Clustering.
Unsupervised Learning

Maria-Florina Balcan

04/06/2015

Reading:

- Chapter 14.3: Hastie, Tibshirani, Friedman.

Additional resources:

- Center Based Clustering: A Foundational Perspective.
  Awasthi, Balcan. Handbook of Clustering Analysis. 2015.

Logistics

- Project:
  - Midway Review due today.
  - Final Report, May 8.
  - Poster Presentation, May 11.
  - Communicate with your mentor TA!

- Exam #2 on April 29th.

Clustering, Informal Goals

Goal: Automatically partition unlabeled data into groups of similar datapoints.

Question: When and why would we want to do this?

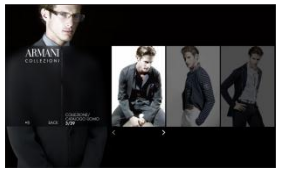
Useful for:

- Automatically organizing data.
- Understanding hidden structure in data.
- Preprocessing for further analysis.
    - Representing high-dimensional data in a low-dimensional space (e.g., for visualization purposes).

Applications (Clustering comes up everywhere…)

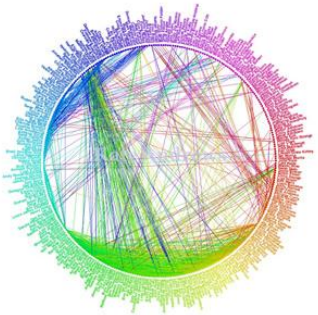
- Cluster news articles or web pages or search results by topic.



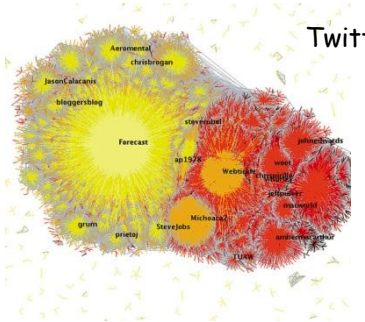


- Cluster protein sequences by function or genes according to expression profile.


- Cluster users of social networks by interest (community detection).



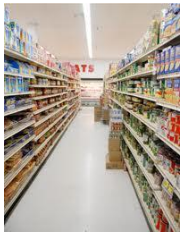
Facebook network



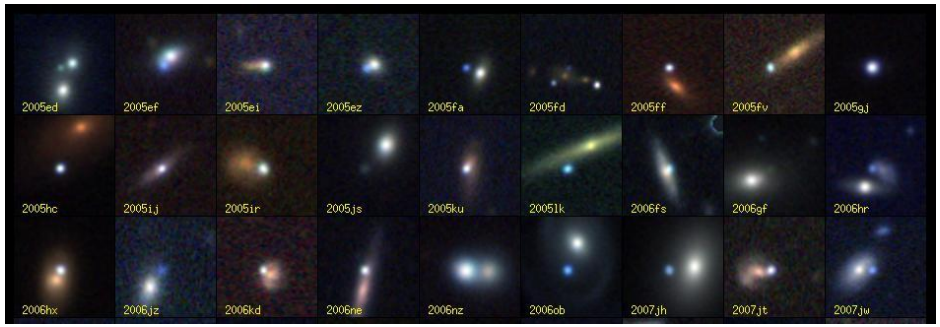
Twitter Network

Applications (Clustering comes up everywhere…)

- Cluster customers according to purchase history.



- Cluster galaxies or nearby stars (e.g. Sloan Digital Sky Survey)



- And many many more applications….

Clustering

Today:

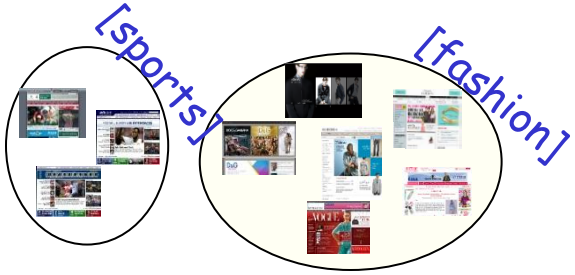
- Objective based clustering
- Hierarchical clustering
- Mention overlapping clusters

[March 4th: EM-style algorithm for clustering for mixture of Gaussians (specific probabilistic model).]

Objective Based Clustering

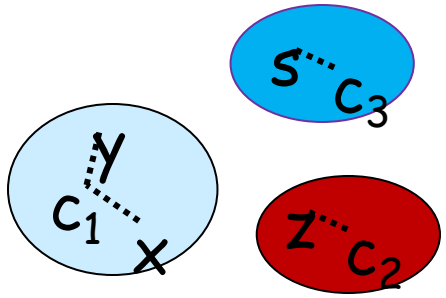
Input: A set S of n points, also a distance/dissimilarity measure specifying the distance d(x,y) between pairs (x,y).

E.g., # keywords in common, edit distance, wavelets coef., etc.



Goal: output a partition of the data.

- k-means: find center pts $c_1, c_2, \ldots, c_k$ to minimize $\sum_{i=1}^{n} \min_{j\in\{1,\ldots,k\}} d^2(\mathbf{x^i}, \mathbf{c_j})$
- k-median: find center pts $\mathbf{c_1}, \mathbf{c_2}, \ldots, \mathbf{c_k}$ to minimize $\sum_{i=1}^{n} \min_{j\in\{1,\ldots,k\}} d(\mathbf{x^i}, \mathbf{c_j})$



- K-center: find partition to minimize the maxim radius

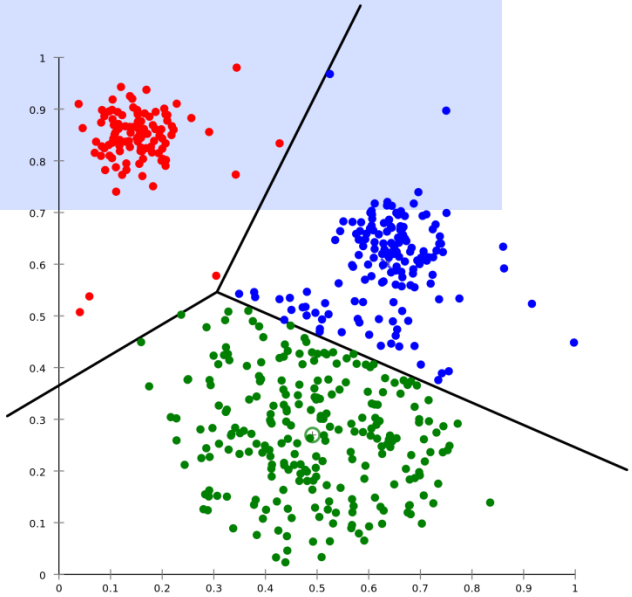
Euclidean k-means Clustering

Input: A set of n datapoints $\mathbf{x^1}, \mathbf{x^2}, \ldots, \mathbf{x^n}$ in $\mathrm{R^d}$
target #clusters k

Output: k representatives $\boldsymbol{c_1}, \mathbf{c_2}, \ldots, \boldsymbol{c_k} \in \mathrm{R^d}$

Objective: choose $\boldsymbol{c_1}, \mathbf{c_2}, \ldots, \boldsymbol{c_k} \in \mathrm{R^d}$ to minimize

$$\sum_{i=1}^{n} \min_{j \in \{1,\ldots,k\}} \left|\left|\mathbf{x^i} - \mathbf{c_j}\right|\right|^2$$



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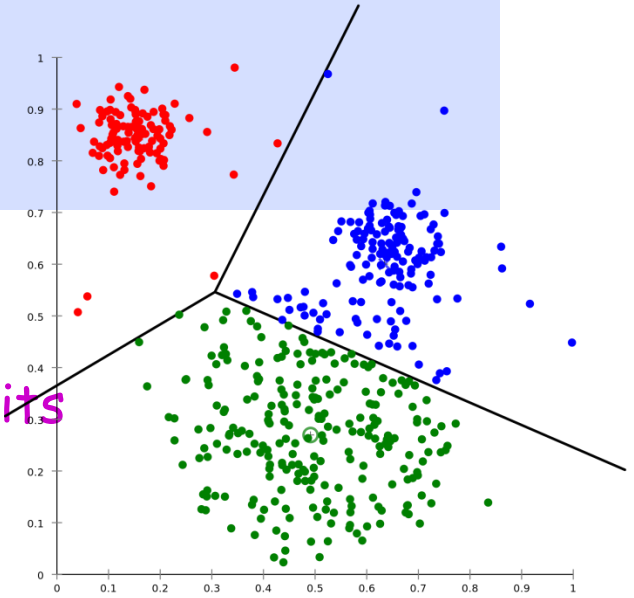
Natural assignment: each point assigned to its closest center, leads to a Voronoi partition.



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Computational complexity:

NP hard: even for $k = 2$ [Dagupta'08] or

$d = 2$ [Mahajan-Nimbhorkar-Varadarajan09]

There are a couple of easy cases…

An Easy Case for k-means: k=1

Input: A set of n datapoints $\mathbf{x^1}, \mathbf{x^2}, \ldots, \mathbf{x^n}$ in R^d

Output: $\boldsymbol{c} \in R^d$ to minimize $\sum_{i=1}^{n} \left|\left|\mathbf{x^i} - \mathbf{c}\right|\right|^2$

Solution: The optimal choice is $\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x^i}$

Idea: bias/variance like decomposition

$$\frac{1}{n}\sum_{i=1}^{n} \left|\left|\mathbf{x^i} - \mathbf{c}\right|\right|^2 = \left|\left|\boldsymbol{\mu} - \mathbf{c}\right|\right|^2 + \frac{1}{n}\sum_{i=1}^{n} \left|\left|\mathbf{x^i} - \boldsymbol{\mu}\right|\right|^2$$

Avg k-means cost wrt c

Avg k-means cost wrt μ

So, the optimal choice for $\mathbf{c}$ is $\boldsymbol{\mu}$.

Another Easy Case for k-means: d=1

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Extra-credit homework question

Hint: dynamic programming in time $O(n^2k)$.

Common Heuristic in Practice: The Lloyd's method

[Least squares quantization in PCM, Lloyd, IEEE Transactions on Information Theory, 1982]

Input: A set of n datapoints $\mathbf{x^1}, \mathbf{x^2}, \ldots, \mathbf{x^n}$ in R^d

Initialize centers $\boldsymbol{c_1}, \mathbf{c_2}, \ldots, \boldsymbol{c_k} \in R^d$ and clusters $C_1, C_2, \ldots, C_k$ in any way.

Repeat until there is no further change in the cost.

- For each j: $C_j \leftarrow \{x \in S$ whose closest center is $\mathbf{c_j}\}$
- For each j: $\mathbf{c_j} \leftarrow$ mean of C_j

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Holding $\boldsymbol{c_1}, \mathbf{c_2}, \ldots, \boldsymbol{c_k}$ fixed, pick optimal $\mathrm{C_1}, \mathrm{C_2}, \ldots, \mathrm{C_k}$

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Note: it always converges.

- the cost always drops and
- there is only a finite #s of Voronoi partitions
  (so a finite # of values the cost could take)

Initialization for the Lloyd's method

Input: A set of n datapoints $\mathbf{x^1}, \mathbf{x^2}, \ldots, \mathbf{x^n}$ in R^d

Initialize centers $\mathbf{c_1}, \mathbf{c_2}, \ldots, \mathbf{c_k} \in R^d$ and clusters $C_1, C_2, \ldots, C_k$ in any way.

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- For each j: $C_j \leftarrow \{x \in S$ whose closest center is $\mathbf{c_j}\}$
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- Initialization is crucial (how fast it converges, quality of solution output)
- Discuss techniques commonly used in practice
  - Random centers from the datapoints (repeat a few times)
  - Furthest traversal
  - K-means ++ (works well and has provable guarantees)

Lloyd's method: Random Initialization

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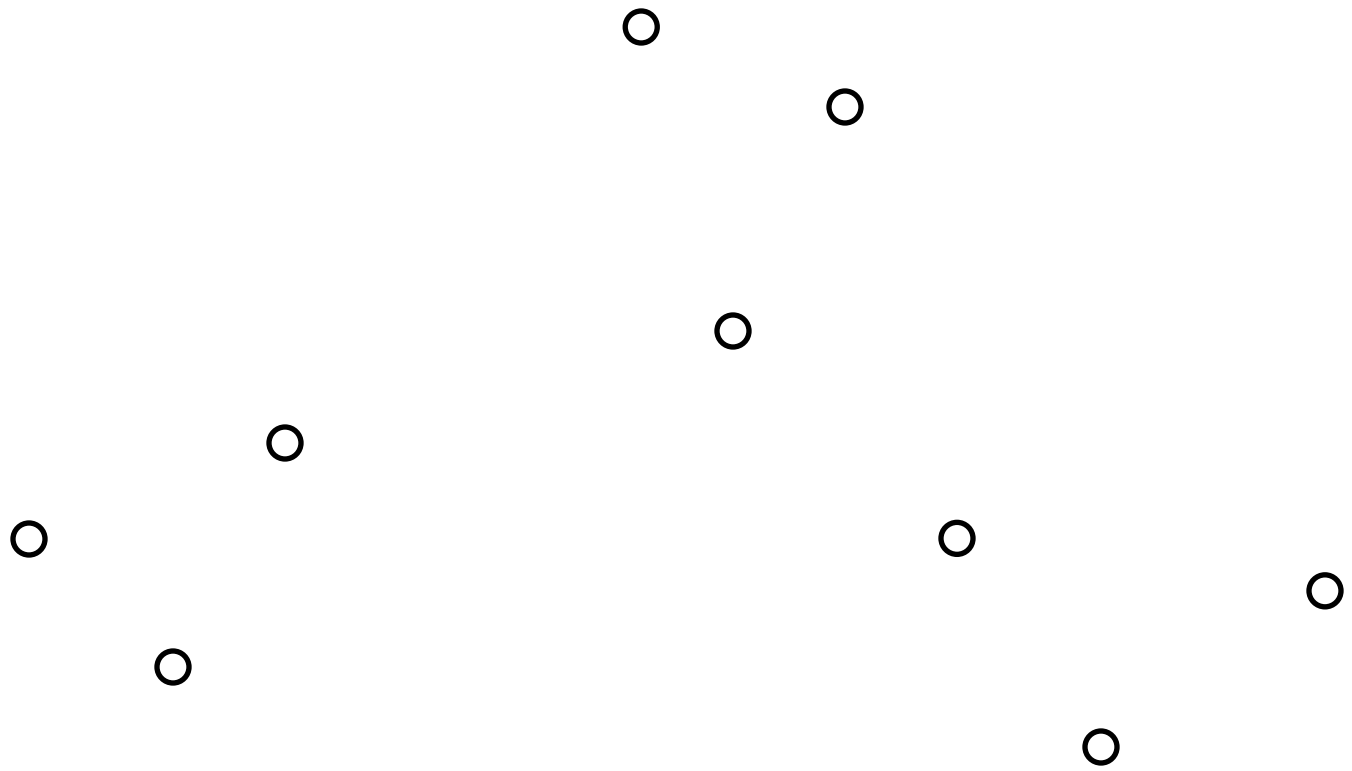
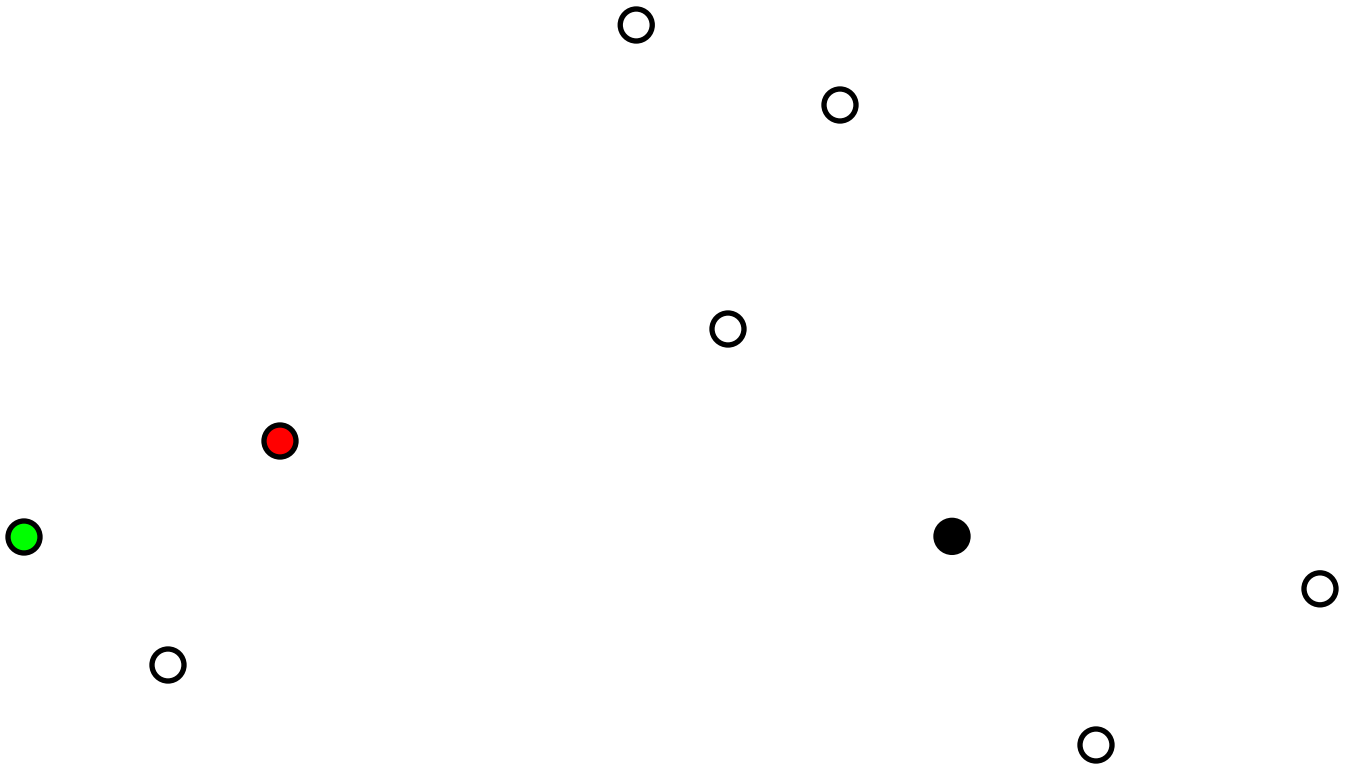
Example: Given a set of datapoints



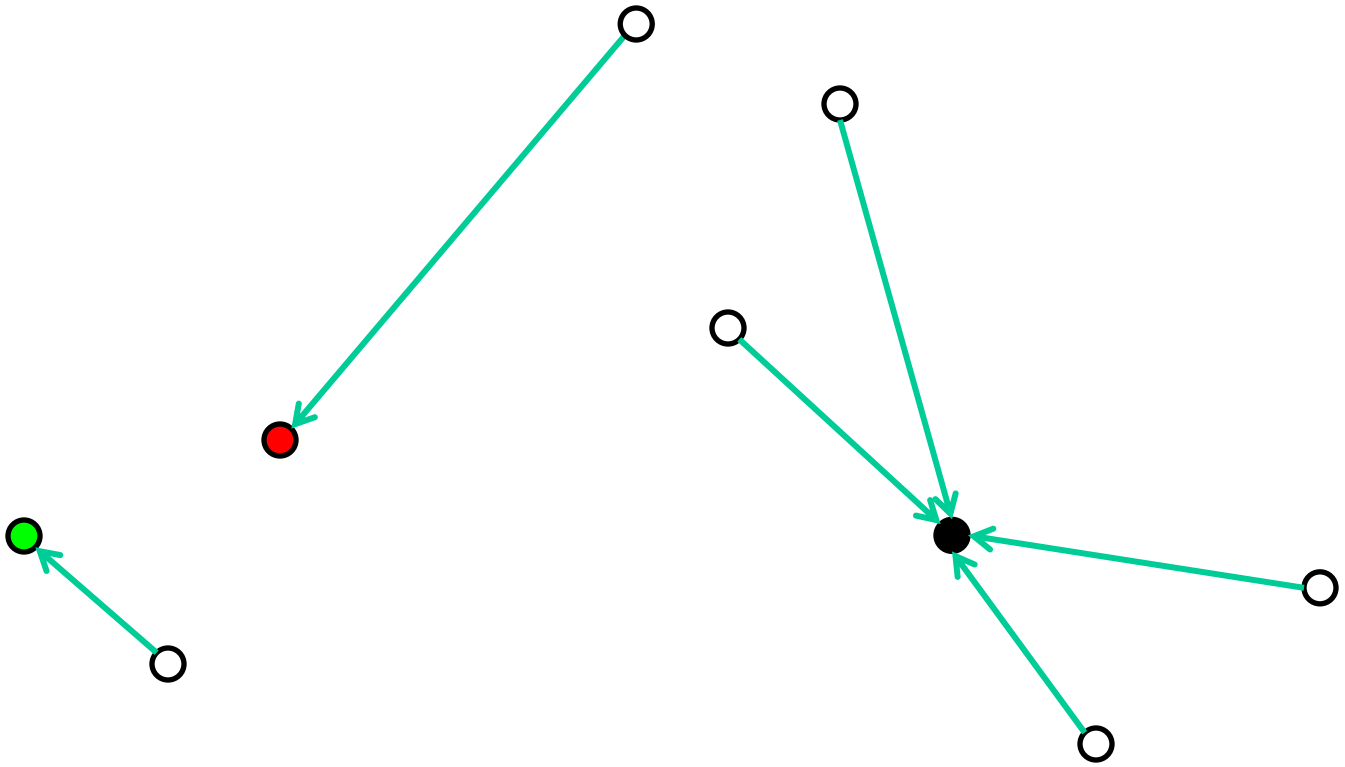
Lloyd's method: Random Initialization

Select initial centers at random



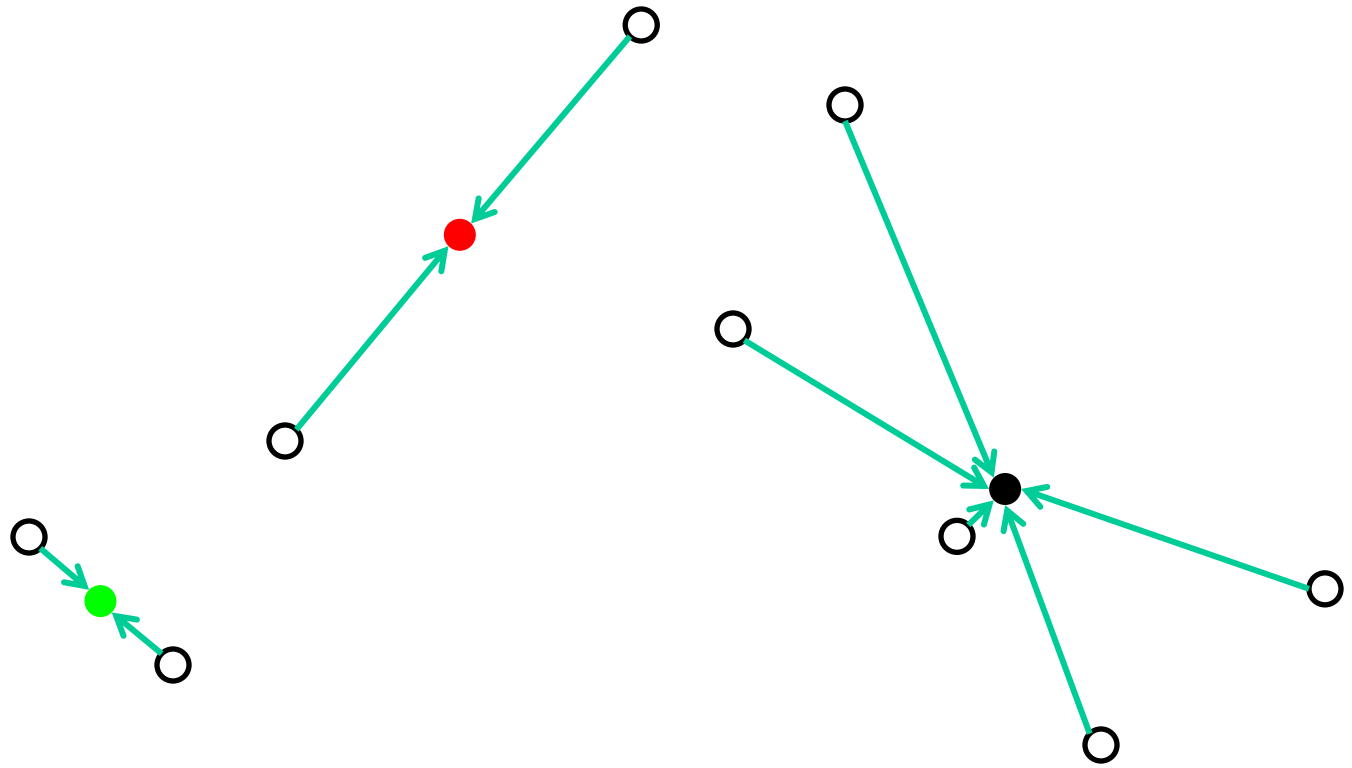
Lloyd's method: Random Initialization

Assign each point to its nearest center



Lloyd's method: Random Initialization

Recompute optimal centers given a fixed clustering



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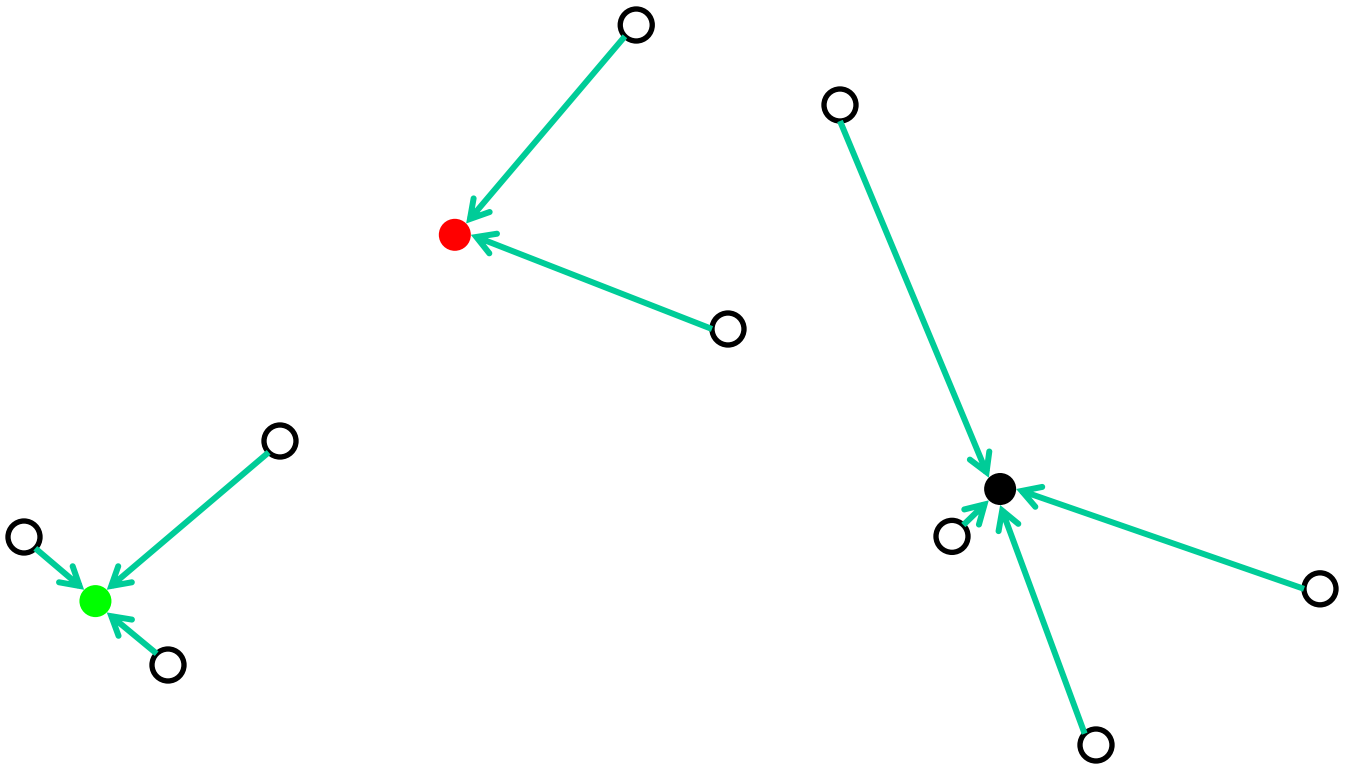

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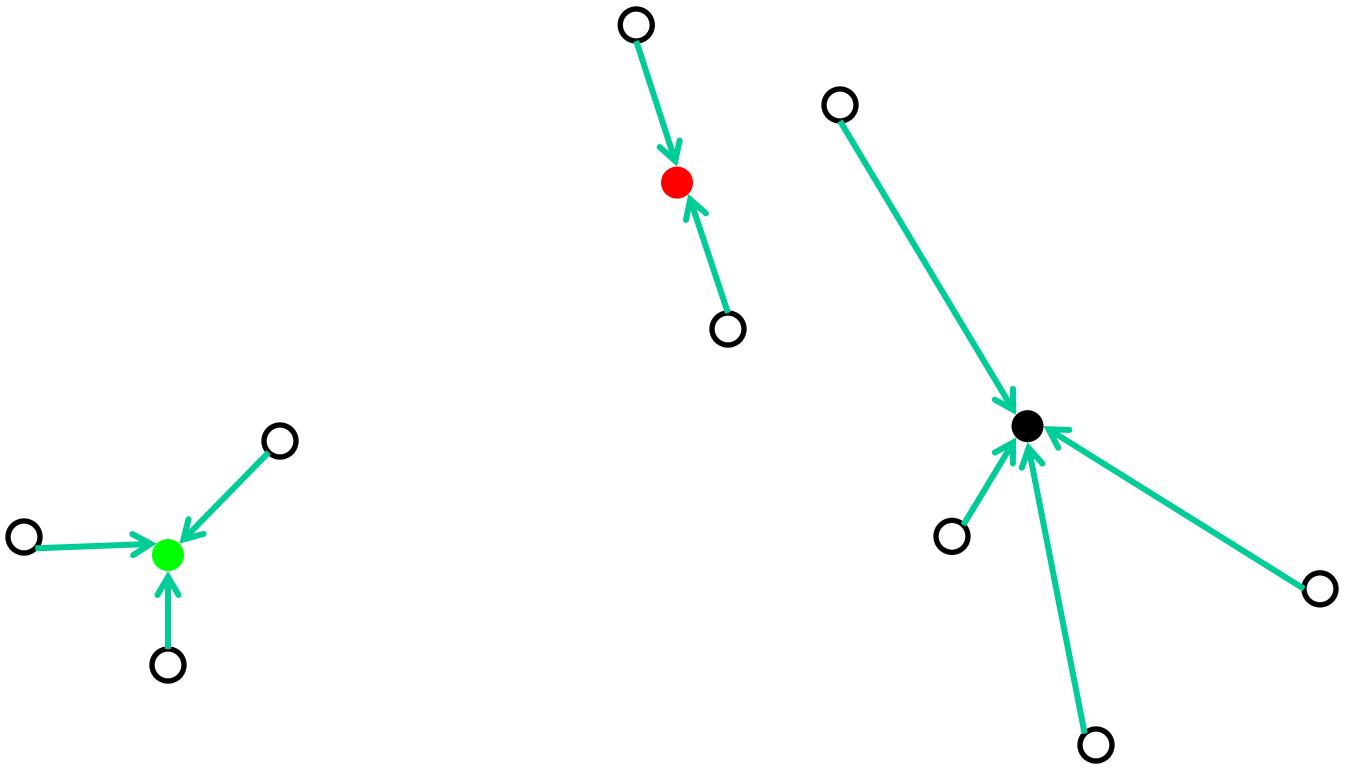

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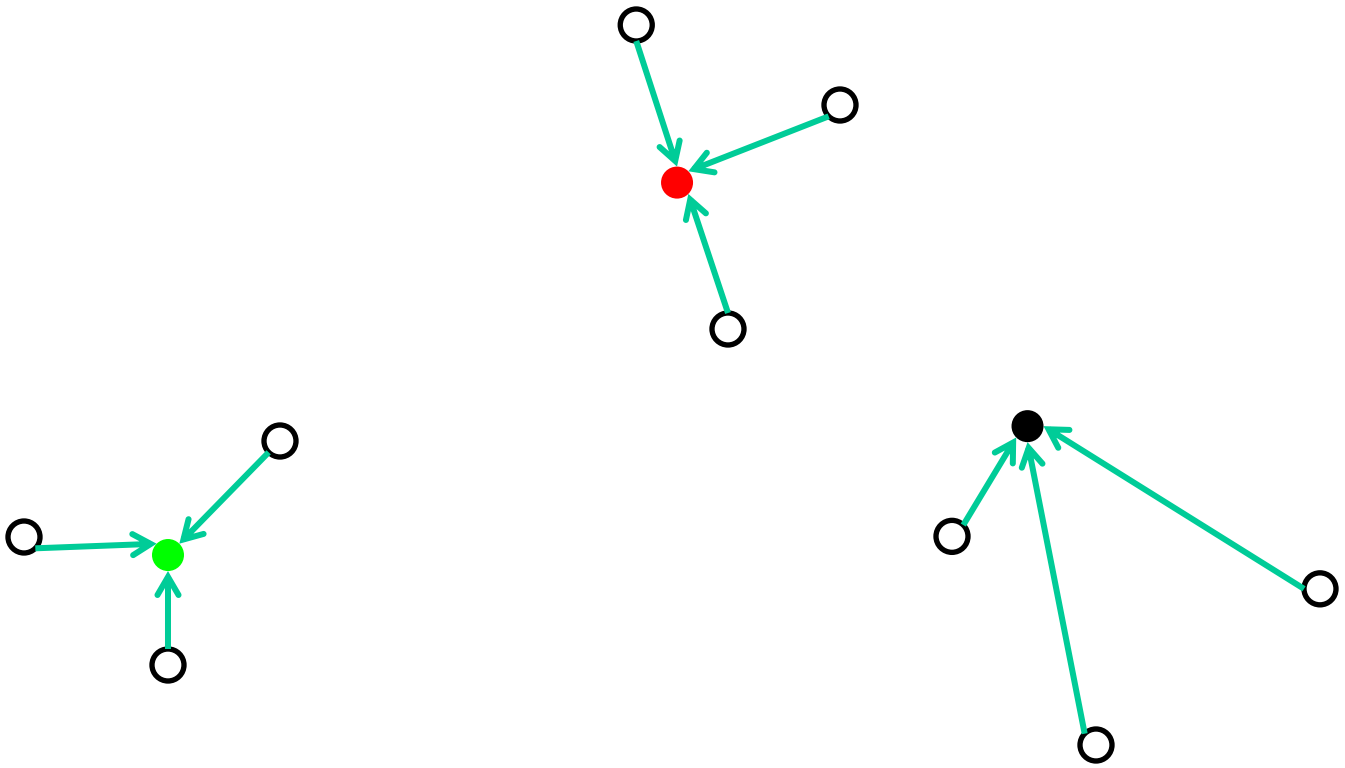

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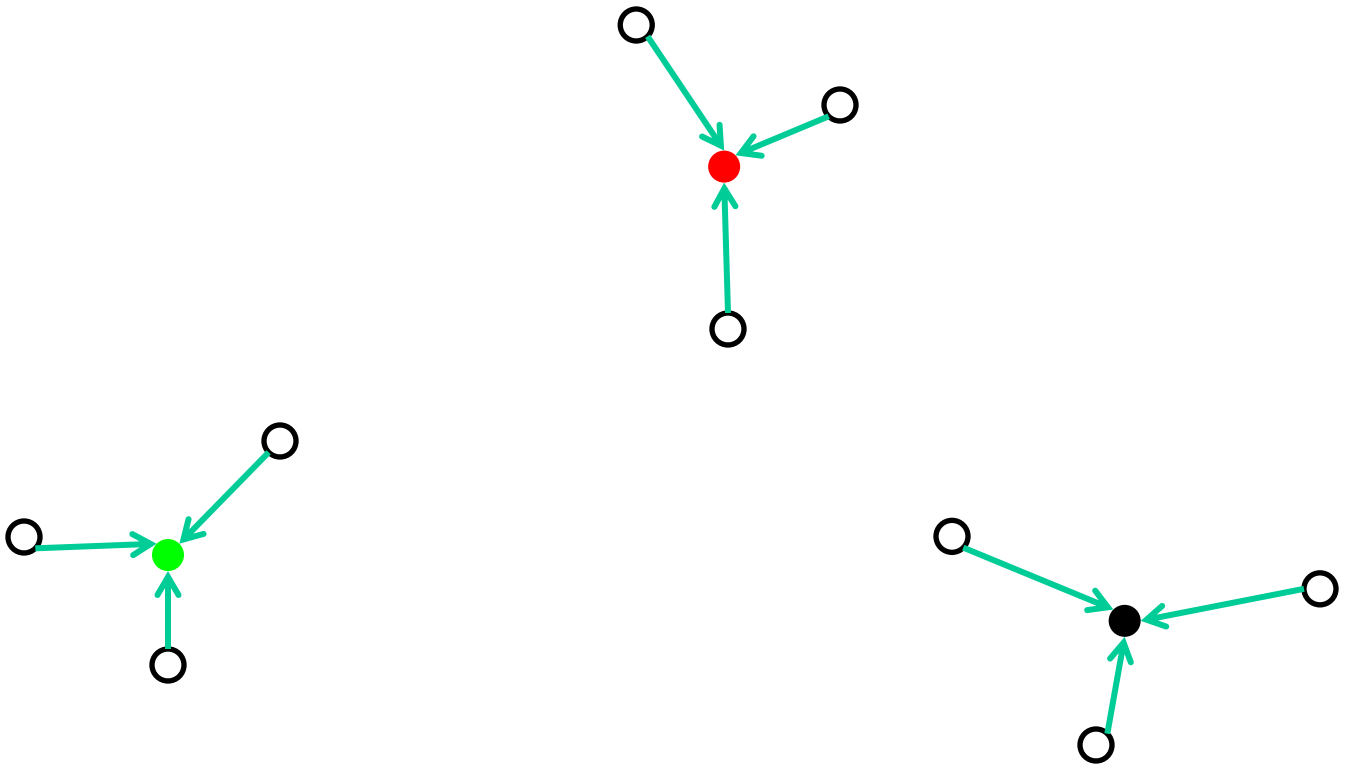
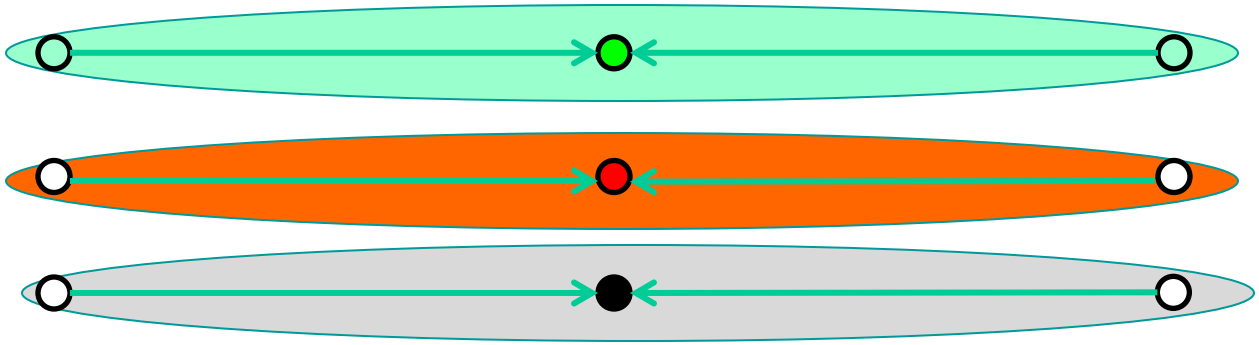


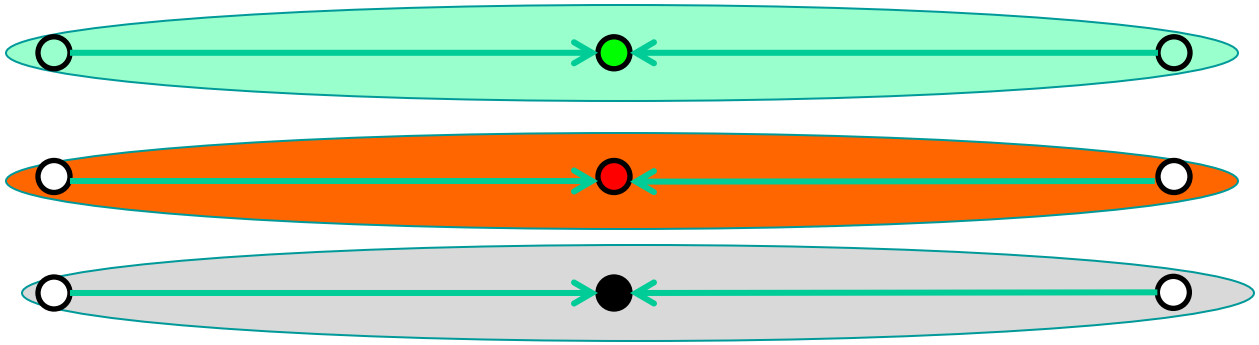
Get a good quality solution in this example.

Lloyd's method: Performance



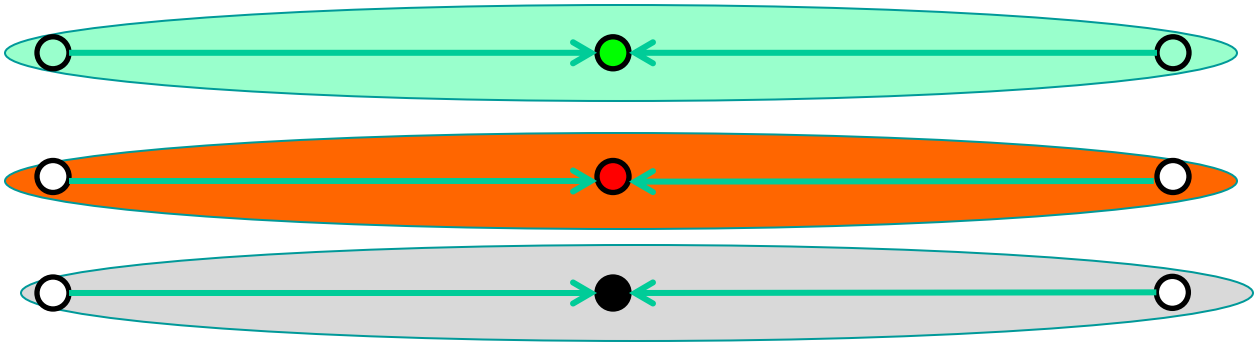
It always converges, but it may converge at a local optimum that is different from the global optimum, and in fact could be arbitrarily worse in terms of its score.

Lloyd's method: Performance

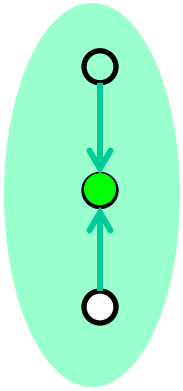


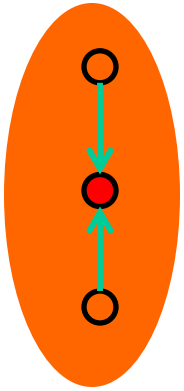
Local optimum: every point is assigned to its nearest center and every center is the mean value of its points.

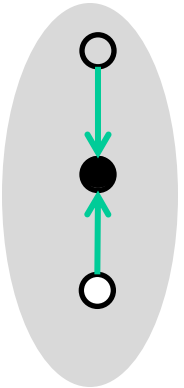
Lloyd's method: Performance



.It is arbitrarily worse than optimum solution….







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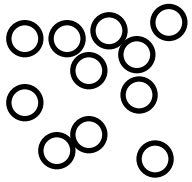
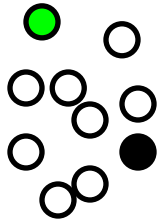
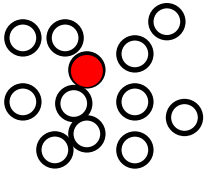
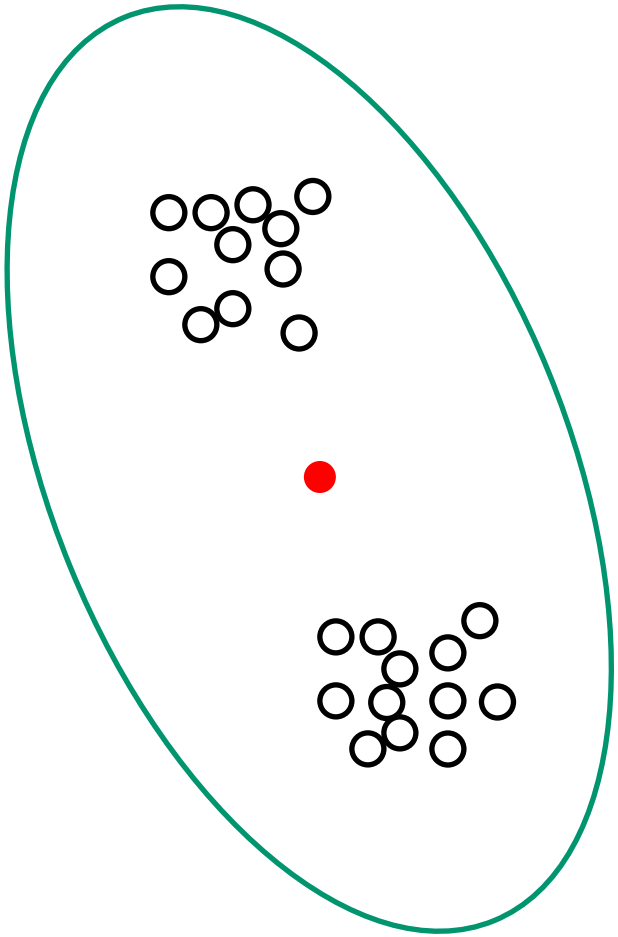


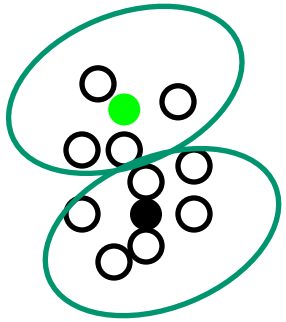




This bad performance, can happen even with well separated Gaussian clusters.

Lloyd's method: Performance





This bad performance, can happen even with well separated Gaussian clusters.

Some Gaussian are combined…..

Lloyd's method: Performance

- If we do random initialization, as k increases, it becomes more likely we won't have perfectly picked one center per Gaussian in our initialization (so Lloyd's method will output a bad solution).
  - For k equal-sized Gaussians, Pr[each initial center is in a different Gaussian] $\approx \frac{k!}{k^k} \approx \frac{1}{e^k}$
  - Becomes unlikely as k gets large.

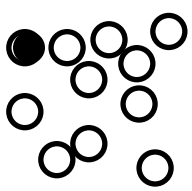
Another Initialization Idea: Furthest Point Heuristic

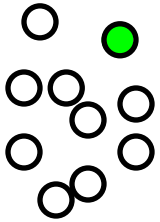
Choose $\mathbf{c_1}$ arbitrarily (or at random).

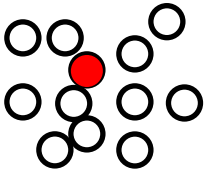
- For $\mathrm{j} = 2, \ldots, \mathrm{k}$
  - Pick $\mathbf{c_j}$ among datapoints $\mathbf{x^1}, \mathbf{x^2}, \ldots, \mathbf{x^d}$ that is farthest from previously chosen $\mathbf{c_1}, \mathbf{c_2}, \ldots, \mathbf{c_{j-1}}$

Fixes the Gaussian problem. But it can be thrown off by outliers….

Furthest point heuristic does well on previous example







Furthest point initialization heuristic sensitive to outliers

Assume k=3

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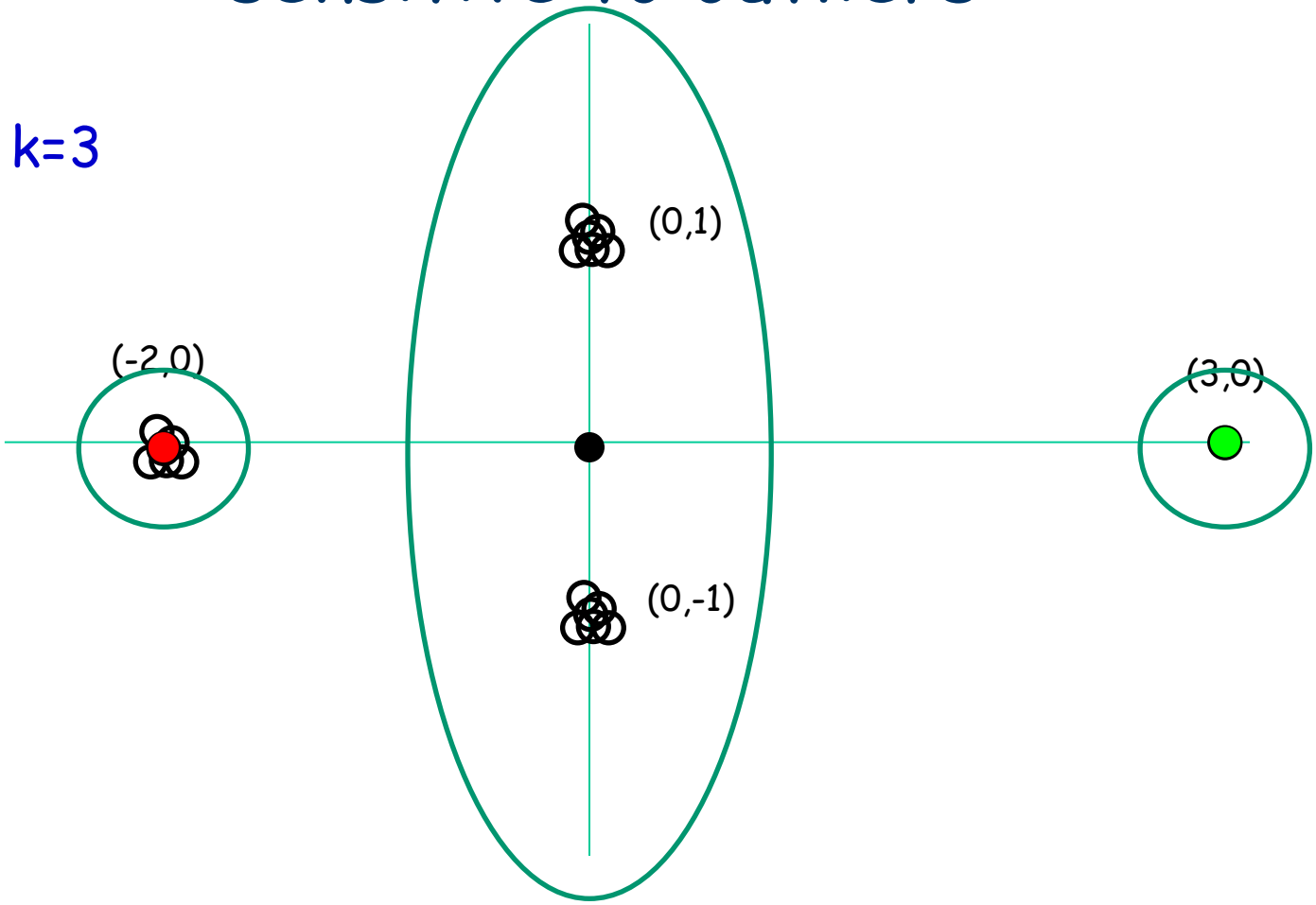


K-means++ Initialization: D^2 sampling [AV07]

- Interpolate between random and furthest point initialization
- Let D(x) be the distance between a point x and its nearest center. Chose the next center proportional to $D^2(x)$.

- Choose c_1 at random.
- For $j = 2, \ldots, k$
  - Pick c_j among $x^1, x^2, \ldots, x^d$ according to the distribution

$$\Pr(c_j = x^i) \propto \min_{j'<j} \left|\left|x^i - c_{j'}\right|\right|^2 \; D^2(x^i)$$

Theorem: K-means++ always attains an $O(\log k)$ approximation to optimal k-means solution in expectation.

Running Lloyd's can only further improve the cost.

K-means++ Idea: D^2 sampling

- Interpolate between random and furthest point initialization
- Let D(x) be the distance between a point x and its nearest center. Chose the next center proportional to $D^{\alpha}(\mathbf{x})$.

  - $\alpha = 0$, random sampling
  - $\alpha = \infty$, furthest point (Side note: it actually works well for k-center)
  - $\alpha = 2$, k-means++

Side note: $\alpha = 1$, works well for k-median

K-means ++ Fix

K-means++/ Lloyd's Running Time

- K-means ++ initialization: $O(nd)$ and one pass over data to select next center. So $O(nkd)$ time in total.
- Lloyd's method

Repeat until there is no change in the cost.

- For each j: $C_j \leftarrow \{x \in S$ whose closest center is $\mathbf{c}_j\}$
  - For each j: $\mathbf{c}_j \leftarrow$ mean of C_j

Each round takes time $O(nkd)$.

- Exponential # of rounds in the worst case [AV07].
- Expected polynomial time in the smoothed analysis model!

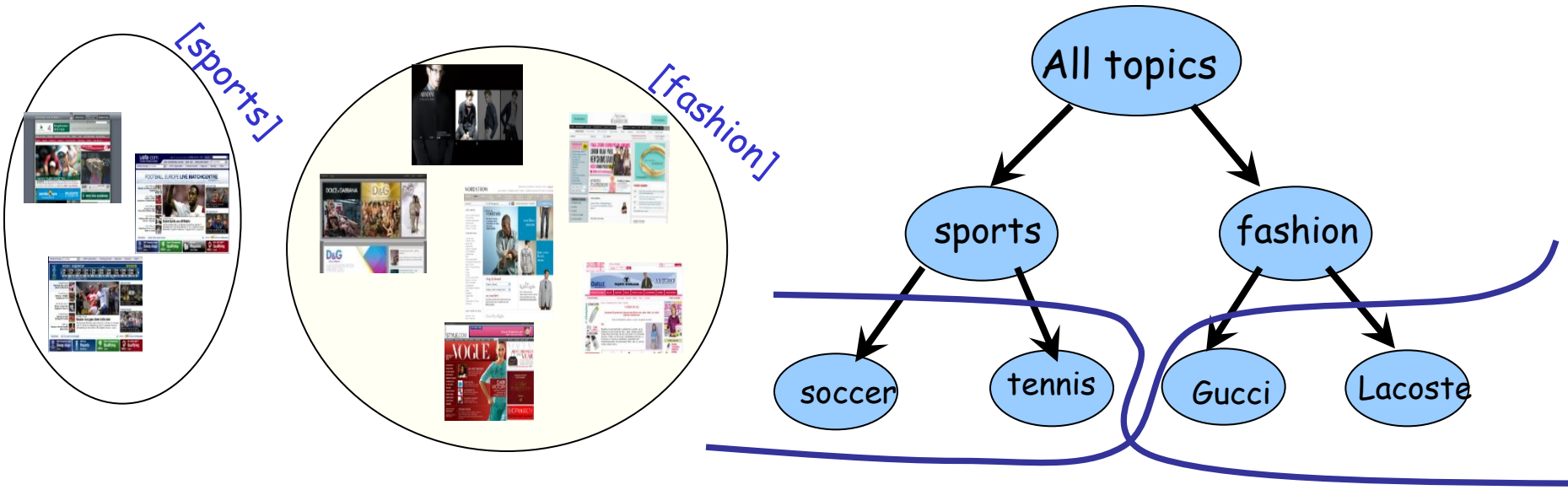
K-means++/ Lloyd's Summary

- K-means++ always attains an $O(\log k)$ approximation to optimal k-means solution in expectation.
- Running Lloyd's can only further improve the cost.
- Exponential # of rounds in the worst case [AV07].
- Expected polynomial time in the smoothed analysis model!
- Does well in practice.

What value of k???

- Heuristic: Find large gap between k -1-means cost and k-means cost.
- Hold-out validation/cross-validation on auxiliary task (e.g., supervised learning task).
- Try hierarchical clustering.

Hierarchical Clustering



- A hierarchy might be more natural.
- Different users might care about different levels of granularity or even prunings.

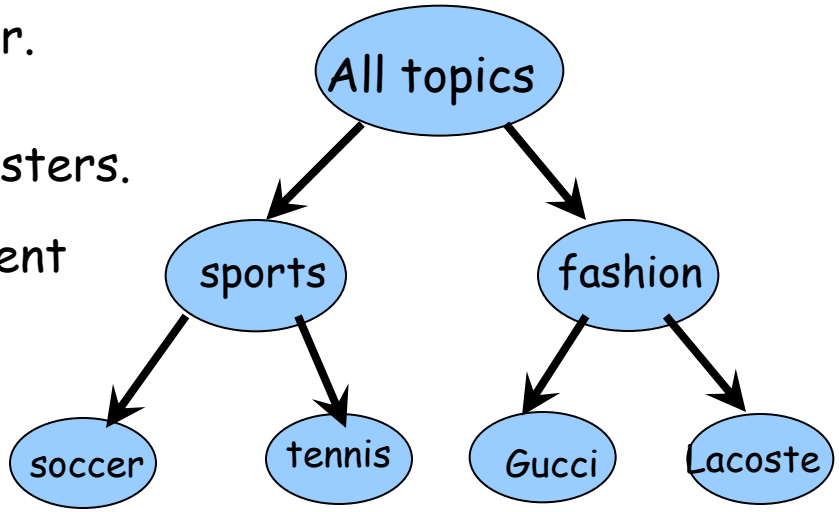
Hierarchical Clustering

Top-down (divisive)

- Partition data into 2-groups (e.g., 2-means)
- Recursively cluster each group.

Bottom-Up (agglomerative)

- Start with every point in its own cluster.
- Repeatedly merge the "closest" two clusters.
- Different defs of "closest" give different algorithms.

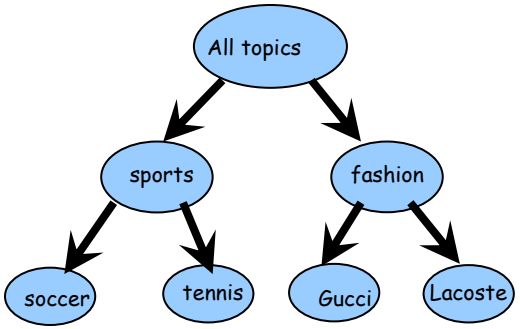


Bottom-Up (agglomerative)

Have a distance measure on pairs of objects.

d(x,y) – distance between x and y

E.g., # keywords in common, edit distance, etc



- Single linkage: $\text{dist}(A, B) = \min_{x \in A, x' \in B'} \text{dist}(x, x')$
- Complete linkage: $\text{dist}(A, B) = \max_{x \in A, x' \in B'} \text{dist}(x, x')$
- Average linkage: $\text{dist}(A, B) = \text{avg}_{x \in A, x' \in B'} \text{dist}(x, x')$
- Wards' method

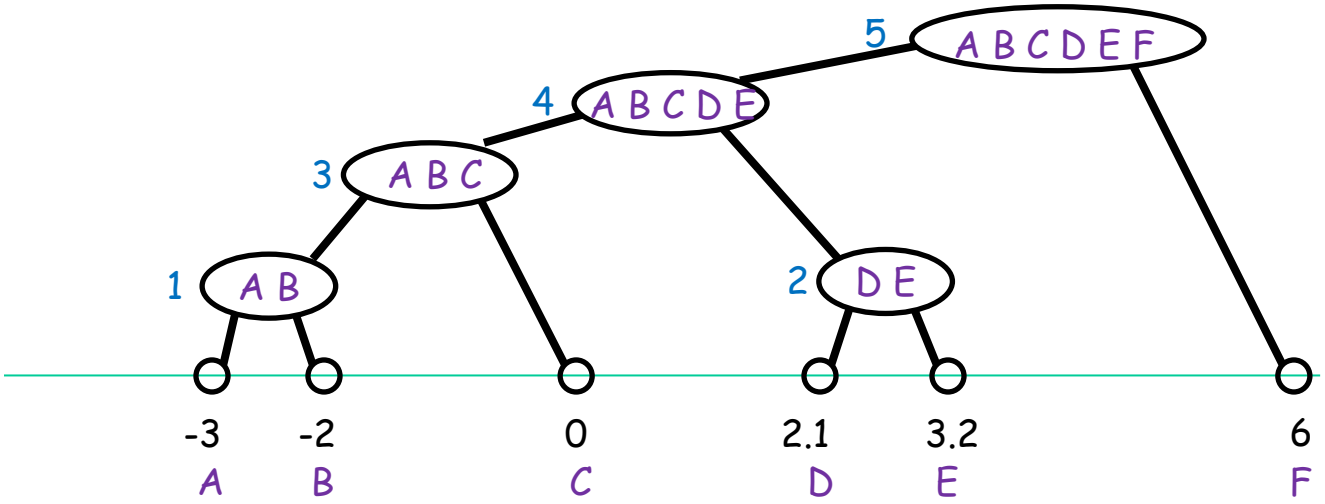
Single Linkage

Bottom-up (agglomerative)

- Start with every point in its own cluster.
- Repeatedly merge the "closest" two clusters.

Single linkage: $\text{dist}(A, B) = \min_{x \in A, x' \in B} \text{dist}(x, x')$

Dendogram



Single Linkage

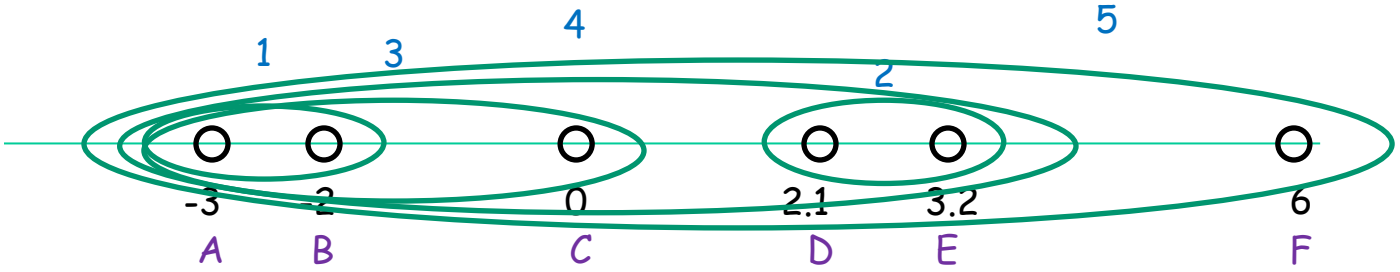
Bottom-up (agglomerative)

- Start with every point in its own cluster.
- Repeatedly merge the "closest" two clusters.

Single linkage: $\text{dist}(A, B) = \min_{x \in A, x' \in B} \text{dist}(x, x')$

One way to think of it: at any moment, we see connected components of the graph where connect any two pts of distance < r.

Watch as r grows (only n-1 relevant values because we only we merge at value of r corresponding to values of r in different clusters).



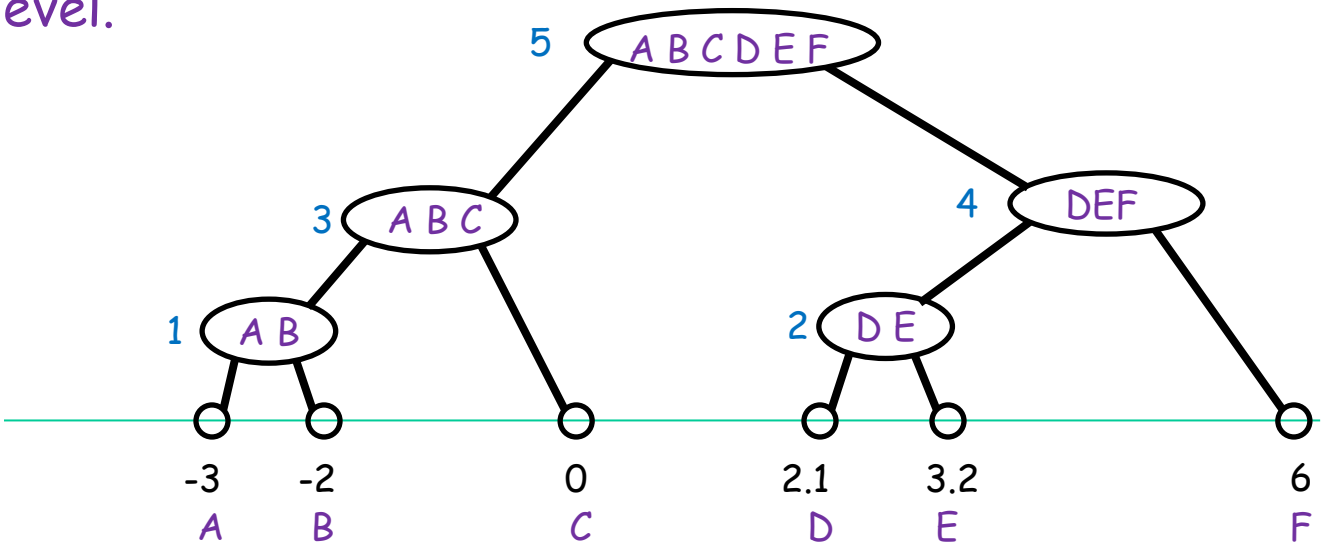
Complete Linkage

Bottom-up (agglomerative)

- Start with every point in its own cluster.
- Repeatedly merge the "closest" two clusters.

Complete linkage: $\text{dist}(A, B) = \max_{x \in A, x' \in B} \text{dist}(x, x')$

One way to think of it: keep max diameter as small as possible at any level.



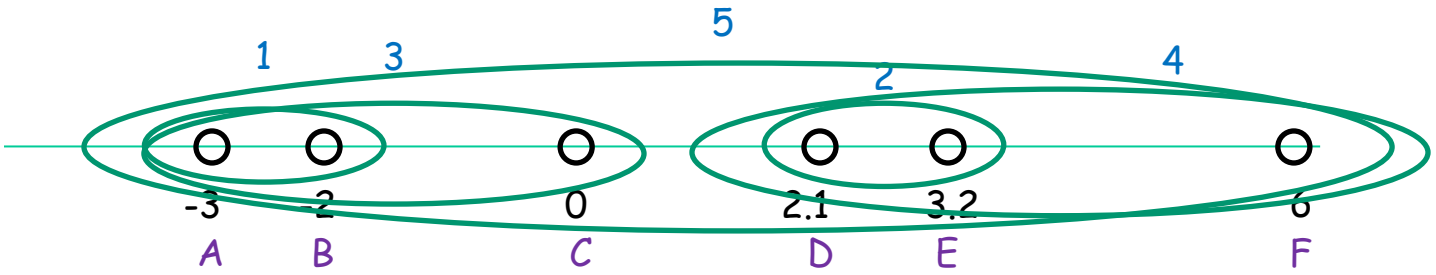
Complete Linkage

Bottom-up (agglomerative)

- Start with every point in its own cluster.
- Repeatedly merge the "closest" two clusters.

Complete linkage: $\text{dist}(A, B) = \max_{x \in A, x' \in B} \text{dist}(x, x')$

One way to think of it: keep max diameter as small as possible.



Ward's Method

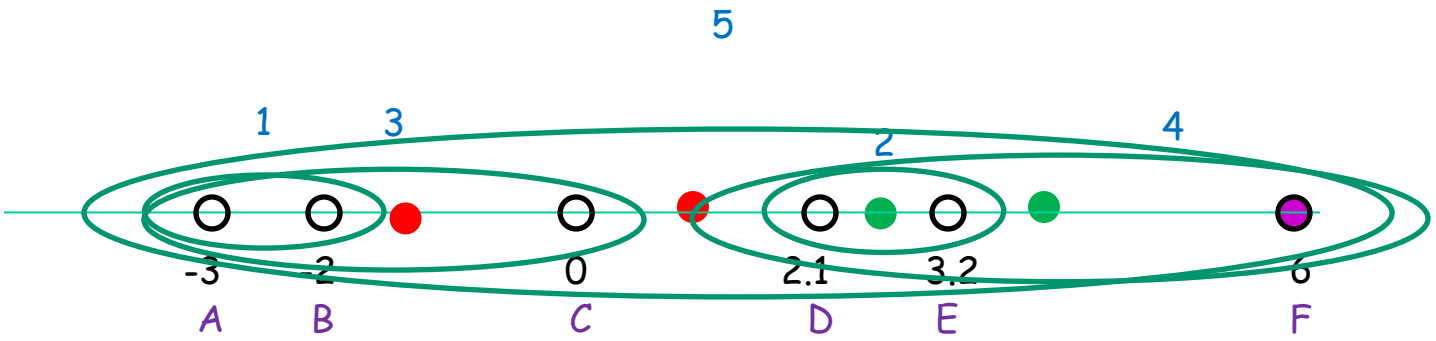
Bottom-up (agglomerative)

- Start with every point in its own cluster.
- Repeatedly merge the "closest" two clusters.

Ward's method: $\mathrm{dist}(C, C') = \frac{|C| \cdot |C'|}{|C| + |C'|} \|\mathrm{mean}(C) - \mathrm{mean}(C')\|^2$

Merge the two clusters such that the increase in k-means cost is as small as possible.

Works well in practice.



Running time

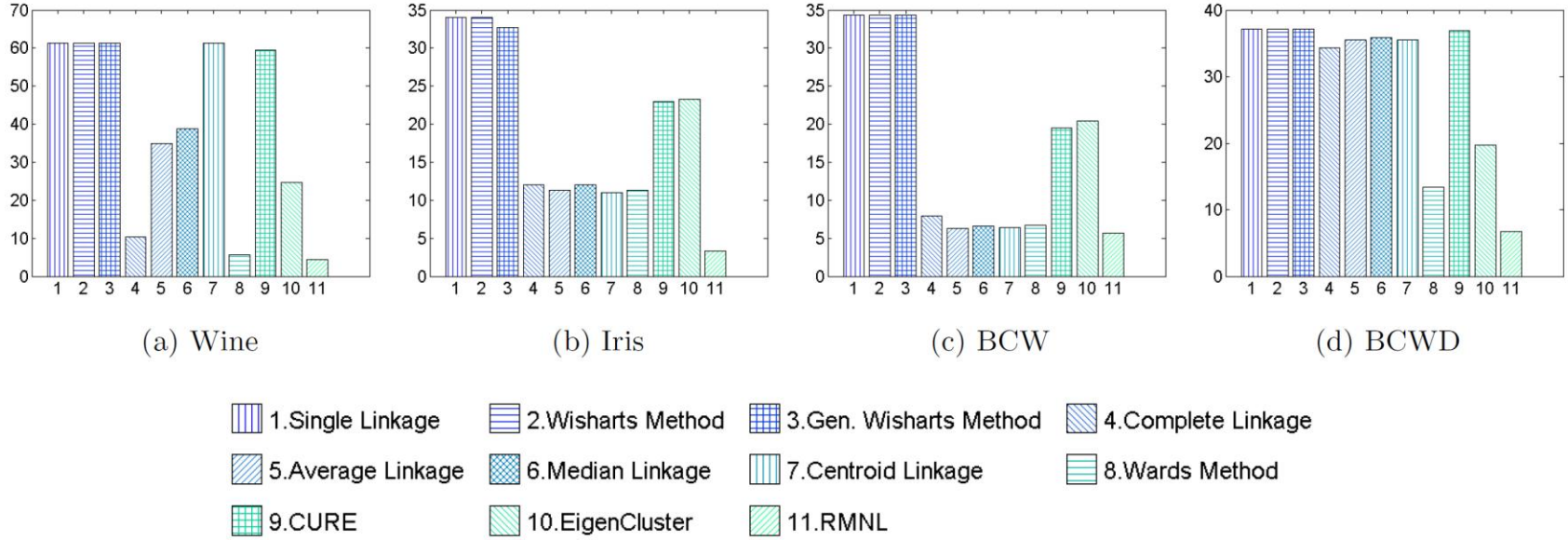
- Each algorithm starts with N clusters, and performs N-1 merges.
- For each algorithm, computing $dist(C, C')$ can be done in time $O(|C| \cdot |C'|)$. (e.g., examining $dist(x, x')$ for all $x \in C, x' \in C'$)
- Time to compute all pairwise distances and take smallest is $O(N^2)$.
- Overall time is $O(N^3)$.

In fact, can run all these algorithms in time $O(N^2 \log N)$.

See: Christopher D. Manning, Prabhakar Raghavan and Hinrich Schütze, Introduction to Information Retrieval, Cambridge University Press. 2008. http://www-nlp.stanford.edu/IR-book/

Hierarchical Clustering Experiments

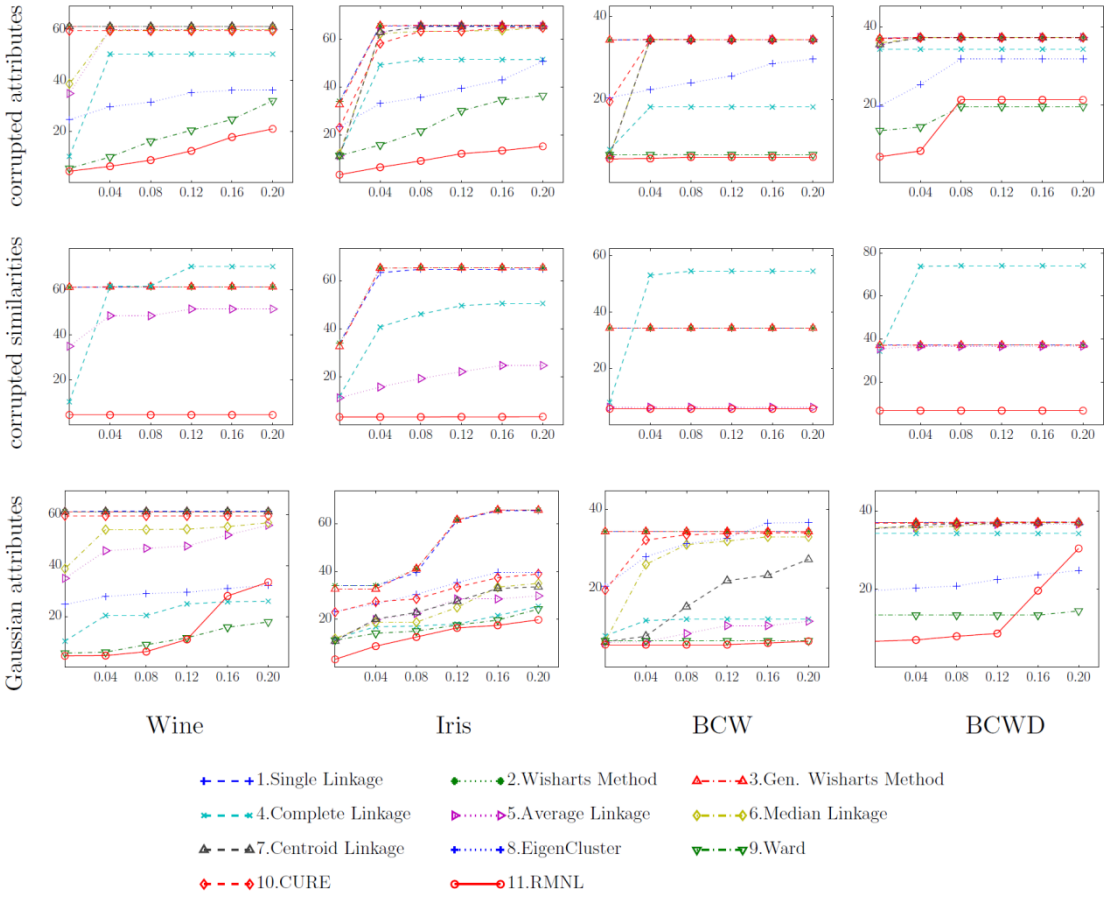
[BLG, JMLR'15]



Ward's method does the best among classic techniques.

Hierarchical Clustering Experiments

[BLG, JMLR'15]



Ward's method does the best among classic techniques.

What You Should Know

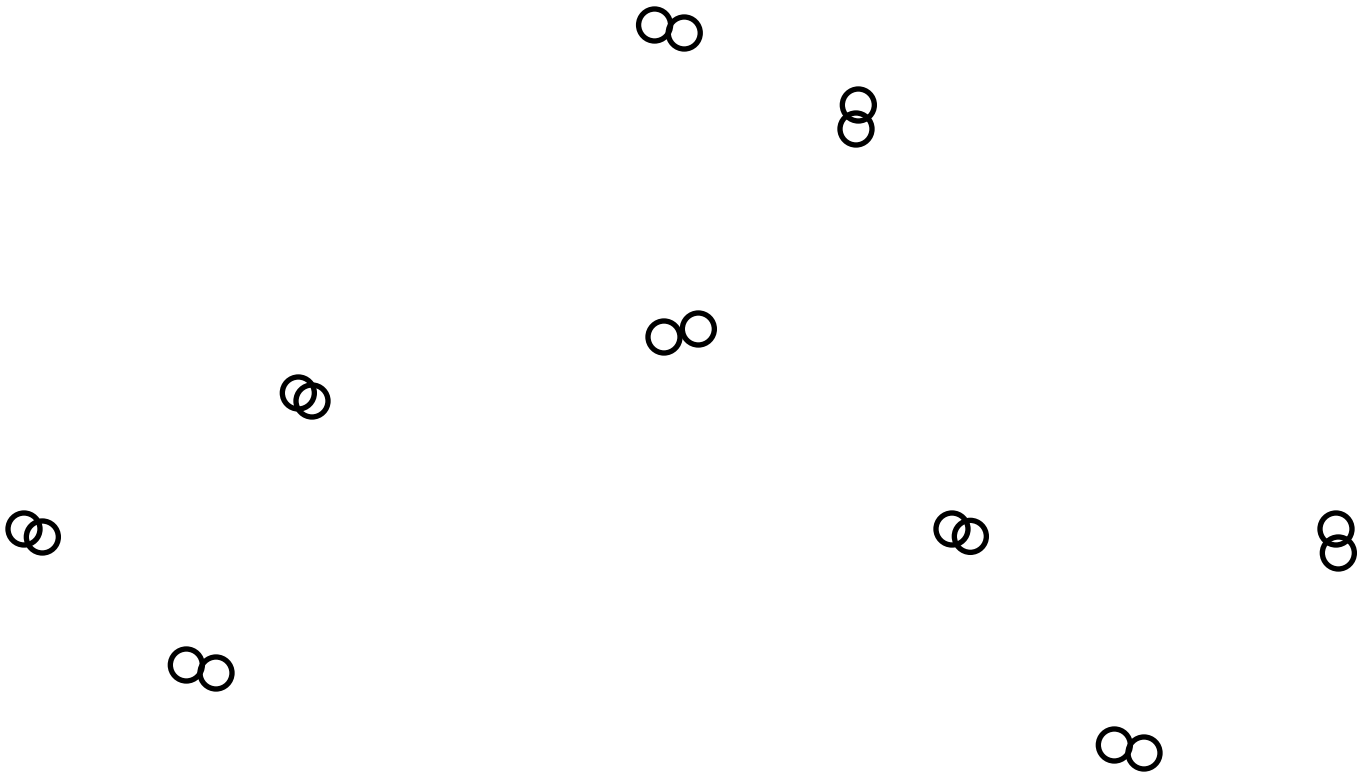
- Partitional Clustering. k-means and k-means ++
  - Lloyd's method
  - Initialization techniques (random, furthest traversal, k-means++)

- Hierarchical Clustering.
  - Single linkage, Complete Linkge, Ward's method

Additional Slides

Smoothed analysis model

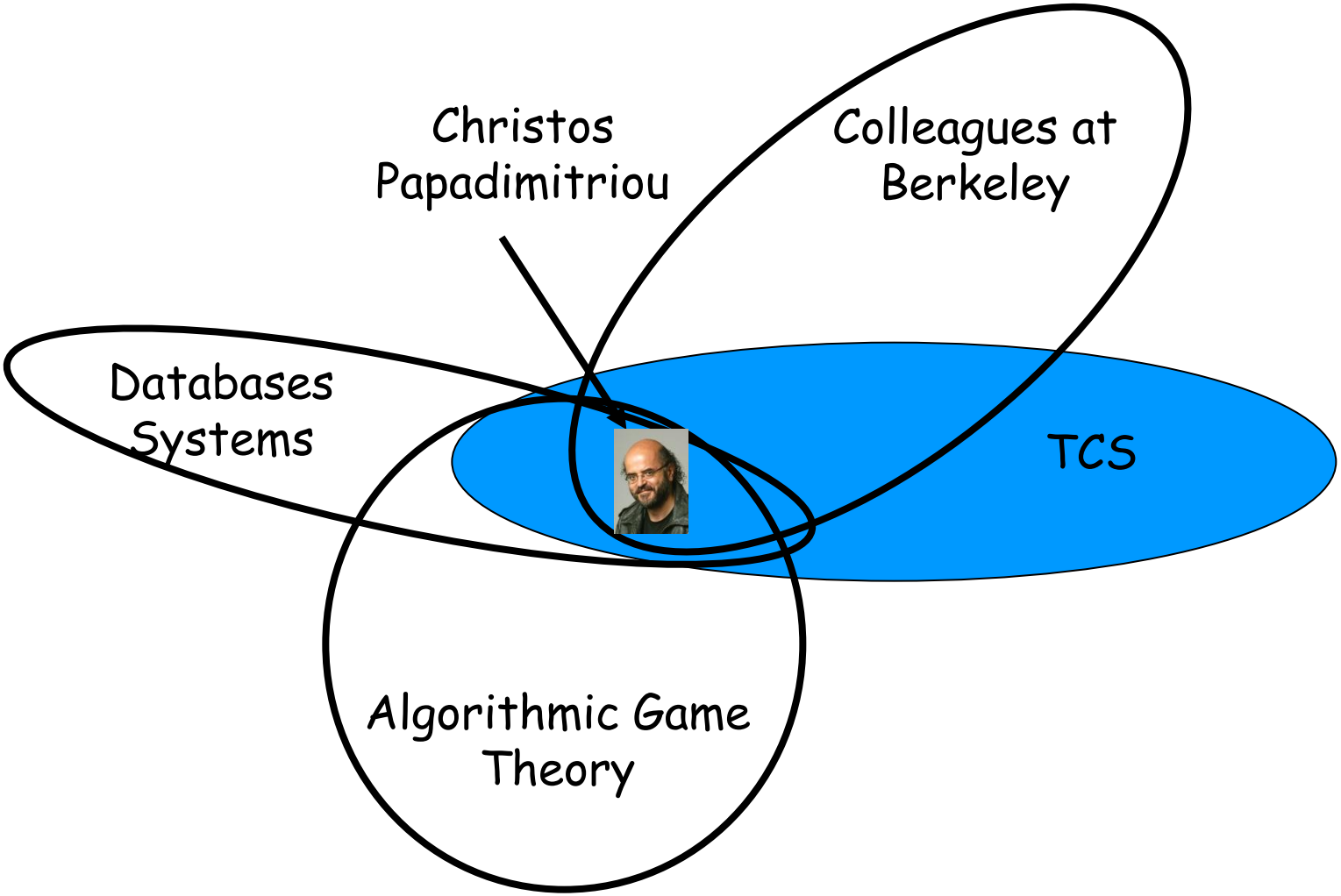
- Imagine a worst-case input.
- But then add small Gaussian perturbation to each data point.



Smoothed analysis model

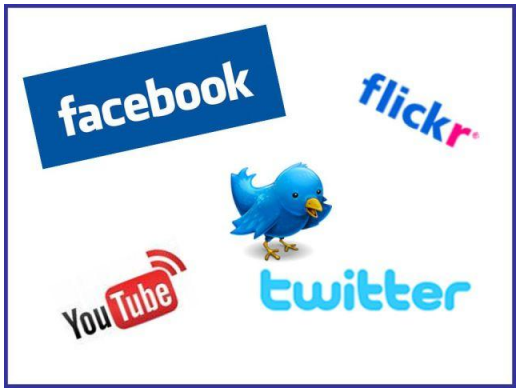
- Imagine a worst-case input.
- But then add small Gaussian perturbation to each data point.
- Theorem [Arthur-Manthey-Roglin 2009]:
  - E[number of rounds until Lloyd's converges] if add Gaussian perturbation with variance σ^2 is polynomial in n, $1/\sigma$.
  - The actual bound is : $O\left(\frac{n^{34}k^{34}d^8}{\sigma^6}\right)$
- Might still find local opt that is far from global opt.

Overlapping Clusters: Communities



Overlapping Clusters: Communities

- Social networks



- Professional networks

- Product Purchasing Networks, Citation Networks, Biological Networks, etc

Overlapping Clusters: Communities