection, etc.)



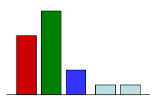
http://www.cs.washington.edu/research/imagedatabase/demo/kmcluster/

Representing Pixels

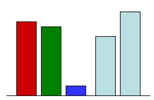
- Basic representation of pixels:
  - 3 dimensional color vector <r, g, b>
  - Ranges: r, g, b in [0, 1]
  - What will happen if we cluster the pixels in an image using this representation?



- Improved representation for segmentation:
  - 5 dimensional vector <r, g, b, x, y>
  - Ranges: x in [0, M], y in [0, N]
  - Bigger M, N makes position more important
  - How does this change the similarities?

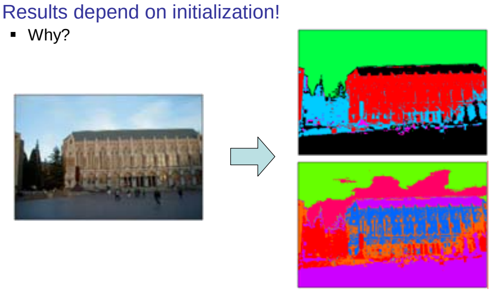


- Note: real vision systems use more sophisticated encodings which can capture intensity, texture, shape, and so on.



K-Means Segmentation

- Results depend on initialization!
  - Why?



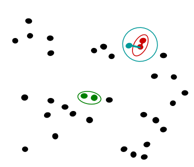
- Note: best systems use graph segmentation algorithms

Other Uses of K-Means

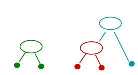
- Speech recognition: can use to quantize wave slices into a small number of types (SOTA: work with multivariate continuous features)
- Document clustering: detect similar documents on the basis of shared words (SOTA: use probabilistic models which operate on topics rather than words)

Agglomerative Clustering

- Agglomerative clustering:
  - First merge very similar instances
  - Incrementally build larger clusters out of smaller clusters
- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there's only one cluster left

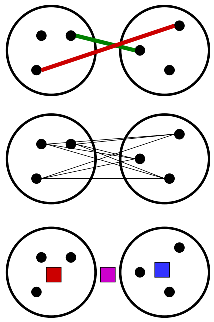


- Produces not one clustering, but a family of clusterings represented by a dendrogram



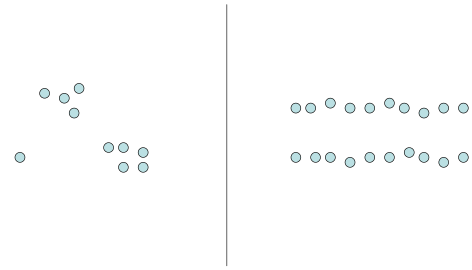
Agglomerative Clustering

- How should we define "closest" for clusters with multiple elements?
- Many options
  - Closest pair (single-link clustering)
  - Farthest pair (complete-link clustering)
  - Average of all pairs
  - Distance between centroids (broken)
  - Ward's method (my pick, like k-means)
- Different choices create different clustering behaviors



Agglomerative Clustering

- Complete Link (farthest) vs. Single Link (closest)



Back to Similarity

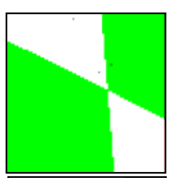
- K-means naturally operates in Euclidean space (why?)
- Agglomerative clustering didn't require any mention of averaging
  - Can use any function which takes two instances and returns a similarity
  - (If your similarity function has the right properties, can adapt k-means too)
- Kinds of similarity functions:
  - Euclidian (dot product)
  - Weighted Euclidian
  - Edit distance between strings
  - Anything else?

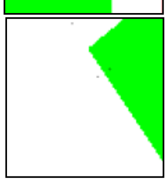
Similarity Functions

- Similarity functions are very important in machine learning
- Topic for next class: kernels
  - Similarity functions with special properties
  - The basis for a lot of advance machine learning (e.g. SVMs)

Case-Based Reasoning

- Similarity for classification
  - Case-based reasoning
  - Predict an instance's label using similar instances
- Nearest-neighbor classification
  - 1-NN: copy the label of the most similar data point
  - K-NN: let the k nearest neighbors vote (have to devise a weighting scheme)
  - Trade-off:
    - Small k gives relevant neighbors
    - Large k gives smoother functions
    - Sound familiar?
- [DEMO]

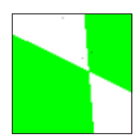




http://www.cs.cmu.edu/~zhuxj/courseproject/knndemo/KNN.html

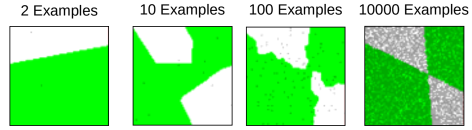
Parametric / Non-parametric

- Parametric models:
  - Fixed set of parameters
  - More data means better settings
- Non-parametric models:
  - Complexity of the classifier increases with data
  - Better in the limit, often worse in the non-limit
- (K)NN is non-parametric



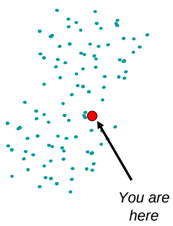
Truth

2 Examples | 10 Examples | 100 Examples | 10000 Examples



Collaborative Filtering

- Ever wonder how online merchants decide what products to recommend to you?
- Simplest idea: recommend the most popular items to everyone
  - Not entirely crazy! (Why)
  - Can do better if you know something about the customer (e.g. what they've bought)
- Better idea: recommend items that similar customers bought
  - A popular technique: collaborative filtering
  - Define a similarity function over customers (how?)
  - Look at purchases made by people with high similarity
  - Trade-off: relevance of comparison set vs confidence in predictions
  - How can this go wrong?



Next Class

- Kernel methods / SVMs
- Basis for a lot of SOTA classification tech