A Computational Theory of Clustering

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Based on work joint with Nina Balcan, Anupam Gupta, and Santosh Vempala

Point of this talk

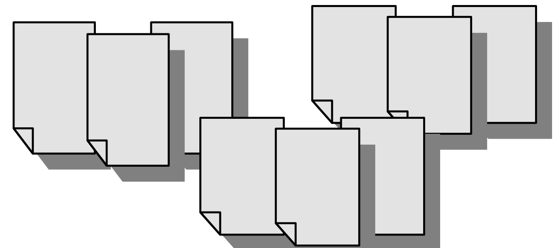
- A new way to theoretically analyze and attack problem of clustering. Fixes a disconnect in previous formulations.

- Interesting theoretical structure. Will show results in this framework, but also many open questions too!

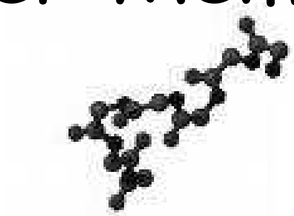
- Motivated by machine learning but you don't need to know any ML for this talk.

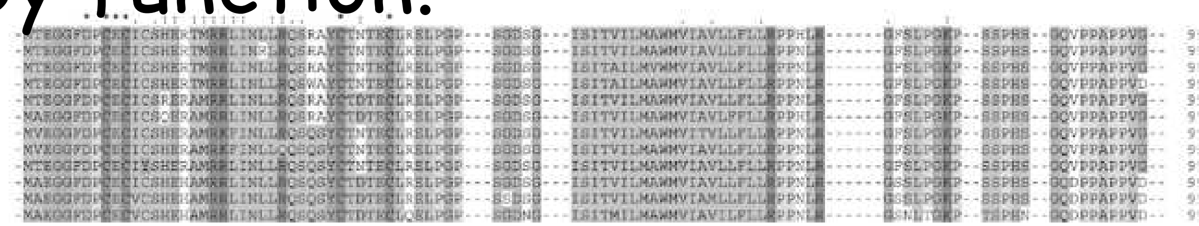
Clustering comes up everywhere

- Given a set of documents or search results, cluster them by topic.



- Given a collection of protein sequences, cluster them by function.



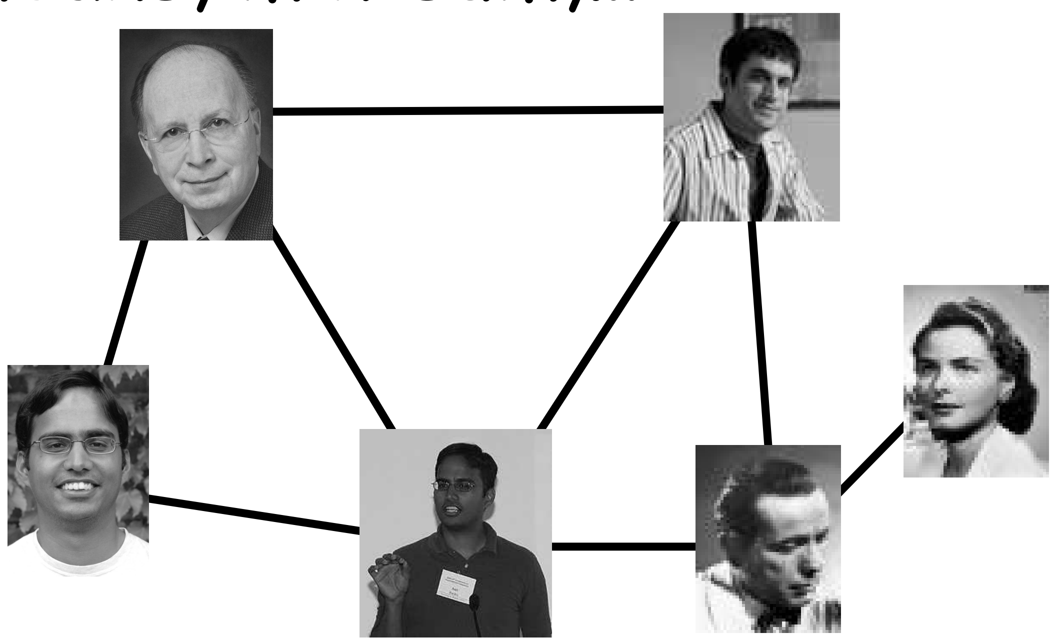


- Given a set of images of people, cluster by who is in them.

- …

Standard theoretical approach

- View data as nodes in weighted graph.
  - Weights based on some measure of similarity (like # keywords in common, edit distance,…)
- Pick some objective to optimize like k-median, k-means, min-sum,…



Standard theoretical approach

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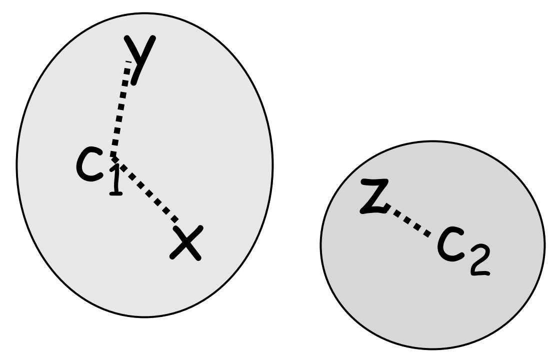
  - Weights based on some measure of similarity (like # keywords in common, edit distance,…)
- Pick some objective to optimize like k-median, k-means, min-sum,…
  - E.g., k-median asks: find center pts $c_1, c_2, \ldots, c_k$ to minimize $\sum_x \min_i d(x,c_i)$



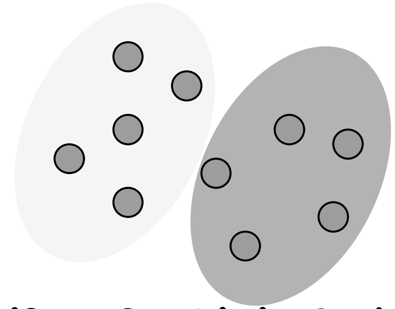
Standard theoretical approach

- View data as nodes in weighted graph.
  - Weights based on some measure of similarity (like # keywords in common, edit distance,…)
- Pick some objective to optimize like k-median, k-means, min-sum,…
- Develop algorithm that approximates this objective. (E.g., best known for k-median is $3+\varepsilon$ approx. Beating $1 + 2/e \approx 1.7$ is NP-hard.)

A bit of a disconnect… isn't our real goal to get the points right??

"We couldn't get a psychiatrist, but perhaps you'd like to talk about your skin. Dr. Perry here is a dermatologist."

Well, but..



- Could say we're implicitly hoping that any c-approx to k-median objective is ε-close pointwise to truth.
- This is an assumption about how the similarity info relates to the target clustering.
- Why not make it explicit?

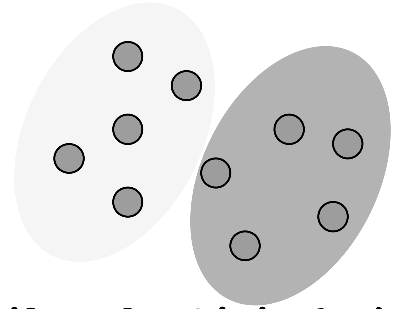
Example of result: for any c>1, this assumption implies structure we can use to get $O(\varepsilon)$-close to truth.

Even for values where getting c-approx is NP-hard!

(Even ε-close, if all clusters are "sufficiently large".)

"Approximate clustering without the approximation"

Well, but..



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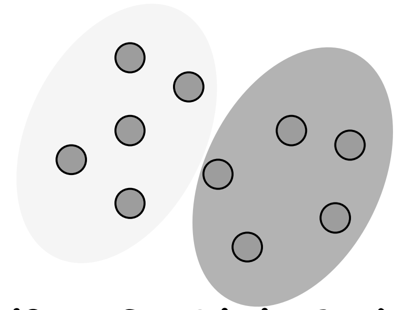
- Why not make it explicit?

More generally: what natural properties of similarity info are sufficient to cluster well, and by what kinds of algorithms?

Give guidance to designers of similarity measures, & about what algs to use given beliefs about them.

Well, but..



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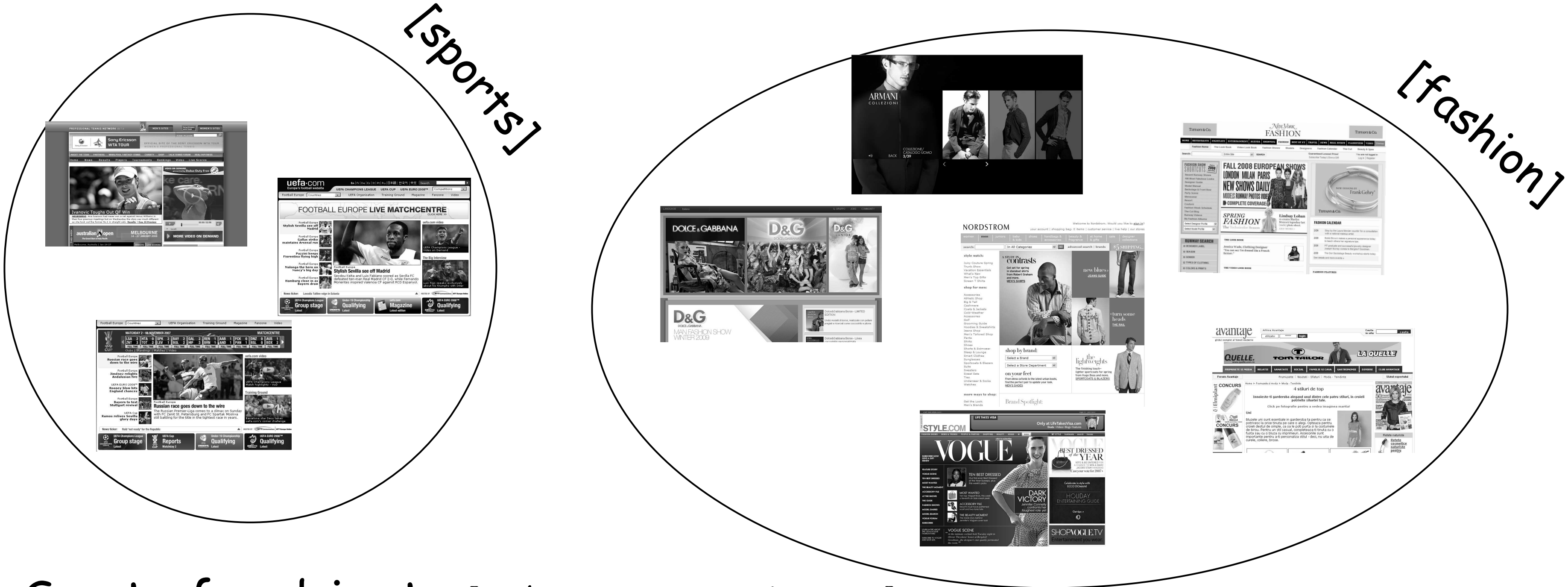
Analogy to learning: what concept classes are learnable and by what algorithms?

General Framework



S set of n objects. [web pages, protein seqs]

$\exists$ ground truth clustering. x, $\ell(x)$ in $\{1,\dots,t\}$. [topic, function]

Goal: clustering h of low error pointwise. $err(h) = \min_\sigma \Pr_{x \in S}[\sigma(h(x)) \neq \ell(x)]$

Given a pairwise similarity function K(x,y) between objects.

Question: how related does K have to be to target to be able to cluster well?

Similarity vs distance

- Using "similarity" instead of distance since don't want to require metric. Usually based on some heuristic.
  - "cosine similarity" between documents (size of intersection / size of union)
  - Smith-Waterman score for bio sequence data.
  - In general, might not even be symmetric.
- In learning, very common as kernel functions. K is a kernel if corresponds to dot-product in implicit space. $K(x,y) = \Phi_K(x) \cdot \Phi_K(y)$. [this is why we use "K"]

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Given a pairwise similarity function $K(x,y)$ between objects.

> Question: how related does K have to be to target to be able to cluster well?

What conditions on a similarity measure would be enough to allow one to **cluster** well?

Will lead to something like a PAC model for clustering.

Alternatively, model data as mixture of Gaussians or other distributions. (Generative model)

Here, we don't want to make distributional assumptions. (compare to learning a linear separator). Can view as advice to designer of similarity function.

What conditions on a similarity measure would be enough to allow one to **cluster** well?

Will lead to something like a PAC model for clustering.

This talk is based on two pieces of work:

- Formulation of framework and analysis of different natural properties [with Nina Balcan and Santosh Vempala]
- Looking specifically at implicit properties used in approximation algorithms [with Nina Balcan and Anupam Gupta]

What conditions on a similarity measure would be enough to allow one to **cluster** well?

[sports]

[fashion]

Protocol

$\exists$ ground truth clustering for S

i.e., each x in S has $\ell(x)$ in $\{1,\ldots,t\}$.

Input S, a similarity function K.

Output Clustering of small error.

$\Rightarrow$

The similarity function K has to be related to the ground-truth.

What conditions on a similarity measure would be enough to allow one to **cluster** well?

Here is a condition that trivially works:

Suppose K has property that:

- $K(x,y) > 0$ for all x,y such that $\ell(x) = \ell(y)$.
- $K(x,y) < 0$ for all x,y such that $\ell(x) \neq \ell(y)$.

If we have such a K, then clustering is easy.

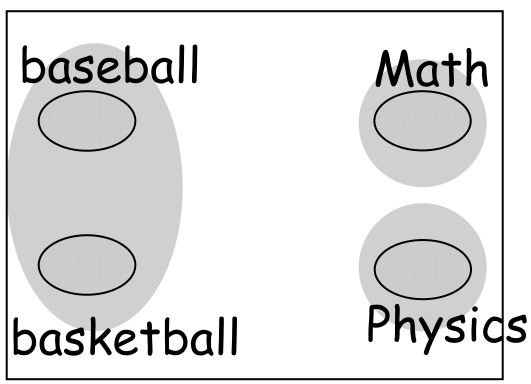
Now, let's try to make this condition a little weaker….

What conditions on a similarity measure would be enough to allow one to **cluster** well?

Suppose K has property that all x are more similar to points y in their own cluster than to any y' in other clusters.

- Still a very strong condition.

Problem: the same K can satisfy for two very different clusterings of the same data!



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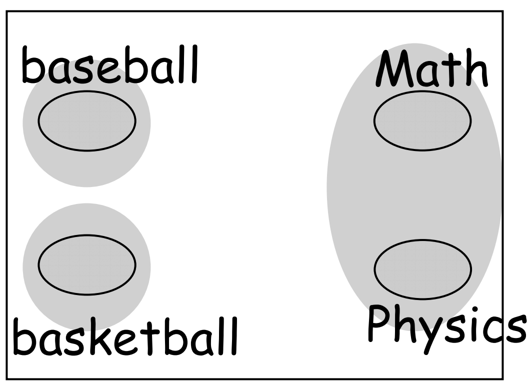
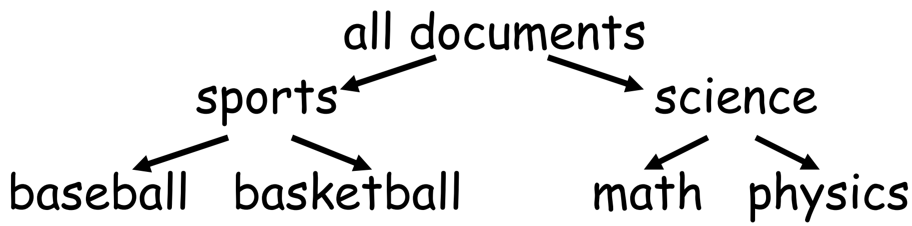
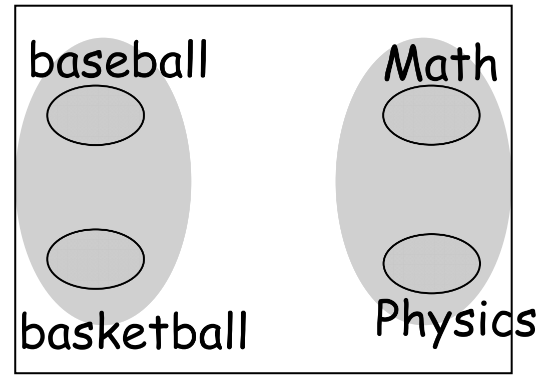


Unlike learning, you can't even test your hypotheses!

Let's weaken our goals a bit…

1. OK to produce a hierarchical clustering (tree) such that correct answer is apx some pruning of it.
   - E.g., in case from last slide:





   - Can view as starting at top and saying "if any of these clusters is too broad, just click and I will split it for you"

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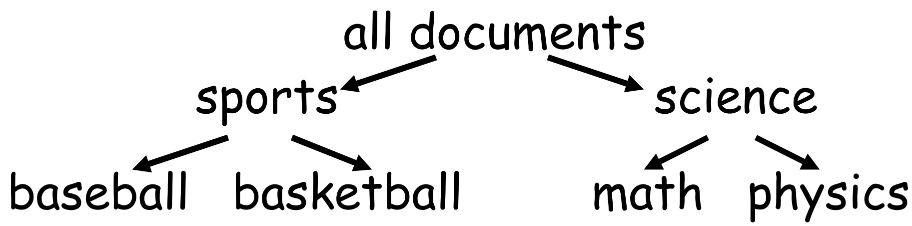
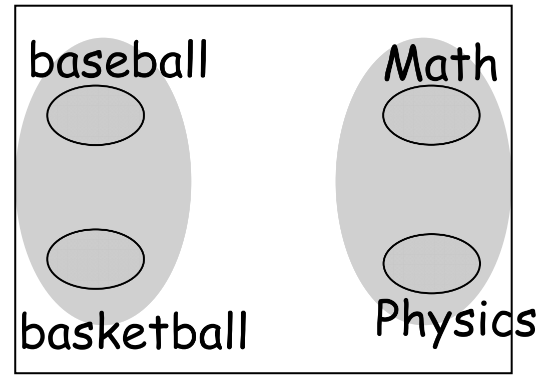




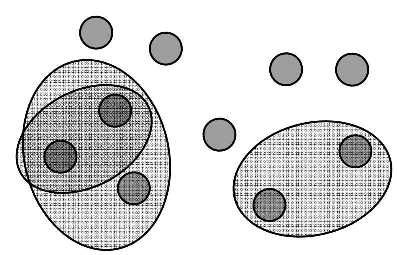
2. OK to output a small # of clusterings such that <u>at least one</u> has low error.
   - Define **clustering complexity** of a property as minimum list length needed to guarantee at least one clustering is ε-close to target.

Then you can start getting somewhere….

1. "all x more similar to all y in their own cluster than to any y' from any other cluster"

is sufficient to get hierarchical clustering such that target is some pruning of tree. (Kruskal's / single-linkage works)

Proof: laminar before $\Rightarrow$ laminar after.



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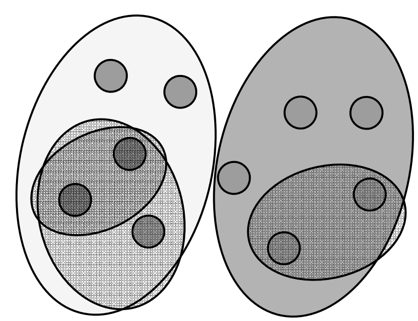

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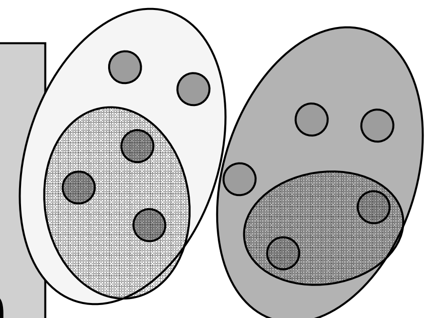
2. Weaker condition: ground truth is "stable":

For all clusters C, C', for all $A \subset C$, $A' \subset C'$: A and A' are not both more similar to each other than to rest of their own clusters.



K(x,y) is attraction between x and y

[E.g., property 1 plus internal noise]

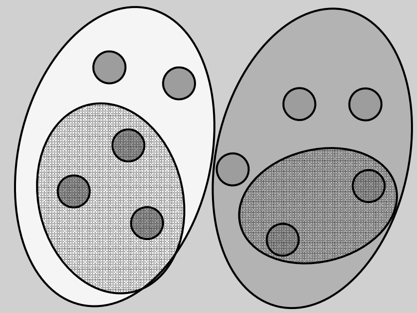
Analysis for slightly simpler version

Assume for all C, C', all $A \subset C$, $A' \subseteq C'$, we have

$$K(A, C-A) > K(A, A'),$$

$\mathrm{Avg}_{x \in A,\, y \in C-A}[K(x,y)]$

and say K is symmetric.



Algorithm: average single-linkage

- Like Kruskal, but at each step merge pair of clusters whose average similarity is highest.

Analysis: (all clusters made are laminar wrt target)

- Failure iff merge C_1, C_2 s.t. $C_1 \subset C$, $C_2 \cap C = \phi$.

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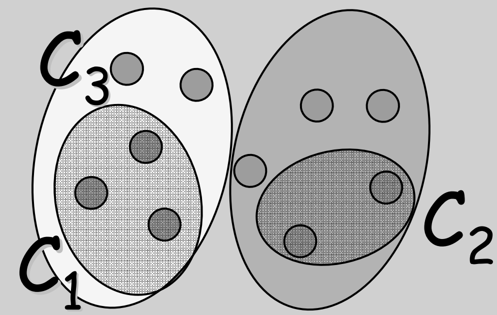

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- Failure iff merge C_1, C_2 s.t. $C_1 \subset C$, $C_2 \cap C = \phi$.
- But must exist $C_3 \subset C$ s.t. $K(C_1, C_3) \geq K(C_1, C-C_1)$, and $K(C_1, C-C_1) > K(C_1, C_2)$. Contradiction.

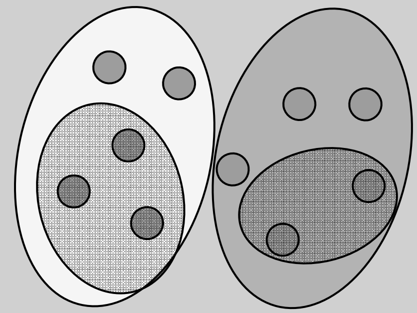
What if asymmetric?

Assume for all C, C', all $A \subset C$, $A' \subseteq C'$, we have

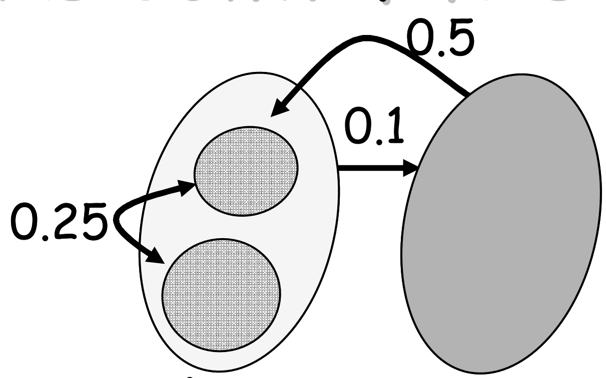
$$K(A, C-A) > K(A, A'),$$

[Think of K as "attraction"] $\mathrm{Avg}_{x \in A,\, y \in C-A}[K(x,y)]$

~~and say K is symmetric.~~



Algorithm breaks down if K is not symmetric:



Instead, run "Boruvka-inspired" algorithm:

- Each current cluster C_i points to $\mathrm{argmax}_{C_j} K(C_i, C_j)$
- Merge directed cycles. (not all components)

Relaxed conditions

Going back to:

"strict separation"

1. "all x more similar to all y in their own cluster than to any z from any other cluster"

Let's consider a relaxed version:

1'. "Exists $S' \subseteq S$, $|S'| \geq (1-\alpha)|S|$, satisfying 1."

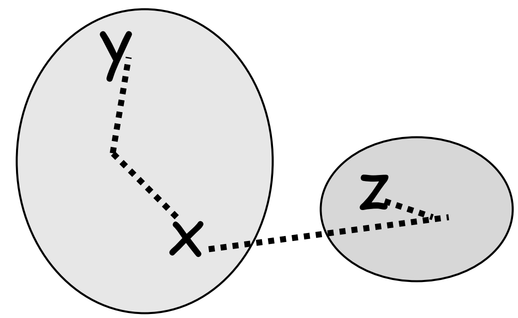
Can show two interesting facts:

A. Can still efficiently get a tree of error α. (assuming all target clusters are large).

B. This property is implied by $(2,\varepsilon)$ k-median property, for $\alpha=4\varepsilon$. (Assume metric. "more similar" = "closer")

Relation to apx k-median assumption

- Suppose any 2-apx k-median solution must be ε-close to the target. (for simplicity, assume target=OPT)
- But doesn't satisfy 1. x is closer to z in other cluster than to y in own cluster.
  - Delete & repeat.
  - Can't repeat > ε n times.
  - Else, move all x's to corresponding z's cluster: at most doubles objective.
    - $d(x,c_z) \leq d(x,z)+cost(z) \leq d(x,y)+cost(z) \leq cost(x)+cost(y)+cost(z)$.



Relation to apx k-median assumption

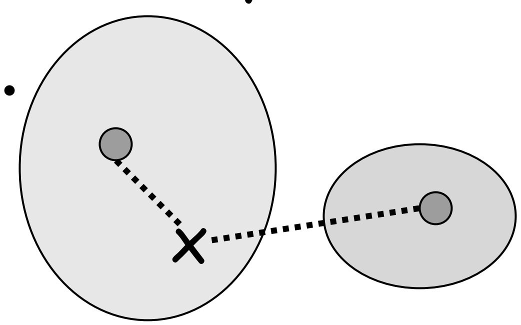
- $(2,\varepsilon)$ k-median property $\Rightarrow$ $O(\varepsilon)$-relaxed separation property.
- $O(\varepsilon)$-relaxed separation property $\Rightarrow$ produce tree s.t. some pruning is $O(\varepsilon)$-close. (assuming all target clusters are large).

- Can actually directly go from (c,ε) k-median property to single $O(\varepsilon)$-close clustering, for any $c>1$. (ε-close if all target clusters are large).
  - Also for k-means, min-sum.

How can we use the (c,ϵ) k-median property to cluster, without solving k-median?

Clustering from (c,ε) k-median prop

- Suppose any c-apx k-median solution must be ε-close to the target. (and for simplicity say target *is* k-median opt, & all cluster sizes > $2\varepsilon n$)
- For any x, let w(x)=dist to own center, $w_2(x)$=dist to 2nd-closest center.
- Let $w_{avg}=avg_x\ w(x)$.
- Then:
  - At most εn pts can have $w_2(x) < (c-1)w_{avg}/\varepsilon$.
  - At most $5\varepsilon n/(c-1)$ pts can have $w(x) \geq (c-1)w_{avg}/5\varepsilon$.
- All the rest (the good pts) have a big gap.



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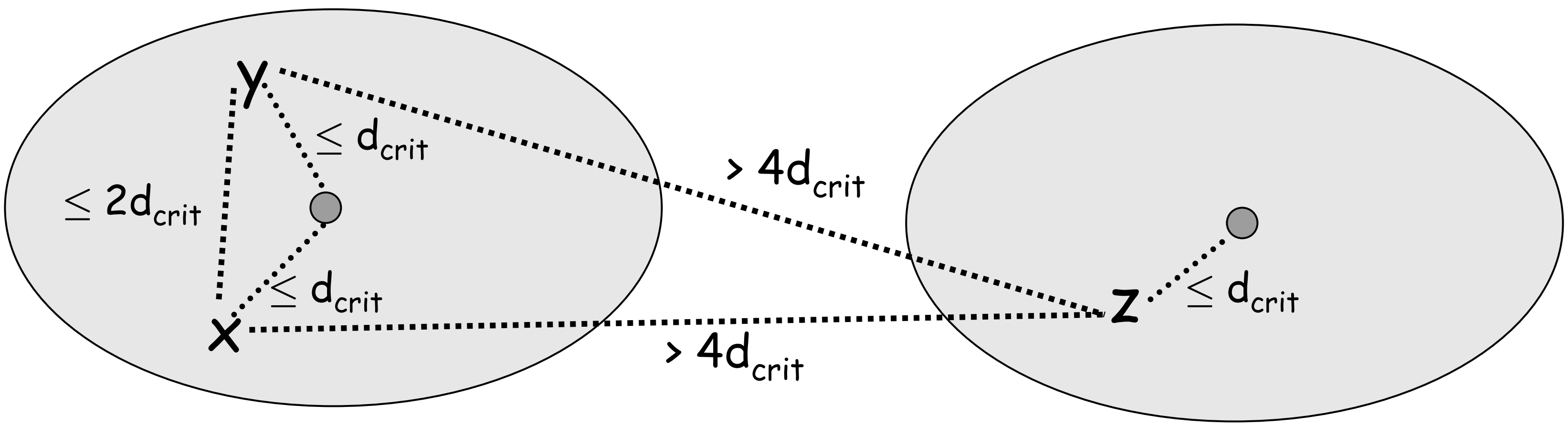
- All the rest (the good pts) have a big gap.
- Define critical distance $d_{crit}=(c-1)w_{avg}/5\varepsilon$.
- So, a $1-O(\varepsilon)$ fraction of pts look like:



Clustering from (c,ε) k-median prop

- So if we define a graph G connecting any two pts within distance $\leq 2d_{crit}$, then:
  - Good pts within cluster form a clique
  - Good pts in different clusters have no common nbrs
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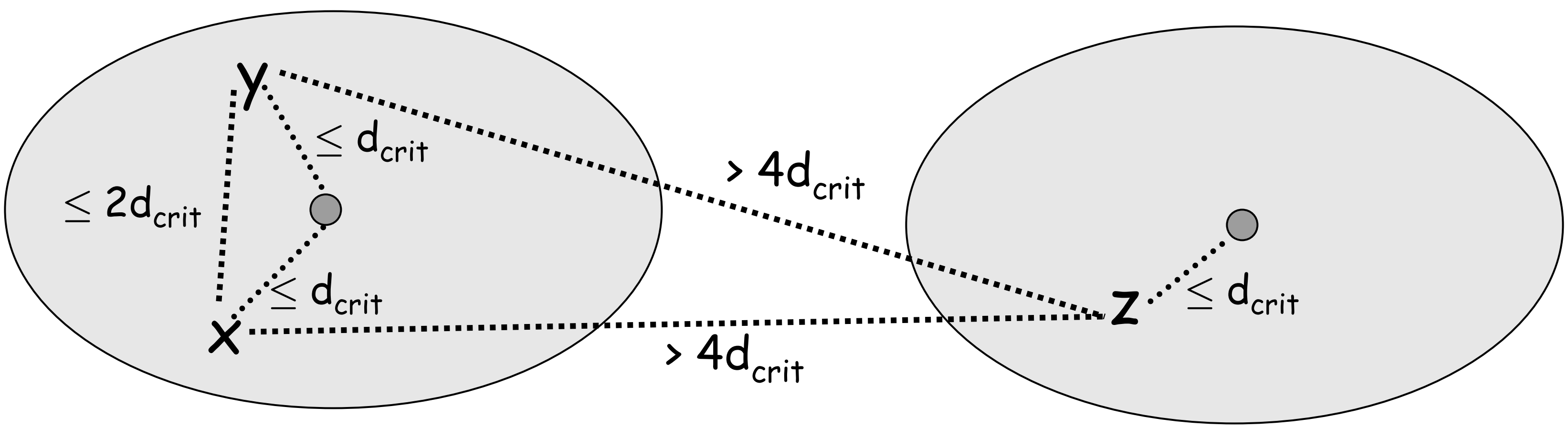

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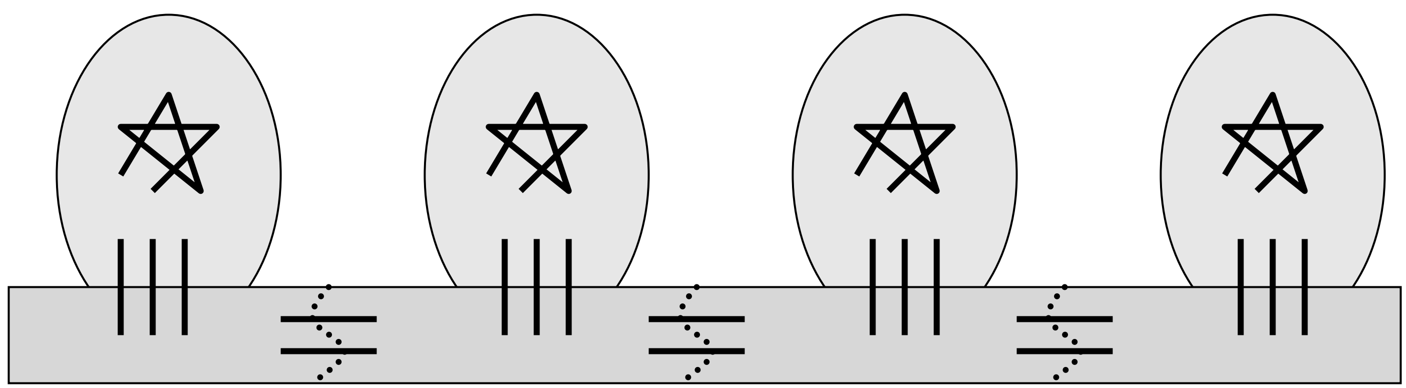
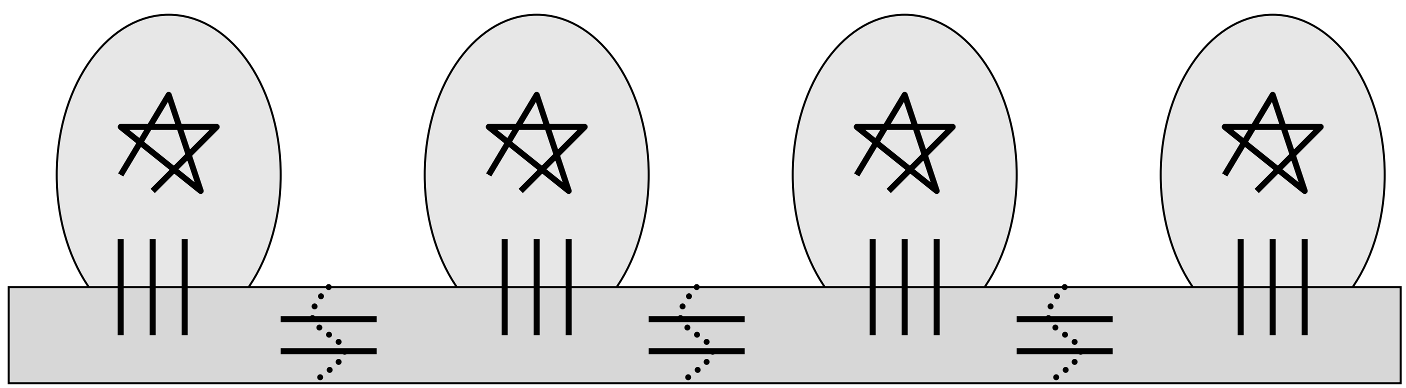


Clustering from (c,ε) k-median prop

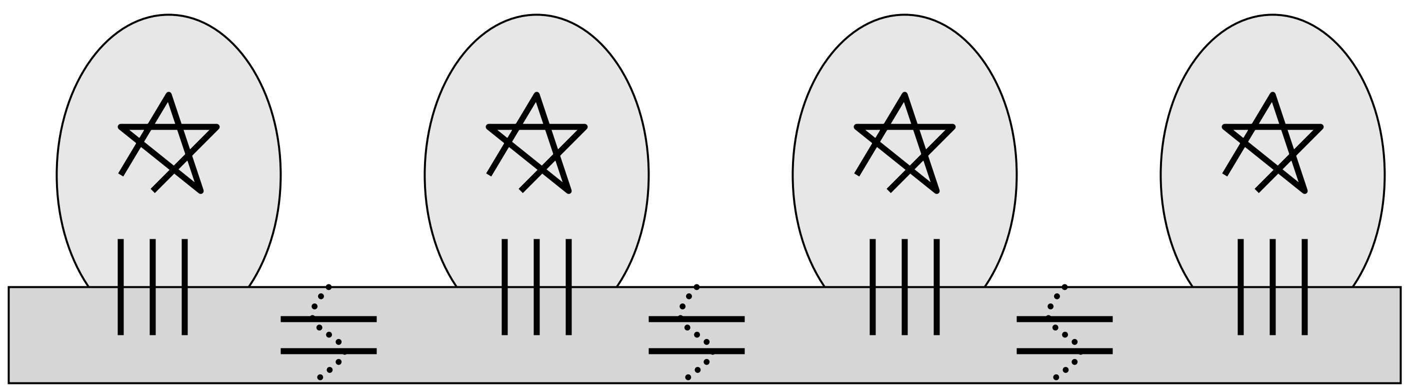
- If all clusters have size > 2b+1, where b = # bad pts = O(εn/(c-1)), then:
  - Create graph H where connect x,y if share > b nbrs in common in G.
  - Output k largest components in H.
- So, the world now looks like:



Clustering from (c,ε) k-median prop

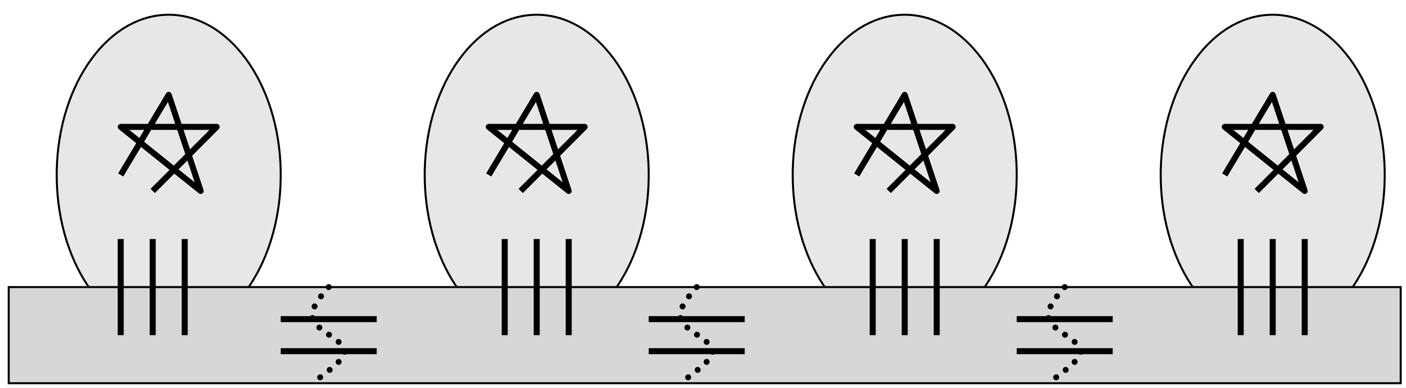
- If clusters not so large, then need to be a bit more careful but can still get error O(ε).
- E.g., now could have some clusters dominated by bad pts....

- So, the world now looks like:



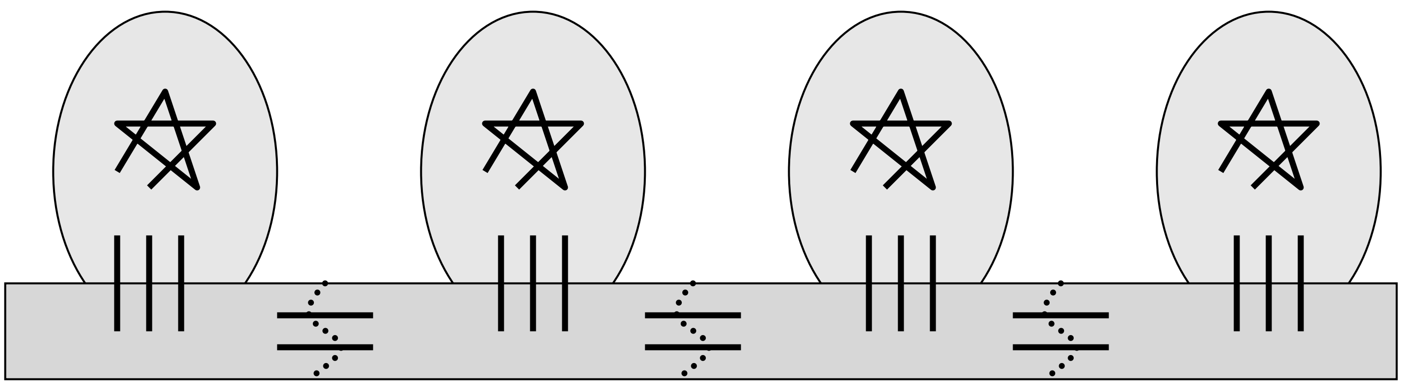
$O(\varepsilon)$-close $\rightarrow$ ε-close

- Back to the large-cluster case: can actually get ε-close. (for any c>1, but "large" depends on c).
- Idea: Really two kinds of bad pts.
  - At most εn "confused": $w_2(x)-w(x) < (c-1)w_{avg}/\varepsilon$.
  - Rest not confused, just far: $w(x) \geq (c-1)w_{avg}/5\varepsilon$.
- Can recover the non-confused ones…



$O(\varepsilon)$-close $\rightarrow$ ε-close

- Back to the large-cluster case: can actually get ε-close. (for any c>1, but "large" depends on c).
- Given output C' from alg so far, reclassify each x into cluster of lowest median distance
  - Median is controlled by good pts, which will pull the non-confused points in the right direction.



Properties Summary

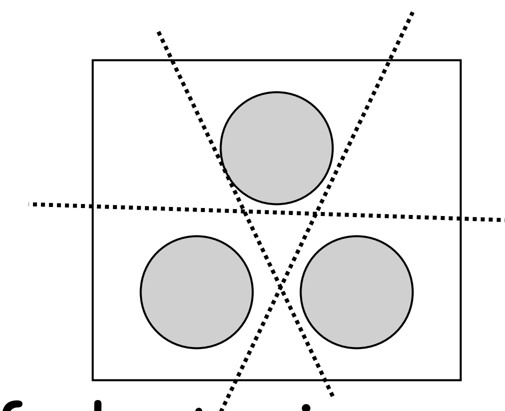
Property	**Model, Algorithm**	**Clustering Complexity**
Strict Separation	Hierarchical, Linkage based	$\Theta(2^k)$
Stability, all subsets. (Weak, Strong, etc)	Hierarchical, Linkage based	$\Theta(2^k)$
Average Attraction (Weighted)	List, Sampling based & NN	$[k^{\Omega(k/\gamma)}, k^{O(k/\gamma^2)}]$
Stability of large subsets	Hierarchical, list and refine (running time $k^{O(k/\gamma^2)}$)	$\Theta(2^k)$
relaxed separation	Hierarchical , list and refine	$\Theta(2^k)$
(c,ε) k-median	Greedy + refining	1

How about weaker conditions?

What if just have: all (most) x satisfy

$E_{x' \in C(x)}[K(x,x')] > E_{x' \in C'}[K(x,x')] + \gamma \quad (\forall C' \neq C(x))$

Not sufficient for hierarchy.



But can produce a small list of clusterings s.t. at least one is good:

§ Upper bound $k^{O(k/\gamma^2 \cdots)}$. [doesn't depend on n]

§ Lower bound $\approx k^{\Omega(k/\gamma)}$.

Upper and lower bounds on "clustering complexity" of this property.

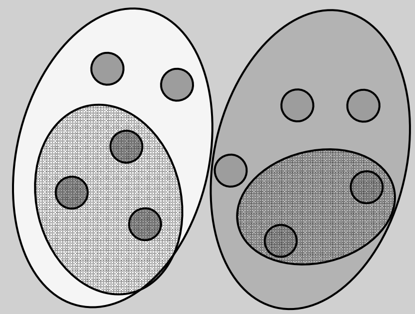
Can also analyze **inductive** setting

- View S as just a random subset from larger instance space X.
- Property holds wrt X.
- Given S, want to:
  - A. produce good clustering of S.
  - B. be able to insert new points in streaming manner as they arrive.

Can also analyze **inductive** setting

Assume for all C, C', all $A \subset C$, $A' \subseteq C'$, we have

$$K(A, C-A) > K(A, A') + \gamma$$



Draw sample S:

- Need to argue that whp $K(A, S \cap C-A)$ is good estimate of $K(A, C-A)$ for all $A \subseteq S$ for suff lg S.
- A sample cplx type argument using "regularity" type results of [AFKK].

Once S is hierarchically partitioned, can insert new points as they arrive.

Like a PAC model for clustering

- PAC learning model: basic object of study is the concept class (a set of functions). Look at which are learnable and by what algs.
- In our case, basic object of study is a property: like a data-dependent concept class. Want to know which allow clustering and by what algs.

Conclusions

What properties of a similarity function are sufficient for it to be useful for **clustering**?

- Target function as ground truth rather than graph as ground truth. Graph is just produced using a heuristic!
- To get interesting theory, helps to relax what we mean by "useful".
- Can view as a kind of PAC model for clustering.
- A lot of interesting directions to explore.

Conclusions

- Natural properties (relations between sim fn and target) that motivate spectral methods?
- Efficient algorithms for other properties? E.g., "stability of large subsets", (c,ε) property for other clustering objectives.
- Other notions of "useful".
  - Produce a small DAG instead of a tree?
  - Others based on different kinds of feedback?
- ...

- A lot of interesting directions to explore.