Clustering:
Overview and K-means algorithm

K-Means illustrations thanks to
2006 student Martin Makowiecki

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Informal goal

- Given set of objects and measure of similarity between them, group similar objects together

- What mean by "similar"?
- What is good grouping?
- Computation time / quality tradeoff

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General types of clustering

- "Soft" versus "hard" clustering
  - Hard: partition the objects
    - each object in exactly one partition
  - Soft: assign degree to which object in cluster
    - view as probability or score
- flat versus hierarchical clustering
  - hierarchical = clusters within clusters

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Applications:

Many
- biology
- astronomy
- computer aided design of circuits
- information organization
- marketing
- …

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Clustering in information search and analysis

- Group information objects
  - ⇒ discover topics
  - ? other groupings desirable
- Clustering versus classifying
  - classifying: have pre-determined classes with example members
  - clustering:
    - get groups of similar objects
    - added problem of labeling clusters by topic
      - e.g. common terms within cluster of docs.

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Example applications in search

- Query evaluation: cluster pruning (§7.1.6)
  - cluster all documents
  - choose representative for each cluster
  - evaluate query w.r.t. cluster reps.
  - evaluate query for docs in cluster(s) having most similar cluster rep.(s)
- Results presentation: labeled clusters
  - cluster only query results
  - e.g. Clusty.com (metasearch)

hard / soft? flat / hier?

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Issues

- What attributes represent items for clustering purposes?
- What is measure of similarity between items?
  - General objects and matrix of pairwise similarities
  - Objects with specific properties that allow other specifications of measure
    - Most common:
      Objects are d-dimensional vectors
      » Euclidean distance
      » cosine similarity
- What is measure of similarity between clusters?

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Issues continued

- Cluster goals?
  - Number of clusters?
  - flat or hierarchical clustering?
  - cohesiveness of clusters?
- How evaluate cluster results?
  - relates to measure of closeness between clusters
- Efficiency of clustering algorithms
  - large data sets => external storage
- Maintain clusters in dynamic setting?
- Clustering methods? - MANY!

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General types of clustering methods

- agglomerative versus divisive algorithms
  - agglomerative = bottom-up
    - build up clusters from single objects
  - divisive = top-down
    - break up cluster containing all objects into smaller clusters
  - both agglomerative and divisive give hierarchies
  - hierarchy can be trivial:

    1 (. .) . . .   2 ((. .) .) . .
    3 (((. .) .) .) .   4 ((((. .) .) .) .)

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General types of clustering methods cont.

- constructive versus iterative improvement
  - constructive: decide in what cluster each object belongs and don't change
    - often faster
  - iterative improvement: start with a clustering and move objects around to see if can improve clustering
    - often slower but better

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Quality of clustering

- In applications quality of clustering depends on how well solves problem at hand
- Algorithm uses measure of quality that can be optimized, but that may or may not do a good job of capturing application needs.
- Underlying graph-theoretic problems usually NP-complete
  - e.g. graph partitioning
- Usually algorithm not finding optimal clustering

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Distance between clusters

Possible definitions:

I. distance between closest pair of objects with one in each cluster
   - called single link

     . . . .
           ^   ^

II. distance between furthest pair objects, one from each cluster
   - called complete linkage

     . . . .
     ^   ^

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Distance between clusters, cont.

Possible definitions:

III. average of pairwise distance between all pairs of objects, one from each
   - more computation

- Generally no representative point for a cluster;
- If Euclidean distance
  - centroid
  - bounding box

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Vector model: K-means algorithm

- Well known, well used
- Flat clustering
- Number of clusters picked ahead of time
- Iterative improvement
- Uses notion of centroid
- Typically uses Euclidean distance

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K-means overview

- Choose k points among set to cluster
  - Call them k centroids
- For each point not selected, assign it to its closest centroid
  - All assignment give initial clustering
- Until "happy" do:
  - Recompute centroids of clusters
    - New centroids may not be points of original set
  - Reassign all points to closest centroid
    - Updates clusters

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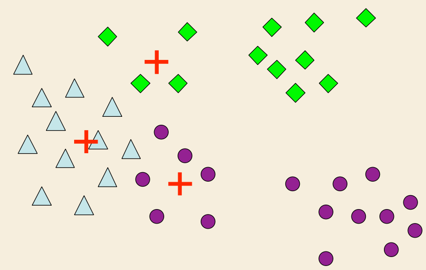
An Example

start: choose centroids and cluster



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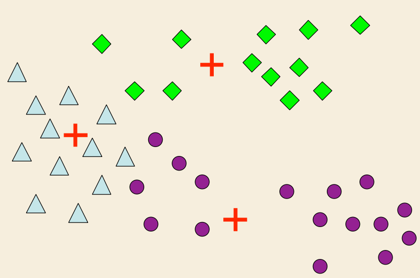
An Example

recompute centroids



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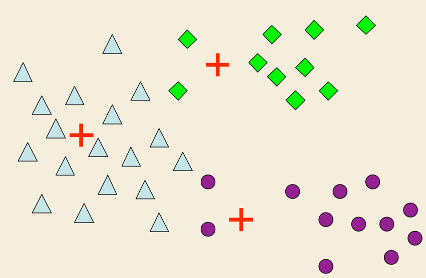
An Example

re-cluster around new centroids



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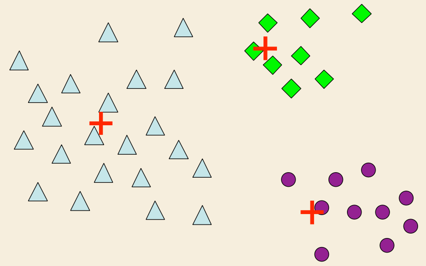
An Example

2nd recompute centroids and re-cluster



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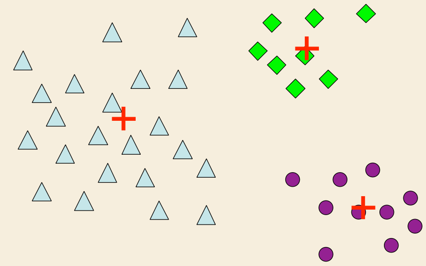
An Example

3rd (final) recompute and re-cluster



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Details for K-means

- Need definition of centroid

  $c_i = 1/|C_i| \sum_{x \in C_i} x$ for i^{th} cluster C_i containing objects x

  notion of sum of objects ?
- Need definition of distance to (similarity to) centroid
- Typically vector model with Euclidean distance
- minimizing sum of squared distances of each point to its centroid = Residual Sum of Squares

$$RSS = \sum_{i=1}^{K} \sum_{x \in C_i} \mathit{dist}(c_i,x)^2$$

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K-means performance

- Can prove RSS decreases with each iteration, so converge
- Can achieve local optimum
  - No change in centroids
- Running time depends on how demanding stopping criteria
- Works well in practice
  - speed
  - quality

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Time Complexity of K-means

- Let t_{dist} be the time to calculate the distance between two objects
- Each iteration time complexity:

  $O(K*n*t_{dist})$

  n = number of objects
- Bound number of iterations I giving

  $O(I*K*n*t_{dist})$
- for m-dimensional vectors:

  O(I*K*n*m)

  m large and centroids not sparse

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Space Complexity of K-means

- Store points and centroids
  - vector model: O((n + K)m)
- External algorithm versus internal?
  - store k centroids in memory
  - run through points each iteration

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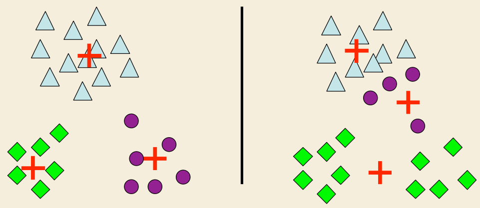
Choosing Initial Centroids

- Bad initialization leads to poor results



Optimal **Not Optimal**

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Choosing Initial Centroids

Many people spent much time examining how to choose seeds

- Random
  - Fast and easy, but often poor results
- Run random multiple times, take best
  - Slower, and still no guarantee of results
- Pre-conditioning
  - remove outliers
- Choose seeds algorithmically
  - run hierarchical clustering on sample points and use resulting centroids
  - Works well on small samples and for few initial centroids

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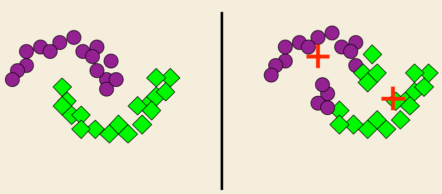
K-means weakness

Non-globular clusters



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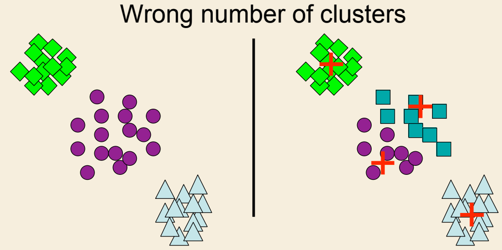
K-means weakness

Wrong number of clusters



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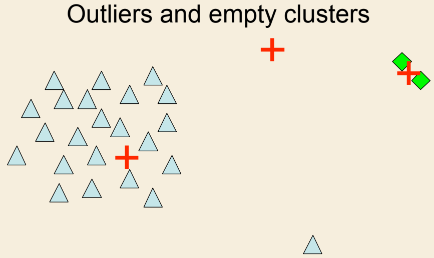
K-means weakness

Outliers and empty clusters



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Real cases tend to be harder

- Different attributes of the feature vector have vastly different sizes
  - size of star versus color
- Can weight different features
  - how weight greatly affects outcome

- Difficulties can be overcome

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