Clustering Algorithms
for general similarity measures

general similarity measure:
specified by object X object similarity matrix

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Types of general clustering methods

- constructive algorithms
- agglomerative versus divisive construction
  - agglomerative = bottom-up
    - build up clusters from single objects
  - divisive = top-down
    - break up cluster containing all objects into smaller clusters
  - both agglom'tive 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 cluster
   – "centroid" similarity

IV. average of pairwise similarity between all pairs of distinct objects, including w/in same cluster
   – "group average" similarity

- 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, group average, centroid
- Uses priority queues to get time complexity
  O((n^2logn)*(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^2logn)*
    (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 τ

```
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)) > τ add v_i to C_max(i)
    else create new cluster {v_i}
}
```

ISSUES?

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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 τ
- depends on order of v_i

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Alternate perspective for single-link algorithm

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

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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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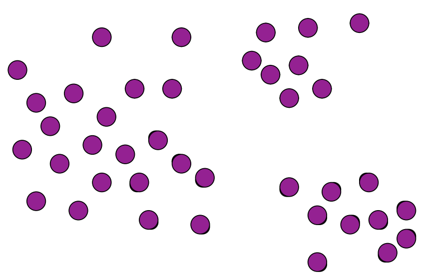
An Example



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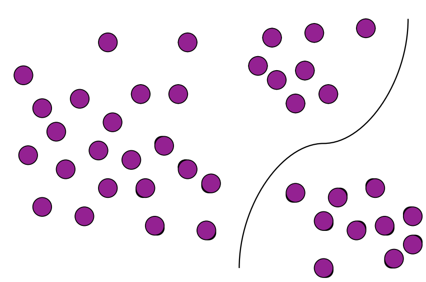
An Example: 1st cut



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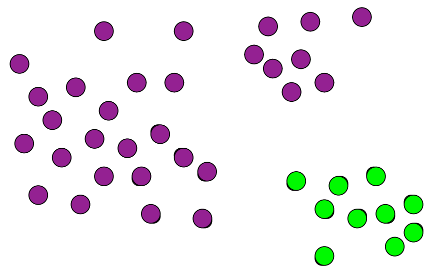
An Example: result of 1st cut



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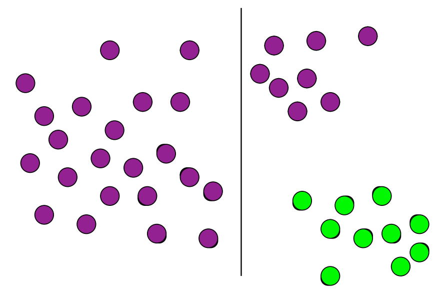
An Example: 2nd cut



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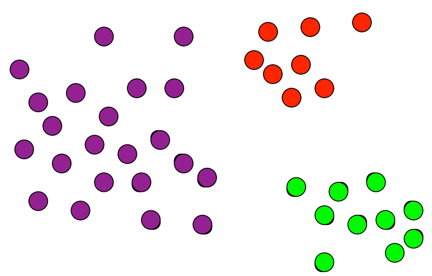
An Example: stop at 3 clusters



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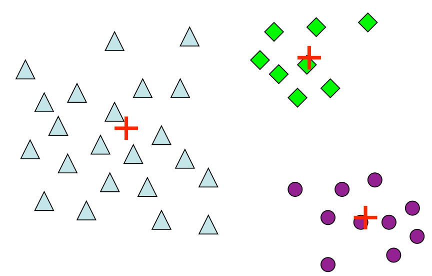
Compare k-means result



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Cut-based optimization

- focus on weak connections between objects in different clusters *rather than* strong connections between objects within a cluster

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

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Inter / Intra cluster costs

Given:

- $V = \{v_1, \ldots, v_n\}$, the set of all objects
- A partitioning clustering $C_1, C_2, \ldots C_k$ of the objects:

$$V = \bigcup_{i=1, \ldots, k} C_i .$$

Define:

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

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

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Cost of a clustering

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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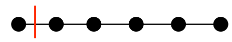
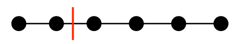
Simple example

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



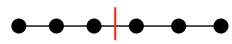
cost UNDEFINED + 1/4

- choice 2:



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

- choice 3:



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

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Second cut-based measure: Conductance

- define:
  s_degree(C_p) = cutcost(C_p)+2*intracost(C_p)
  - model as graph, similarity = edge weights
  - s_degree is sum over all vertices in C_p of weights of edges touching vertex
- conductance (C_p) =

$$\frac{\text{cutcost}(C_p)}{\min\{\text{s\_degree}(C_p),\ \text{s\_degree}(V-C_p)\}}$$

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Optimization using conductance

- Choices:
  - minimize $\sum^{k}_{p=1}$ conductance (C_p)
  - minimize $\text{MAX}^{k}_{p=1}$ conductance (C_p)
- Observations
  - conductance (C_p) = conductance $(V-C_p)$
  - Finding a cut (C, V-C) with minimum conductance is NP-hard

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Simple example

- six objects
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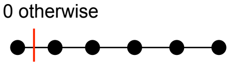
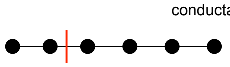
- similarity 0 otherwise
- choice 1:



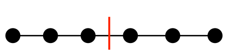
conductance 1/min(1,9) = 1

- choice 2:



conductance 1/min(3, 7) = 1/3

- choice 3:



conductance1/min(5, 5) = 1/5 *prefer balance

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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 total relative cut cost, choose C_i with largest cutcost(C_i) / intracost(C_i)

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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

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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:
  - divisive algorithm can minimize a cut-based cost
    - total relative cut cost, conductance use external and internal measures
  - k-means maximizes only similarity within a cluster
    - ignores cost of cuts

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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

spectrum of a graph is list of eigenvalues, with multiplicity, of its adjacency matrix

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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)
   - variety of definitions of L
     - e.g. Laplacian L=I-E if similarity is edge/no edge
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 =

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

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Properties of cluster F-score

- always ≤ 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. $\{C_i\}$ = $\text{F-score}_{\{Ci\}}(\{K_j\})$
  - treat $\{K_j\}$ as if are classes and compute F-score of $\{C_i\}$ w.r.t. $\{K_j\}$ = $\text{F-score}_{\{Kj\}}(\{C_i\})$
  - ➢ $\text{F-score}_{\{Ci\}}(\{K_j\}) = \text{F-score}_{\{Kj\}}(\{C_i\})$

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another related external measure Rand index

$$\frac{(\#\text{ similar pairs in the same cluster} + \#\text{ dissimilar pairs in the different clusters})}{N\,(N-1)/2}$$

percentage pairs that are correct

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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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