Clustering. Unsupervised Learning

Maria-Florina Balcan 04/06/2015

Reading:

· Chapter 14.3: Hastie, Tibshirani, Friedman.

<u>Additional resources:</u>

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

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.



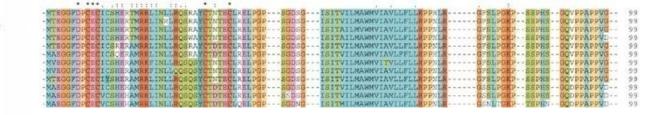




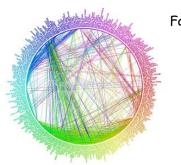


Cluster protein sequences by function or genes according to expression

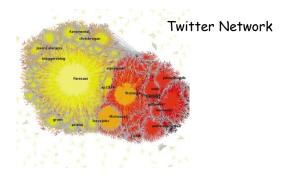
profile.



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



Facebook network



Applications (Clustering comes up everywhere...)

Cluster customers according to purchase history.





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



Image segmentation (clustering pixels)



Clustering

Today:

- Objective based clustering
 Hierarchical clustering
- soft Mention overlapping clusters

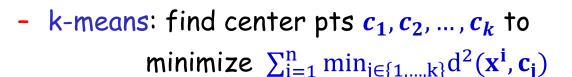
[March 4th: EM-style algorithm for clustering for mixture of Gaussians (specific probabilistic model).]

distance metric learning $d(x_1, x_2) = (x_1-x_2)^T A(x_1-x_2)$. Objective Based Clustering

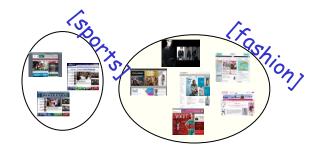
Input: A set 5 of n points, also a distance/dissimilarity measure specifying the distance d(x,y) between pairs (x,y).

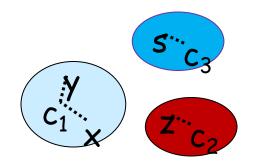
E.g., # keywords in common, edit distance, wavelets coef., etc.

Goal: output a partition of the data.



- k-median: find center pts $c_1, c_2, ..., c_k$ to minimize $\sum_{i=1}^{n} \min_{i \in \{1,...,k\}} d(\mathbf{x}^i, \mathbf{c}_i)$





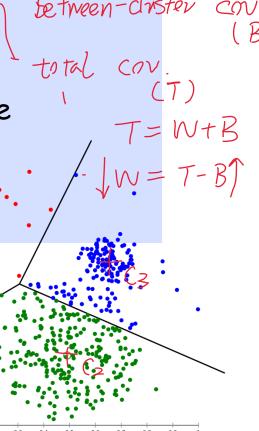
K-center: find partition to minimize the maxim radius

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

Output: k representatives $c_1, c_2, ..., c_k \in \mathbb{R}^d$

Objective: choose $c_1, c_2, ..., c_k \in \mathbb{R}^d$ to minimize

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



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

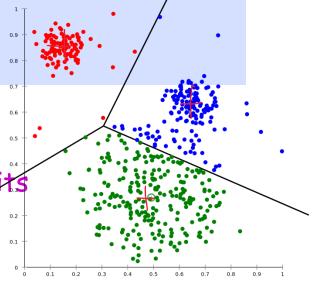
Output: k representatives $c_1, c_2, ..., c_k \in \mathbb{R}^d$

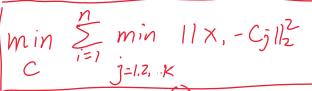
many local
minimum
G

Objective: choose $c_1, c_2, ..., c_k \in \mathbb{R}^d$ to minimize

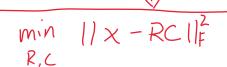
 $\sum_{i=1}^{n} \min_{j \in \{1,\dots,k\}} \left| \left| x^i - c_j \right| \right|^2$

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





min
$$\sum_{k=1}^{\infty} \sum_{j=1}^{\infty} |I| \times i - C_j |I|^2$$
 , $\gamma_{ij} = \begin{cases} 1, \times i \in G_j \\ 0, \text{ otherwise} \end{cases}$

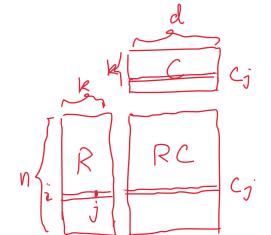


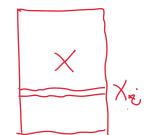
$$|t\alpha|_{z}^{2}=\langle a,a\rangle=\alpha^{T}a$$

$$||A||_F^2 = \langle A, A \rangle = T_r(A^T A)$$

$$= T_r(AA^T)$$

$$\gamma_{ij} = \begin{cases} 1, & \text{if } G_i \\ 0, & \text{otherwise} \end{cases}$$





R: Indicator matrix

Input: A set of n datapoints $x^1, x^2, ..., x^n$ in R^d target #clusters k

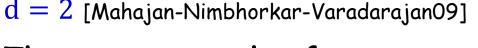
Output: k representatives $c_1, c_2, ..., c_k \in \mathbb{R}^d$

Objective: choose $c_1, c_2, ..., c_k \in \mathbb{R}^d$ to minimize

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

Computational complexity:

NP hard: even for k = 2 [Dagupta'08] or d = 2 [Mahaian Nimbhankan Vanadanaian 00]



There are a couple of easy cases...



An Easy Case for k-means: k=1

Input: A set of n datapoints $x^1, x^2, ..., x^n$ in R^d

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

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

Idea: bias/variance like decomposition

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

Avg k-means cost wrt c

Avg k-means cost wrt μ

So, the optimal choice for c is μ .

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 x¹, x², ..., xn in Rd
    Initialize centers c₁, c₂, ..., ck ∈ Rd and clusters C₁, C₂, ..., Ck in any way.
    Repeat until there is no further change in the cost.
    E-step • For each j: Cj ←{x ∈ S whose closest center is cj}
    M-step • For each j: cj ←mean of Cj
```

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 $x^1, x^2, ..., x^n$ in R^d

Initialize centers $c_1, c_2, ..., c_k \in \mathbb{R}^d$ and clusters $C_1, C_2, ..., C_k$ in any way. $1/X - \mathbb{RCI}_F^2$

Repeat until there is no further change in the cost.

- For each j: $C_j \leftarrow \{x \in S \text{ whose closest center is } c_j\}$
- For each $j: c_j \leftarrow \text{mean of } C_j \leftarrow G_j = \frac{1}{|C_j|} \sum_{x \in C_j} X_i$ $C_j = \left\{ x_i \mid j = \underset{k=1}{\text{arg min } 1/x_i C_k} | |_{2_j}^2 \sum_{i=1,2,...,n} X_i \right\}$

Holding $c_1, c_2, ..., c_k$ fixed, pick optimal $C_1, C_2, ..., C_k$

Holding $C_1, C_2, ..., C_k$ fixed, pick optimal $c_1, c_2, ..., c_k$

Common Heuristic: The Lloyd's method

```
\label{eq:continuous_set} \begin{split} \textbf{Input:} \ \textit{A} \ \textit{set of } n \ \textit{datapoints} \ \mathbf{x^1, x^2, ..., x^n} \ \textit{in} \ R^d \\ \textbf{Initialize} \ \textit{centers} \ \mathbf{c_1, c_2, ..., c_k} \in R^d \ \textit{and} \\ \textit{clusters} \ \textit{C_1, C_2, ..., C_k} \ \textit{in any way}. \end{split}
```

Repeat until there is no further change in the cost.

- For each j: (C_j) ← {x ∈ S whose closest center is c_j }
- ^{2.} C For each j: c_j ← mean of C_j

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)

Common Heuristic: The Lloyd's method

min
$$1/X - RC11_F^2 = Q(R,C)$$
.
S-t.. $R \in \{0,1\}^{n \times k}$, $R = 1_n$

$$I_{R} = \left\{ \left\{ \right\} \right\}_{R}, \quad I_{n} = \left\{ \left\{ \right\} \right\}_{n}$$

t-th iteration.

$$R^{(t-1)}$$
, $C^{(t-1)}$

$$Q(R^{(t)}, C^{(t-1)}) \leq Q(R^{(t-1)}, C^{(t-1)})$$

2.
$$C^{(+)} = avg \min_{C} Q(R^{(+)}, C)$$

 $Q(R^{(+)}, C^{(+)}) \leq Q(R^{(+)}, C^{(+-1)})$

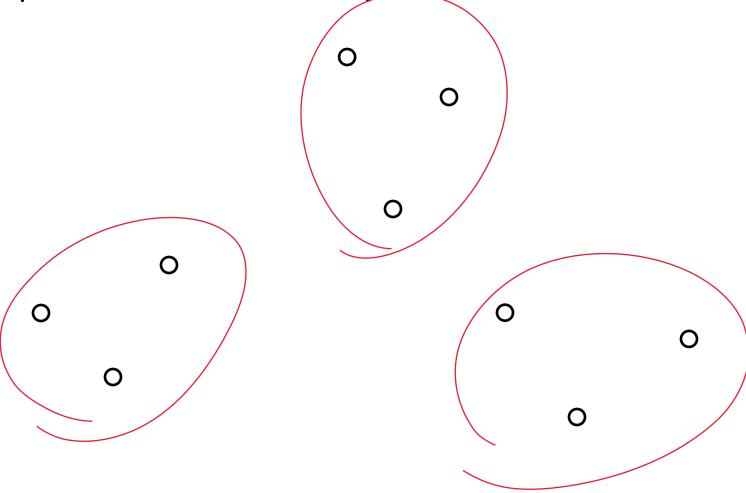
$$\Rightarrow$$
 Q(R⁽⁺⁾, C⁽⁺⁾) \leq Q(R⁽⁺⁻⁾, C⁽⁺⁻⁾)

Initialization for the Lloyd's method

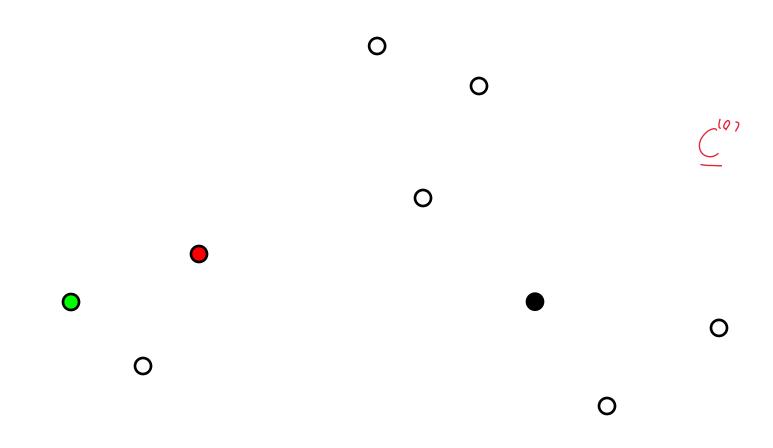
```
\label{eq:continuous_set_of_n_def} \begin{subarray}{ll} \textbf{Input: A set of $n$ datapoints $x^1, x^2, ..., x^n$ in $R^d$ \\ \hline & \textbf{Initialize centers $c_1, c_2, ..., c_k \in R^d$ and \\ & clusters $C_1, C_2, ..., C_k$ in any way. \\ \hline & \textbf{Repeat until there is no further change in the cost.} \\ \end{subarray}
```

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

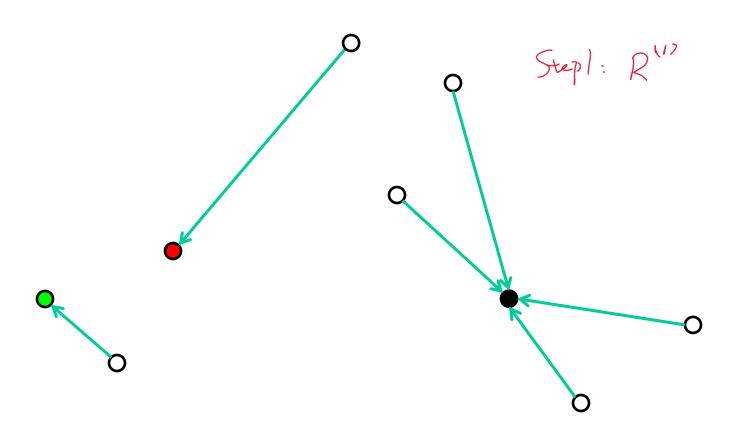
Example: Given a set of datapoints



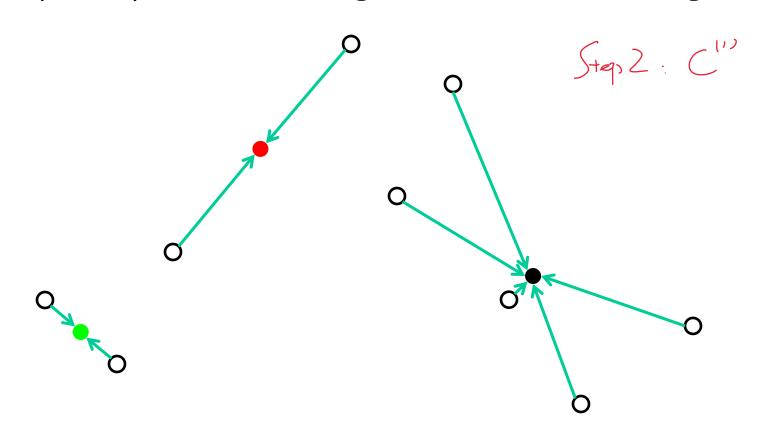
Select initial centers at random



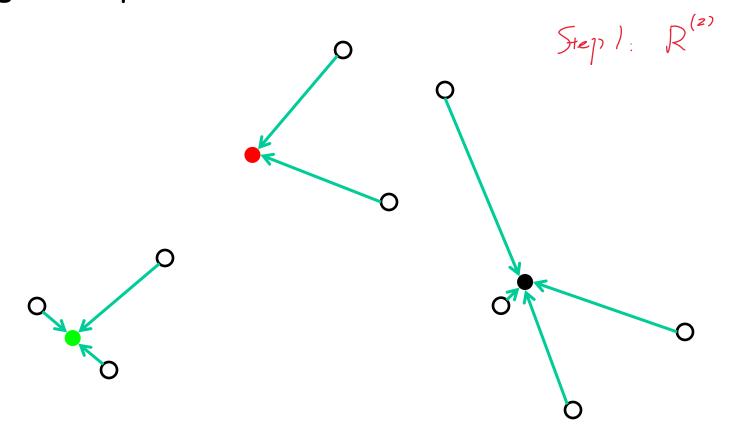
Assign each point to its nearest center



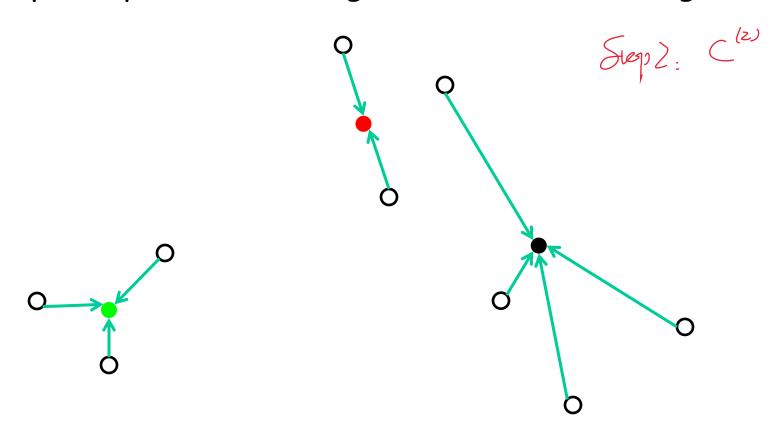
Recompute optimal centers given a fixed clustering



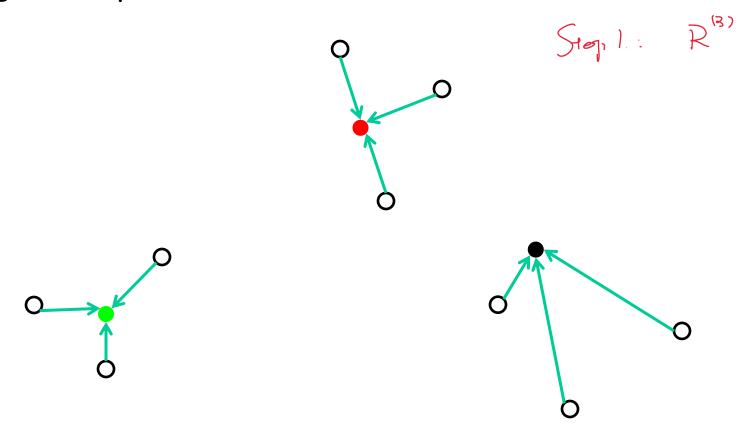
Assign each point to its nearest center



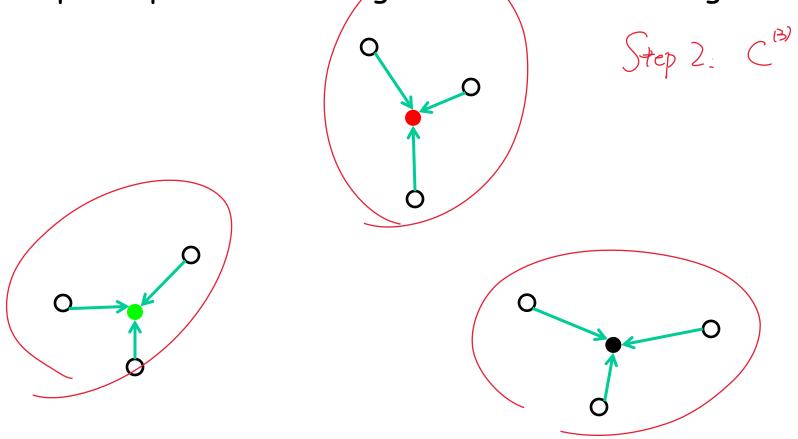
Recompute optimal centers given a fixed clustering



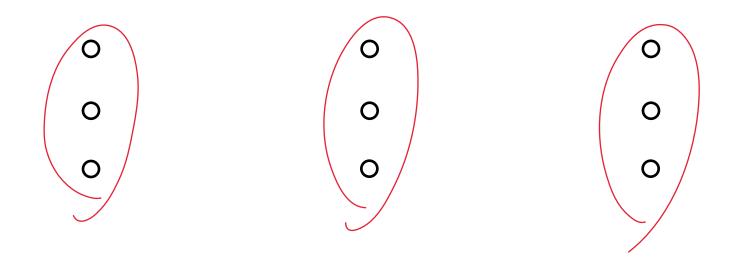
Assign each point to its nearest center



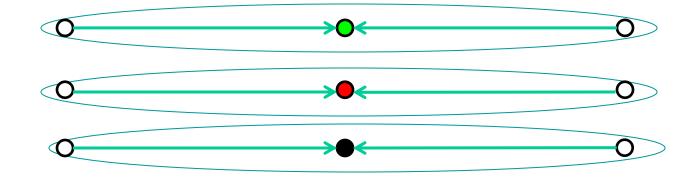
Recompute optimal centers given a fixed clustering



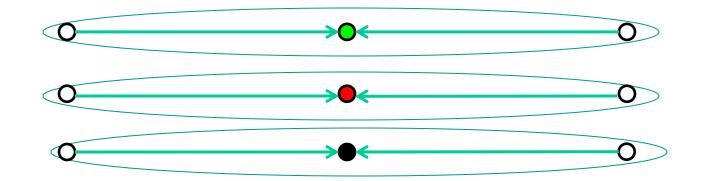
Get a good quality solution in this example.



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.

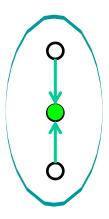


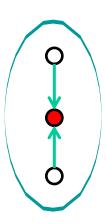
Local optimum: every point is assigned to its nearest center and every center is the mean value of its points.

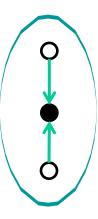


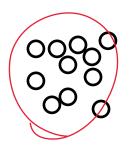
.It is arbitrarily worse than optimum solution....

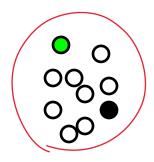


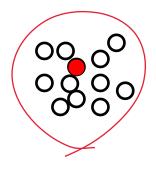




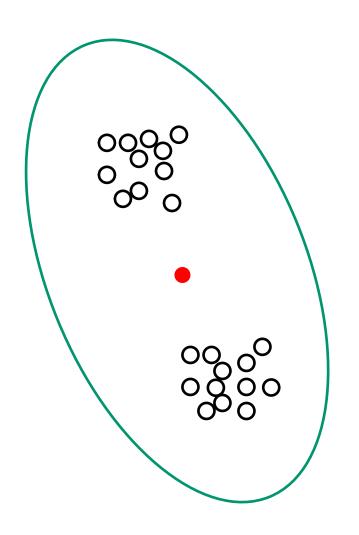


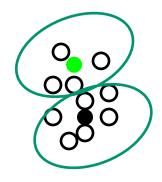






This bad performance, can happen even with well separated Gaussian clusters.





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

Some Gaussian are combined.....



- 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). $L(k-1) \cdot (k-2) \cdot (k-2) \cdot (k-1) \cdot (k-2) \cdot (k-2$
 - For k equal-sized Gaussians, Pr[each initial center is in a different Gaussian] $\approx \frac{k!}{k^k} \approx \frac{1}{e^k}$ $(k+k-1) = O(k^k)$
 - Becomes unlikely as k gets large.

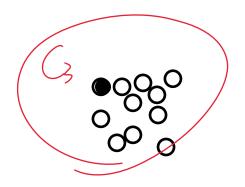
Another Initialization Idea: Furthest Point Heuristic

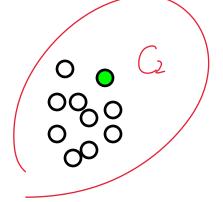
Choose c_1 arbitrarily (or at random).

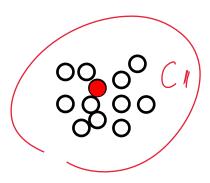
- For j = 2, ..., k
 - Pick c_j among datapoints $x^1, x^2, ..., x^d$ that is farthest from previously chosen $c_1, c_2, ..., c_{j-1}$

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

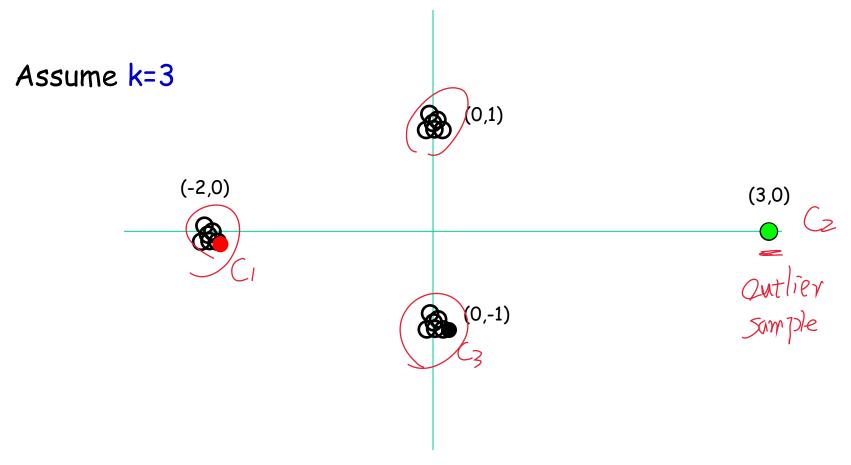
Furthest point heuristic does well on previous example



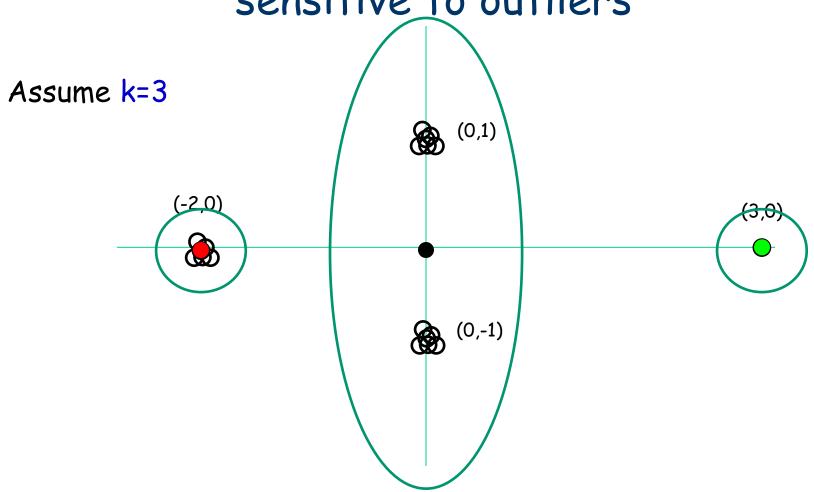




Furthest point initialization heuristic sensitive to outliers



Furthest point initialization heuristic sensitive to outliers



K-means++ Initialization: D² 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, ..., k
 - Pick c_i among $x^1, x^2, ..., x^n$ 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: D² 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 $D^{\alpha}(x)$.
 - $\alpha = 0$, random sampling
 - $\alpha = \infty$, furthest point (Side note: it actually works well for k-center)
 - $\alpha = 2$, k-means++

$$||a||_{\alpha} = \left(\sum_{j=1}^{d} |a_{j}|^{\alpha}\right)^{\frac{1}{\alpha}}$$

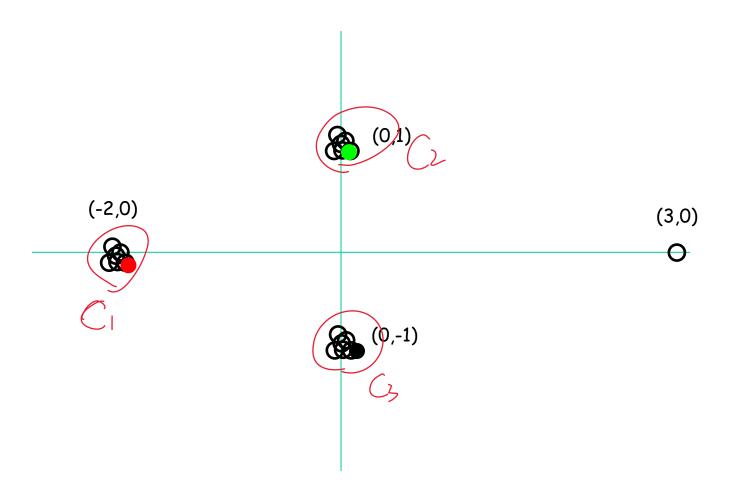
$$||a||_{\alpha} = \sum_{j=1}^{d} |a_{j}|^{\alpha}$$

$$||a||_{\alpha} = \sum_{j=1}^{d} |a_{j}|$$

$$||a||_{\alpha} = \sum_{j=1}^{d} |a_{j}|$$

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

Q(R,c) = 11x- RC 1/2

Repeat until there is no change in the cost.

For each $j: C_j \leftarrow \{x \in S \text{ whose closest center is } c_j\}$

For each $j: c_j \leftarrow \text{mean of } C_j$

Each round takes

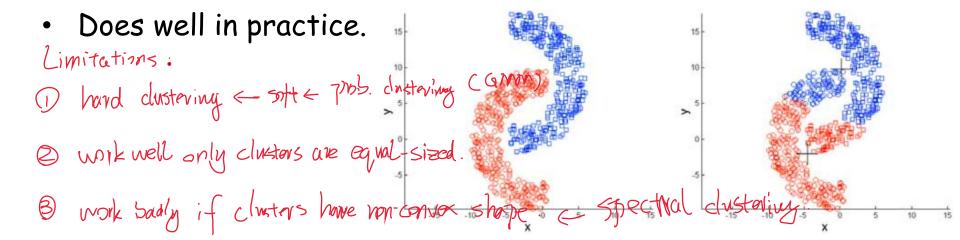
time O(nkd). (T, #iter)

In total: O(nkd) + O(Tnkd)

- 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!



kernel trick

Kernel K-means

= Tr(AA?

min $11X-RCI_F^2 = Q(R,C)$.

S.t. RESPUBLIK, RIK=In.

 $C = (R^T R)^{-1} R^T X$ $= DR^T \times$

 $minQ(R) = 11 \times - RDR^{T} \times 11_{F}^{2}$

R

= < X - RDR X, X - RDR X)

 $= \langle \times, \times \rangle - 2 \langle \times, RDR^T \times \rangle + \langle RDR^T \times, RDR^T \times \rangle$

- EX, ROR'X)

< X RDRXX

 $k(\langle x; x_{3} \rangle) = \langle \phi(x_{1}), \phi(x_{3}) \rangle$

11A1/2= < A. A) $T_{V}(ABC) = T_{V}(CAB)$ =7,(ATA)

= Tr(BCA)

RDRTBORT = RDR7 $= T_r(FXX^TF)$

 $< \times$, $RDR^{T} \times >$ $= T_{r}(x^{T}RDR^{T}x) = T_{r}(x^{T}FF^{T}x)$

 $(F = R(R^TR)^{-\frac{1}{2}})$ weighted indicator

= To (XT RDRT RDRTX)

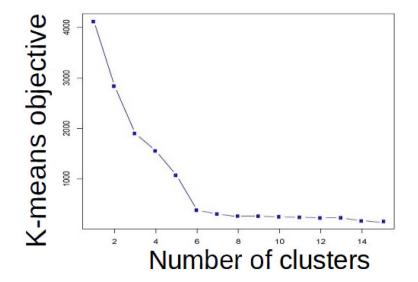
RDRT

Gram.

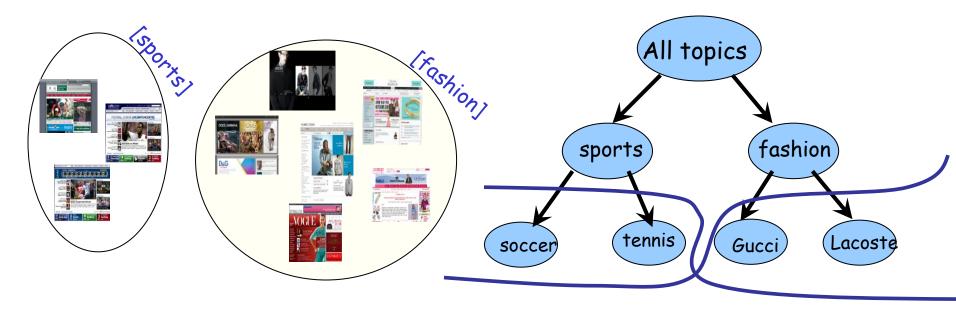
max Tr (FTXXF) S.t. FF=I

What value of k???

- Heuristic: Find large gap between k -1-means cost and k-means cost.
- According to information criteria (AIC, BIC, etc.)
- Try hierarchical clustering.



Hierarchical Clustering

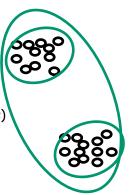


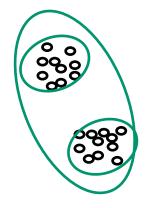
- A hierarchy might be more natural.
- Different users might care about different levels of granularity or even prunings.

Hierarchical Clustering

Top-down (divisive)

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



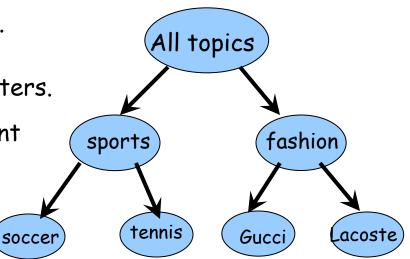


Bottom-Up (agglomerative)

Start with every point in its own cluster.

Repeatedly merge the "closest" two clusters.

 Different defs of "closest" give different algorithms.

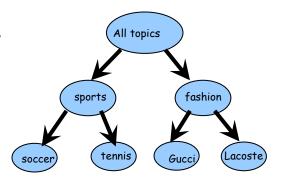


Bottom-Up (agglomerative)

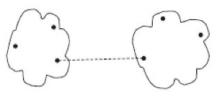
Have a distance measure on pairs of objects.

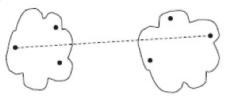
d(x,y) - distance between x and y

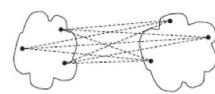
E.g., # keywords in common, edit distance, etc



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







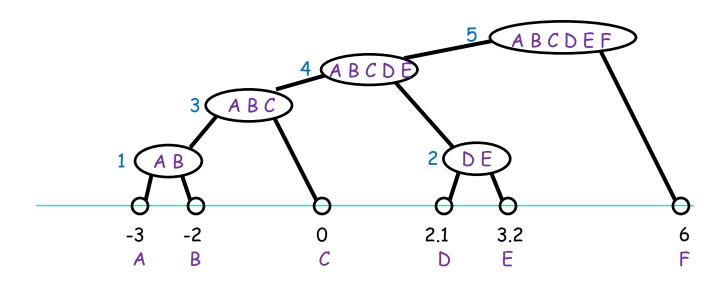
Single Linkage

Bottom-up (agglomerative)

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

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

Dendogram



Single Linkage

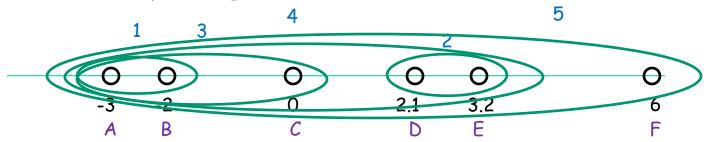
Bottom-up (agglomerative)

- Start with every point in its own cluster.
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Single linkage:
$$dist(A, B) = \min_{x \in A, x' \in B} dist(x, x')$$

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).



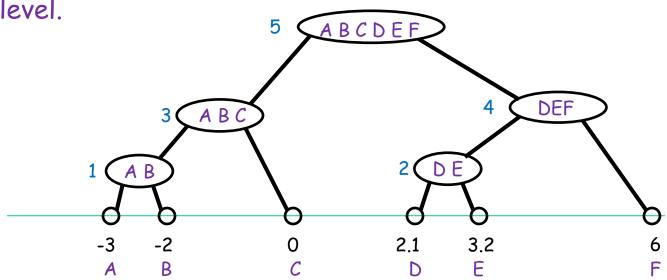
Complete Linkage

Bottom-up (agglomerative)

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

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

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



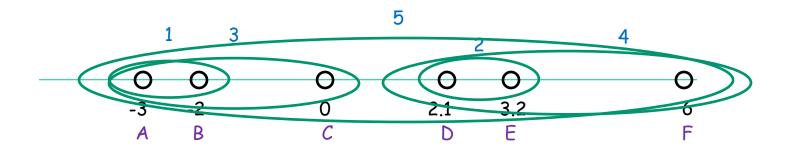
Complete Linkage

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Ward's Method

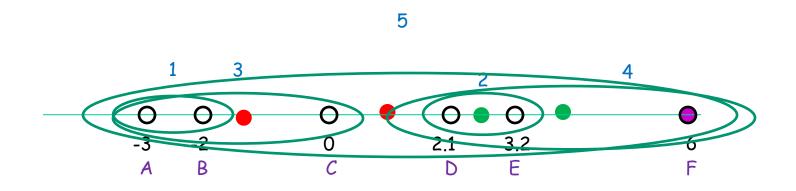
Bottom-up (agglomerative)

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

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

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

Works well in practice.



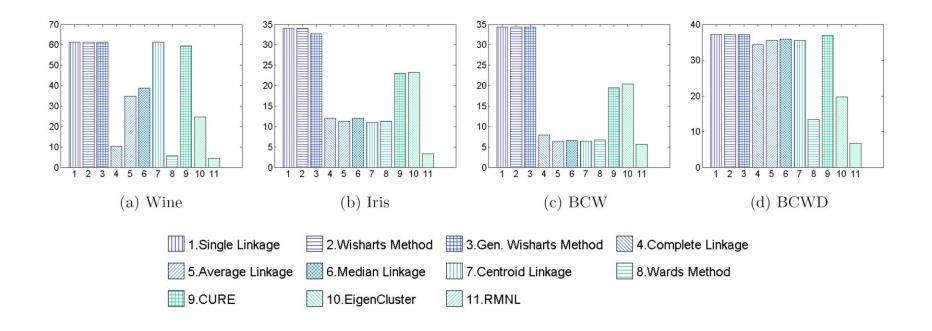
Running time

- 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 $O(N^2 \log N)$.

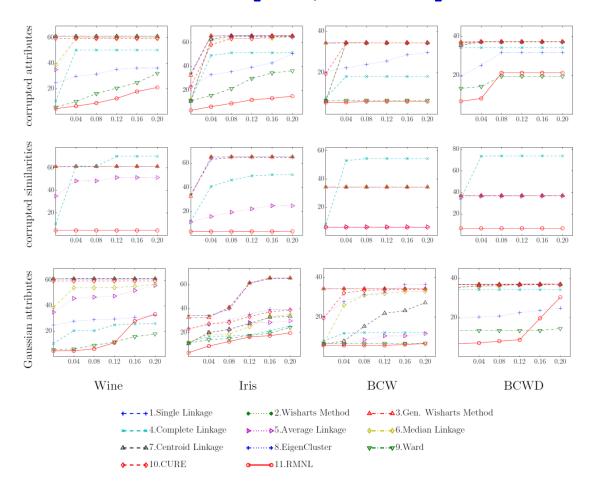
See: Christopher D. Manning, Prabhakar Raghavan and Hinrich Schütze, Introduction to Information Retrieval, Cambridge University Press. 2008. http://www-nlp.stanford.edu/IR-book/

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

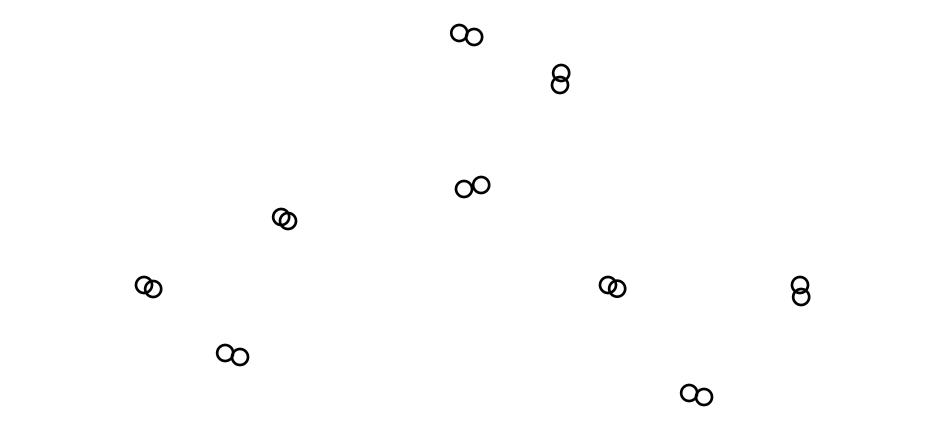
- Partitional Clustering. k-means and k-means ++
 - Lloyd's method
 - Initialization techniques (random, furthest traversal, k-means++)

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

Additional Slides

Smoothed analysis model

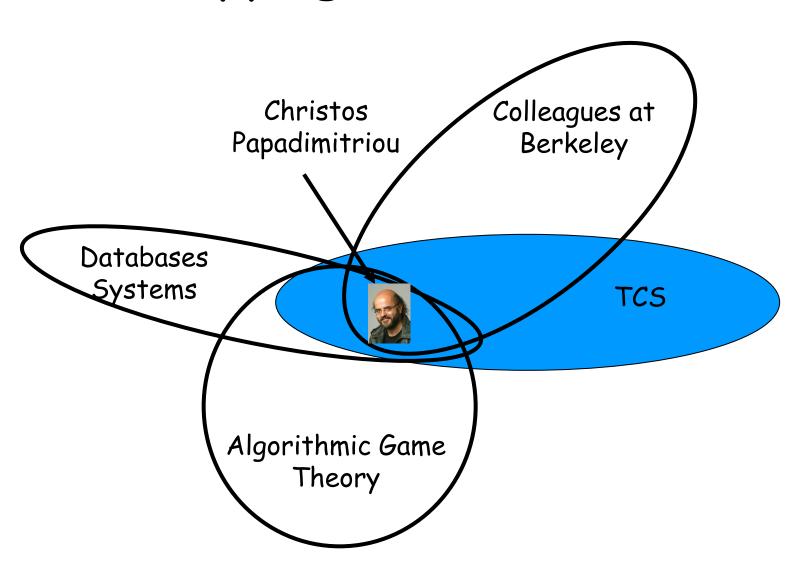
- Imagine a worst-case input.
- But then add small Gaussian perturbation to each data point.



Smoothed analysis model

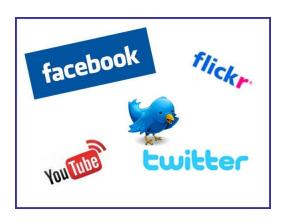
- Imagine a worst-case input.
- But then add small Gaussian perturbation to each data point.
- Theorem [Arthur-Manthey-Roglin 2009]:
 - E[number of rounds until Lloyd's converges] if add Gaussian perturbation with variance σ^2 is polynomial in n, $1/\sigma$.
 - The actual bound is : $O\left(\frac{n^{34}k^{34}d^8}{\sigma^6}\right)$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

