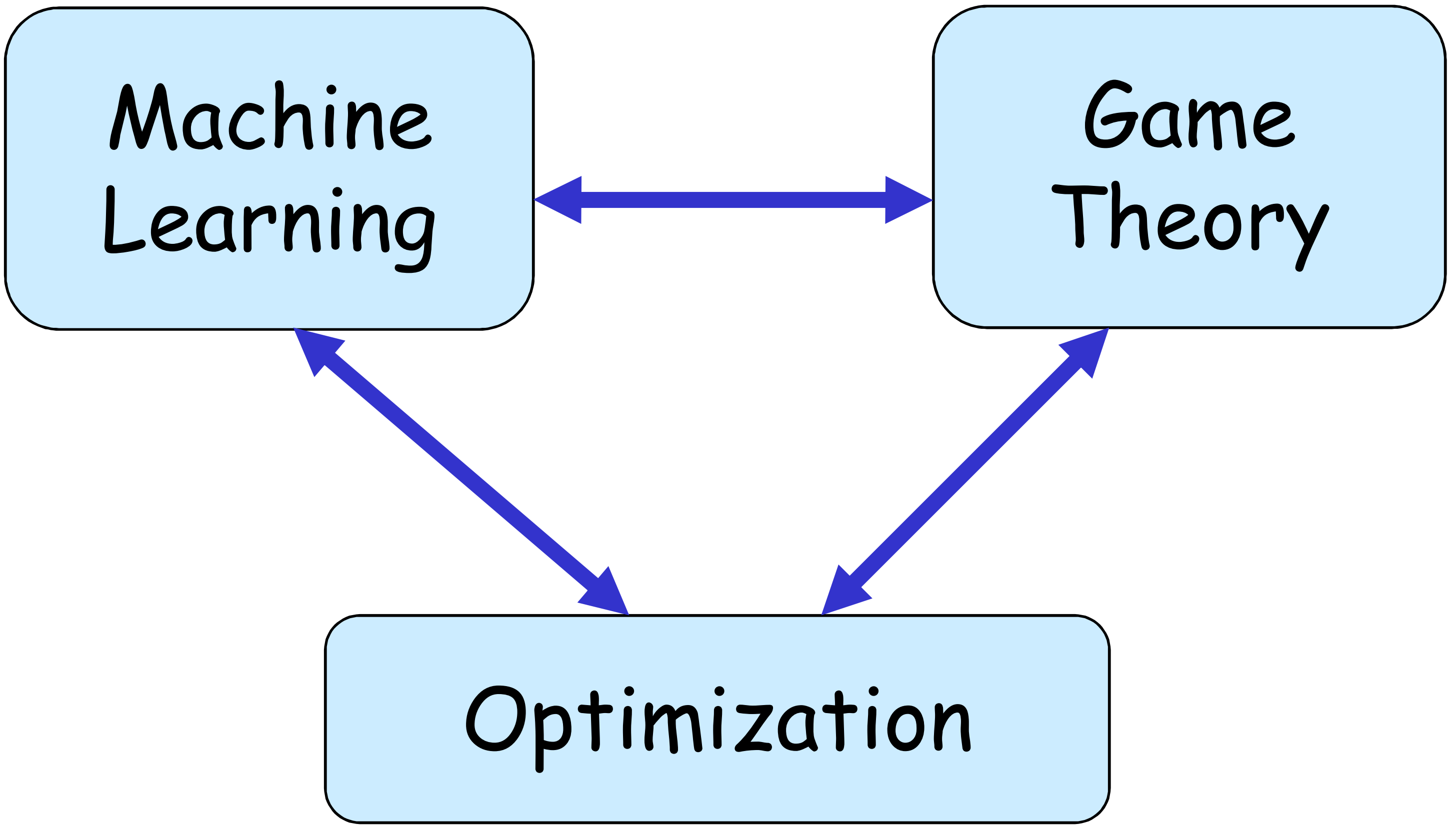
Approximate Clustering without the Approximation Algorithm

& a new angle on Optimization

Avrim Blum
Carnegie Mellon University

Indo-US Symposium on Machine Learning, Game Theory and Optimization 2010



3 great areas that go great together

Approximate Clustering without the Approximation Algorithm

& a new angle on Optimization

Avrim Blum
Carnegie Mellon University

Based on work joint with Nina Balcan, Pranjal Awasthi, Anupam Gupta, Or Sheffet, and Santosh Vempala

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Theme of this talk

- What if worst-case instances are hard, even to apx, but don't want to make distributional assumptions?

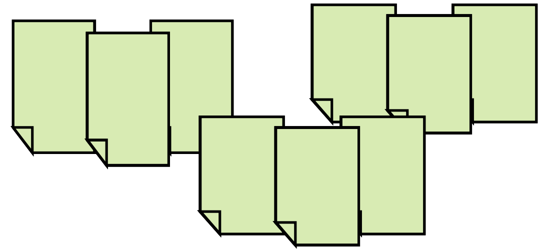
- Often there are assumptions will need to make anyway when it comes time to use your solution.

- If make these explicit up front, can give alg more to work with, and sometimes get around computational hardness barriers.

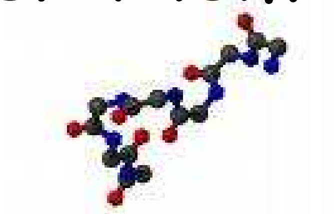
Clustering

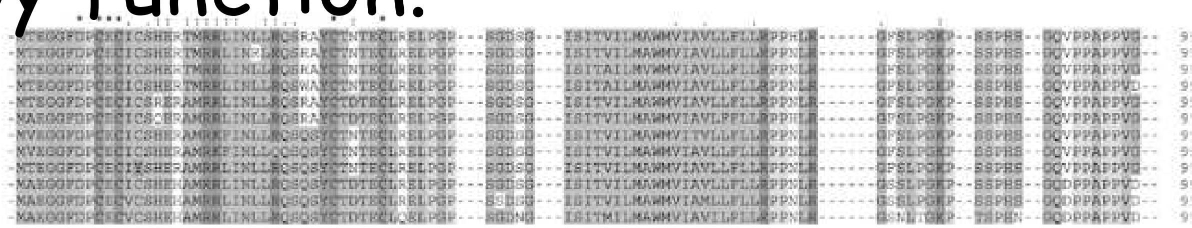
Clustering comes up in many places

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



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



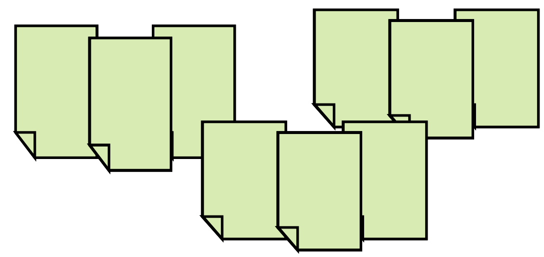


- Given a set of images of people, cluster by who is in them.

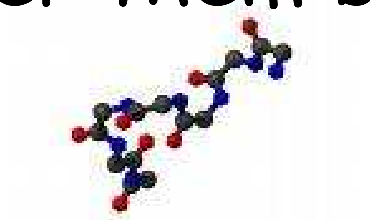
- …

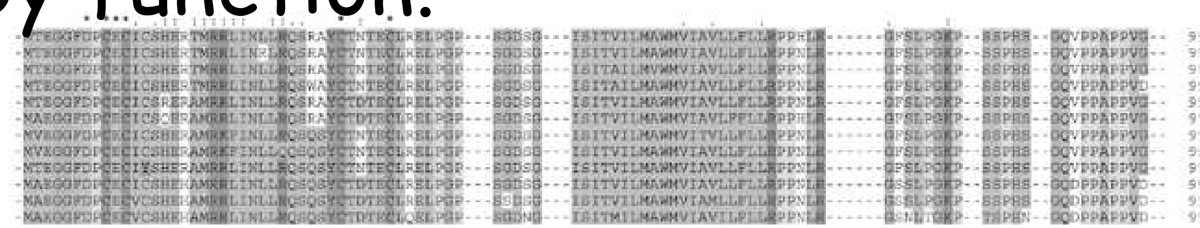
Standard approach

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



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





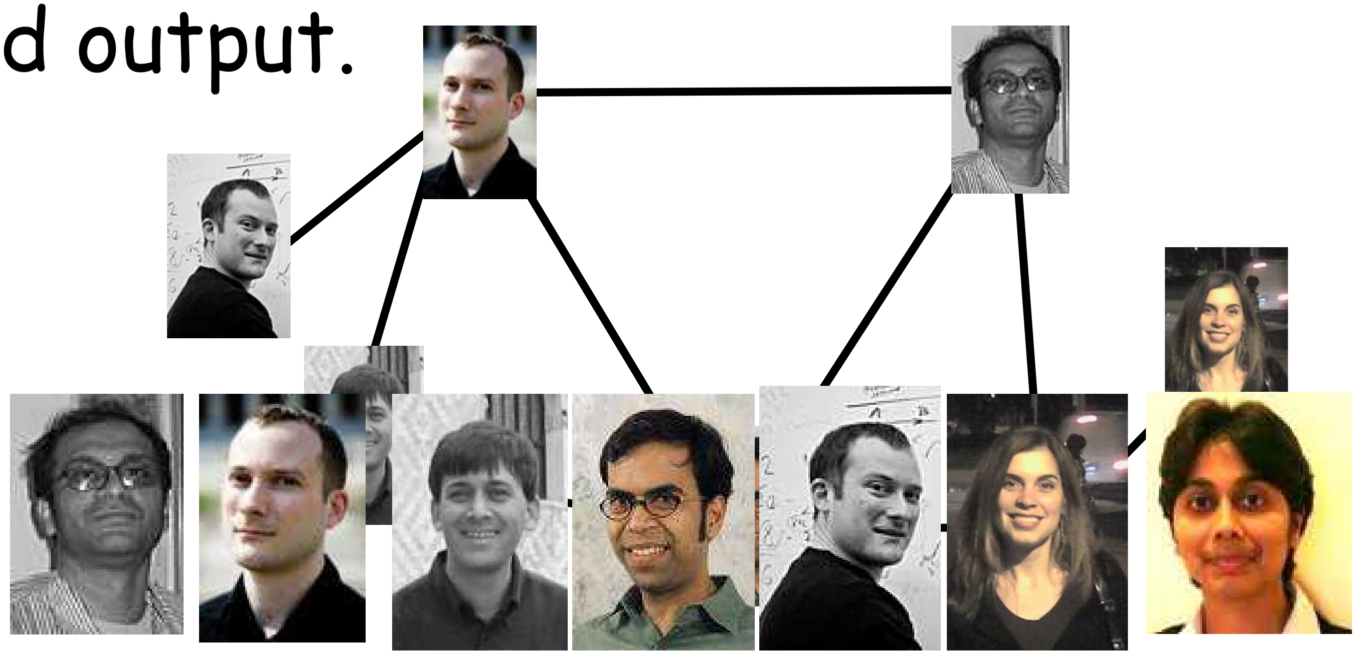
- Given a set of images of people, cluster by who is in them.

- …

Standard approach

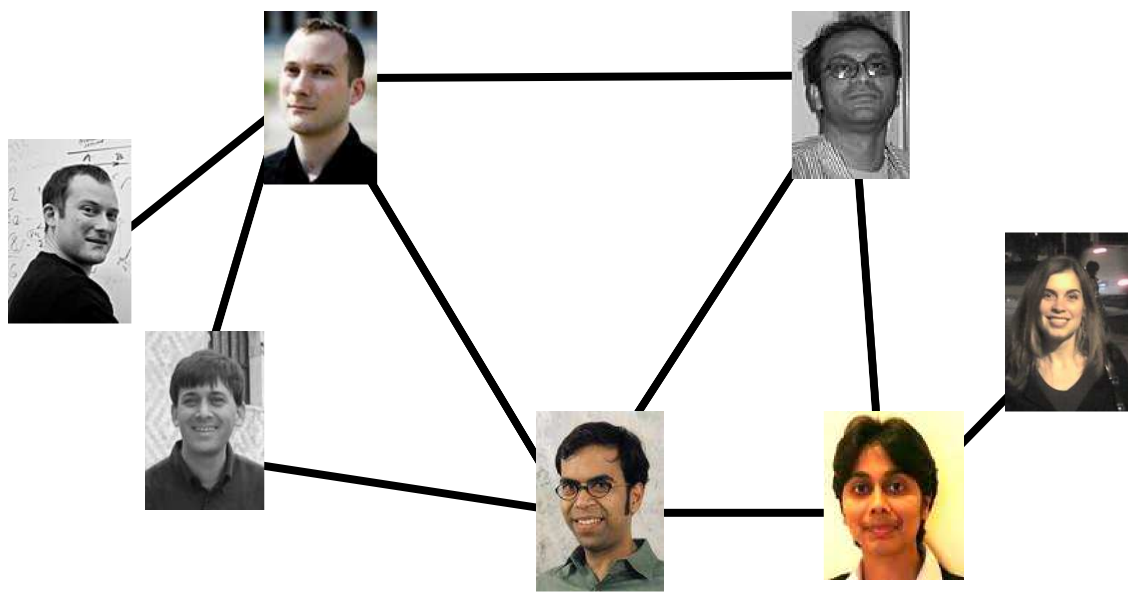
- Come up with some measure of similarity
  (like # keywords in common, edit distance,...)
- Use to view data as nodes in weighted graph

- Run clustering algorithm on graph. Hope it gives a good output.



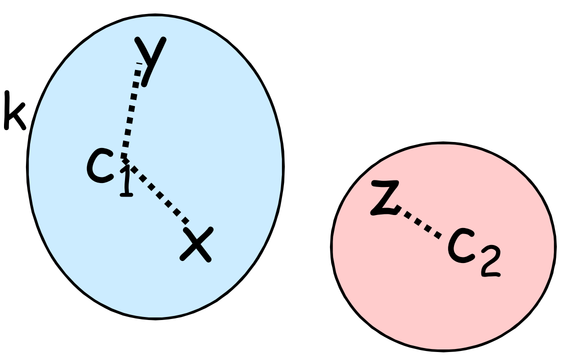
Standard theoretical approach

- Come up with some measure of similarity (like # keywords in common, edit distance,…)
- Use to view data as nodes in weighted graph
- Pick some objective to optimize like k-median, k-means, min-sum,…



Standard theoretical approach

- Come up with some measure of similarity (like # keywords in common, edit distance,…)
- Use to view data as nodes in weighted graph
- 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 $\sum_x \min_i d(x,c_i)$
  - k-means asks: find $c_1, c_2, \ldots, c_k$ to minimize $\sum_x \min_i d^2(x,c_i)$



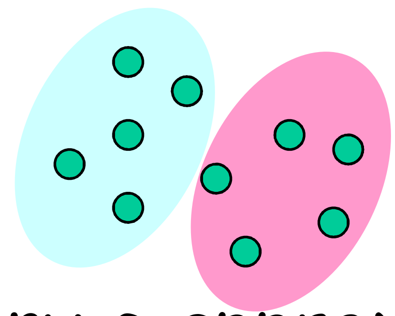
Standard theoretical approach

- Come up with some measure of similarity (like # keywords in common, edit distance,...)
- Use to view data as nodes in weighted graph
- Pick some objective to optimize like k-median, k-means, min-sum,...
- Develop algorithm to (approx) optimize this objective. (E.g., best known for k-median is $3+\varepsilon$ approx [AGKMMP04]. Beating $1 + 1/e$ is NP-hard [JMS02].)

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 in error to truth.
- This is an assumption about how the distance measure relates to the target clustering.
- Why not make it explicit?

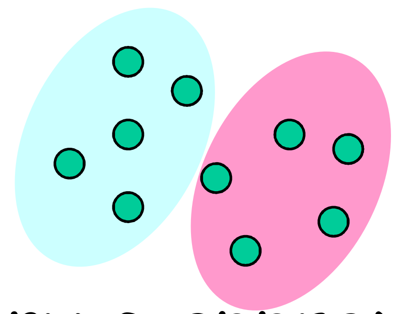
Example of result: for any $c>1$, this property implies structure we can use to get $O(\varepsilon)$ error.

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

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

As well as if we could approximate to NP-hard value!

Well, but..



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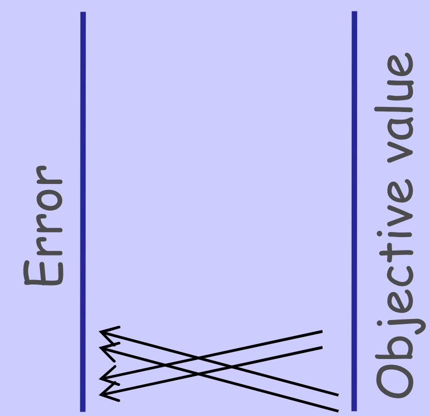
- This is an assumption about how the distance measure relates to the target clustering.
- Why not make it explicit?

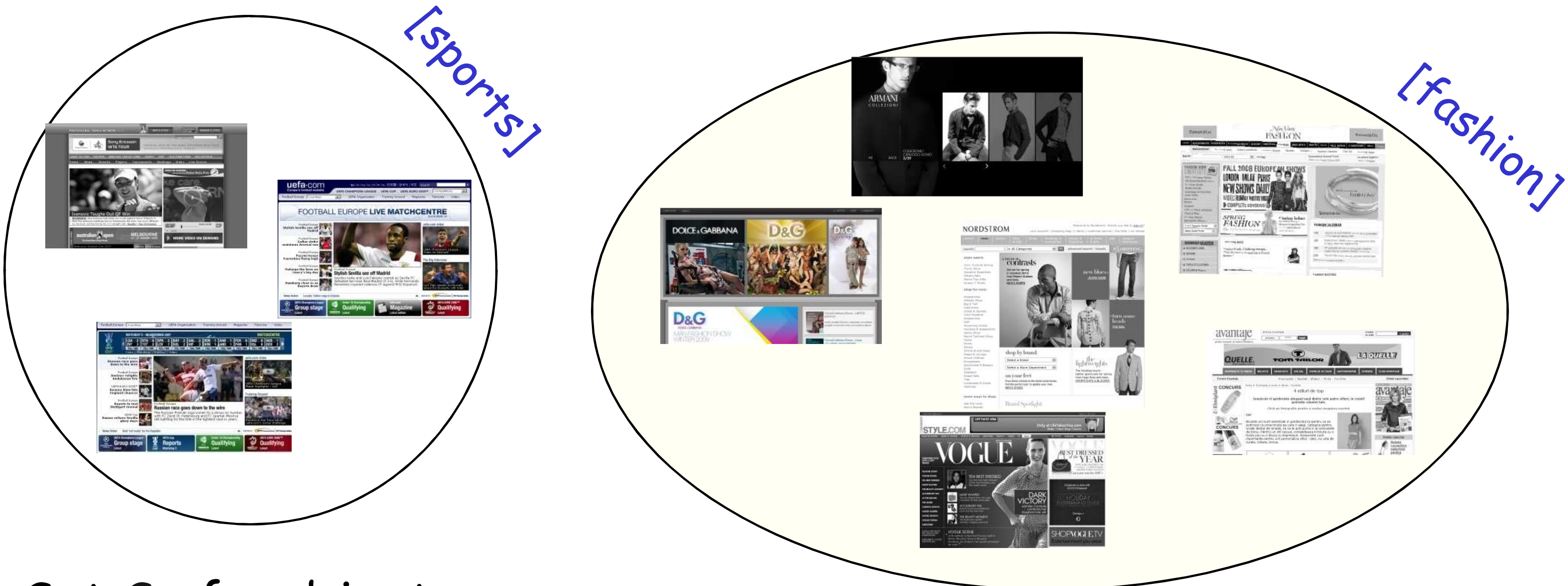
More generally: have one objective you can measure, and a different one you care about.

Implicitly assuming they are related.

Let's make it explicit.



Formal Setup



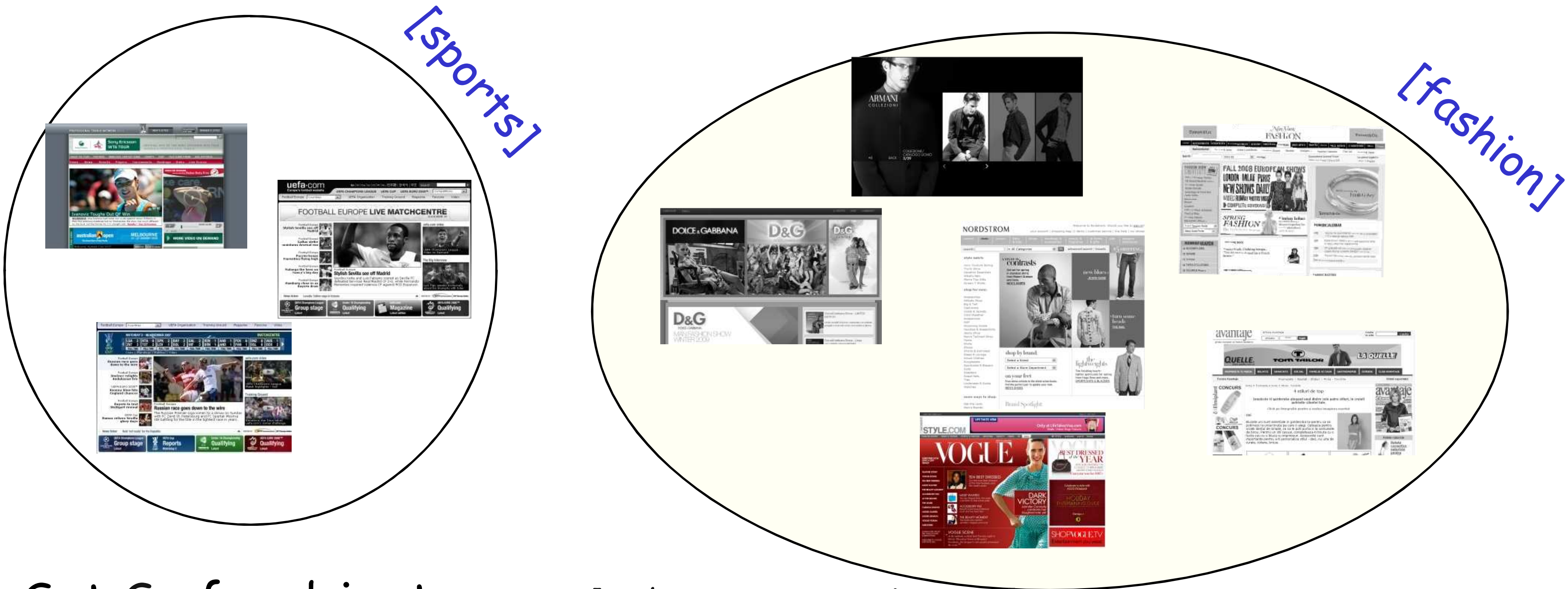
Set S of n objects. [web pages, protein seqs]

Ground truth clustering. $C_1^*, C_2^*, \ldots, C_k^*$. [true clustering by topic]

Goal: clustering $C_1, \ldots, C_k$ of low error. $\text{error}(C) = \min_{\sigma \in S_k} \frac{1}{n} \sum_{i=1}^{k} |C_i^* - C_{\sigma(i)}|$

error(C) = fraction of pts need to reassign in order to match true target clustering (up to re-indexing of clusters)

Formal Setup



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Given a distance metric d(x,y) on objects.

Satisfies (c,ε)-approximation-stability for objective Φ if any c-approximation to Φ has error at most ε.

Approximation-stability

- Instance is (c,ε)-apx-stable for objective Φ: any c-approximation to Φ has error $\leq \varepsilon$.
- Focus on Φ = "k-median objective".
  - (Also results for k-means, min-sum)

How are we going to use this to cluster well if we don't know how to get a c-approximation?

(c,ε) k-median stability

We're assuming any c-apx k-median solution must be ε-close to the target, $c>1$.

Two approaches that don't work:

1. Hope that $(1.1,\varepsilon)$ stable $\Rightarrow$ $(3,O(\varepsilon))$ stable
   - But for any $c_1 < c_2$ can construct dataset and target s.t. all c_1 apx to k-median have error $< \varepsilon$, but exists c_2 apx that has error 0.49.

(c,ε) k-median stability

We're assuming any c-apx k-median solution must be ε-close to the target, $c>1$.

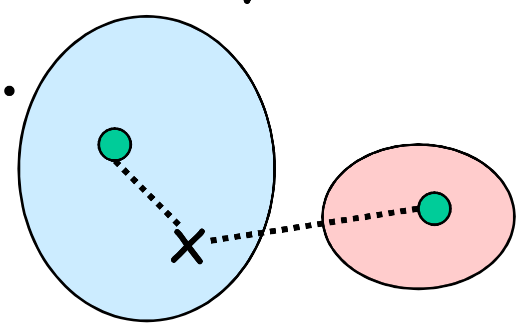
Two approaches that don't work:

1. Hope that $(1.1,\varepsilon)$ stable $\Rightarrow$ $(3,O(\varepsilon))$ stable
2. Hope that c-apx is easy under (c,ε) stability
   - Unfortunately, c-apx is as hard as in general case. (if min cluster size small vs εn – will get back to this…)

Instead, want to skip this proxy, just use properties implied by assumption.

Clustering from (c,ε) k-median stability

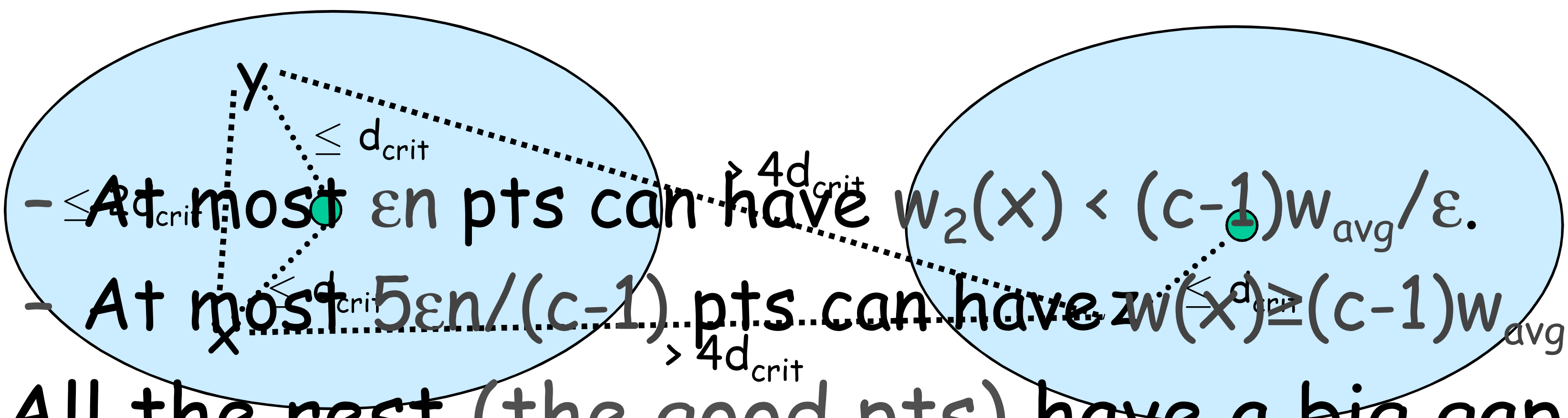
- Suppose any c-apx k-median solution must be ε-close to the target. (and for simplicity say target *is* k-median opt, & all cluster sizes > $2\varepsilon n$)
- For any x, let $w(x)$=dist to own center, $w_2(x)$=dist to 2nd-closest center.
- Let $w_{avg}=\text{avg}_x\, w(x)$. [$OPT = n \cdot w_{avg}$]



- 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.

Clustering from (c,ε) k-median stability

- Define critical distance $d_{crit}=(c-1)w_{avg}/5\varepsilon$.
- So, a $1\text{-}O(\varepsilon)$ fraction of pts look like:



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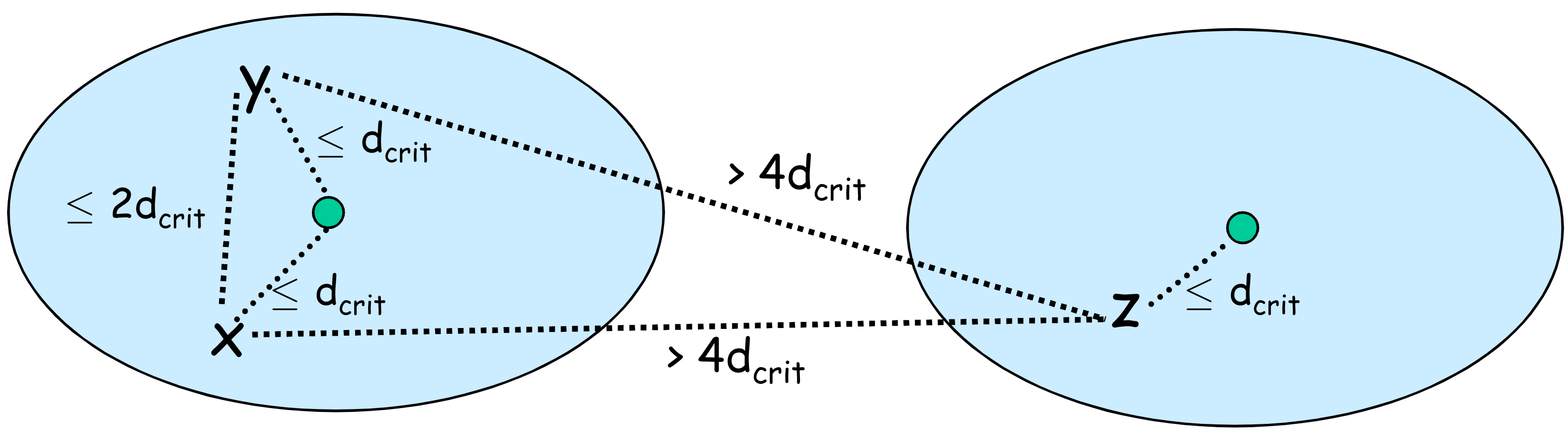
Clustering from (c,ε) k-median stability

- 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
- So, a $1-O(\varepsilon)$ fraction of pts look like:



Clustering from (c,ϵ) k-median stability

- So if we define a graph G connecting any two pts within distance $\leq 2d_{crit}$, then:
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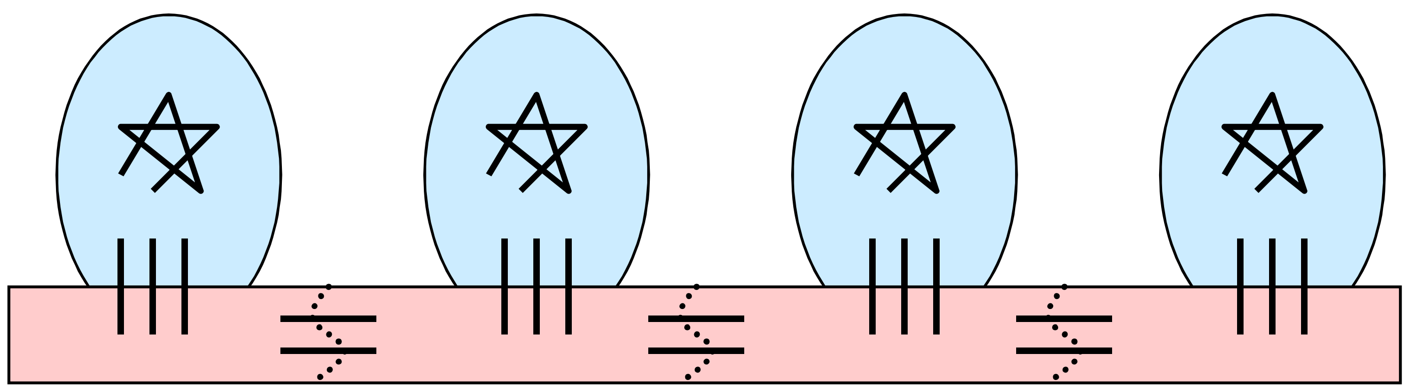
- So, the world now looks like:

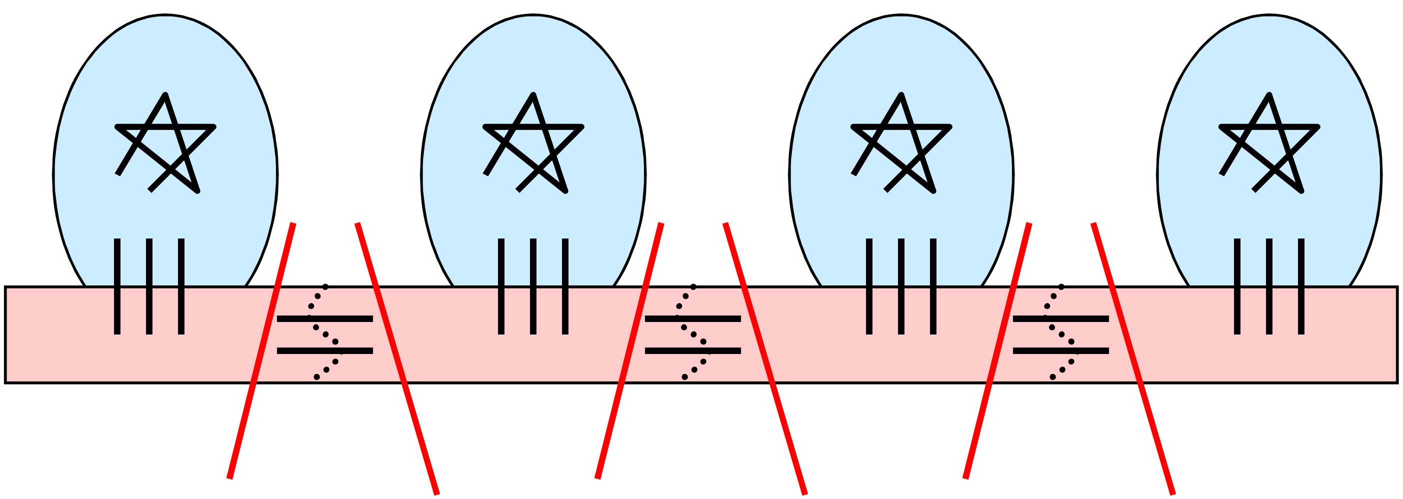


Clustering from (c,ε) k-median stability

- If furthermore all clusters have size > 2b+1, where b = # bad pts = $O(\varepsilon n/(c-1))$, then:
  - Create graph H where connect x,y if share > b nbrs in common in G.
  - Output k largest components in H.

(only makes mistakes on bad points)

- So, the world now looks like:

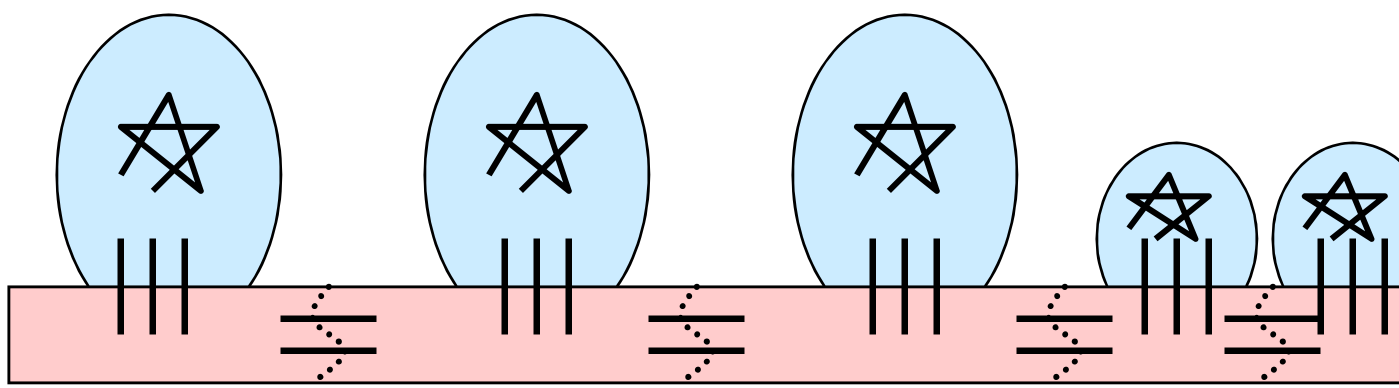


Clustering from (c,ε) k-median stability

If clusters not so large, then need to be a bit more careful but can still get error $O(\varepsilon/(c-1))$.

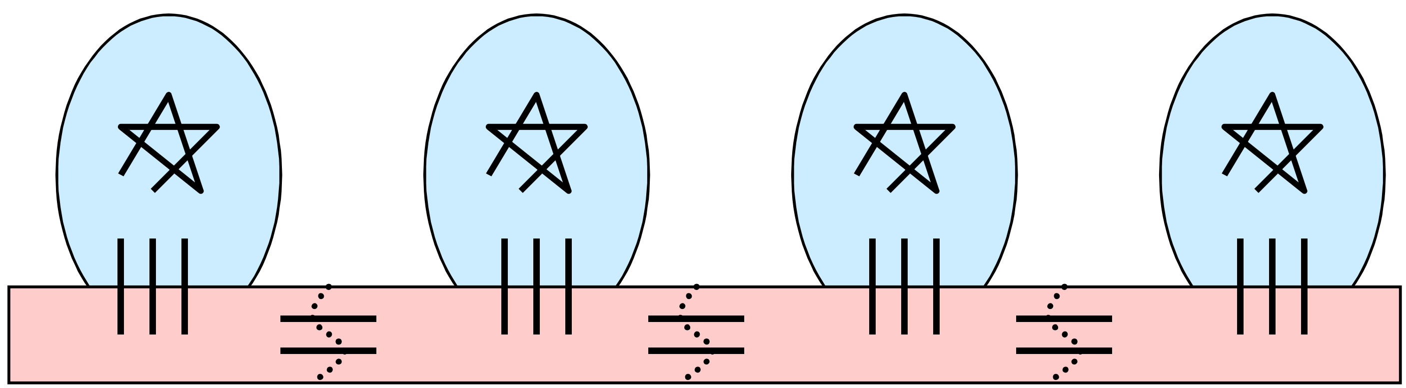
Could have some clusters dominated by bad pts…

Actually, just need to modify algorithm a bit, but analysis more involved.



$O(\varepsilon)$-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…



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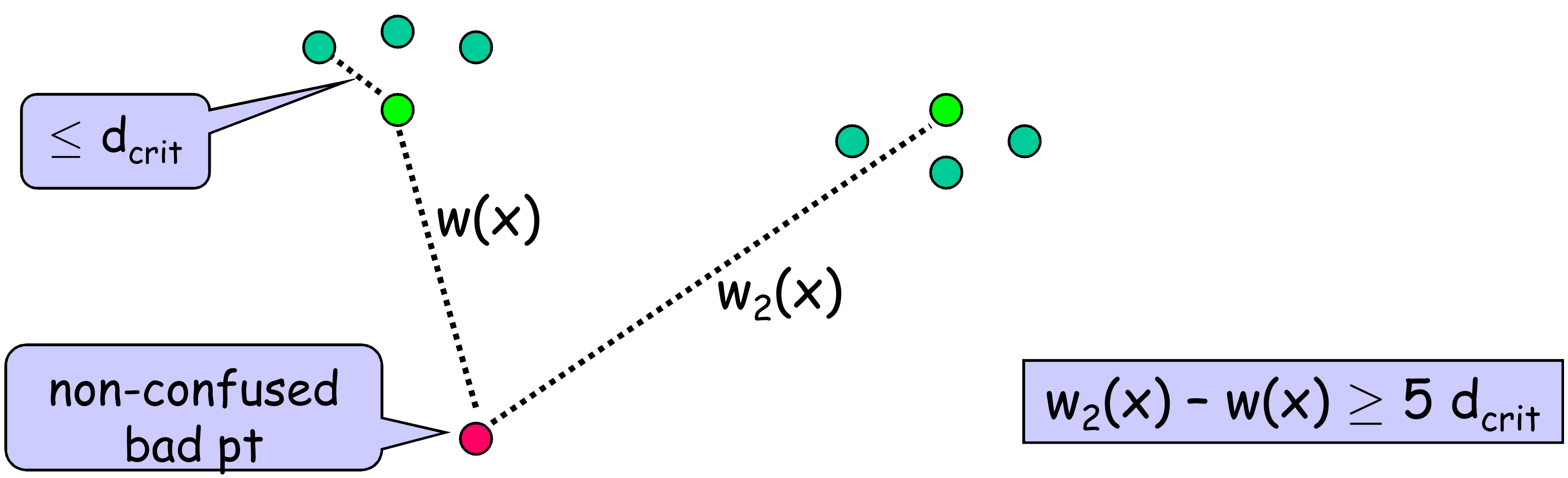

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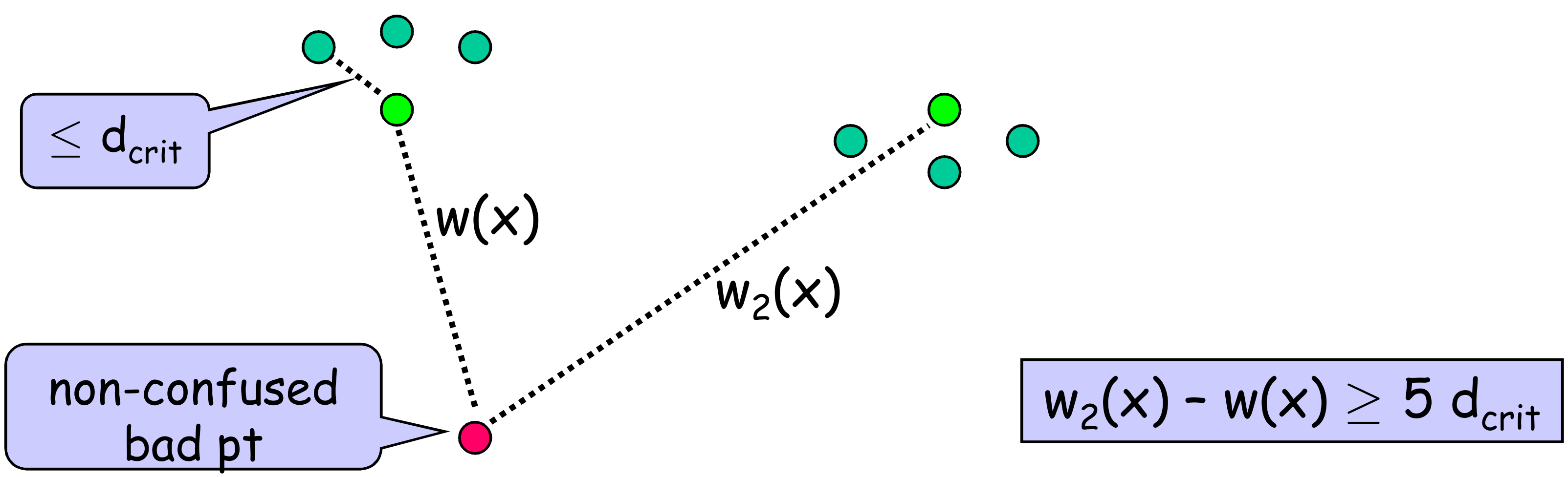
  - Given output C′ from alg so far, reclassify each x into cluster of lowest median distance
  - Median is controlled by good pts, which will pull the non-confused points in the right direction.



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A bit like 2-rounds of k-means/Lloyd's algorithm

Stepping back…

- Assumption that any c-apx to k-median is ε-close allows us to get ε-close (for large clusters) or O(ε)-close (for general cluster sizes)

- Can also get similar guarantees for k-means, min-sum objectives.

See [Balcan-Braverman09] for best results

Stepping back…

- Assumption that any c-apx to k-median is ε-close allows us to get ε-close (for large clusters) or $O(\varepsilon)$-close (for general cluster sizes)

Useful in practice?

- [Voevodski-Balcan-Roglin-Teng-Xia UAI'10]
  - Show how algorithm can be adapted to be very fast in setting of 1-vs-all queries.
  - Apply to protein sequence clustering problems (Pfam, SCOP databases)
  - Fast and high accuracy.

Extensions

[Awasthi-B-Sheffet'10]

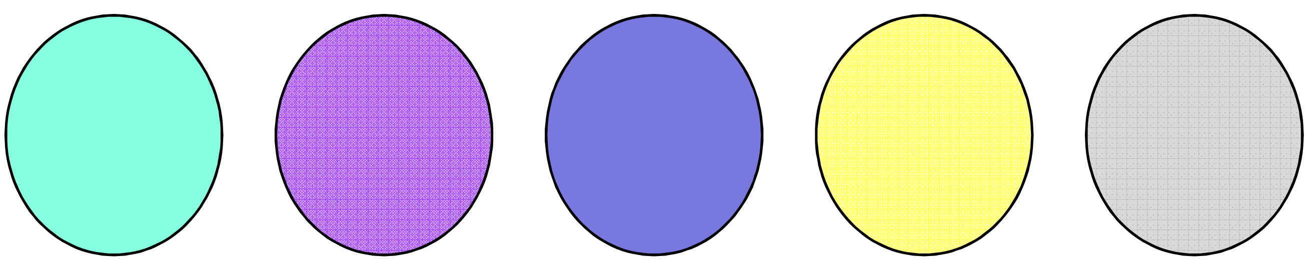
All ε-far solutions are not c-approximations

$\Downarrow$

All k-1 clusterings are not c-approximations

(strictly weaker condition in the "large clusters" case)

Under this condition, can get a PTAS: 1+α apx in polynomial time (exponential in 1/α, 1/(c-1))



Extensions

[Awasthi-B-Sheffet'10]

All ε-far solutions are not c-approximations

↓

All k-1 clusterings are not c-approximations

Implications:

- Under approx stability, get exactly ϵ-close in "large clusters" case for k-means too.
- Only need clusters of size $\geq 2\epsilon n$ vs $\Omega(\epsilon n/(c-1))$.

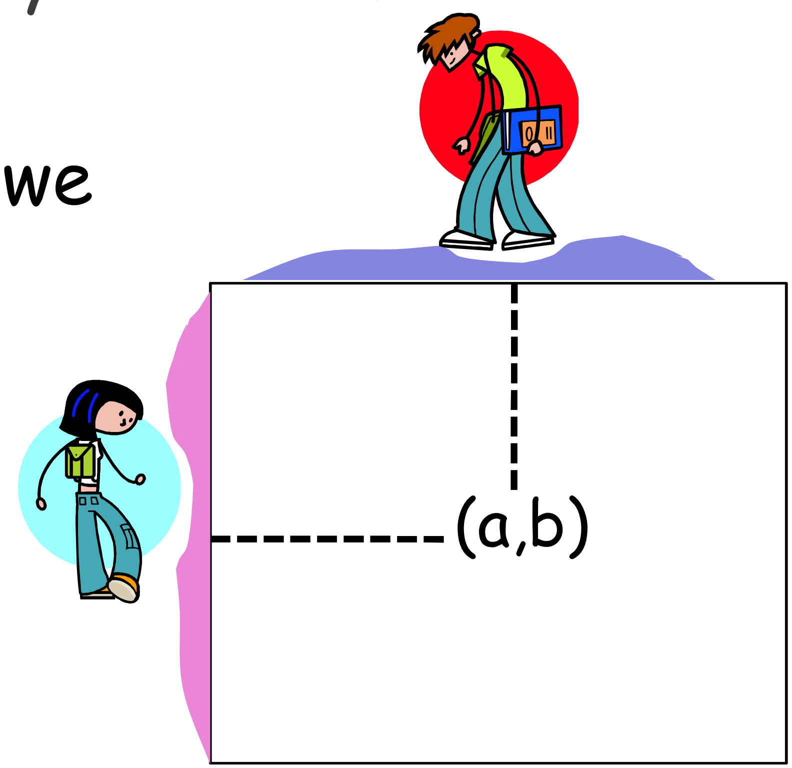
Other problems?

One proposal: Nash equilibria.

So, what's a Nash equilibrium?

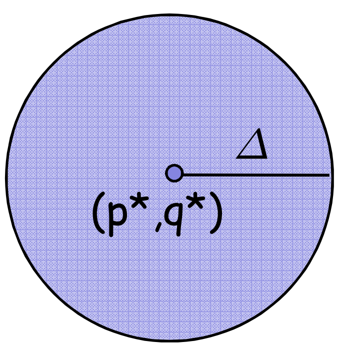
Nash equilibrium

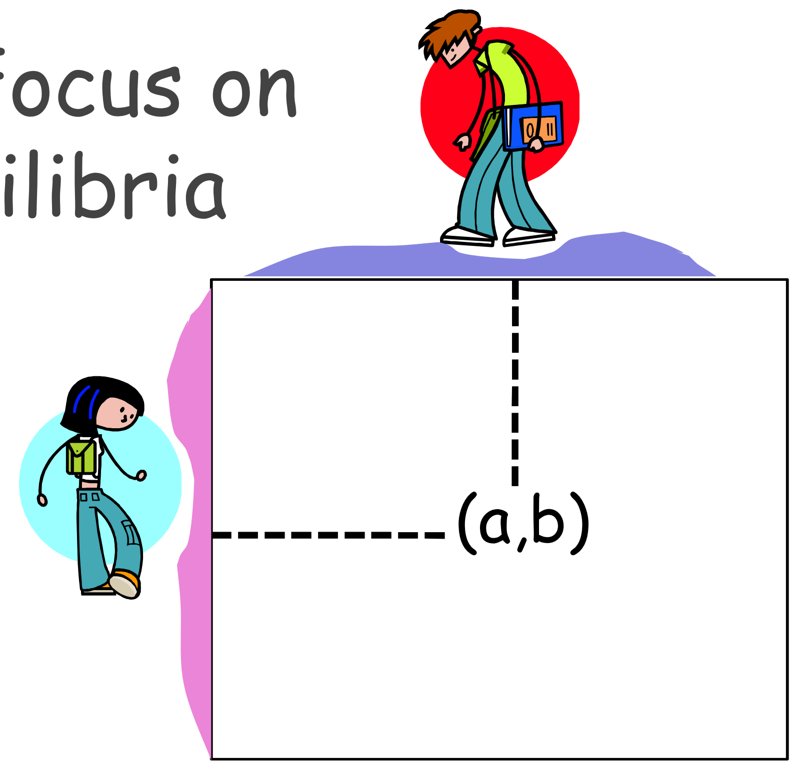
- Set of (randomized) strategies for players in a multiagent interaction (i.e., game) such that no one has any incentive to deviate.
- Appears to be computationally hard to find even in 2-player n-action games.
- A lot of interest in whether we can compute ϵ-equilibria efficiently (best general alg: time $n^{O((\log n)/\epsilon^2)}$)



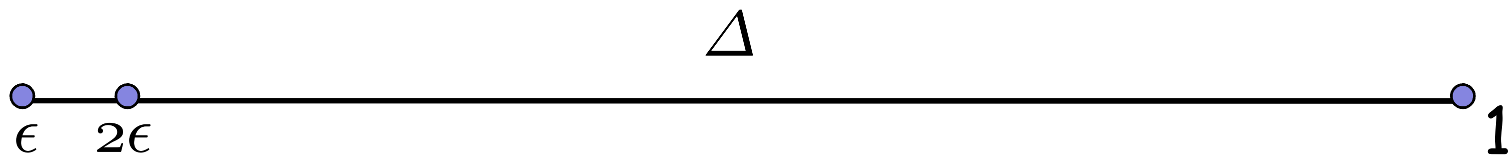
Nash equilibrium

- Why do we want to find an (apx) equilibrium?
  - One reason: predict long-term behavior (e.g, proposing design of new system), which we believe will be at (apx) equilibrium.
- In that case, natural to focus on cases where all (apx) equilibria are close to each other.



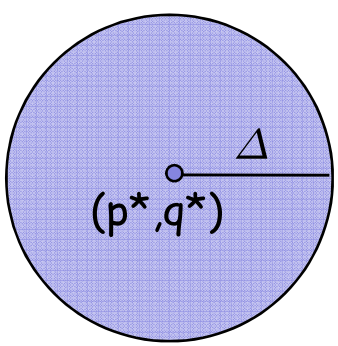


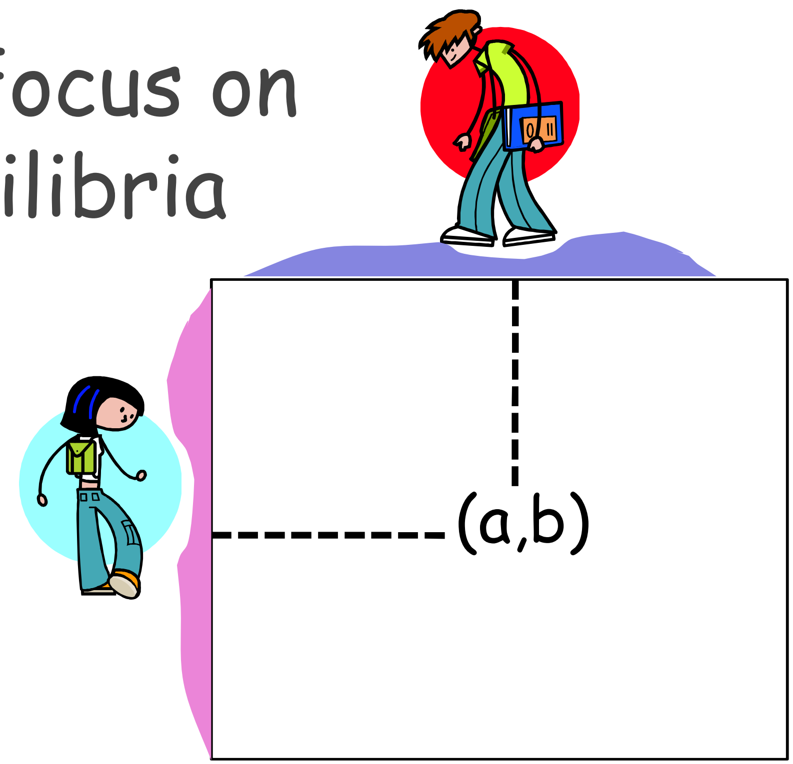
Nash equilibrium



So, what can we say?

- In that case, natural to focus on cases where all (apx) equilibria are close to each other.





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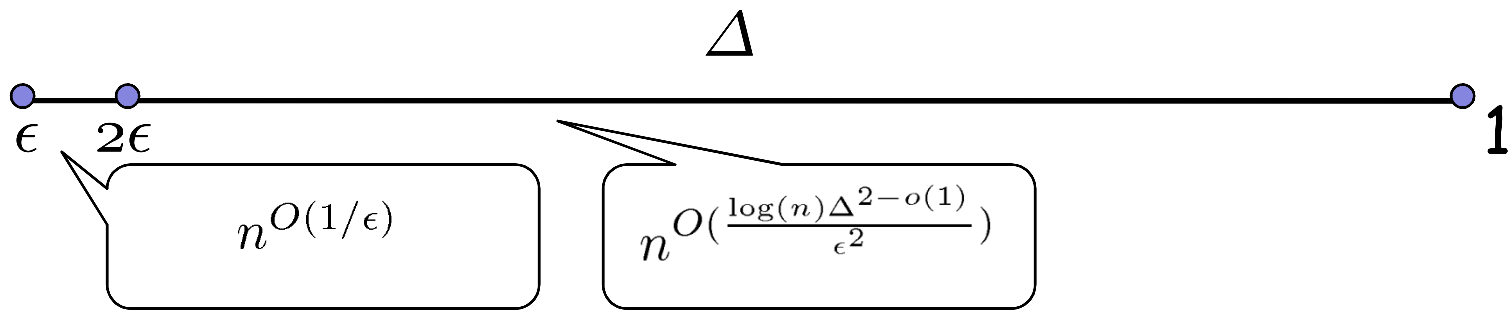

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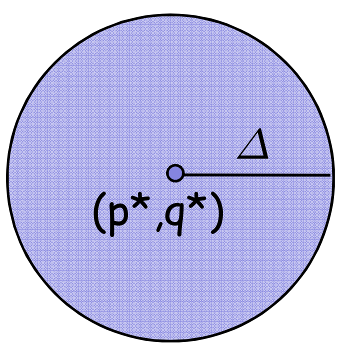

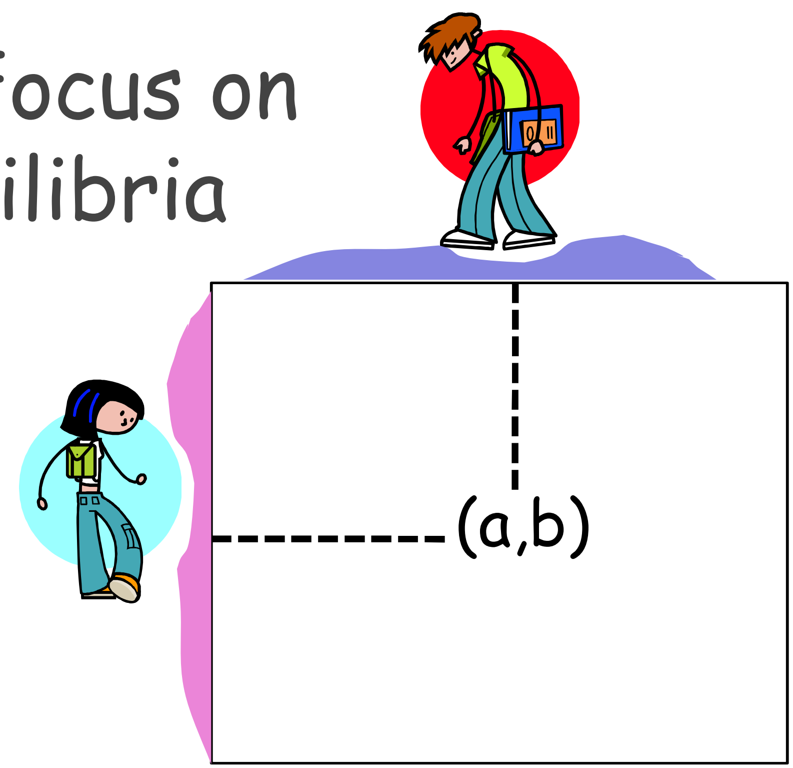

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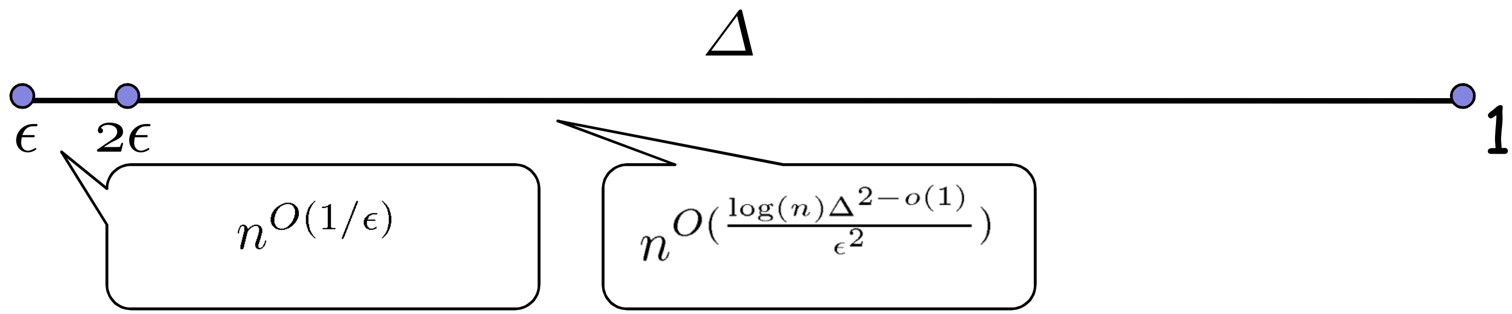
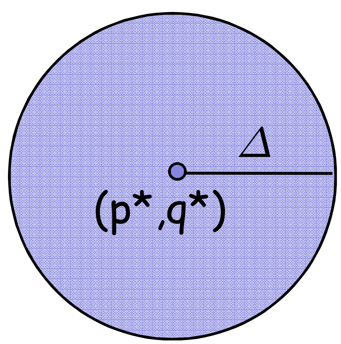
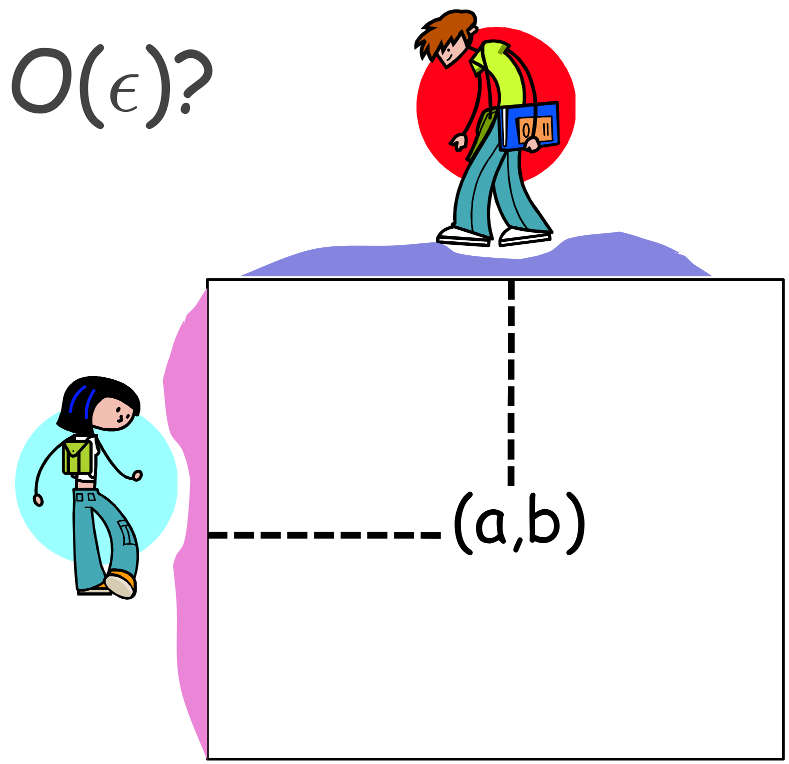
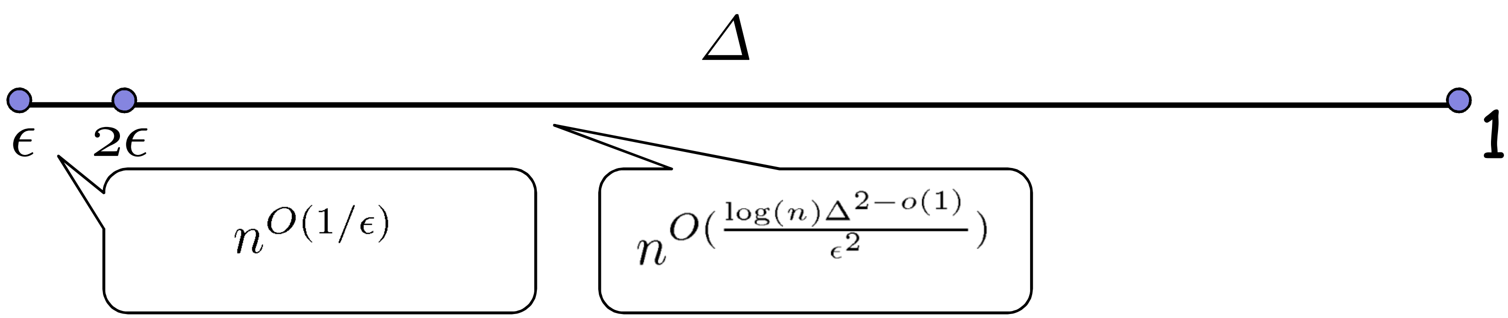


- Get poly-time for all $\Delta = O(\epsilon)$?





Nash equilibrium

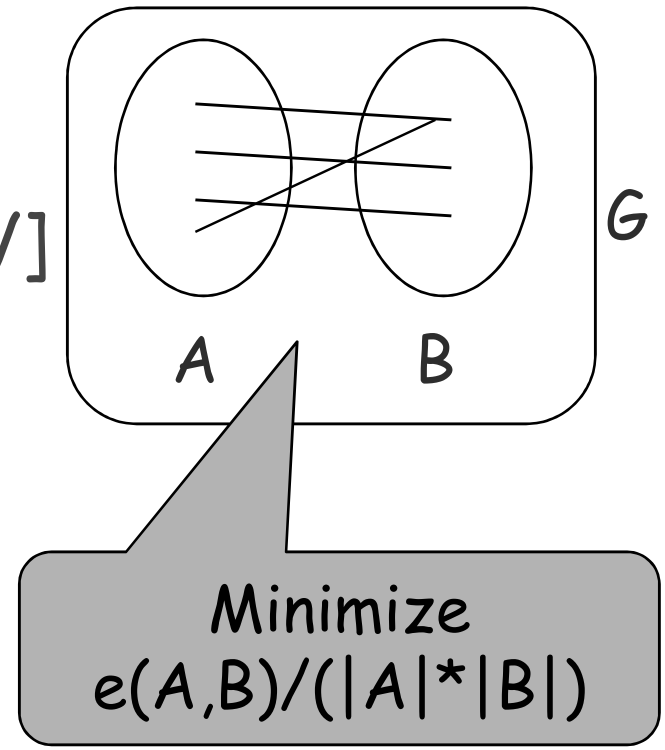


- Get poly-time for all $\Delta = O(\epsilon)$?
- Recent work of [Balcan-Braverman]:
  - $\Delta = O(\epsilon^{1/4})$ as hard as general case for poly-time.
  - Extensions to reversed-quantifier condition.
  - Connections to perturbation-stability.

Other problems where approach might make sense?

A few ideas:

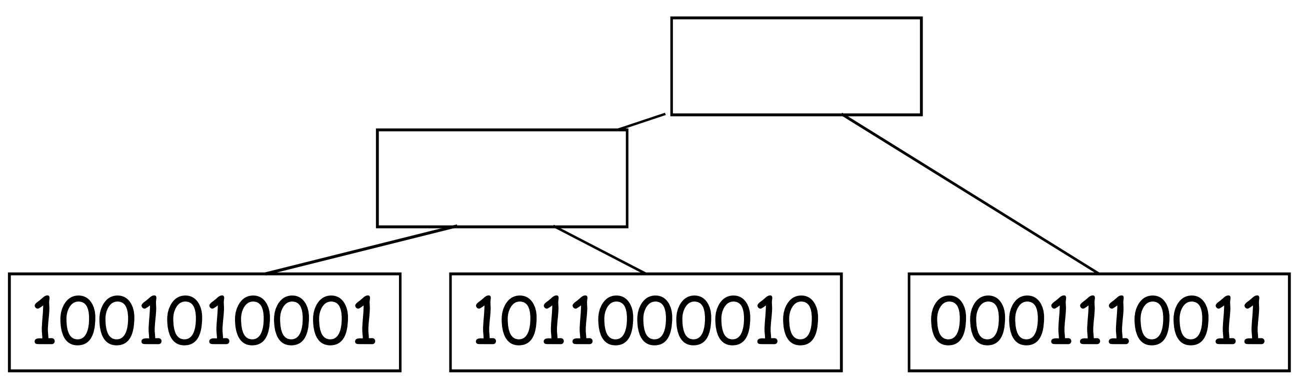
- Sparsest cut
  - Best apx is $O((\log n)^{1/2})$ [ARV]
  - What if assume any 10-apx has error $\leq \epsilon$?



Other problems where approach might make sense?

A few ideas:

- Evolutionary tree reconstruction
  - Often posed as a Steiner-tree-like problem.
  - To have confidence in solution, would hope that near-optimal answers are close in structure.
  - Brings up related Q: what if only part of input is stable. Maybe can identify & output solution for that?



Summary

For clustering, can say "if data has the property that a 1.1 apx to [pick one: k-median, k-means, min-sum] would be sufficient to cluster well, then we can cluster well" …even though you might think NP-hardness results for approximating these objectives would preclude this.

Suggests an approach to other optimization problems where objective function may be a proxy for something else, or esp care about stable instances

- Nash equilibria
- Market equilibria?
- Sparsest cut? Evolutionary trees?

Many interesting problems to explore!