Clustering Algorithms: Divisive hierarchical and flat

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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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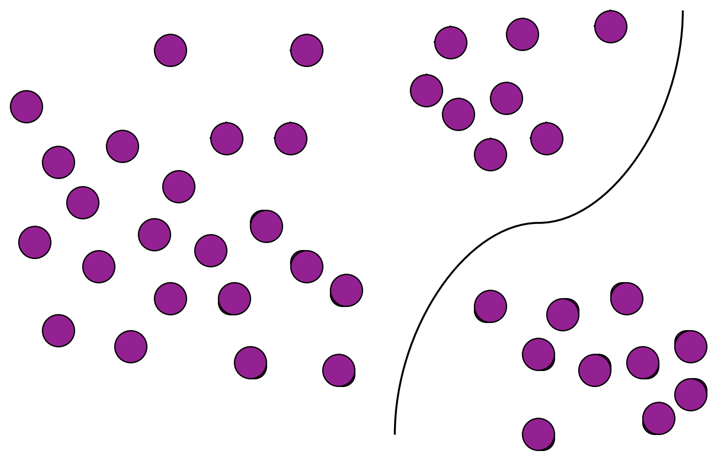
An Example: 1^{st} cut



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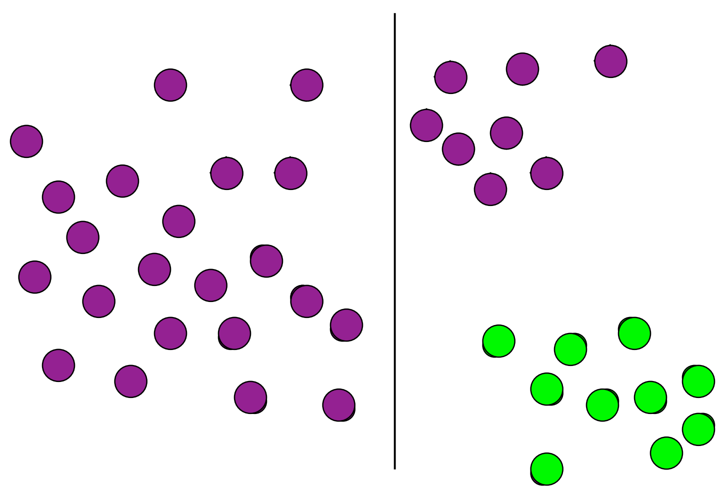
An Example: 2^{nd} cut



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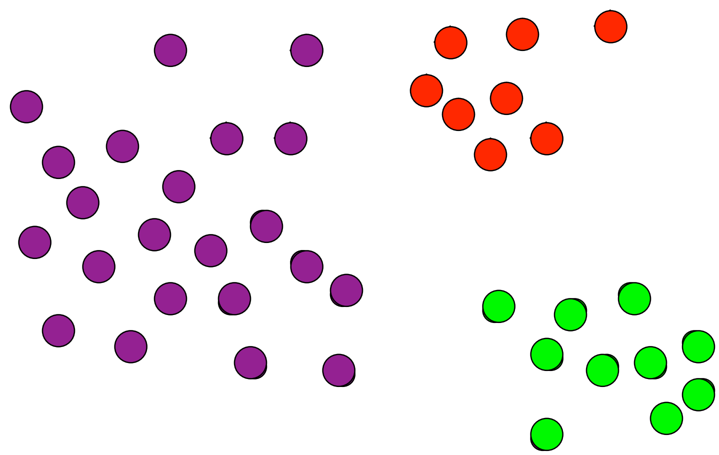
An Example: stop at 3 clusters



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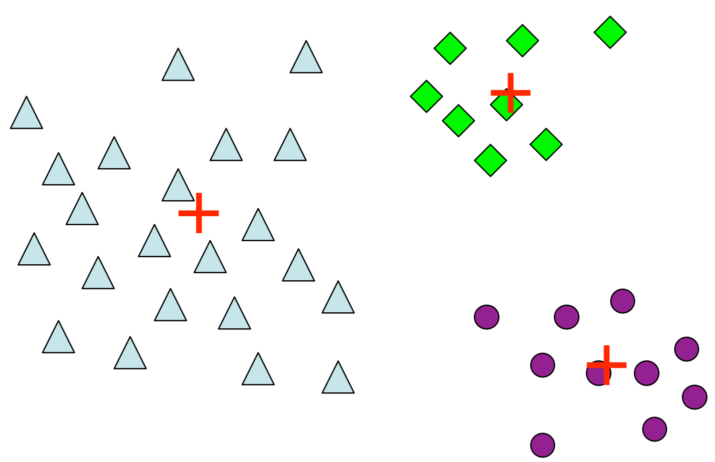
Compare k-means result



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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:

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

Define:

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

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

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Cost of a clustering

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

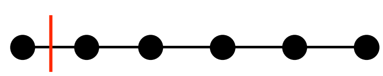
min-max cut optimization

Find clustering $C_1, \dots, C_k$ that minimizes

cost$(C_1, \dots, C_k)$

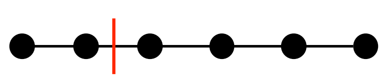
Simple example

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



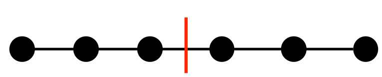
cost UNDEFINED + 1/4

- choice 2:



cost 1/1 + 1/3 = 4/3

- choice 3:



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

Iterative Improvement Algorithm

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

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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

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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:
  - min-max cut algorithm minimizes a cut-based cost
  - k-means maximizes only similarity within a cluster
    - ignores cost of cuts

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Another method: Spectral clustering

Brief overview

Given:

- k: number of clusters
- nxn object-object sim. matrix S of non-neg. values

Compute:

1. Laplacian matrix L from S (straightforward computation)
   - are variations in def. Laplacian
2. eigenvectors corresponding to k smallest eigenvalues
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 min-max cut

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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 min-max cut, choose C_i with largest cutcost(C_i) / intracost(C_i)

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External measures

- comparing two clusterings as to similarity
- if one clustering "correct", one clustering by an algorithm, measures how well algorithm doing

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one measure motivated by F-score in IR: combining *precision* and *recall*

- Given:

a "correct" clustering $S_1, \ldots S_k$ of the objects ($\equiv$ relevant)
a computed clustering $C_1, \ldots C_k$ of the objects ($\equiv$ retrieved)

- Define:

precision of C_x w.r.t $S_q = p(x,q) = |S_q \cap C_x| \;/\; |C_x|$

fraction of computed cluster that is "correct"

recall of C_x w.r.t $S_q = r(x,q) = |S_q \cap C_x| \;/\; |S_q|$

fraction of a "correct" cluster found in a computed cluster

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Fscore of C_x w.r.t $S_q = F(x,q) =$

$$2r(x,q)*p(x,q) \;/\; (\, r(x,q) + p(x,q)\,)$$

combine precision and recall (Harmonic mean)

Fscore of $\{C_1, C_2, \ldots C_k\}$ w.r.t $S_q = F(q) =$

$$\max_{x = 1,\ldots,k} F(x,q)$$

score of best computed cluster for S_q

Fscore of $\{C_1, C_2, \ldots C_k\}$ w.r.t $\{S_1, S_2, \ldots S_k\}$ = *desired measure

$$\sum_{q = 1, \ldots, k} (|S_q| / n)\, *F(q)$$

weighted average of best scores over all correct clusters

always ≤ 1

- Perfect match of computed clusters to correct clusters gives Fscore of 1

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