Clustering

Overview

- Supervised vs. Unsupervised Learning
- Curse of Dimensionality
- K-means
  - Algorithm
  - Choosing K (# of clusters)

- Hierarchical clustering
  - Algorithm
  - Choosing K (# of clusters)

Unsupervised Learning

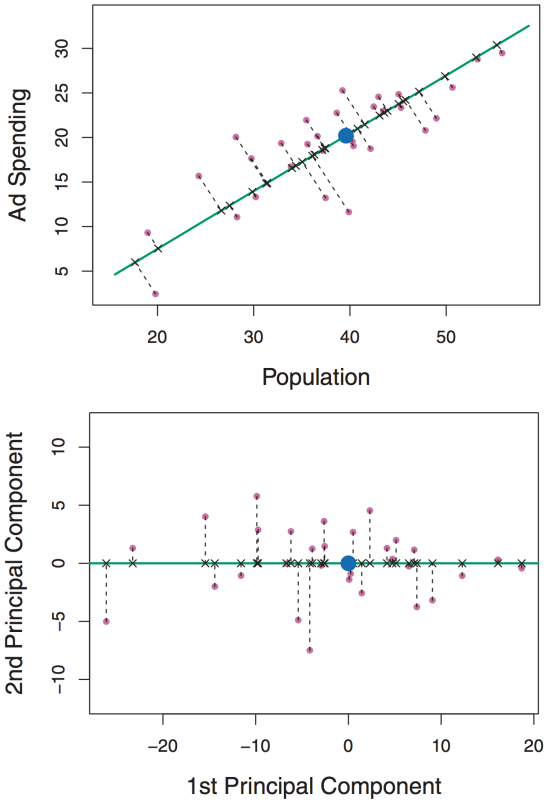
- No response variable, y
  - Just based on predictors, X_1, X_2, X_3, …, X_p
- A fuzzy endeavor...
  - Not cross-validating to choose best "model" in usual sense
  - Not cross-validating to know how well you're doing
- Can be useful as
  - ✓ preprocessing step for supervised learning
  - ✓ better understand features

Unsupervised Learning

Two most common and contrasting unsupervised techniques

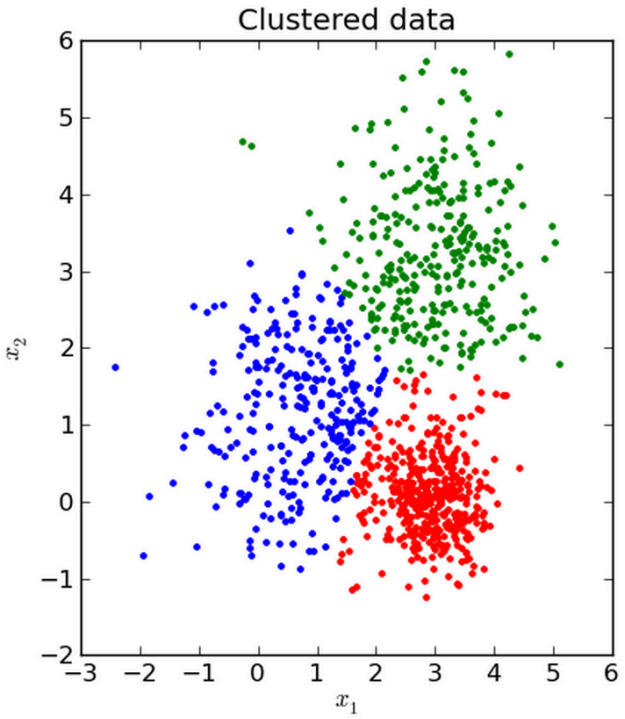
PCA

Low-dim representation of data that explains good fraction of variance



Clustering

Find homogenous subgroups among data



Supervised Learning

- **The label is the supervisor!**

  No label ⇔ Not supervised

  – K-means clustering is not supervised learning, nor is hierarchical clustering

  – PCA is not supervised learning

  ⇒Though again, both can be used in supervised learning!

- Supervised Learning

  – Linear, Logistic, Lasso, Ridge

  – Decision Trees, Bagging, Random Forest, Boosting

  – SVM

  – kNN

Curse of Dimensionality

First let's take a detour and re-visit Linear Regression and k-th Nearest Neighbor

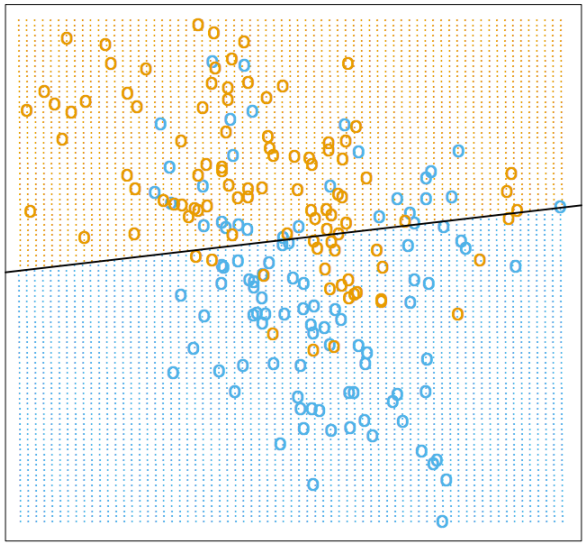
Linear Models

- Very structured
- Stable but possibly inaccurate
- Low Variance, High Bias

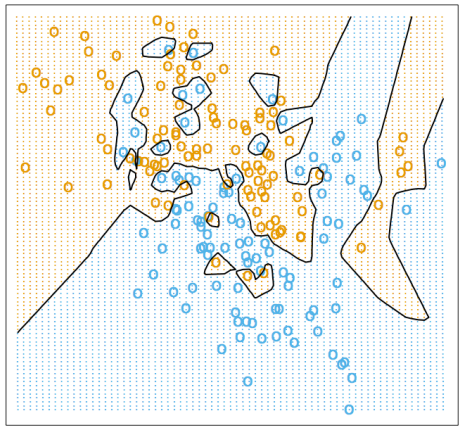
k-th Nearest Neighbor

- Very mildly structural
- Often accurate, but unstable
- High Variance, Low Bias

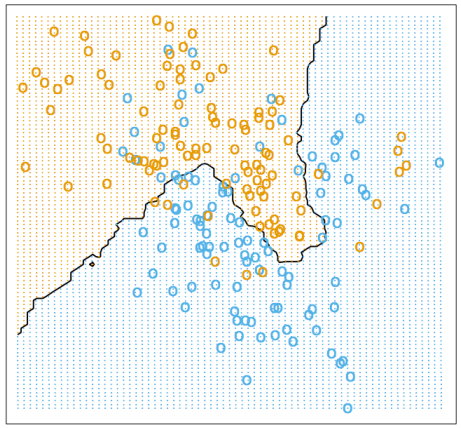
Linear Regression with 0/1 Response



1-Nearest Neighbor



15-Nearest Neighbor

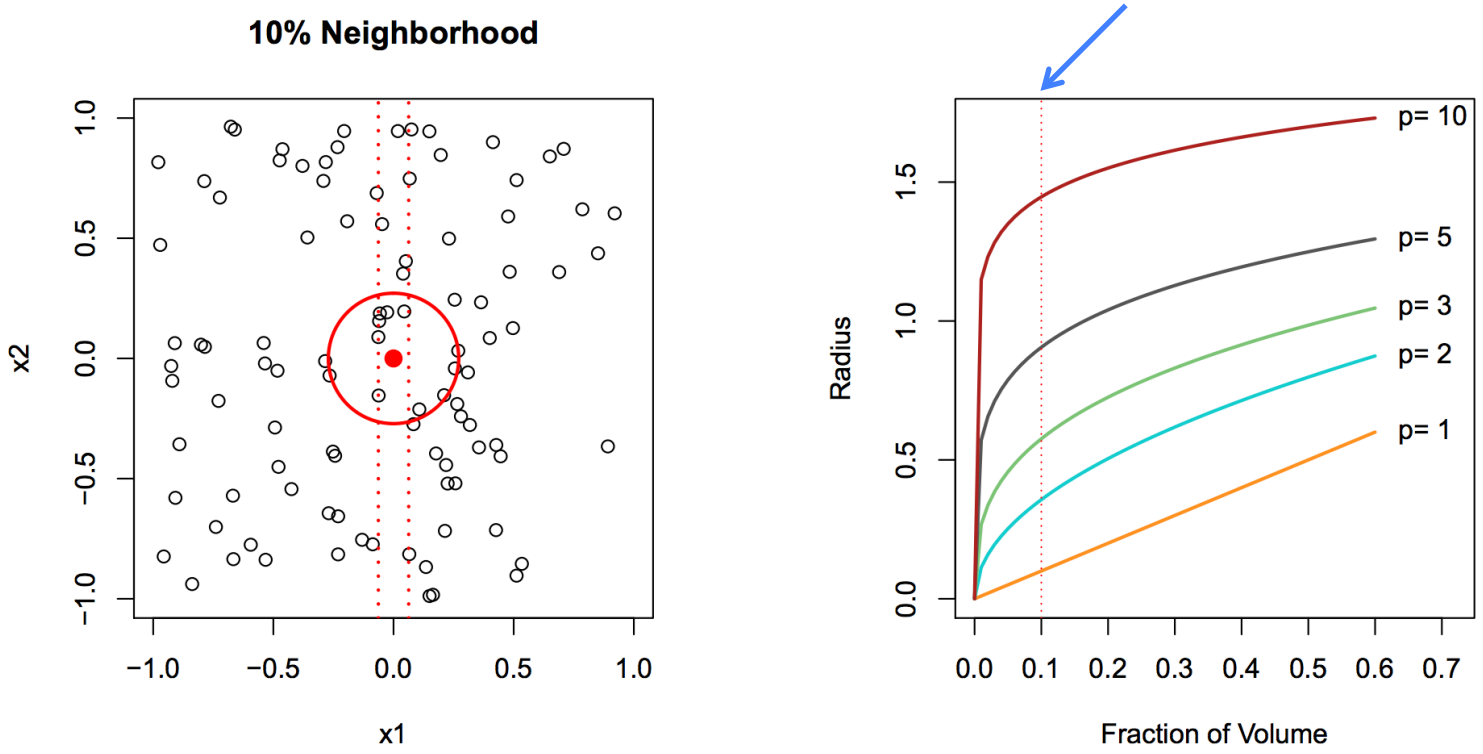


Curse of Dimensionality

- kNN is problematic in high-dim spaces
  - Though can be pretty good for $p \leq 4$ and N on the large side
- Nearest neighbors can be "far" in high dimensions
- Need to get a reasonable fraction of the N values of y_i to average to bring down the variance

Okay….what's "far"?
To start, let's consider 10% to be a reasonable fraction

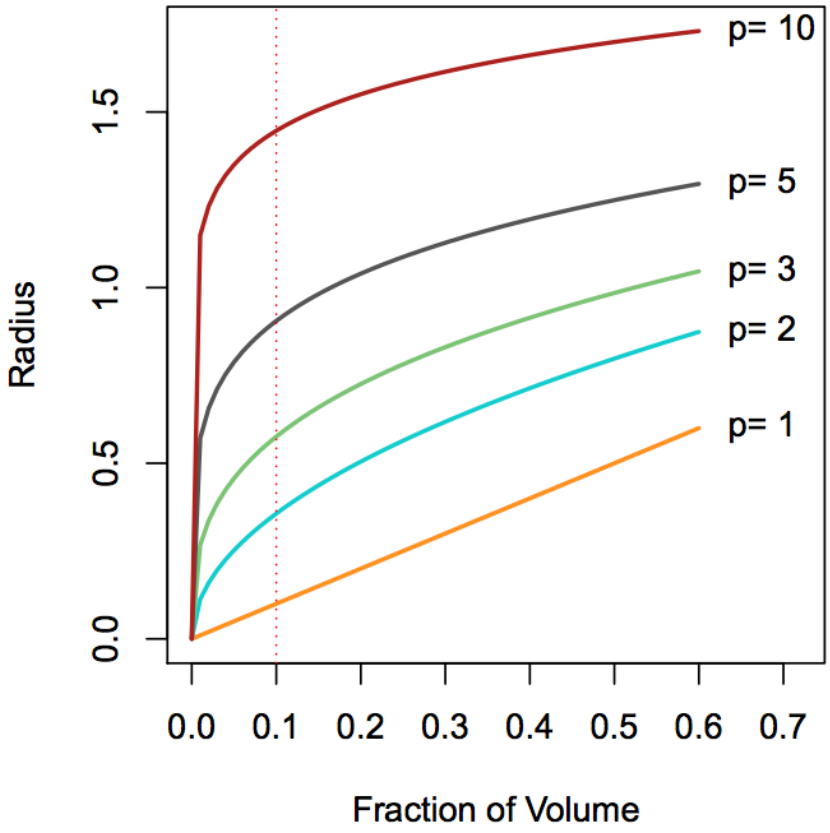
Curse of Dimensionality



- p = 1 just involves variable x1
- p = 2 involves x1 and x2
  - Notice radius of circle in 2 dimensions is much bigger than radius in 1 dimension

Curse of Dimensionality

Can you work out some of the points on the plot?



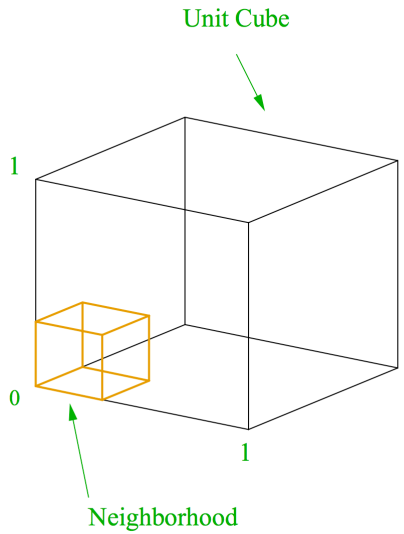
Dimension	Volume of a ball of radius R	Radius of a ball of volume V
0	1	All balls have volume 1
1	$2R$	$V/2$
2	πR^2	$\frac{V^{1/2}}{\sqrt{\pi}}$
3	$\frac{4}{3}\pi R^3$	$\left(\frac{3V}{4\pi}\right)^{1/3}$
4	$\frac{\pi^2}{2}R^4$	$\frac{(2V)^{1/4}}{\sqrt{\pi}}$
5	$\frac{8\pi^2}{15}R^5$	$\left(\frac{15V}{8\pi^2}\right)^{1/5}$
6	$\frac{\pi^3}{6}R^6$	$\frac{(6V)^{1/6}}{\sqrt{\pi}}$
7	$\frac{16\pi^3}{105}R^7$	$\left(\frac{105V}{16\pi^3}\right)^{1/7}$
8	$\frac{\pi^4}{24}R^8$	$\frac{(24V)^{1/8}}{\sqrt{\pi}}$
9	$\frac{32\pi^4}{945}R^9$	$\left(\frac{945V}{32\pi^4}\right)^{1/9}$
10	$\frac{\pi^5}{120}R^{10}$	$\frac{(120V)^{1/10}}{\sqrt{\pi}}$

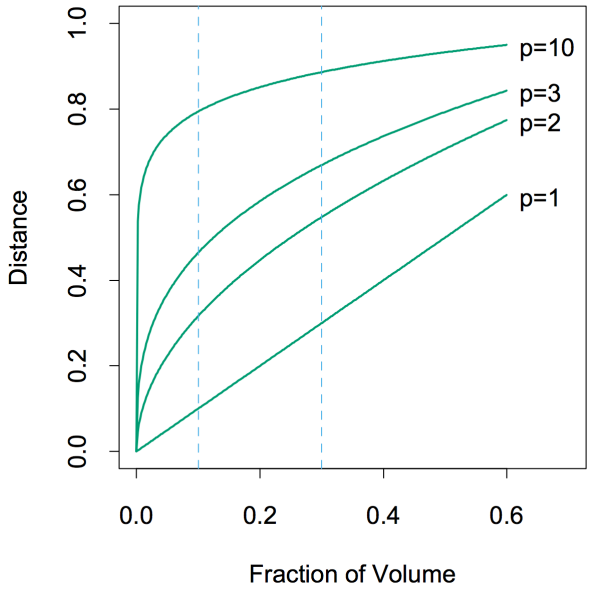
Curse of Dimensionality

Another way to think about dimensionality and its curse

- Hyper-cubical neighborhood about target point to capture fraction ***v*** of the the unit volume
- Expected edge length will be:

$$e_p(v) = v^{1/p}$$

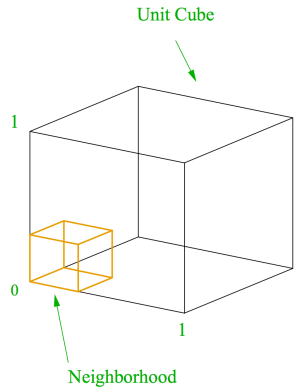


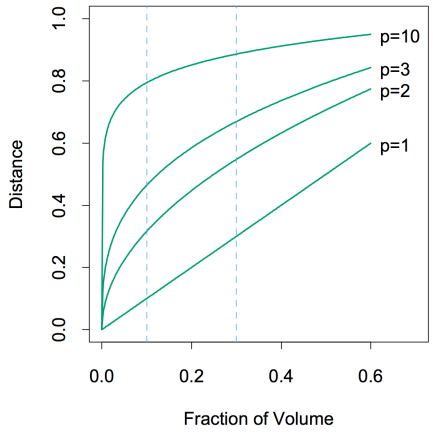


Can you work out out the 10% neighborhood for the unit cube case?

How much more data do we need to compensate for increasing dimensions (p)?

Curse of Dimensionality





Expected edge length

$$e_p(v) = v^{1/p}$$

Sampling density proportional to

$$N^{1/p}$$

p is dimensions of input space
N is number of points

Edge length example: Suppose interested in a v = 10% neighborhood

p = 1 → edge = (0.1)^1 = 0.1
p = 10 → edge = (0.1)^(1/10) = 0.794

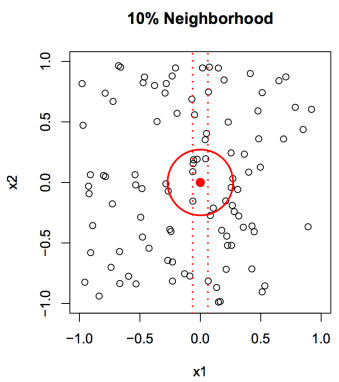
Sampling density example: How to achieve equivalent density in higher dimensions

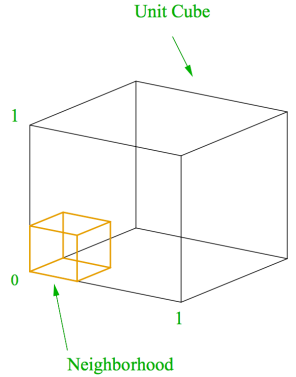
If $N_1 = 100$ represents dense sample for a single dim feature space
To achieve same density for 10 inputs, we need $N_{10} = 100^{10}$ points

Curse of Dimensionality - Takeaways

- kNN, or any method involving this sort of distancing, suffers majorly from curse of dimensionality
  - Nearest neighbors "far" in high dimensions (even for p = 10)
  - As we'll see, k-means and hierarchical clustering fall prey to curse.

- We can mathematically think of idea of "far" and sparsity of points in high dimensions using both radii approach and hypercube approaches





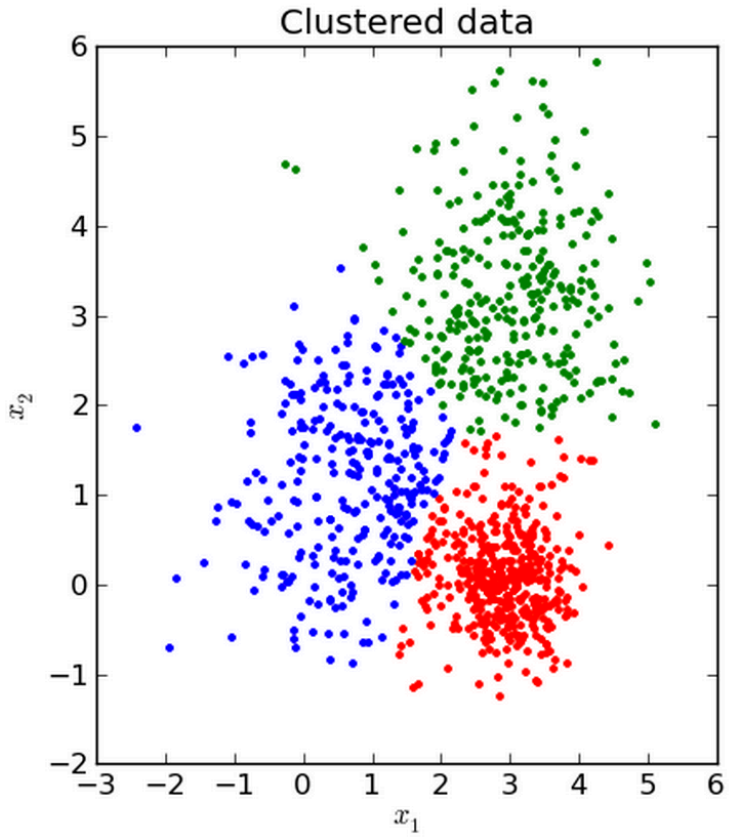
- It takes **a lot** of data to make up for increase in dimensions

Expected edge length $e_p(v) = v^{1/p}$

Sampling density $\propto$ to $N^{1/p}$

What is clustering?

Divide data into distinct subgroups such that observations within each group are quite similar



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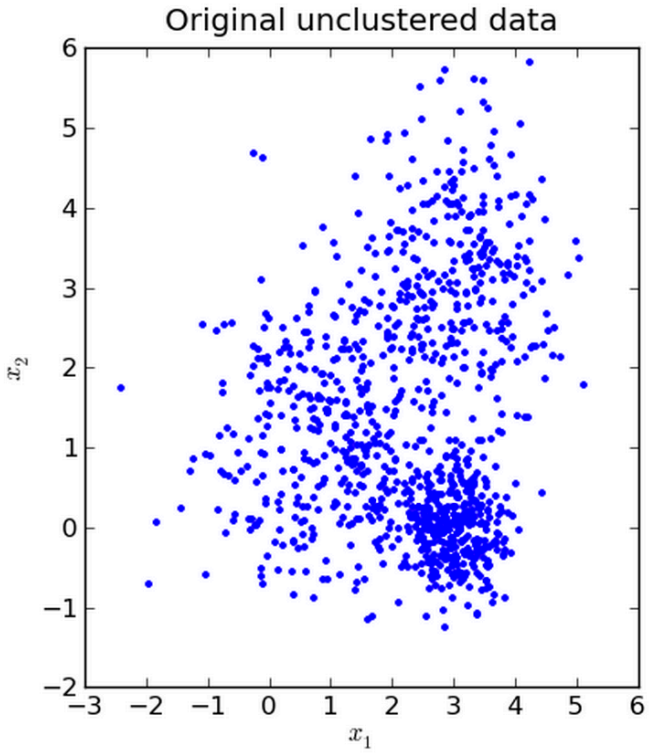
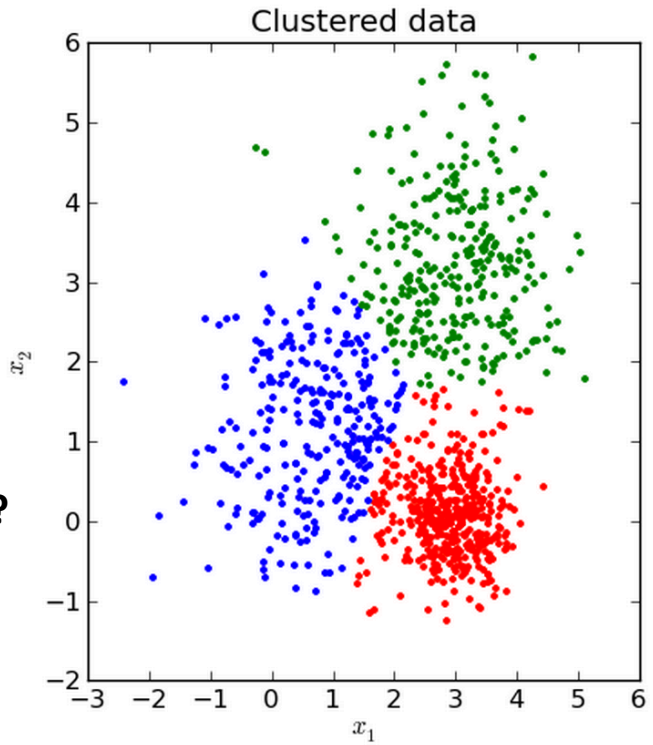


How many subgroups?

What's considered similar?

How am I even doing this?



Two most popular approaches

K-means

Hierarchical clustering

We'll go over

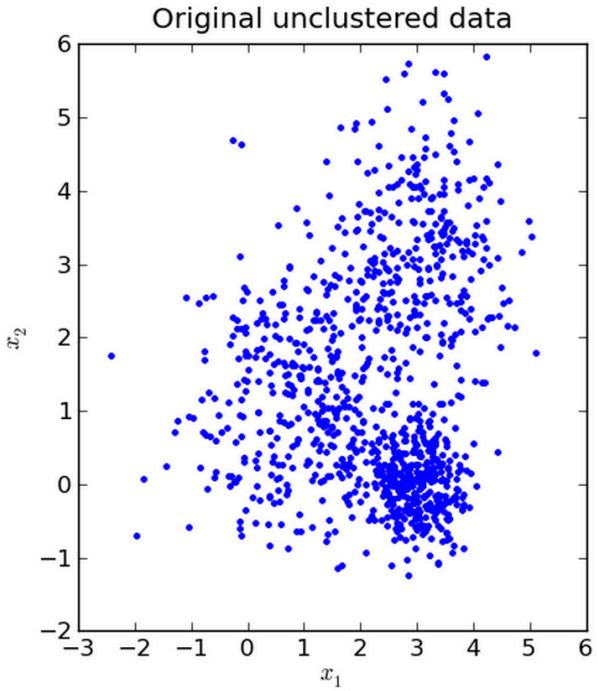
- Algorithm
- Choosing K
- Special considerations

K-means

Idea: Want "within-cluster variation" to be small

Suppose: A fixed K, say K=3. Want to assign each of *n* data point to one of 3 clusters, such that "within-cluster variation" is smallest

- There are K^n possible choices! Pretty unwieldy



K-means

- Again, want to partition data into K subgroups while minimizing within-cluster variation
- More formally….

$$\underset{C_1,\ldots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} \text{WCV}(C_k) \right\}$$

where WCV for k-th cluster is the sum of all the pairwise Euclidean distances

$$\text{WCV}(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

$|C_k|$ is number of observations in k-th cluster

K-means

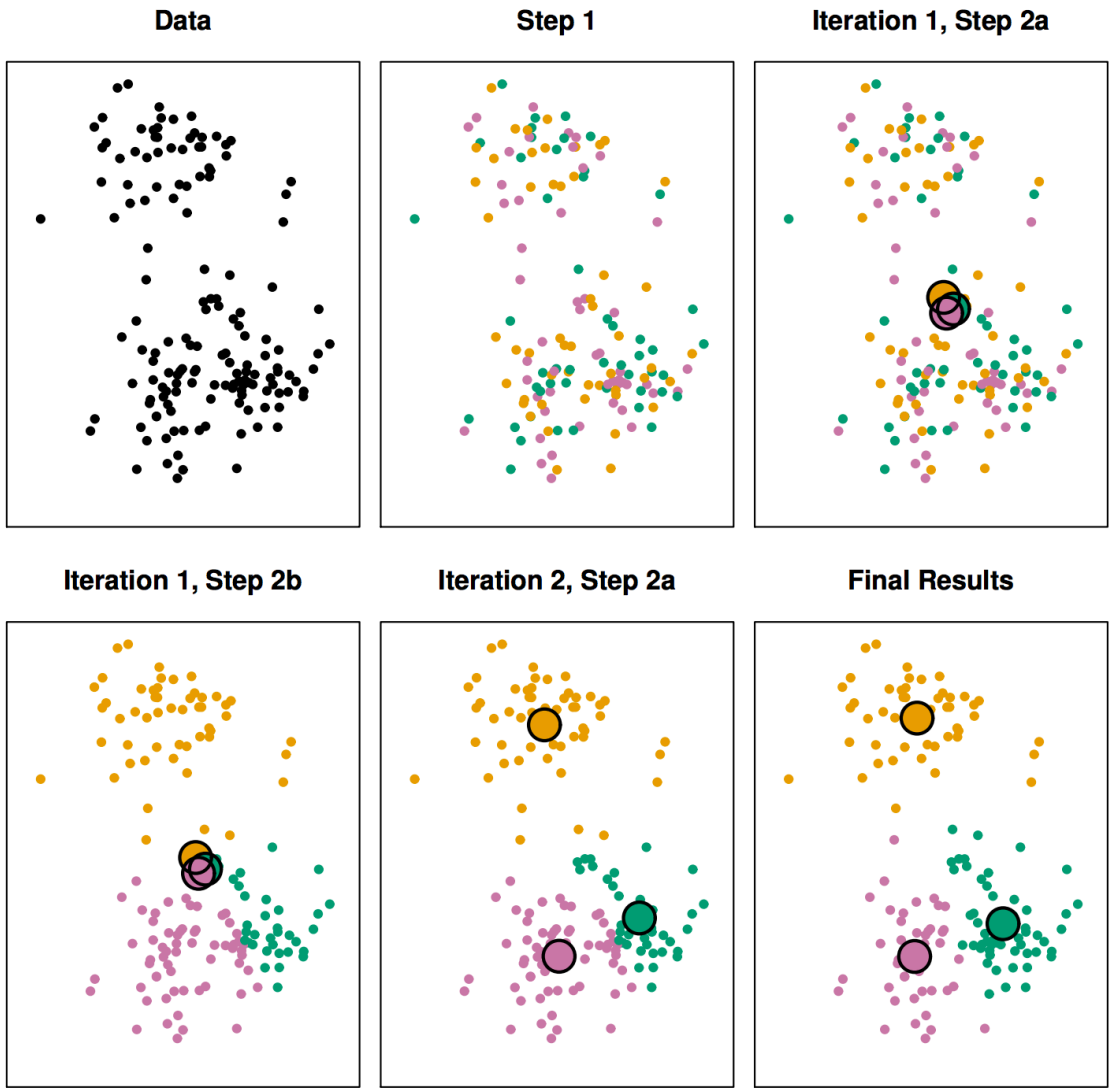
Altogether, we're picking C_1, … C_K such that

$$\underset{C_1,\ldots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

But again the problem is that there are K^n ways.
Too many!

K-means algorithm

For K=3…



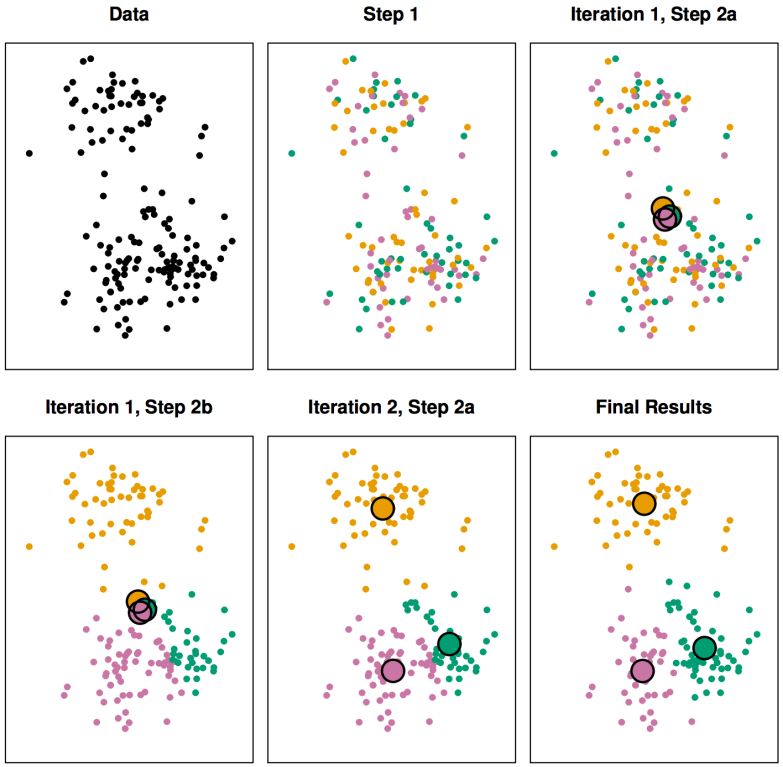
K-means algorithm

(1) Randomly assign number, from 1 to K, to each data point.

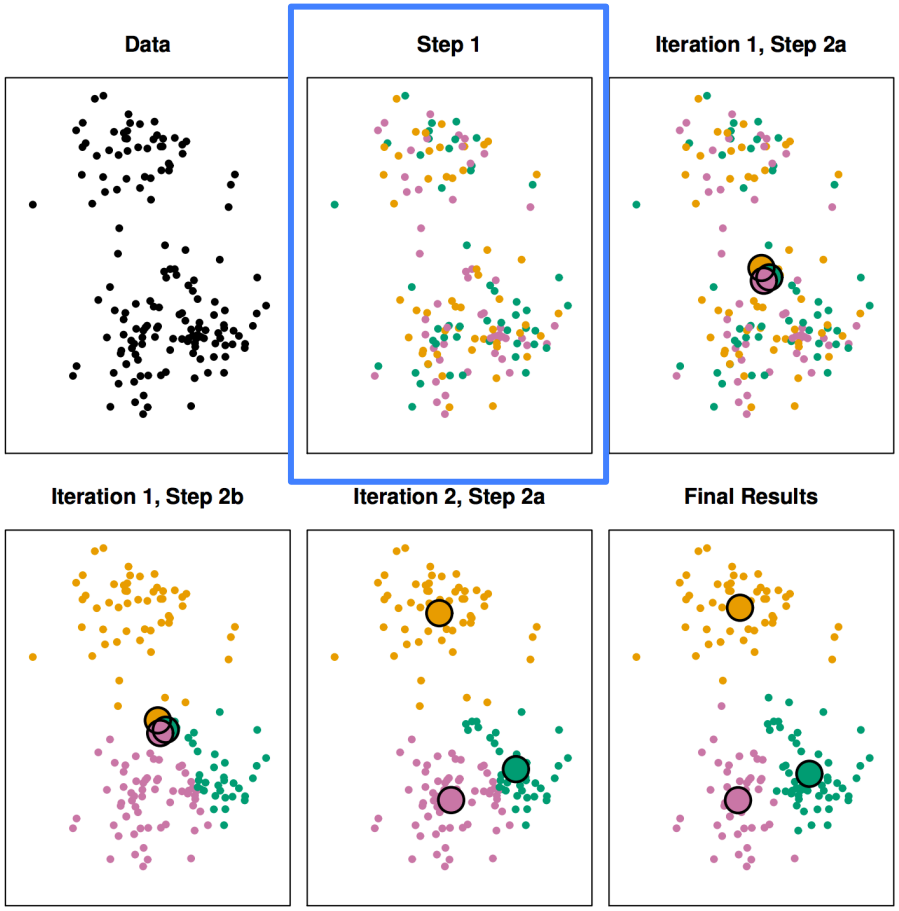
(2) Repeat until cluster assignments stop changing

a. For each of K clusters, compute cluster **centroid** by taking vector of p feature means

b. Assign data point to cluster for which centroid is closest (Euclidean)



K-means algorithm



Finds local optimum!

Results depend on random initialization

Solution

Try multiple initializations and pick one with lowest

$$\underset{C_1,\ldots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

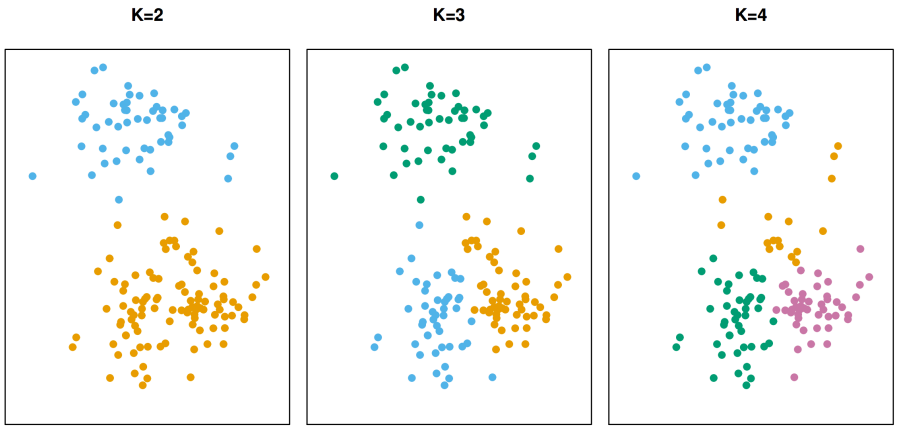
* Also could consider smarter initializations such as kmeans++ http://en.wikipedia. org/wiki/K-means%2B%2B

Choosing K

- No easy answer
- A fuzzy endeavor
  - May just want K similar groups
  - But more often, want something useful or interpretable that exposes some interesting aspect of data
    - Presence/absence of natural distinct groups
    - Descriptive statistics about groups
  - Ex. Are there certain segments of my market that tend to be alike?
    - Ex. middle-aged living in suburbs who log-in infrequently

Choosing K

- Fuzziness aside, there are many methods we can employ to choose K
- We'll go over three popular ones
  - "Elbow" method
  - GAP statistic
  - Silhouette Coefficient

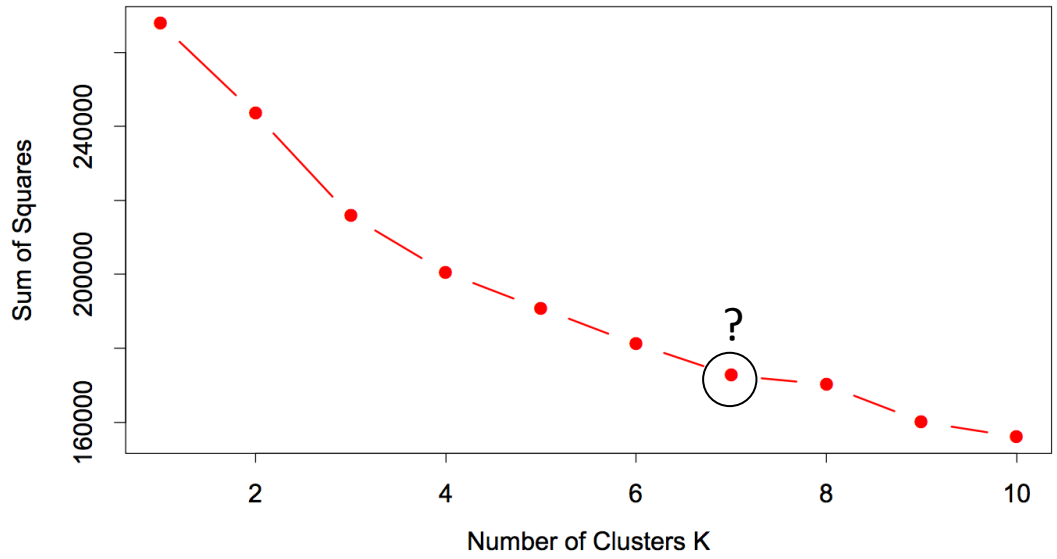


Choosing K – "Elbow" method

- Same Idea: Choose a number of clusters so that adding another cluster doesn't give us that much more

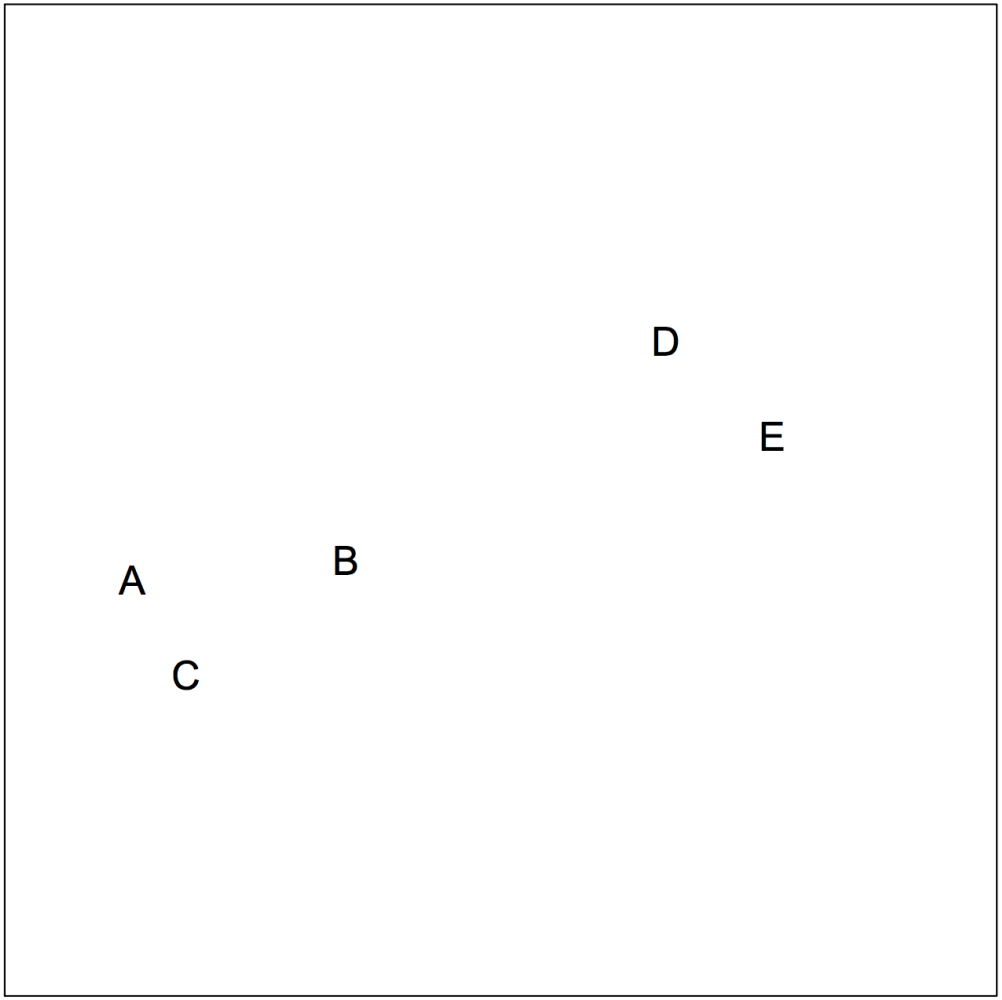
$$W(C) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')=k}||x_i - x_{i'}||^2$$

Within Cluster Point Scatter
A natural loss function is the sum pairwise distances of the points within each cluster, summed over all clusters.



Hierarchical Clustering

Hierarchical Clustering



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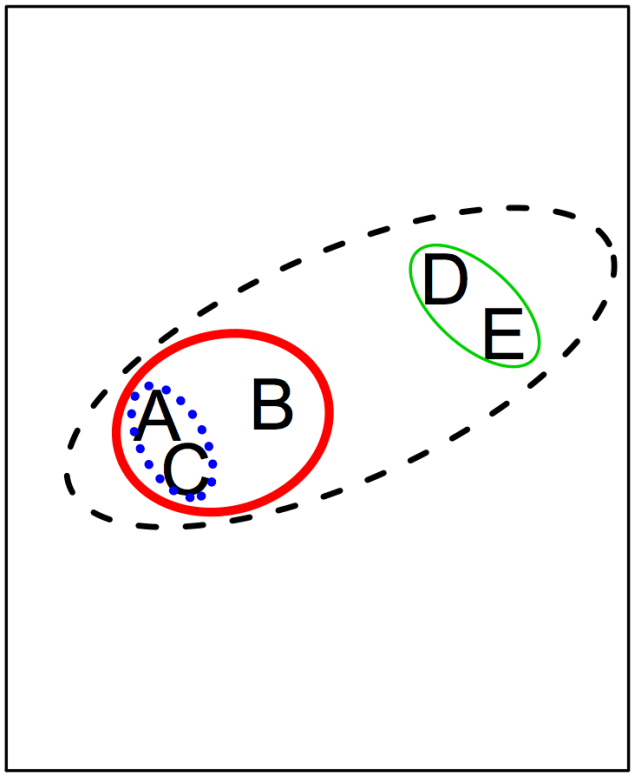
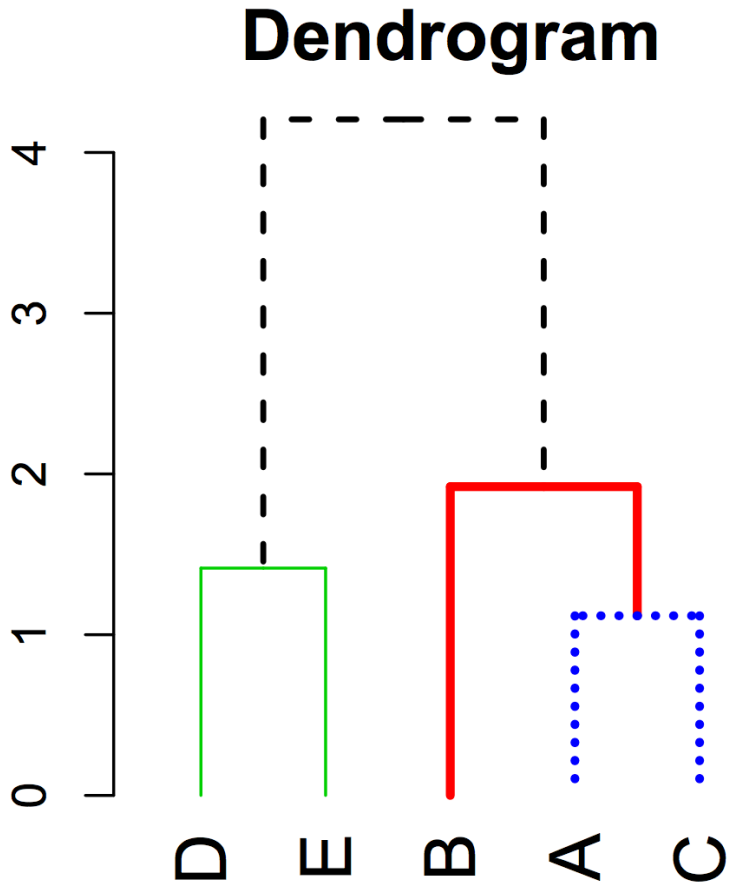




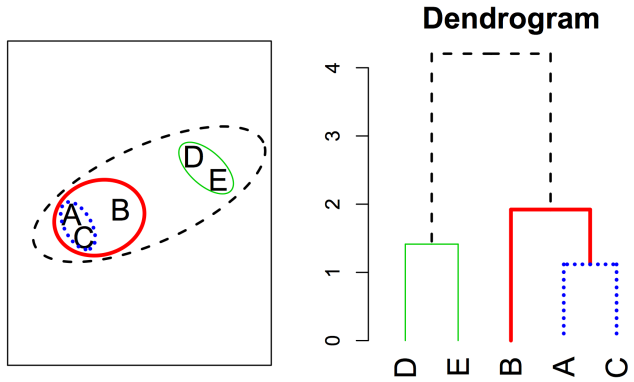
Hierarchical Clustering

Algorithm

(1) Each point as its own cluster

(2) Merge closest clusters

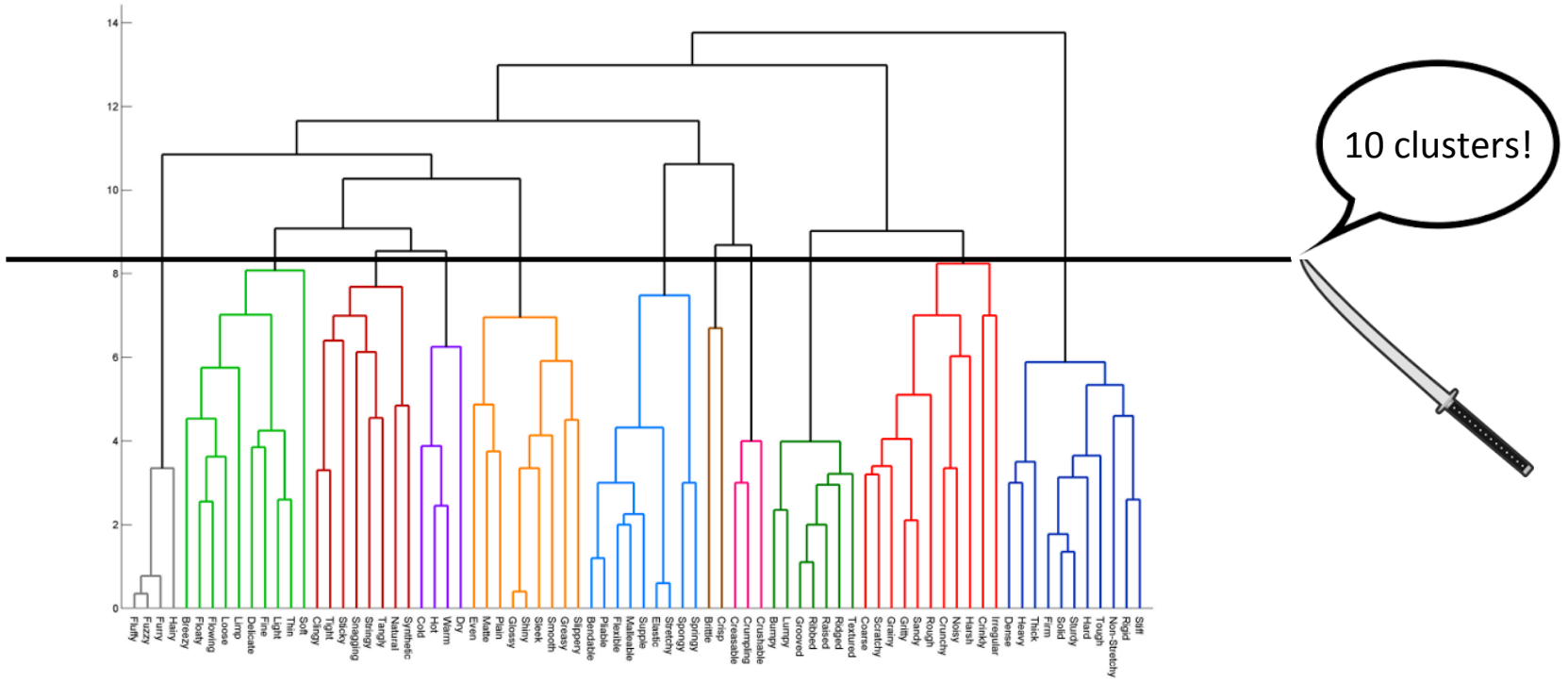
(3) End when all points in single cluster



Notice

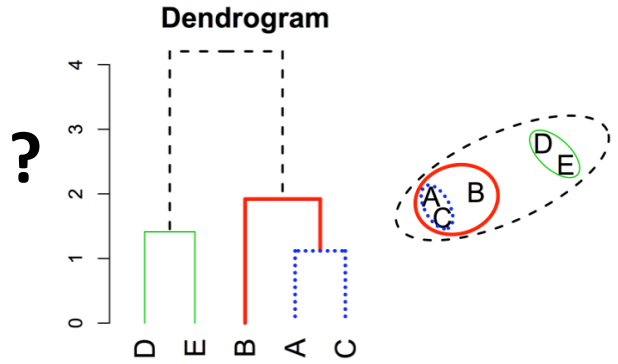
- Skipped over the notion of “distance” between clusters
- Height of fusion tells you how close clusters are!
  - A and C are pretty close, at around 1.2
  - Red and Green are not that close, fusing at around 4.1

Varying K



- In contrast to K-means, don't have to choose K from the start!
  - Depending on where precisely we cut, we have anywhere from 1 to n clusters
- Choosing K: Can again use Elbow Method, Gap Statistic, Silhouette
  - But notice the heights give you sense of separation of clusters depending on cut.

Distance between two clusters?



☺ Tends to be balanced → (more commonly used)

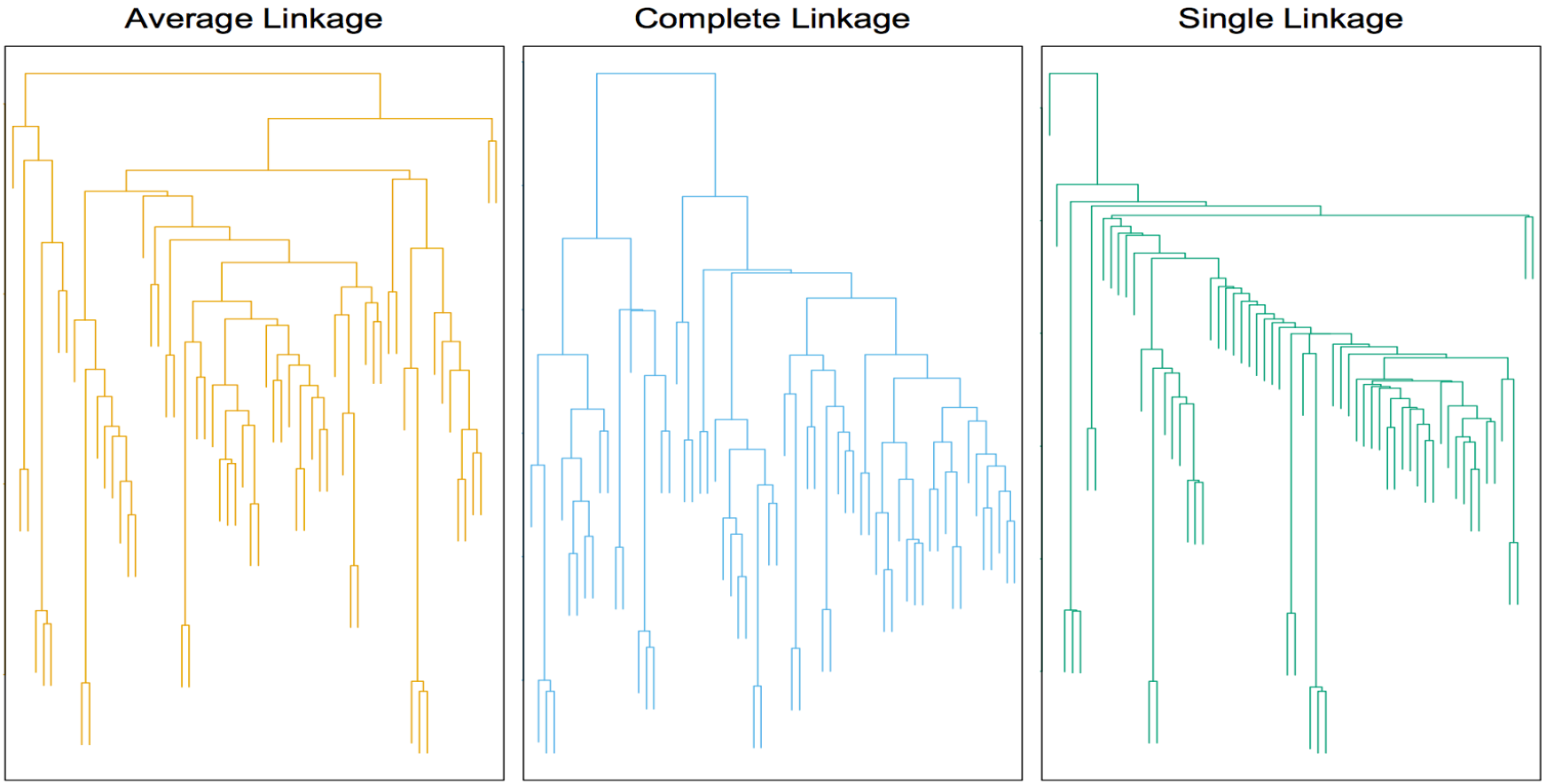
Extended trailing clusters → (less commonly used)

☺ Tends to be balanced → (more commonly used)

(not as commonly used, though popular in Genomics)

Linkage	*Description*
Complete	Maximal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *largest* of these dissimilarities.
Single	Minimal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *smallest* of these dissimilarities. Single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.
Average	Mean intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *average* of these dissimilarities.
Centroid	Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B. Centroid linkage can result in undesirable *inversions*.

Distance between two clusters?



- Not too sensitive to outliers
- Compromise between complete linkage and single

- Less sensitive to outliers
- May violate to “closeness”

- More sensitive to outliers
- Handles irregular shapes fairly naturally

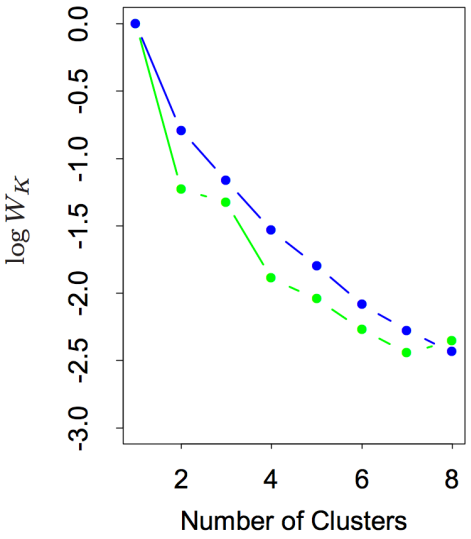
Questions

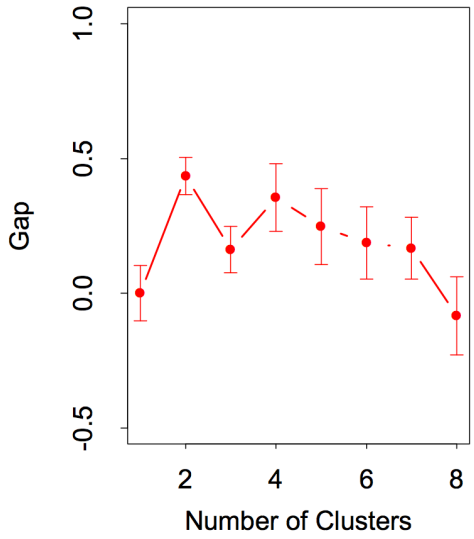
- What is the curse of dimensionality?
  - Why is it particularly bad for kNN and clustering?
  - Pick either the radius or cube interpretation and provide a volume based explanation of the curse
- Describe the K-means algorithm in steps
- Describe the Hierarchical clustering algorithm in steps
  - What is the height of the dendrogram?
  - Contrast with K-means
- Choosing K is no trivial task! What are ways of choosing K?
  - Describe Elbow method
  - Bonus (more advanced, can get away with just Elbow method): Describe GAP statistic, Silhouette Coefficient

Appendix

Choosing K – GAP Statistic

- Arguably best method!
- Idea: Compare within-cluster scatter $W_1, \ldots, W_k$ to uniformly distributed rectangle containing data. Find largest gap.
  - Notice as number of clusters increase, within cluster scatter decreases
  - What happens when number of clusters is number of points?





Three Steps to the Gap Statistic

(1) Observed vs. Expected value of log(W_k) over 20 simulations from uniform data

(2) Translate curves so that log(W_k) = 0 for k=1

(3) Gap statistic K* is smallest K producing gap within one standard deviation of gap at K+1

Choosing K – Silhouette Coefficient

General method for interpreting and validating clusters of data

For each observation i:

- a(i) = average dissimilarity of i with all other data points within same cluster
  - A measure of how well i is assigned to the cluster
  - The smaller a(i) is, the better the assignment
- b(i) = lowest average dissimilarity of i to any other cluster, of which i is not member.
  - Other cluster can be thought of as a "neighboring cluster"

silhouette(i) = [b(i) – a(i)] / max{a(i), b(i)}

-1 < silhouete(i) < 1

Want a(i) small, b(i) large → Want silhouette large

- near 1, dense and well separated
- near 0, overlapping clusters; could well belong to another cluster
- near -1, misclustered

Silhouette Coefficient

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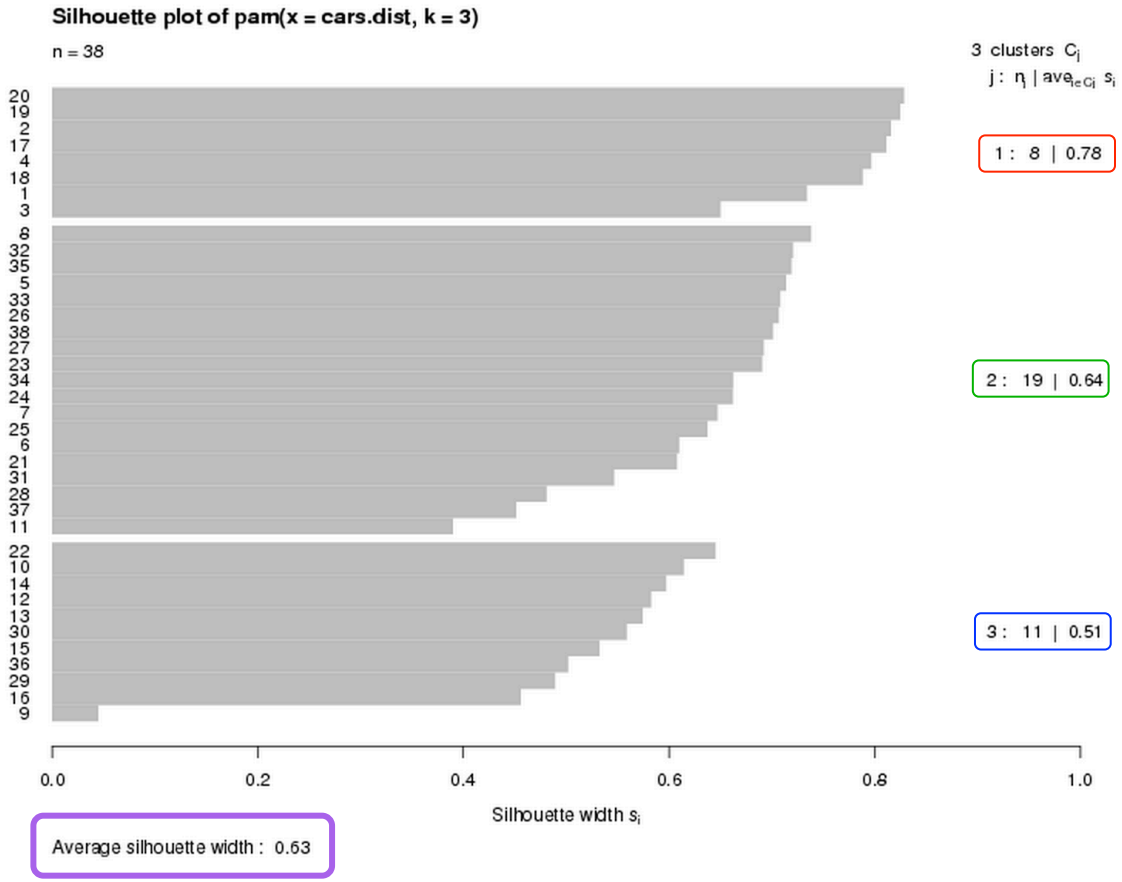

38 data points

3 clusters

- 1st cluster has 8 data points and average silhouette of 0.78
- 2nd cluster has 19 points, 0.64
- 3rd cluster has 11 points, 0.51
- Overall average silhouette **0.63**

Guidelines for Overall Avg Silhouette

Range	Interpretation
0.71 – 1.0	Strong structure found
0.51 – 0.7	Reasonable structure
0.26 – 0.5	Structure weak/artificial
< 0.25	No substantial structure

Some Additional Considerations

- Standardize features?
  - Yes, probably.
  - How to deal with categorical?
- Outliers can be problematic
  - Especially using squared Euclidean as a distance metric
  - What if small subset of observations quite different from all others?
    - Kmeans and hierarchical clustering FORCES every data-point into clusters, potentially distorting clusters
    - Mixture models ('soft clustering') are attractive alternative as they accommodate outliers
- Generally not very robust
  - Can test by clustering subsets of data

K-means – a few more notes

Simple, elegant method, but can be problematic in a lot of ways

- Only intended for **quantitative** features (think centroid calculation for categorical data) and squared **Euclidean** distance (which is not robust to outliers)

One alternative is K-medoids

- Worth reading up a bit more about http://web.stanford.edu/~hastie/local.ftp/Springer/OLD/ESLII_print4.pdf page 515
- Computationally more intensive (requires large proximity matrix computation)
- But, handles categorical features more naturally (though still must define distance metric for mixed data rather carefully), and more robust to outliers.

Within Cluster Point Scatter

$$W(C) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')=k} d(x_i, x_{i'})$$

Within Cluster Point Scatter

A natural loss function is the sum pairwise distances of the points within each cluster, summed over all clusters. In particular, we could specify d(xi, xi') to be Euclidean

---

Let $d_{ii'} = d(x_i, x_{i'})$

$$T = \frac{1}{2}\sum_{i=1}^{N}\sum_{i'=1}^{N} d_{ii'} = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\left(\sum_{C(i')=k} d_{ii'} + \sum_{C(i')\neq k} d_{ii'}\right)$$

Total Point Scatter

$$T = W(C) + B(C)$$

$$B(C) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')\neq k} d_{ii'}$$

Between Cluster Point Scatter

Within Cluster Point Scatter

It can be shown that

$$
\begin{aligned}
W(C) &= \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')=k}||x_i - x_{i'}||^2 \\
&= \sum_{k=1}^{K} N_k \sum_{C(i)=k}||x_i - \bar{x}_k||^2,
\end{aligned}
$$

where

$\bar{x}_k = (\bar{x}_{1k}, \ldots, \bar{x}_{pk})$ is mean vector associated with k-th cluster

$N_k = \sum_{i=1}^{N} I(C(i) = k)$