# Clustering Algorithms
for general similarity measures

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## Types of general 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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## Similarity between clusters

Possible definitions:

I. similarity between most similar pair of objects with one in each cluster
   – called single link

. . . .   . . . .
^   ^

II. similarity between least similar pair objects, one from each cluster
   – called complete linkage

. . . .   . . . .
^   ^

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## Similarity between clusters, cont.

Possible definitions:

III. average of pairwise similarity between all pairs of objects, one from each
   – more computation

- Generally no representative point for a cluster;
  – compare K-means
- If using Euclidean distance as metric
  – centroid
  – bounding box

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## General Agglomerative

- Uses any computable cluster similarity measure sim($C_i$, $C_j$)
- For n objects $v_1$, …, $v_n$, assign each to a singleton cluster $C_i$ = {$v_i$}.
- repeat {
  - identify two most similar clusters $C_j$ and $C_k$ (could be ties – chose one pair)
  - delete $C_j$ and $C_k$ and add ($C_j$ U $C_k$) to the set of clusters

  } until only one cluster
- Dendrograms diagram the sequence of cluster merges.

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## Agglomerative: remarks

- *Intro. to IR* discusses in great detail for cluster similarity:
  - single-link, complete-link, avg. of all pairs, centroid
- Uses priority queues to get time complexity O(($n^2$logn)*(time to compute cluster similarity))
  - one priority queue for each cluster: contains similarities to all other clusters plus bookkeeping info
  - time complexity more precisely:

    **O(**($n^2$) *(time to compute object-object similarity) + ($n^2$logn)*
    (time to compute sim(cluster$_z$, cluster$_j$ U cluster$_k$)
    if know sim(cluster$_z$, cluster$_j$ )
    and sim(cluster$_z$, cluster$_k$)) **)**
- Problem with priority queue?

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## Single pass agglomerative-like

Given arbitrary order of objects to cluster: $v_1, \ldots v_n$ and threshold $\tau$

Put $v_1$ in cluster $C_1$ by itself
For i = 2 to n {
for all existing clusters $C_j$
calculate sim($v_i$, $C_j$);
record most similar cluster to $v_i$ as $C_{max(i)}$
if sim($v_i$, $C_{max(i)}$) > $\tau$ add $v_i$ to $C_{max(i)}$
else create new cluster {$v_i$}
}

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## Issues

- put $v_i$ in cluster after seeing only $v_1, \ldots v_{i-1}$
- not hierarchical
- tends to produce large clusters
  - depends on $\tau$
- depends on order of $v_i$

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## Alternate perspective for single-link algorithm

- Build a minimum spanning tree (MST) - graph alg.
  - edge weights are pair-wise similarities
  - since in terms of similarities, not distances, really want maximum spanning tree
- For some threshold $\tau$, remove all edges of similarity < $\tau$
- Tree falls into pieces => clusters
- Not hierarchical, but get hierarchy for sequence of $\tau$

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## Hierarchical Divisive: Template

1. Put all objects in one cluster
2. Repeat until all clusters are singletons
   a) choose a cluster to split
      - what criterion?
   b) replace the chosen cluster with the sub-clusters
      - split into how many?
      - how split?
      - “reversing” agglomerative => split in two

- cutting operation: cut-based measures seem to be a natural choice.
  - focus on similarity across cut - lost similarity
- not necessary to use a cut-based measure

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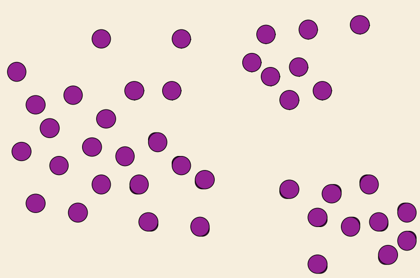
## An Example



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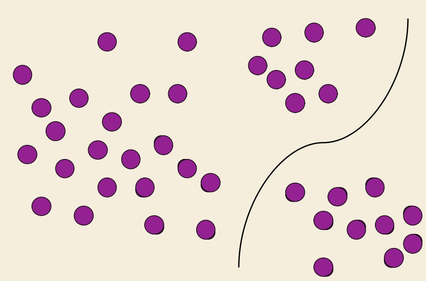
## An Example: 1st cut



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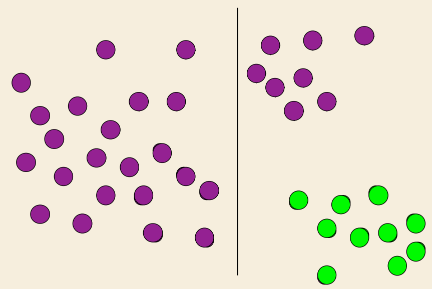
## An Example: $2^{nd}$ cut



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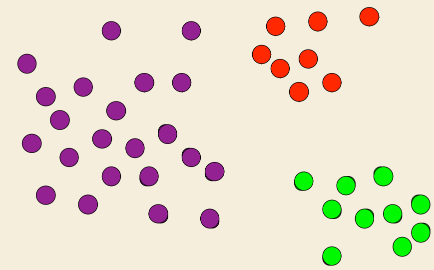
## An Example: stop at 3 clusters



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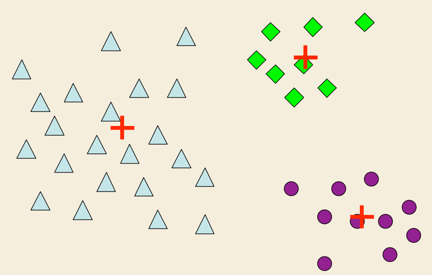
## Compare k-means result



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## Cut-based optimization

- weaken the connection between objects in different clusters *rather than* strengthening connection between objects within a cluster

- Are many cut-based measures
- We will look at one

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## Inter / Intra cluster costs

Given:

- $V = \{v_1, \dots, v_n\}$, the set of all objects
- A partitioning clustering $C_1, C_2, \dots C_k$ of the objects:
  $V = \cup_{i=1,\dots,k} C_i$ .

Define:

- cutcost $(C_p) = \sum_{\substack{v_i \text{ in } C_p \\ v_j \text{ in } V-C_p}} \text{sim}(v_i, v_j)$.

- intracost$(C_p) = \sum_{v_i, v_j \text{ in } C_p} \text{sim}(v_i, v_j)$.

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## Cost of a clustering

total relative cut cost $(C_1, \dots, C_k)$ =

$$\sum_{p=1}^{k} \frac{\text{cutcost}\ (C_p)}{\text{intracost}\ (C_p)}$$

- contribution each cluster:
  ratio external similarity to internal similarity

## Optimization

Find clustering $C_1, \dots, C_k$ that minimizes total relative cut cost$(C_1, \dots, C_k)$

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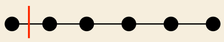
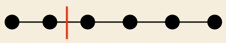
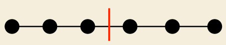
## Simple example

- six objects
- similarity 1 if edge shown
- similarity 0 otherwise
- choice 1: 

  cost UNDEFINED + 1/4
- choice 2: 

  cost 1/1 + 1/3 = 4/3
- choice 3:

  cost 1/2 + 1/2 = 1 *prefer balance



## Hierarchical divisive revisited

- can use one of cut-based algorithms to split a cluster
- how choose cluster to split next?
  - if building entire tree, doesn't matter
  - if stopping a certain point, choose next cluster based on measure optimizing
    - e.g. for total relative cut cost, choose $C_i$ with largest cutcost($C_i$) / intracost($C_i$)



## Divisive Algorithm:
## Iterative Improvement; no hierarchy

1. Choose initial partition $C_1, \ldots, C_k$
2. repeat {

    unlock all vertices

    repeat {

        choose some $C_i$ at random

        choose an unlocked vertex $v_j$ in $C_i$

        move $v_j$ to that cluster, if any, such that move gives maximum decrease in cost

        lock vertex $v_j$

    } until all vertices locked

}until converge



## Observations on algorithm

- heuristic
- uses randomness
- convergence usually improvement < some chosen threshold between outer loop iterations
- vertex "locking" insures that all vertices are examined before examining any vertex twice
- there are many variations of algorithm
- can use at each division of hierarchical divisive algorithm with k=2
  - more computation than an agglomerative merge



## Compare to k-means

- Similarities:
  - number of clusters, k, is chosen in advance
  - an initial clustering is chosen (possibly at random)
  - iterative improvement is used to improve clustering
- Important difference:
  - divisive algorithm can minimize a cut-based cost
    - total relative cut cost uses external and internal measures
  - k-means maximizes only similarity within a cluster
    - ignores cost of cuts



## Eigenvalues and clustering

General class of techniques for clustering a graph using eigenvectors of adjacency matrix (or similar matrix) called

Spectral clustering

First described in 1973

## Spectral clustering: *brief* overview

Given: k: number of clusters
nxn object-object sim. matrix S of non-neg. val.s

Compute:

1. Derive matrix L from S (straightforward computation)
   - e.g. Laplacian: are variations in def.
2. find eigenvectors corresp. to k smallest eigenval.s of L
3. use eigenvectors to define clusters
   - variety of ways to do this
   - all involve another, simpler, clustering
     - e.g. points on a line

Spectral clustering optimizes a cut measure
similar to total relative cut cost

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## Comparing clusterings

- Define external measure to
  - comparing two clusterings as to similarity
  - if one clustering "correct", one clustering by an algorithm, measures how well algorithm doing
    - refer to "correct" clusters as classes
      - "gold standard"
    - refer to computed clusters as clusters
- External measure independent of cost function optimized by algorithm

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## One measure: motivated by F-score in IR

- Given:
  - a set of classes $S_1, \ldots S_k$ of the objects
    use to define relevance
  - a computed clustering $C_1, \ldots C_k$ of the objects
    use to define retrieval
- Consider pairs of objects
  - pair in same class, call "similar pair" ≡ relevant
  - pair in different classes ≡ irrelevant
  - pair in same clusters ≡ retrieved
  - pair in different clusters ≡ not retrieved
- Use to define precision and recall

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## Clustering f-score

*precision* of the clustering w.r.t the gold standard =

$$\frac{\#\text{ similar pairs in the same cluster}}{\#\text{ pairs in the same cluster}}$$

*recall* of the clustering w.r.t the gold standard =

$$\frac{\#\text{ similar pairs in the same cluster}}{\#\text{ similar pairs}}$$

*f-score* of the clustering w.r.t the gold standard =

$$\frac{2*\text{precision}*\text{recall}}{\text{precision} + \text{recall}}$$

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## Properties of cluster F-score

- always $\leq 1$
- Perfect match computed clusters to classes gives F-score = 1
- Symmetric
  - Two clusterings $\{C_i\}$ and $\{K_j\}$, neither "gold standard"
  - treat $\{C_i\}$ as if are classes and compute F-score of $\{K_j\}$ w.r.t. $\{C_i\}$ = F-score$_{\{Ci\}}(\{K_j\})$
  - treat $\{K_j\}$ as if are classes and compute F-score of $\{C_i\}$ w.r.t. $\{K_j\}$ = F-score$_{\{Kj\}}(\{C_i\})$

$\Rightarrow$ F-score$_{\{Ci\}}(\{K_j\})$ = F-score$_{\{Kj\}}(\{C_i\})$

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## Clustering: wrap-up

- many applications
  - application determines similarity between objects
- menu of
  - cost functions to optimizes
  - similarity measures between clusters
  - types of algorithms
    - flat/hierarchical
    - constructive/iterative
  - algorithms within a type

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