Search Engines

WS 2009 / 2010

Lecture 12, Thursday January 28th, 2010
(Clustering, Clustering, Clustering)

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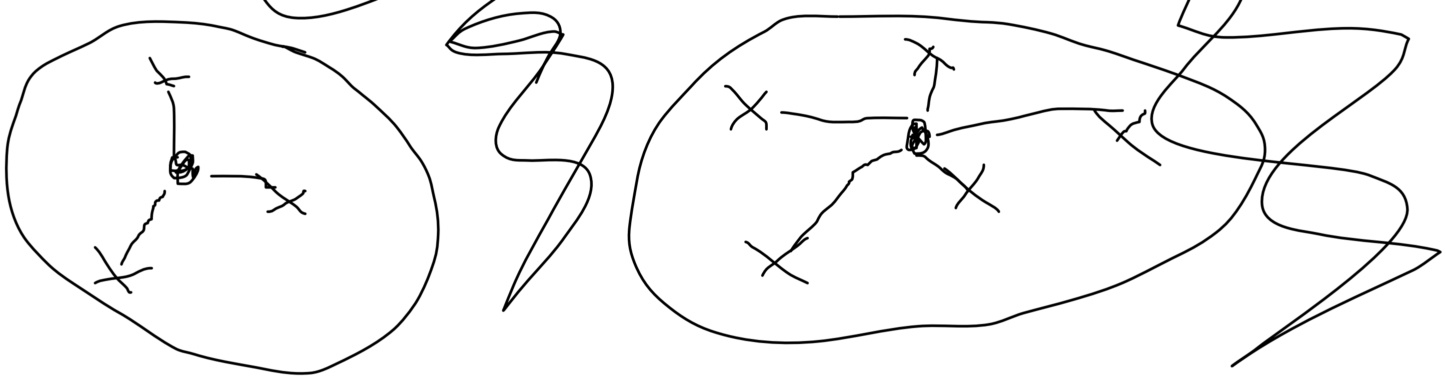
Overview of Today's Lecture

- Learn how to cluster
  - What is clustering and how is it different from classification?
  - The simplest of all clustering algorithms: k-means
  - Hierarchical clustering
  - A very nice impossibility result (Kleinberg, NIPS 2002)
    - No single clustering algorithms can achieve all desirable goals at the same time

      (a bit like Heisenberg's uncertainty principle)

What is Clustering

- Given a set of points, find a "good" partitioning



- Difference to classification:
  - Classification is supervised
    - we need training data where we know the classes
  - Clustering is unsupervised
    - we are just given the objects / points

When is a Clustering "Good" ?

- Many different ways to define quality
  - quality relative to a ground truth:
    - define precision and recall as usual
  - without a ground truth, just data-dependent:
    - intuitively, a clustering is good if it has
      - high intra-cluster similarity
      - low inter-cluster similarity
    - one formalization of this: RSS = residual sum of squares
      - Centroid of a cluster = average of points in the cluster
      - assume clusters $C_1,\ldots,C_k$ with centroids $\mu_1,\ldots,\mu_k$
      - then $RSS = \Sigma_{i=1,\ldots,k} \Sigma_{x \text{ in } Ci} |x - \mu_i|^2$

K-Means

- The simplest of all clustering algorithms
  - used a lot in practice (because of its simplicity, like Naive Bayes)
  - k-means tries to minimize RSS from last slide
  - assume we know the optimal centroids
    - (A) then best to assign each point to its nearest centroid
  - assume we know the optimal clustering
    - (B) then best to take centroid = average of points in cluster
  - but initially we know neither the centroids nor the clustering
    - so guess some initial centroids
    - from that compute clustering according to (A)
    - from that compute centroids according to (B)
    - and so on ... DEMO

Proof of optimality of (A) and (B)

RSS

$$RSS = \sum_{i=1}^{2} \sum_{x \in C_i} |x - \mu_i|^2$$

(A) decreases RSS : obvious!

(B) decreases RSS :

which μ minimizes $\sum_{i=1}^{m} |x_i - \mu|^2 =: R$

$$\frac{\partial R}{\partial \mu} = \sum_{i=1}^{m} -2(x_i - \mu) = -2\left(\sum_{i=1}^{m} x_i - m \cdot \mu\right) = 0$$

$$\Longrightarrow \mu = \sum_{i=1}^{m} x_i / m$$

K-Means — Code

- Code live in a VNC session ...
  - with points = integers — Exercise: points = text
- Possible abort criteria
  - after a fixed number of iterations
    - simple, but how to guess a good number?
  - until assignment of points to clusters remains constant
    - very reasonable, but can take very long for large data sets
  - terminate when RSS falls below given threshold
    - makes sense, but RSS may never fall below given threshold
    - combine with bound on number of iterations
  - terminate when decrease in RSS falls below given threshold
    - good, because we stop when we are close to convergence
    - must also combine with bound on number of iterations

K-Means — Convergence

- Proof of convergence to a local optimum
  - RSS decreases in assignment step (A)
    - this follows from our optimality proof for (A)
  - RSS decreases in centroid computation step (B)
    - this follows from our optimality proof for (B)
  - stop when there is no more decrease
  - only finitely many clusterings → termination
  - however, we must pay attention to proper tie breaking
    - tie = two centroids are equally close
    - for example, always prefer centroid with smaller index
    - otherwise may cycle forever between clusters of equal quality

K-Means — Time Complexity

- The time complexity is
  - each assigment step (A) takes time $O(n \cdot k)$
    - where n = #points and k = #clusters
  - each centroid computation step (B) takes time $O(n)$
  - so with I iterations we get $O(I \cdot n \cdot k)$
  - but this assumes that adding two points takes time $O(1)$
    - not true for vectors in high-dimensional space
    - however, these vectors are usually sparse (e.g. docs)
    - then cost of addition is O(#non-zero entries)
    - however, the centroids quickly become not sparse!
    - simple trick: centroid truncation
      - set components with small values to zero

K-Means — Choice of K

- Idea: try to base it on RSS
  - Idea 1: choose the K with smallest RSS
    - bad idea, because RSS is always minimized for $K = n$
  - Idea 2: choose K with smallest $RSS + \lambda \cdot K$
    - makes sense: RSS becomes larger as K becomes smaller
    - λ is a tuning parameter
    - now we have shifted the problem to finding a good λ
    - but for a given application, λ is often a constant while the best K may vary from instance to instance
    - this formula has an information-theoretic justification

Hierarchical Clustering

- General bottom-up idea:
  - start with clustering, where each point is its own cluster
  - iteratively merge the two clusters that are "closest"
  - natural visualization of hierarchy as a dendrogram

Which Clusters To Merge

- Similarity measure between clusters sim(C_i, C_j)
  - in each step merge C_i and C_j with smallest sim(C_i, C_j)
- Four common similarity measures
  - Single-Link: similarity of closest points
  - Complete-Link: similarity of farthest points
  - Centroid: average inter-similarity
  - Group-Average: average of all similarities

Single-Link and Complete-Link

- Single-Link Problem
  - only the closest pair counts → tendency to straggly clusters

- Complete-Link Problem
  - high sensitivity even to single outlier

- Graph-theoretic interpretation
  - let $s_k = sim(C_i, C_j)$ in k-th merging step
  - let G_k be the graph with an edge between all points with $d \leq s_k$
  - then single-link clusters = connected components of G_k
  - and complete-link clusters = maximal cliques of G_k

Hierarchical Clustering — Time Complexity

- Naive algorithm
  - assume we proceed until we have k clusters
  - compute all pairwise distances for all cluster pairs
    - this is on the order of n^2 (n = #points)
  - so that gives a total time complexity of $O(k \cdot n^2)$
  - n^2 is prohibitive for large data
- Improvement
  - using a priority queue we can achieve $O(k \cdot n \cdot \log n)$
  - this is ok; recall that k-means needs $O(I \cdot k \cdot n)$
  - for single-link we can even achieve $O(k \cdot n)$
  - we will not go into the details of these algorithms here
    - read in the references in case you are interested

An Impossibility Theorem for Clustering

- Naive but valid question:
  - Can't there a single clustering that is always the best?
  - Each clustering algorithm we know has some drawbacks
  - but that does not answer our question
    - maybe just no one has been smart enough yet?
  - let's formulate three natural properties which every clustering algorithm should have

Three Properties ...

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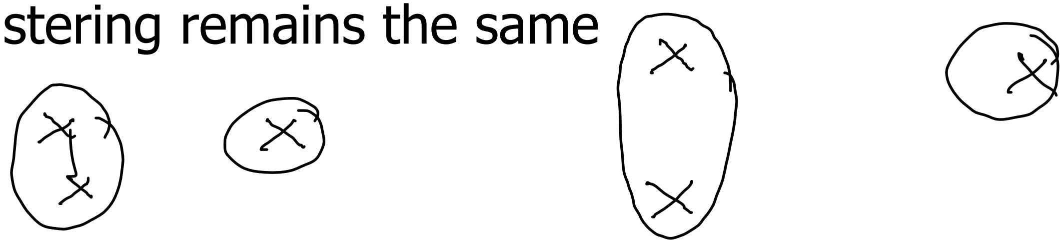
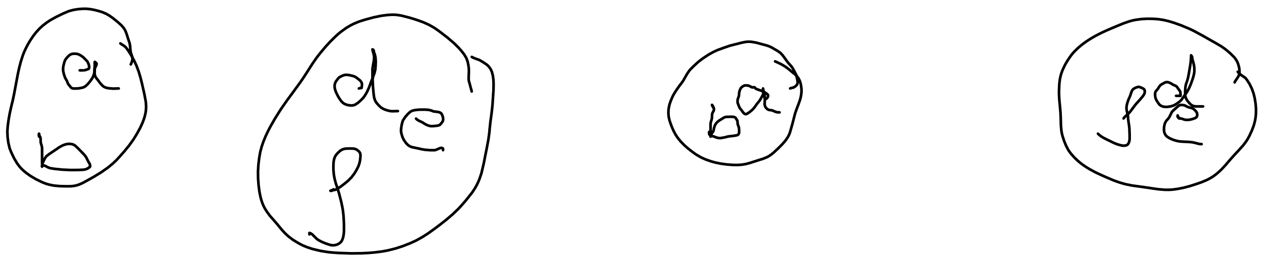
- ... every clustering algorithm should have
  - **Scale Invariance:** when we multiply all distances by a constant factor, the clustering remains the same



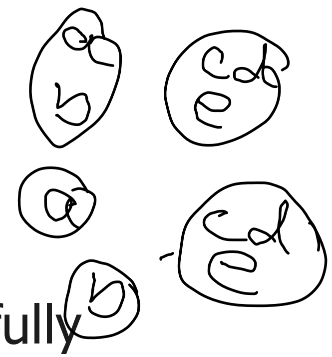
  - **Richness:** each possible partioning is achieved on some dataset

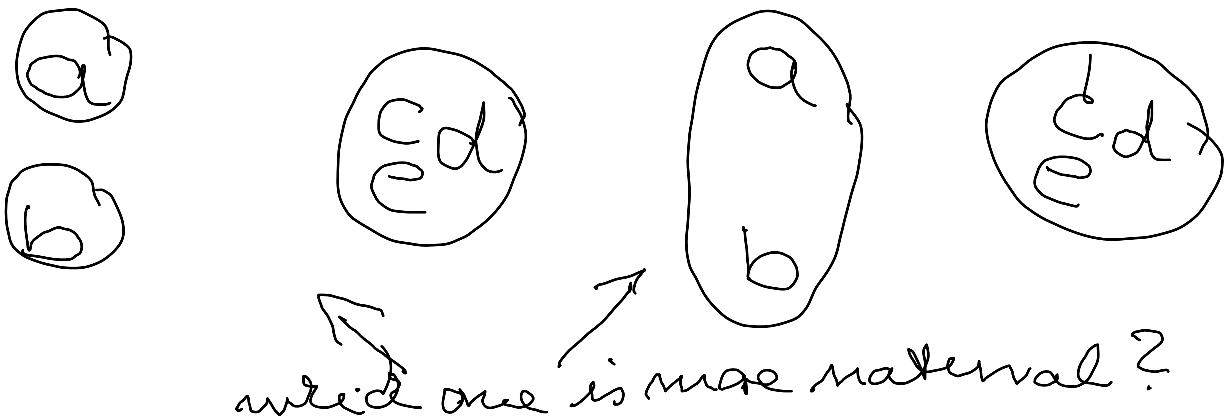
  - **Consistency:** if we shrink the intra-cluster distances and increase the inter-cluster distances, the clustering stays the same



Impossibility theorem

- No clustering algorithm can achieve all three!
  - here is the basic proof idea
  - define an antichain as a set of partionings where no partioning is a refinement of another partioning
  - then proof that Scale-Invariance + Consistency imply that the set of achievable partionings is an antichain thus contradicting Richness
  - here is some intuition which you will only be able to fully understand after you have understood the proof:





Proof of Impossibility Theorem 1

Let A be any clustering algorithm which satisfies SCALE-INVARIANCE and CONSISTENCY

Assume (by way of contradiction) that $\exists\, \Gamma_1, \Gamma_2$ where $\Gamma_1 \leq \Gamma_2$, both prod. by A

$\exists\, \alpha, \beta$ with the following property

if all intra-cluster dist $\leq \alpha$, all inter-cluster dist $\geq \beta$ $\Longrightarrow$ A always prod Γ_1

where $\alpha < \beta$. Follows from CONSISTENCY. For example $(1, 5)$ i.e. α, β

$\exists\, \beta, \gamma$ with the following property

if all intra ... $\leq \beta$, all inter $\geq \gamma$ $\Longrightarrow$ A produces Γ_2

Follows from CONSISTENCY + SCALE e.g. $(5, 10)$

Proof of Impossibility Theorem 2

$(1, 5) \Rightarrow \Gamma_1$ (1)

$(5, 10) \Rightarrow \Gamma_2$ (2)

Now take clustering Γ_2 and bring all intra-cluster distances of $\Gamma_1 \leq 1$.

(1) $\Rightarrow$ A produces Γ_1

(2) $\Rightarrow$ A produces Γ_2 ↯

Proof of Impossibility Theorem 3

References

- K-Means and Hierarchical Clustering
  - Again, the Wikipedia articles are ok
    http://en.wikipedia.org/wiki/K-means
    http://en.wikipedia.org/wiki/Hierarchical_clustering
  - Here is the textbook which I also consulted
    Introduction to Information Retrieval
- The impossibility theorem
  - The NIPS 2002 paper by Jon Kleinberg
    An impossibility theorem for Clustering