CPSC 340: Machine Learning and Data Mining

Hierarchical Clustering

Fall 2017

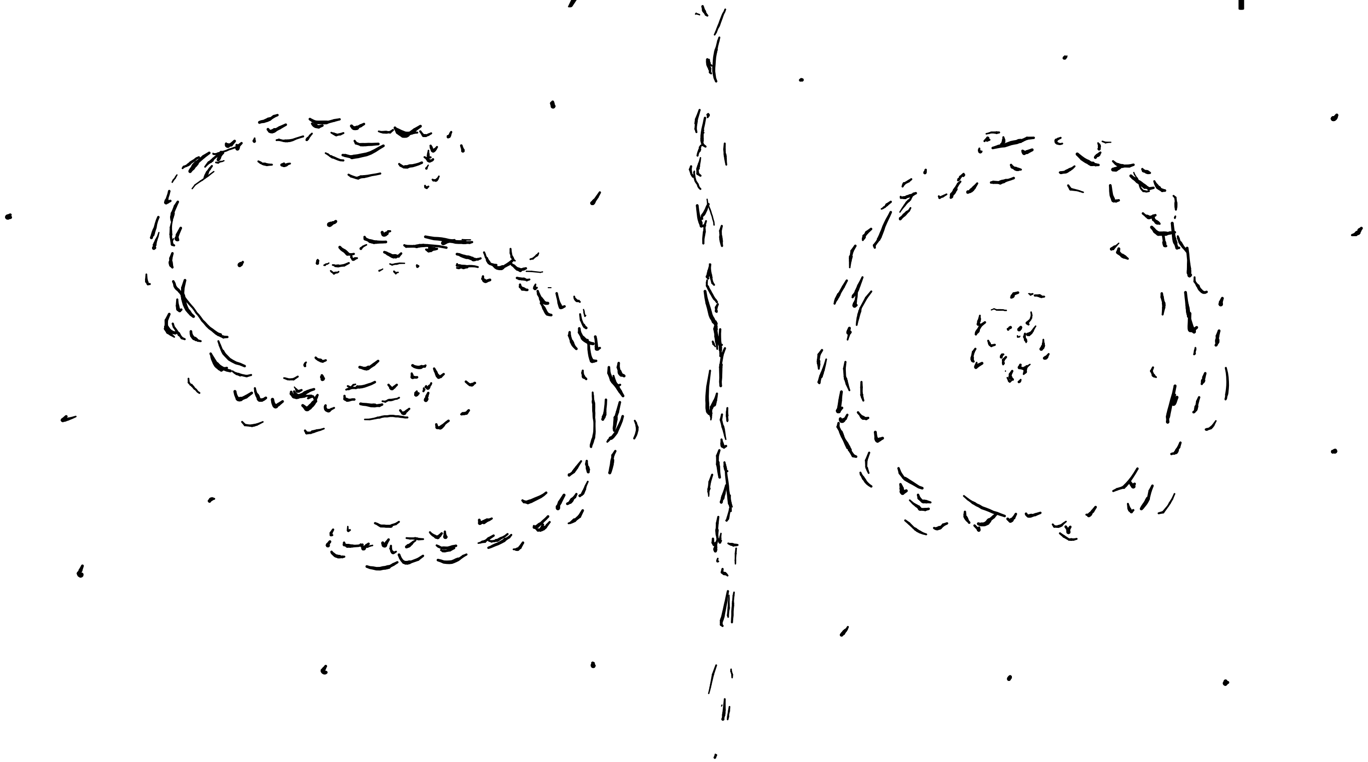
Admin

- Assignment 1 is due Friday.
  - Follow the assignment guidelines naming convention (a1.zip/a1.pdf).

- Assignment 0 grades posted on Connect.

Last Time: Density-Based Clustering

- We discussed density-based clustering:
  - Non-parametric clustering method.
  - Based on finding connected regions of dense points.
  - Can find non-convex clusters, and doesn't cluster all points.



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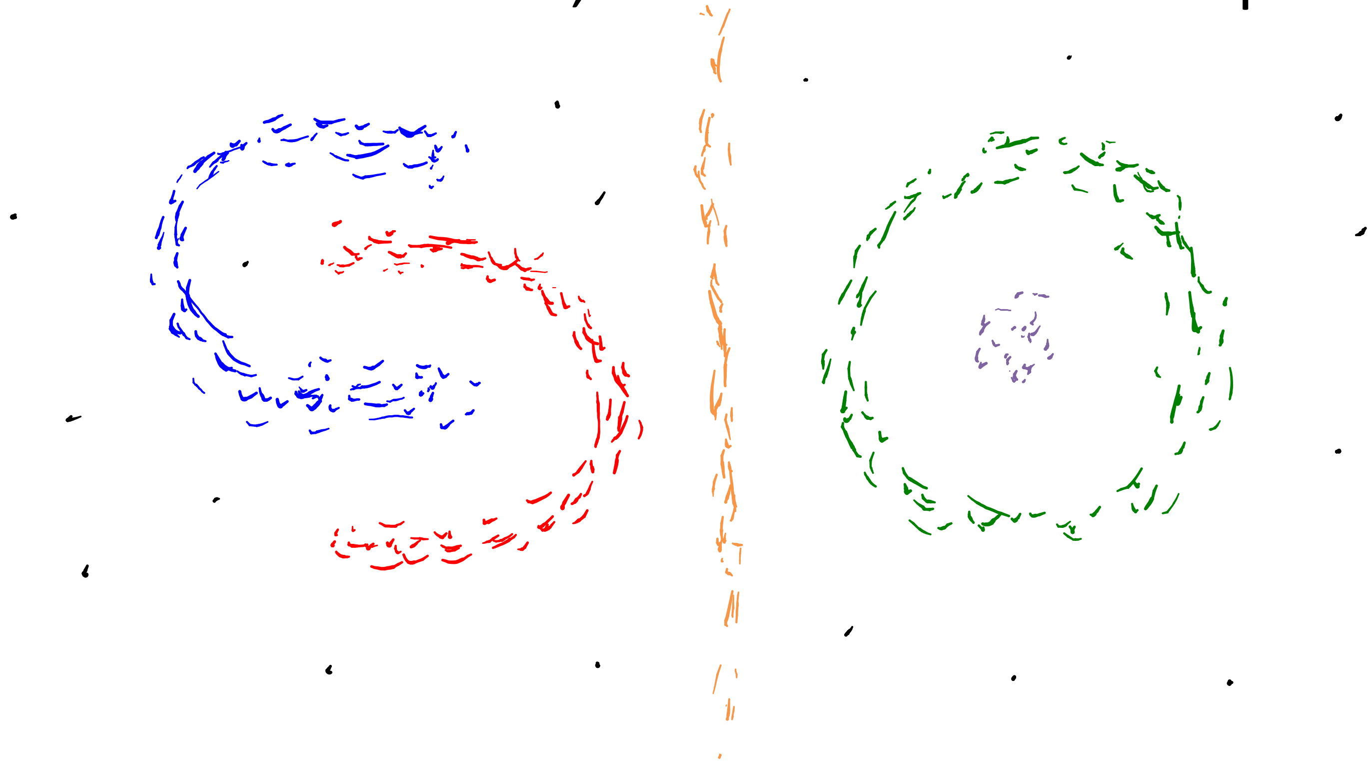
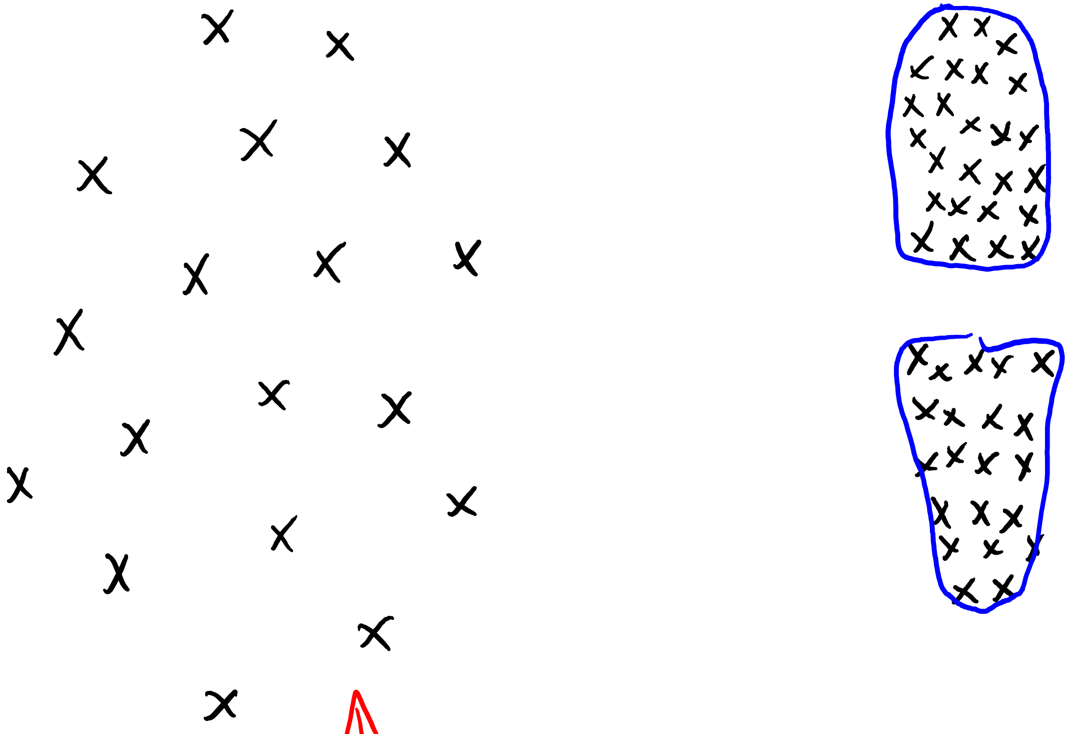


Differing Densities

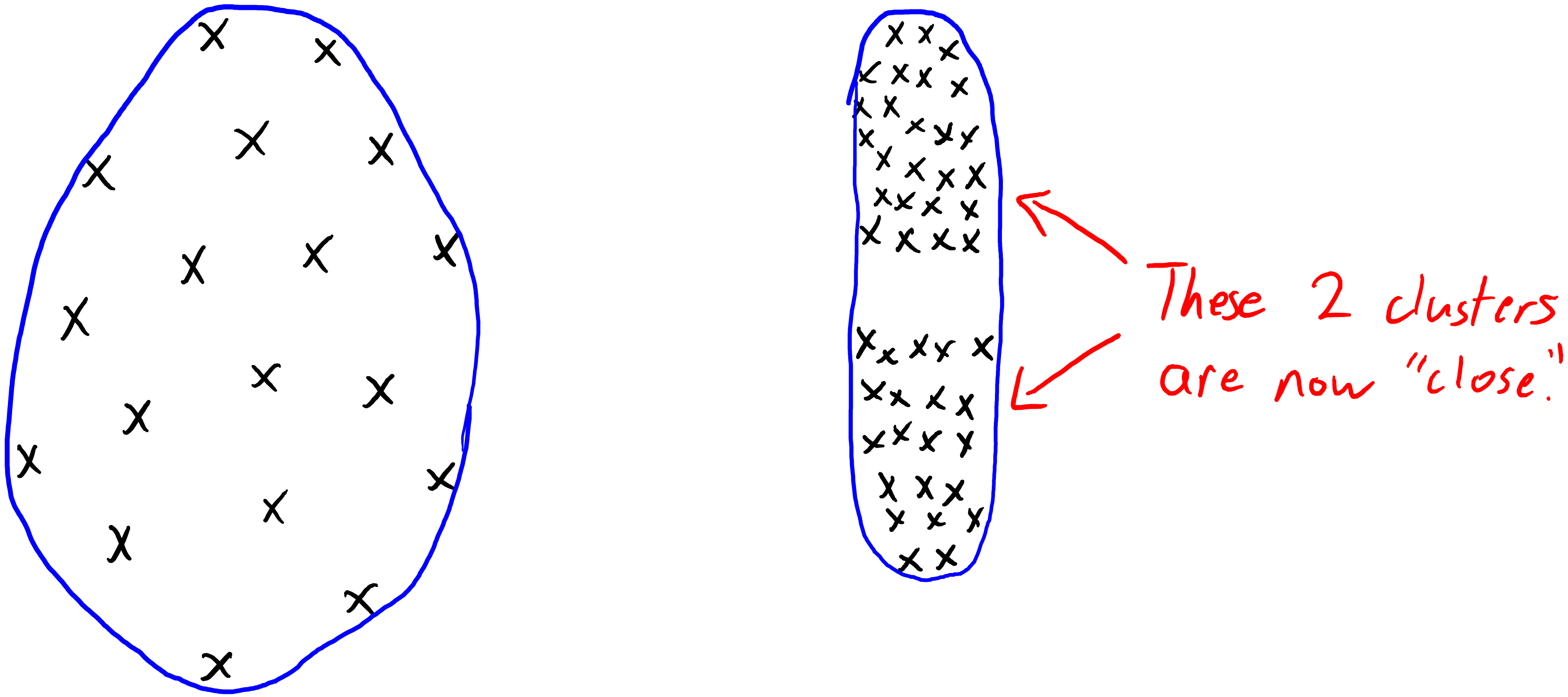
- Consider density-based clustering on this data:



It missed this cluster.

Differing Densities

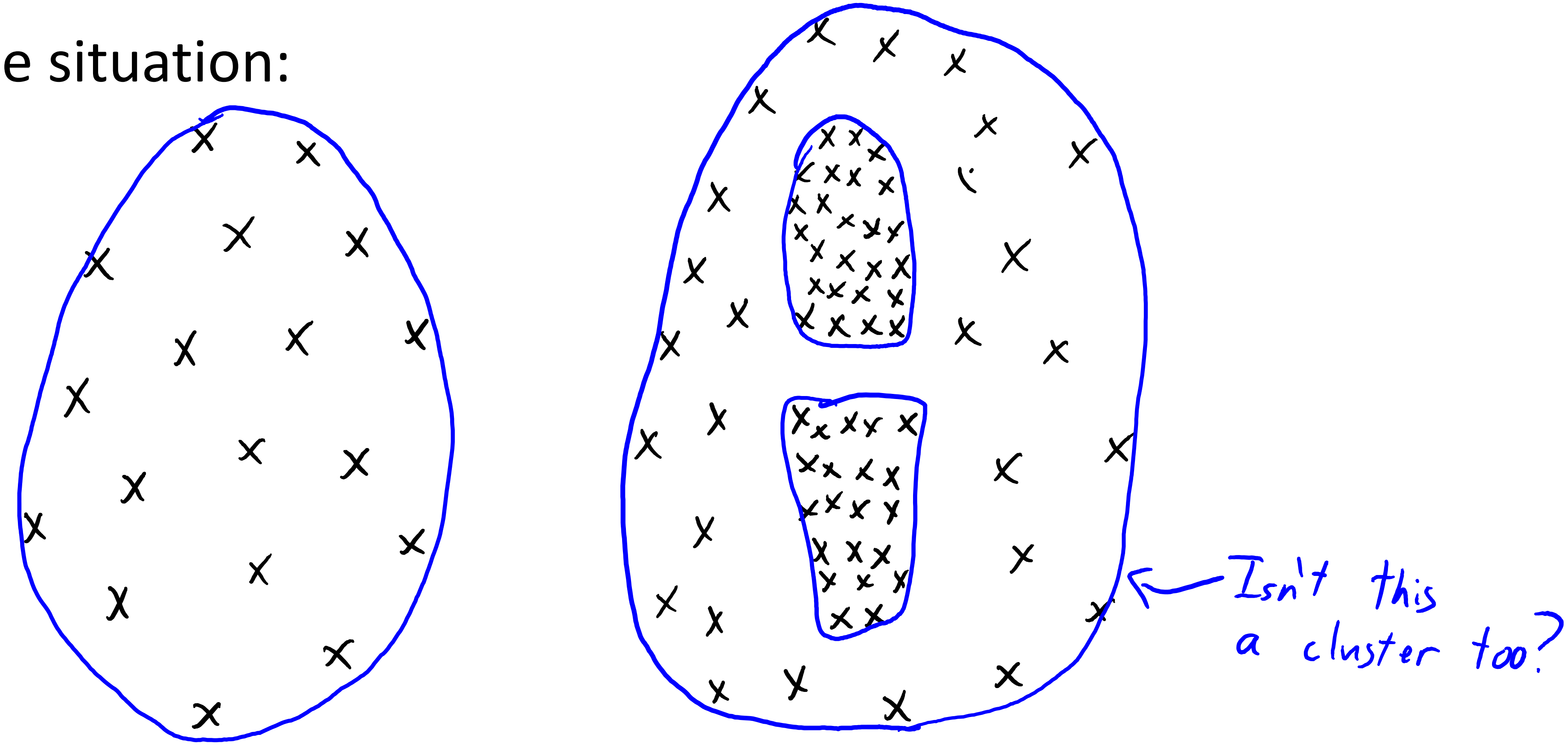
- Increase epsilon and run it again:



- There may be no density-level that gives you 3 clusters.

Differing Densities

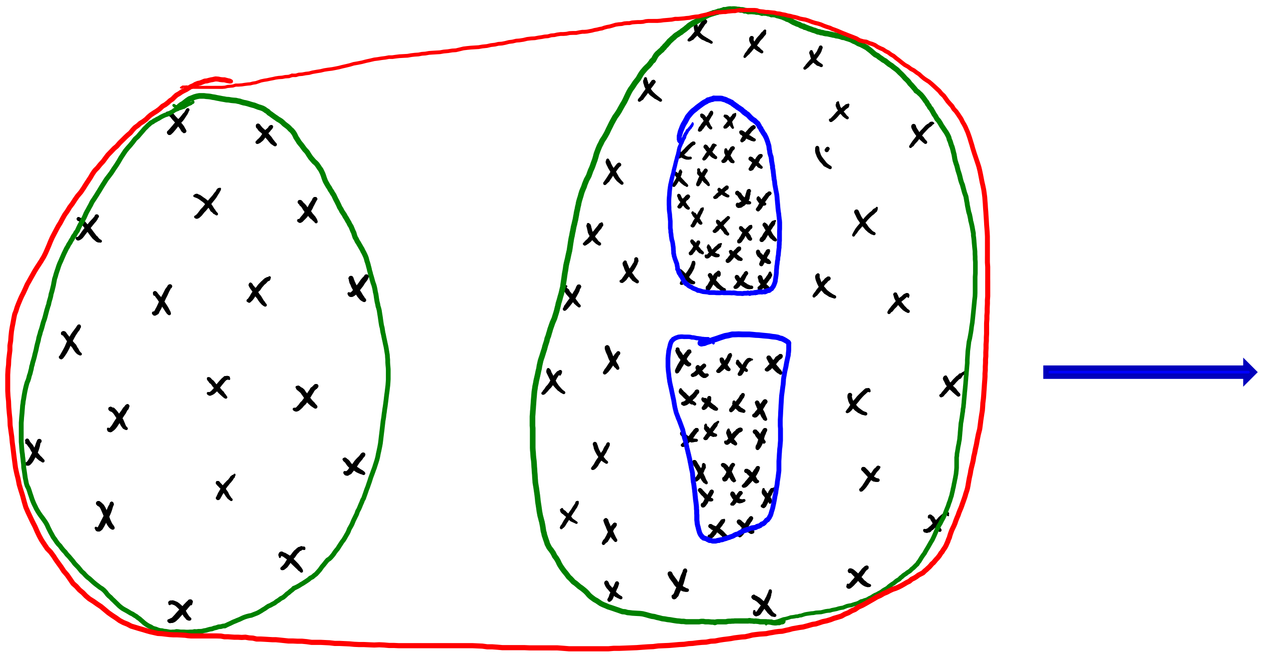
- Here is a worse situation:

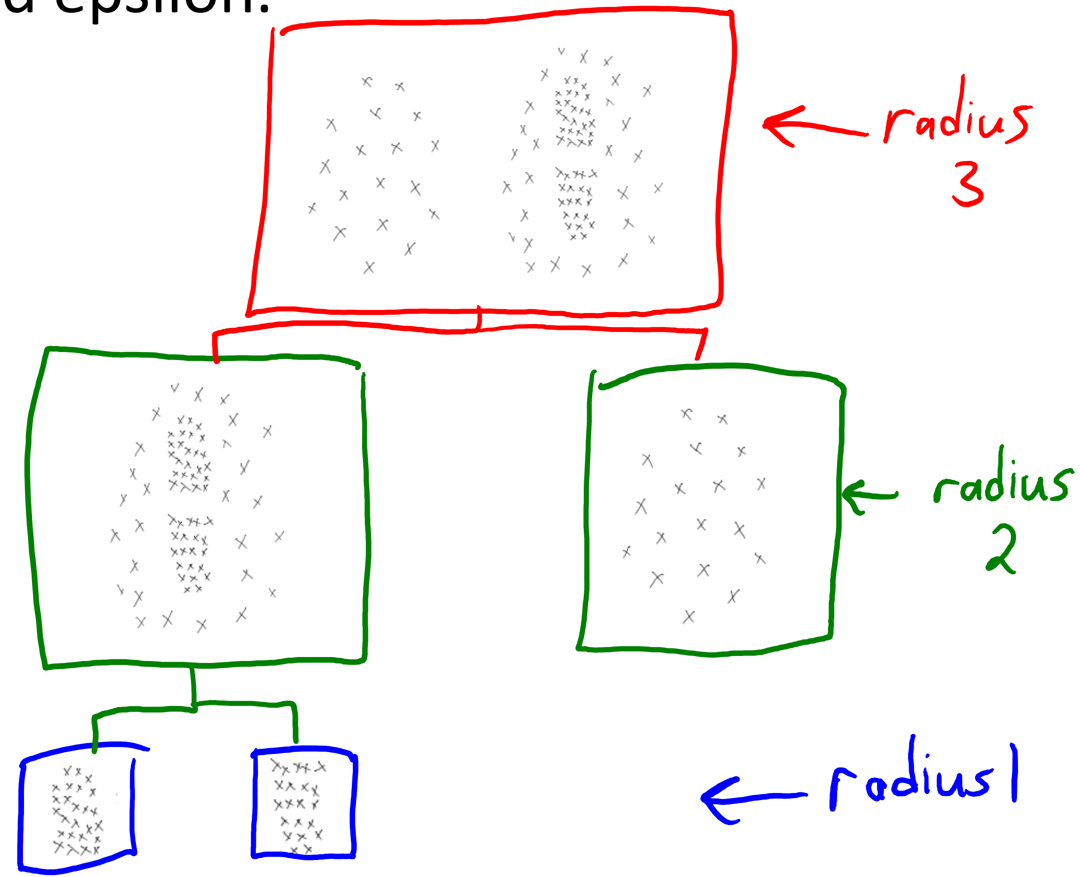


- Now you need to choose between coarse/fine clusters.
- Instead of fixed clustering, we often want hierarchical clustering.

Density-Based Hierarchical Clustering

- A simple way to make a hierarchical DBSCAN:
  - Fix minNeighbours, record clusters as you vary epsilon.
  - Much more information than using a fixed epsilon.





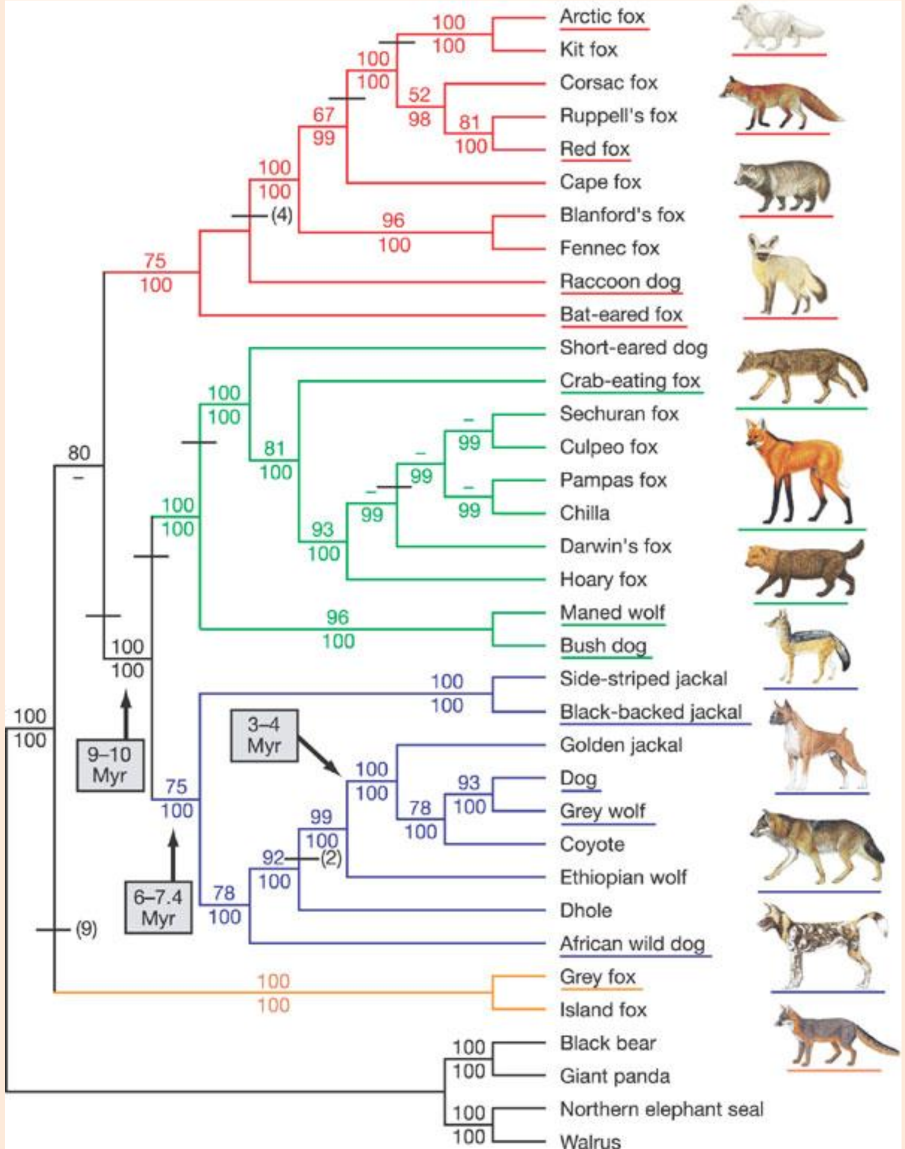
  - Output is a tree of different clustering.

Application: Phylogenetics

- We sequence genomes of a set of organisms.
- Can we construct the “tree of life”?

- Comments on this application:
  - On the right are individuals.
  - As you go left, clusters merge.
  - Merges are ‘common ancestors’.

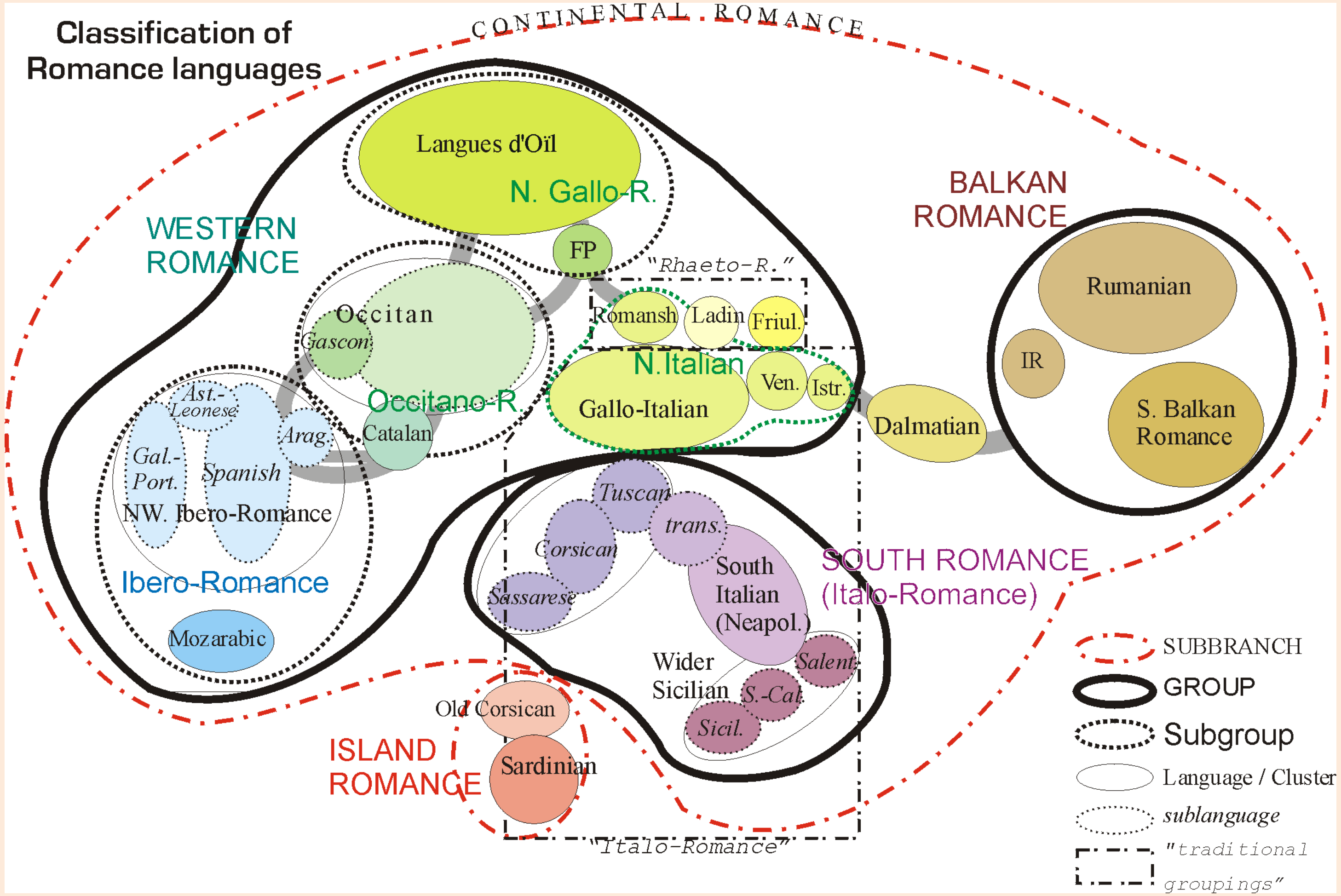
- More useful information in the plot:
  - Line lengths: chose here to approximate time.
  - Numbers: #clusterings across bootstrap samples.
  - ‘Outgroups’ (walrus, panda) are a sanity check.



http://www.nature.com/nature/journal/v438/n7069/fig_tab/nature04338_F10.html

Application: Phylogenetics

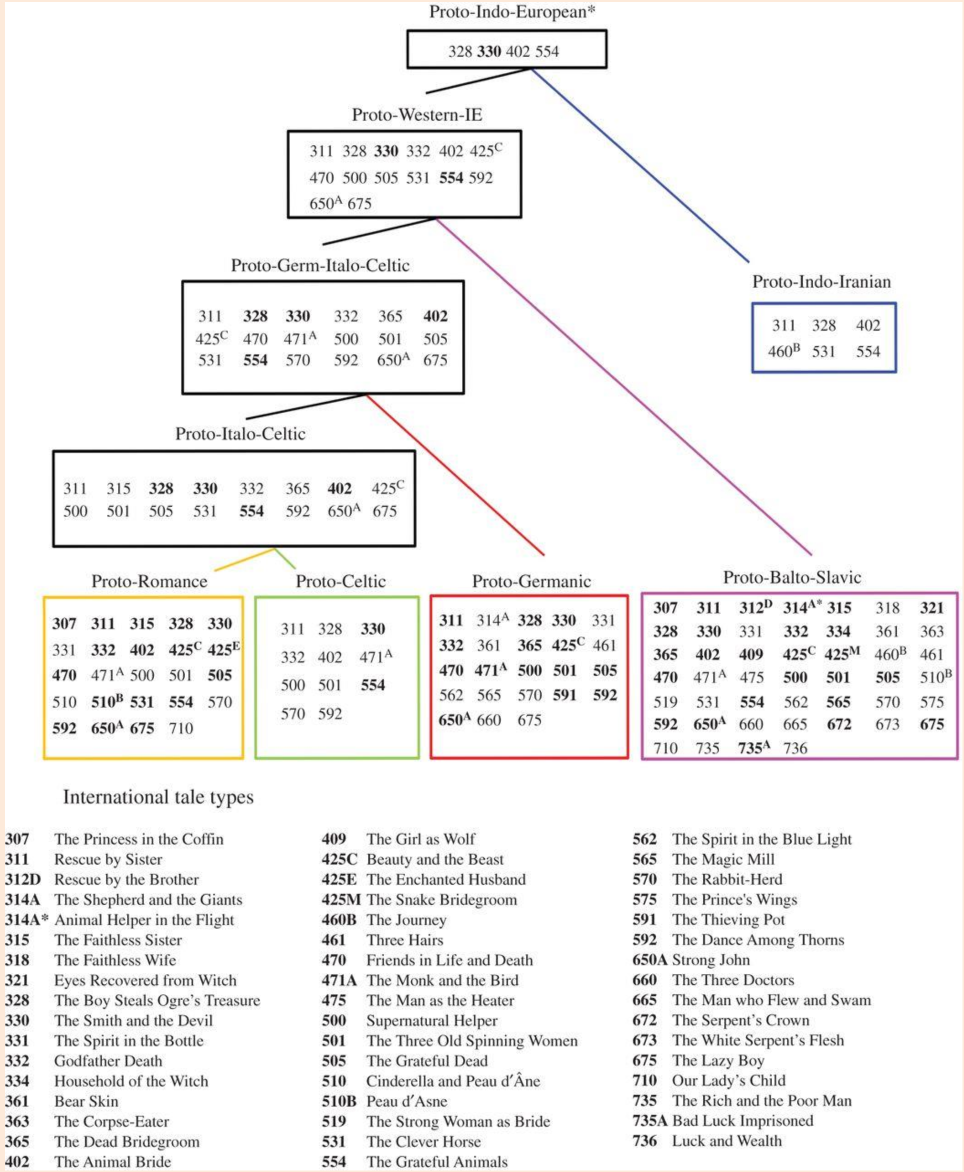
- Comparative method in linguistics studies evolution of languages:



https://en.wikipedia.org/wiki/Comparative_method_(linguistics)

Application: Phylogenetics

- January 2016: evolution of fairy tales.
  - Evidence that “Devil and the Smith” goes back to bronze age.
  - “Beauty and the Beast” published in 1740, but might be 2500-6000 years old.

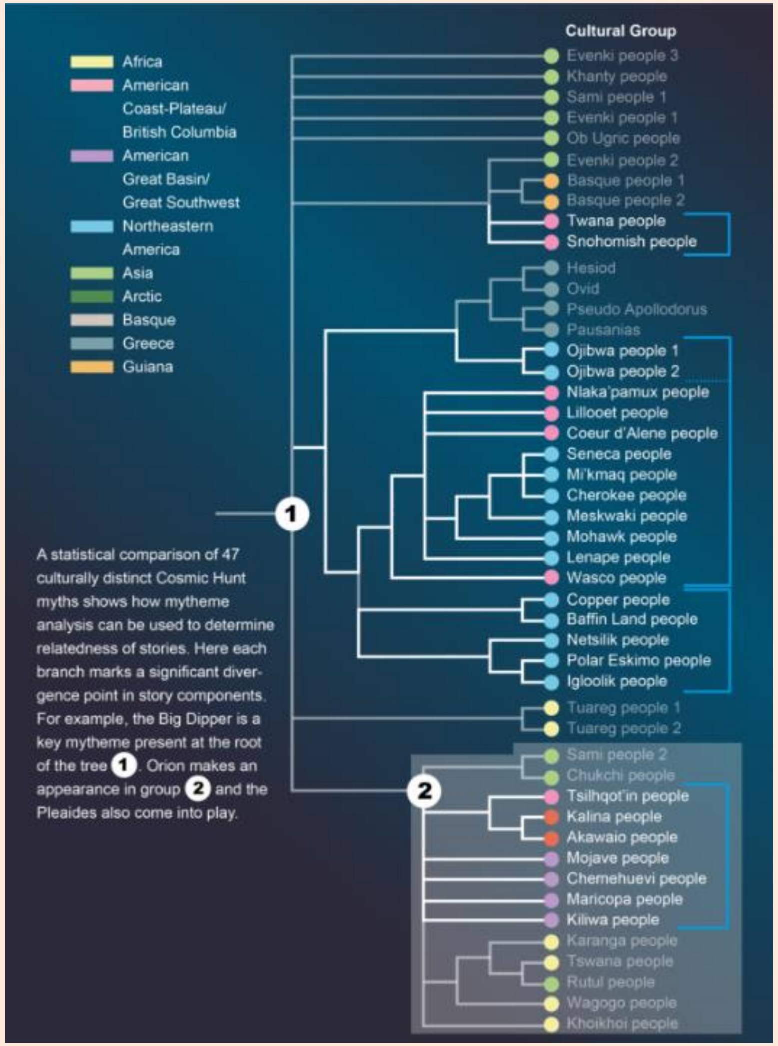


http://rsos.royalsocietypublishing.org/content/3/1/150645

Application: Phylogenetics

- January 2016: evolution of fairy tales.
  - Evidence that “Devil and the Smith” goes back to bronze age.
  - “Beauty and the Beast” published in 1740, but might be 2500-6000 years old.

- September 2016: evolution of myths.
  - “Comic hunt” story:
    - Person hunts animal that becomes constellation.
      - Previously known to be at least 15,000 years old.
    - May go back to paleololithic period.



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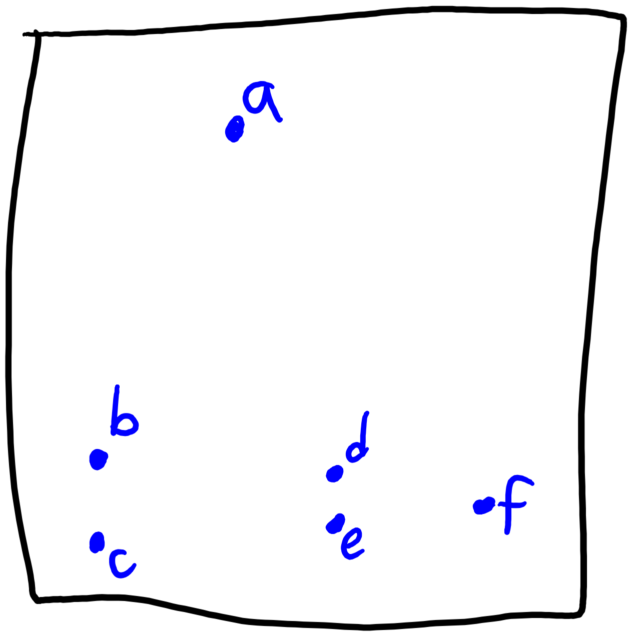
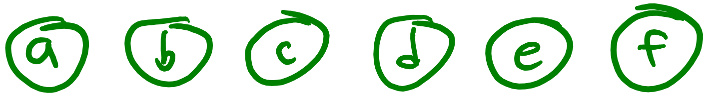
Agglomerative (Bottom-Up) Clustering

- More common hierarchical method: agglomerative clustering.
  1. Starts with each point in its own cluster.





https://en.wikipedia.org/wiki/Hierarchical_clustering

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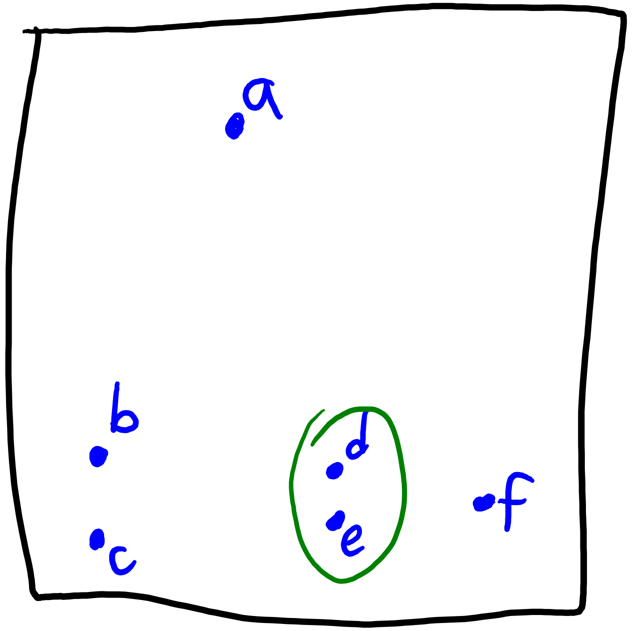

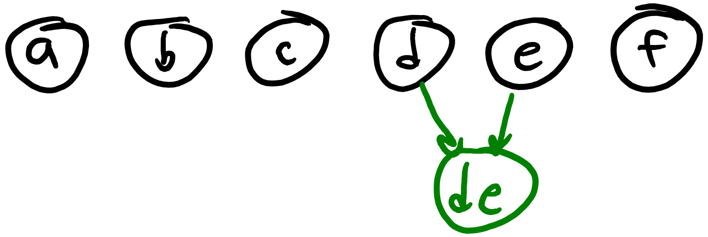

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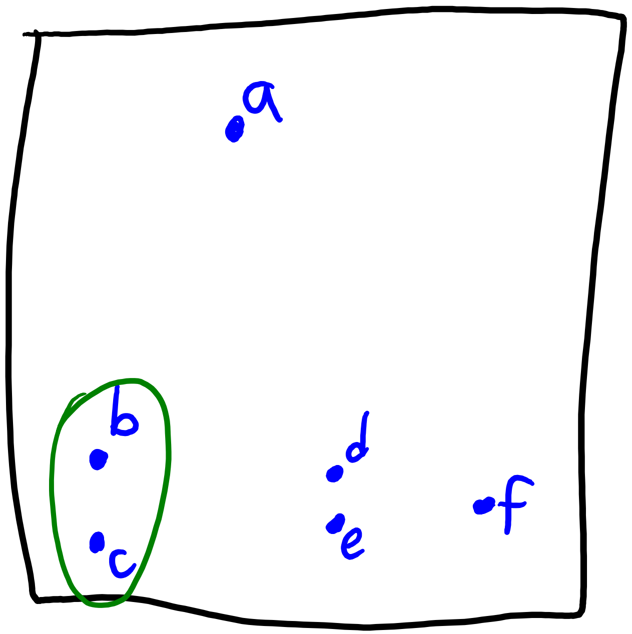

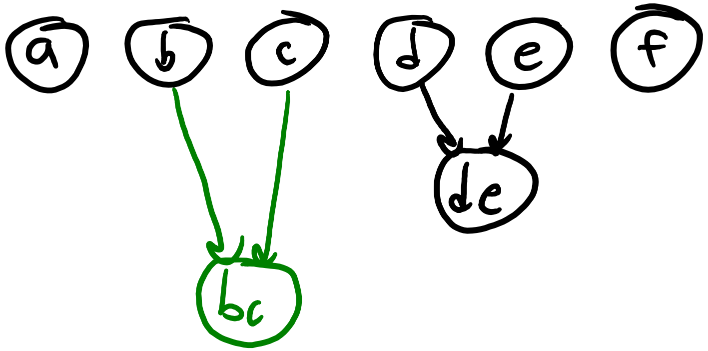

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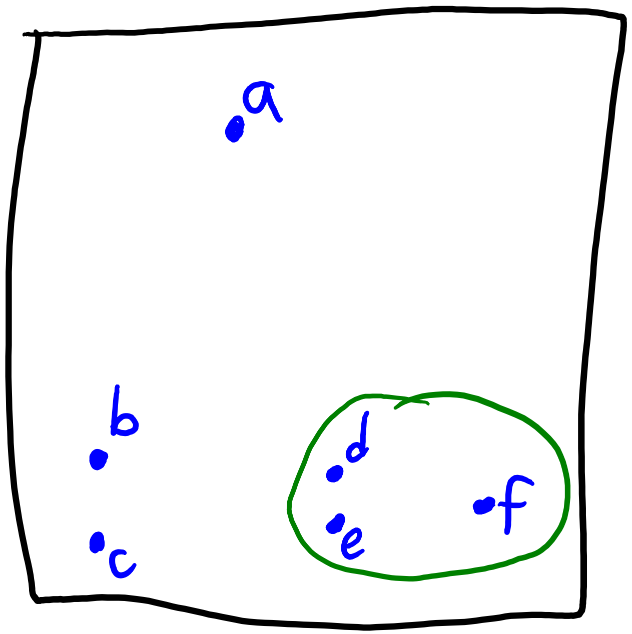

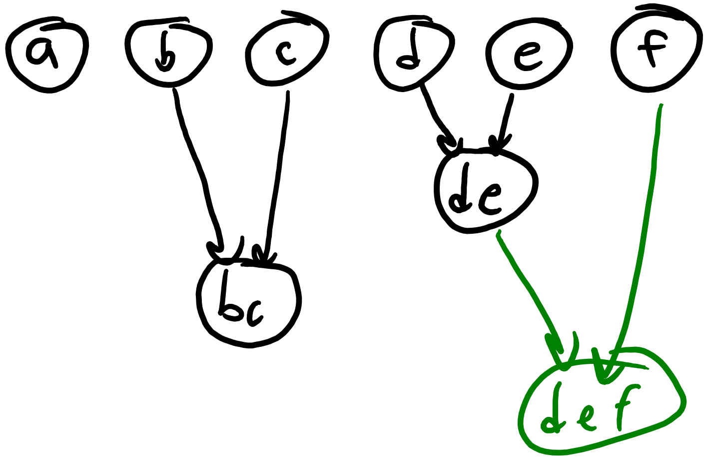

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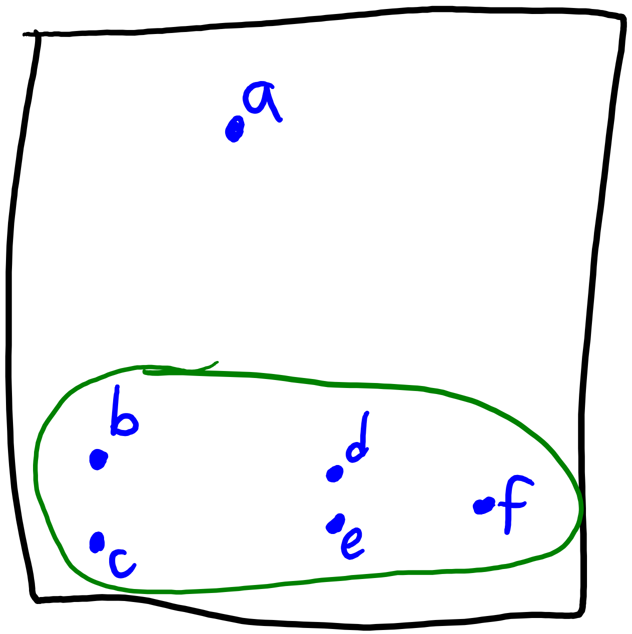

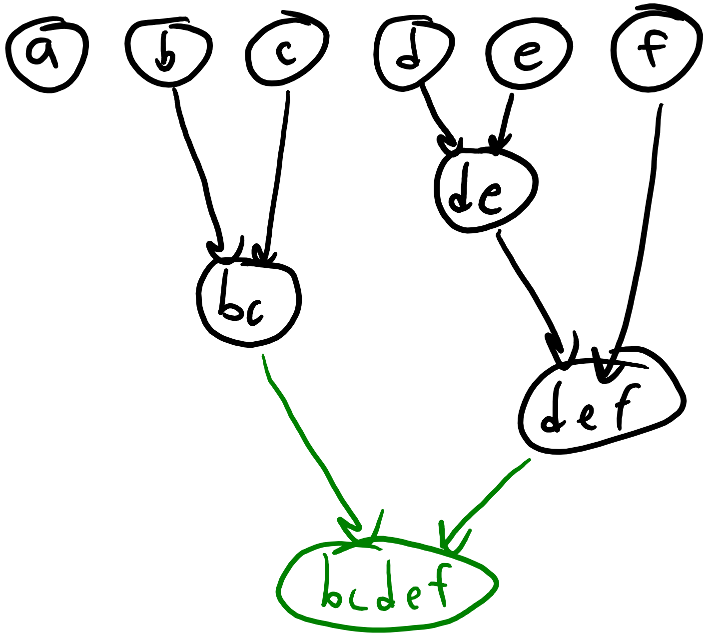

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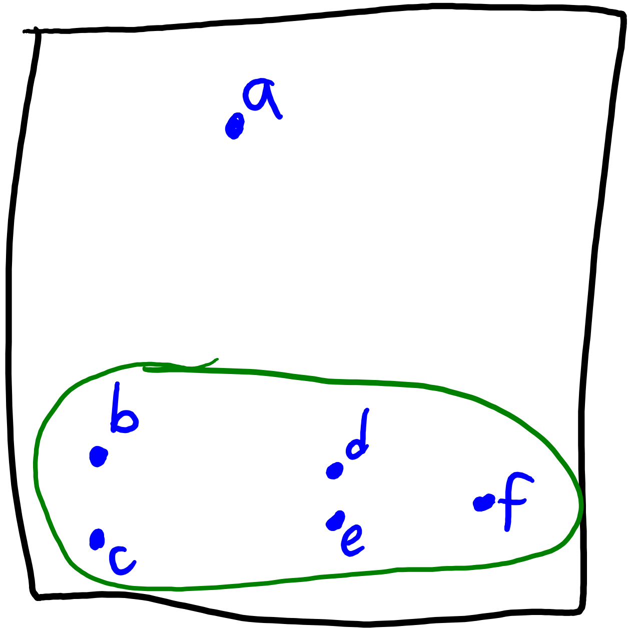
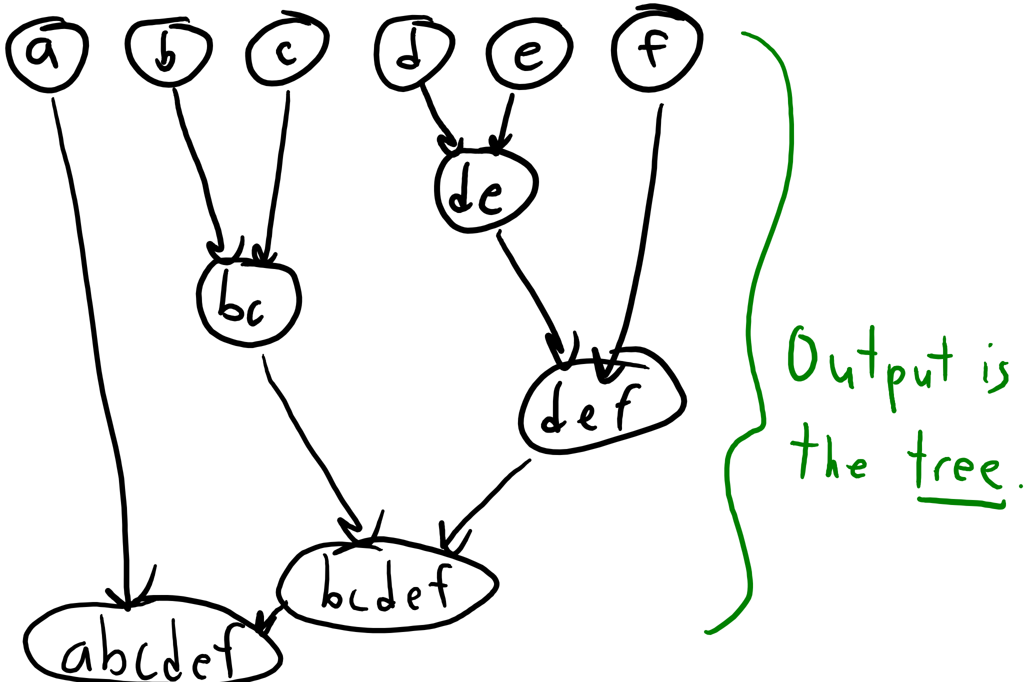
Agglomerative (Bottom-Up) Clustering

- More common hierarchical method: agglomerative clustering.
  1. Starts with each point in its own cluster.
  2. Each step merges the two “closest” clusters.
  3. Stop with one big cluster that has all points.





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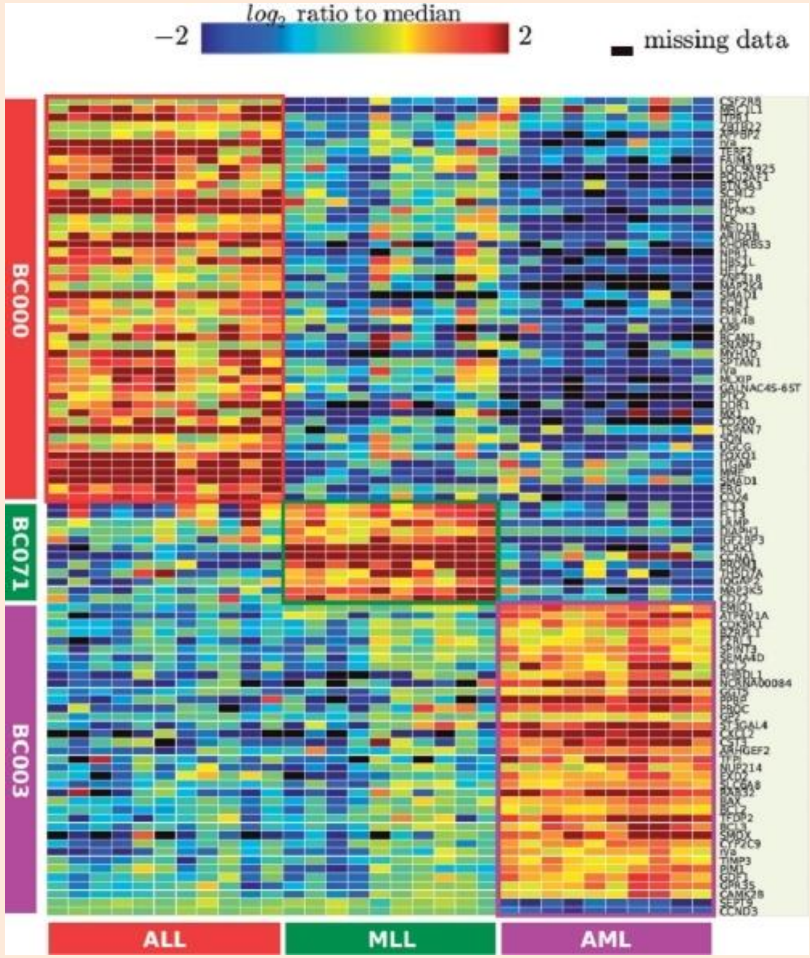
Agglomerative (Bottom-Up) Clustering

- Reinvented by different fields under different names ("UPGMA").
- Needs a "distance" between two clusters.
- A standard choice: distance between means of the clusters.
  - Not necessarily the best, many choices exist (bonus slide).
- Cost is $O(n^3d)$ for basic implementation.
  - Each step costs $O(n^2d)$, and each step might only cluster 1 new point.

Other Clustering Methods

- Mixture models:
  - Probabilistic clustering.
- Mean-shift clustering:
  - Finds local “modes” in density of points.
- Bayesian clustering:
  - A variant on ensemble methods.
  - Averages over models/clustering, weighted by “prior” belief in the model/clustering.
- Biclustering:
  - Simultaneously cluster objects and features.
- Spectral clustering and graph-based clustering:
  - Clustering of data described by graphs.

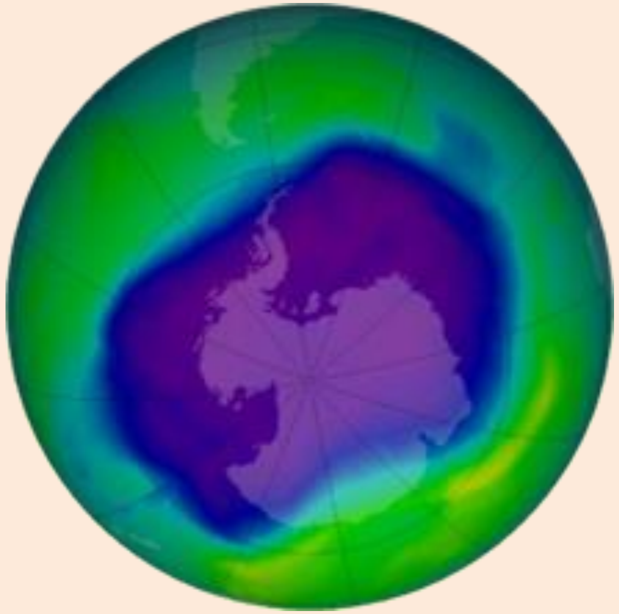


http://openi.nlm.nih.gov/detailedresult.php?img=2731891_gkp491f3&req=4

(pause)

Motivating Example: Finding Holes in Ozone Layer

- The huge Antarctic ozone hole was “discovered” in 1985.

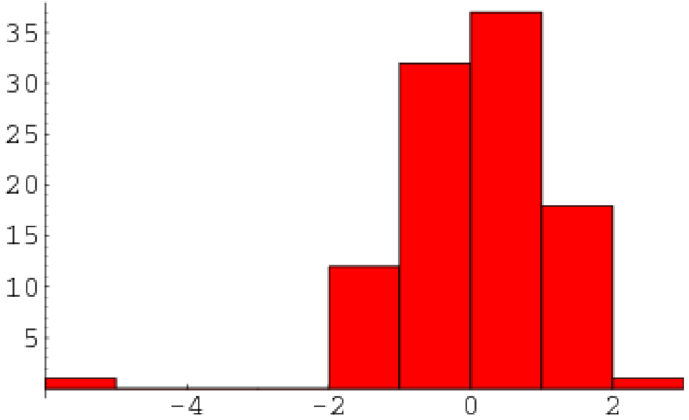


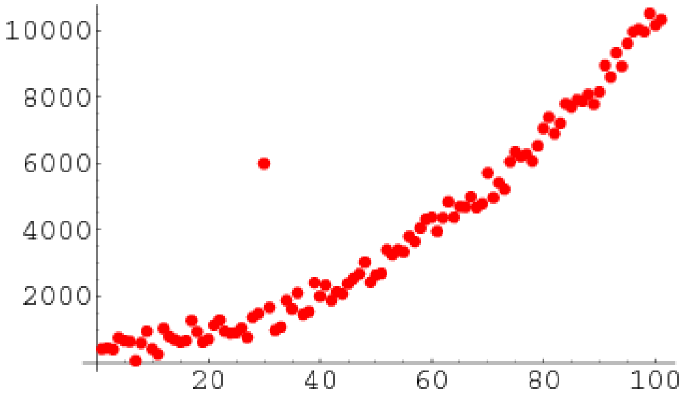
- It had been in satellite data since 1976:
  – But it was flagged and filtered out by quality-control algorithm.

https://en.wikipedia.org/wiki/Ozone_depletion

Outlier Detection

- Outlier detection:
  - Find observations that are “unusually different” from the others.
  - Also known as “anomaly detection”.
  - May want to remove outliers, or be interested in the outliers themselves (security).





- Some sources of outliers:
  - Measurement errors.
  - Data entry errors.
  - Contamination of data from different sources.
  - Rare events.

http://mathworld.wolfram.com/Outlier.html

Applications of Outlier Detection

- Data cleaning.
- Security and fault detection (network intrusion, DOS attacks).
- Fraud detection (credit cards, stocks, voting irregularities).

Transaction Date	Posted Date	Transaction Details	Debit	Credit
Aug. 27, 2015	Aug. 28, 2015	BEAN AROUND THE WORLD VANCOUVER, BC	$10.95	

- Detecting natural disasters (underwater earthquakes).
- Astronomy (find new classes of stars/planets).
- Genetics (identifying individuals with new/ancient genes).

Classes of Methods for Outlier Detection

1. Model-based methods.
2. Graphical approaches.
3. Cluster-based methods.
4. Distance-based methods.
5. Supervised-learning methods.

- Warning: this is the topic with the most ambiguous “solutions”.

But first…

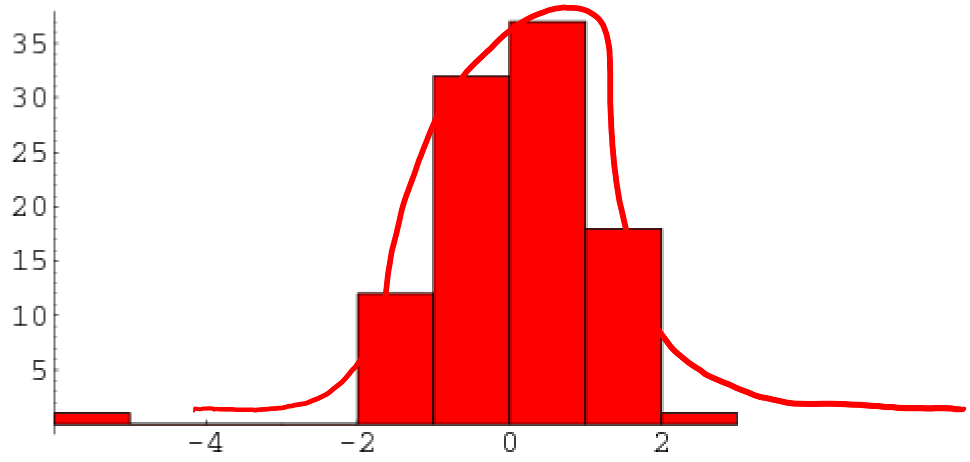
- Usually it's good to do some basic sanity checking…

Egg	Milk	Fish	Wheat	Shellfish	Peanuts	Peanuts	Sick?
0	0.7	0	0.3	0	0	0	1
0.3	0.7	0	0.6	-1	3	3	1
0	0	0	"sick"	0	1	1	0
0.3	0.7	1.2	0	0.10	0	0.01	-1
900	0	1.2	0.3	0.10	0	0	1

  - Would any values in the column cause a Python/Julia "Type" error?
  - What is the range of numerical features?
  - What are the unique entries for a categorical feature?
  - Does it look like parts of the table are duplicated?
- These types of simple errors are VERY common in real data.

Model-Based Outlier Detection

- Model-based outlier detection:
  1. Fit a probabilistic model.
  2. Outliers are examples with low probability.



- Example:
  – Assume data follows normal distribution.
  – The z-score for 1D data is given by:

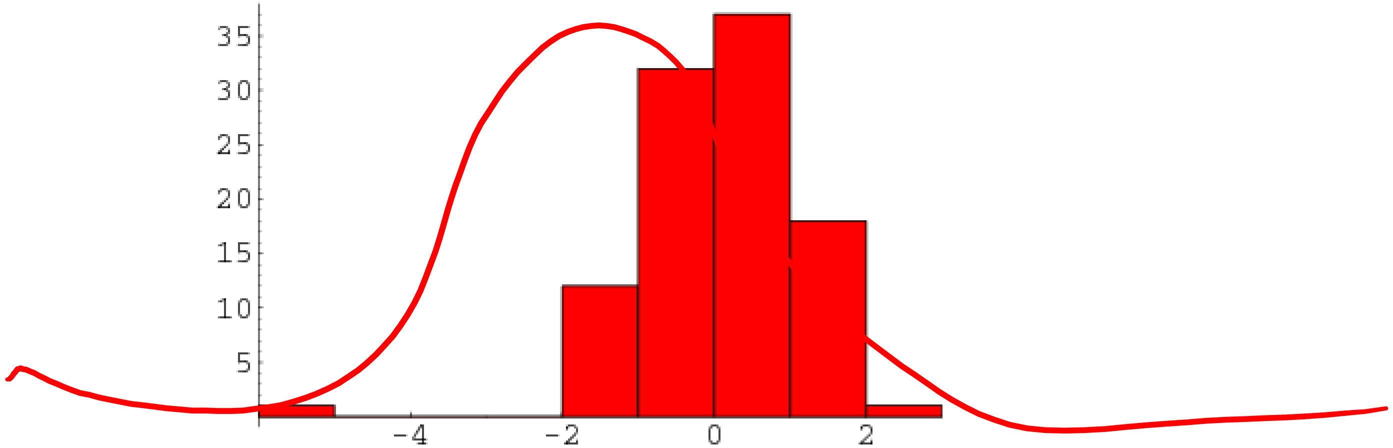
$$z_i = \frac{x_i - \mu}{\sigma} \quad \text{where } \mu = \frac{1}{n}\sum_{i=1}^{n} x_i \quad \text{and } \sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2}$$

  – "Number of standard deviations away from the mean".
  – Say "outlier" is |z| > 4, or some other threshold.

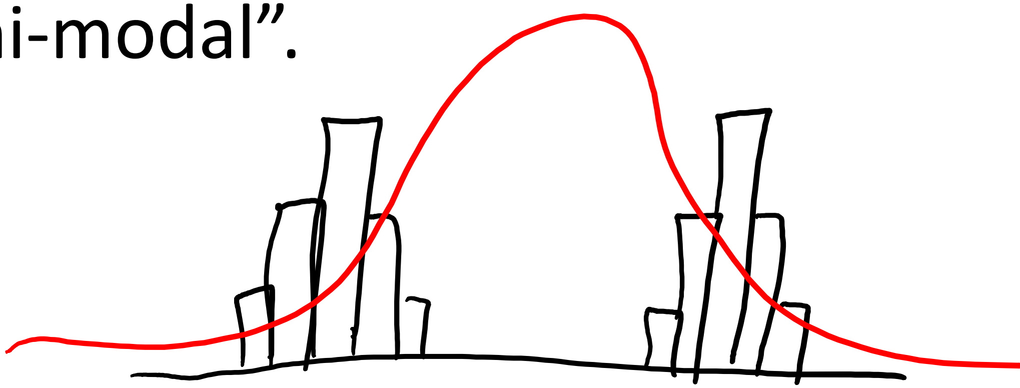
http://mathworld.wolfram.com/Outlier.html

Problems with Z-Score

- Unfortunately, the mean and variance are sensitive to outliers.



  - Possible fixes: use quantiles, or sequentially remove worse outlier.
- The z-score also assumes that data is “uni-modal”.
  - Data is concentrated around the mean.



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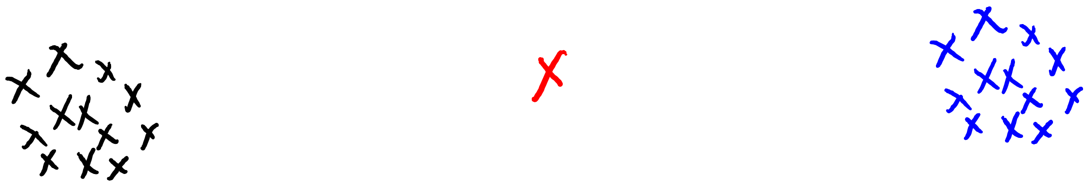
Global vs. Local Outliers

- Is the red point an outlier?

Global vs. Local Outliers

- Is the red point an outlier? What if we add the blue points?



Global vs. Local Outliers

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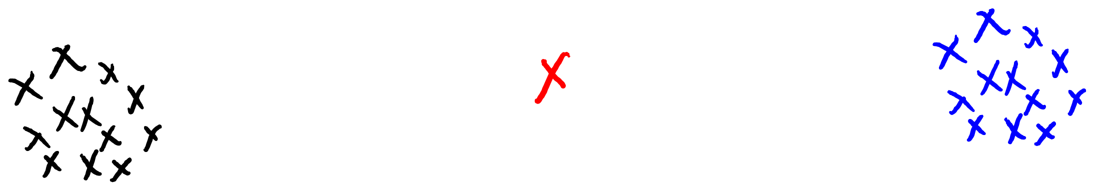

- Red point has the lowest z-score.
  - In the first case it was a “global” outlier.
  - In this second case it’s a “local” outlier:
    - Within normal data range, but far from other points.
- It’s hard to precisely define “outliers”.

Global vs. Local Outliers

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  - Can we have outlier groups?

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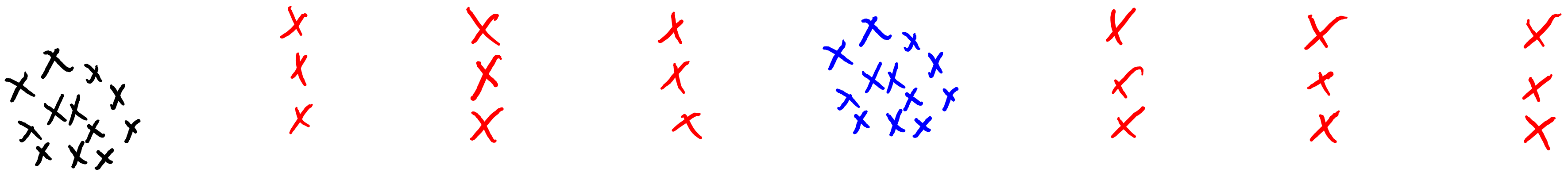

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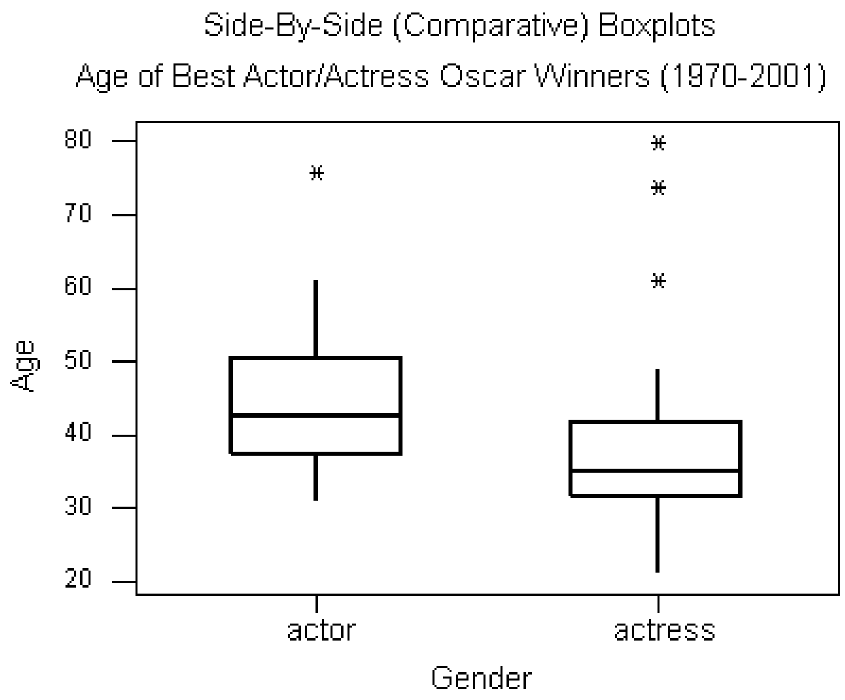
    - Within normal data range, but far from other points.
- It's hard to precisely define "outliers".
  - Can we have outlier groups? What about repeating patterns?

Graphical Outlier Detection

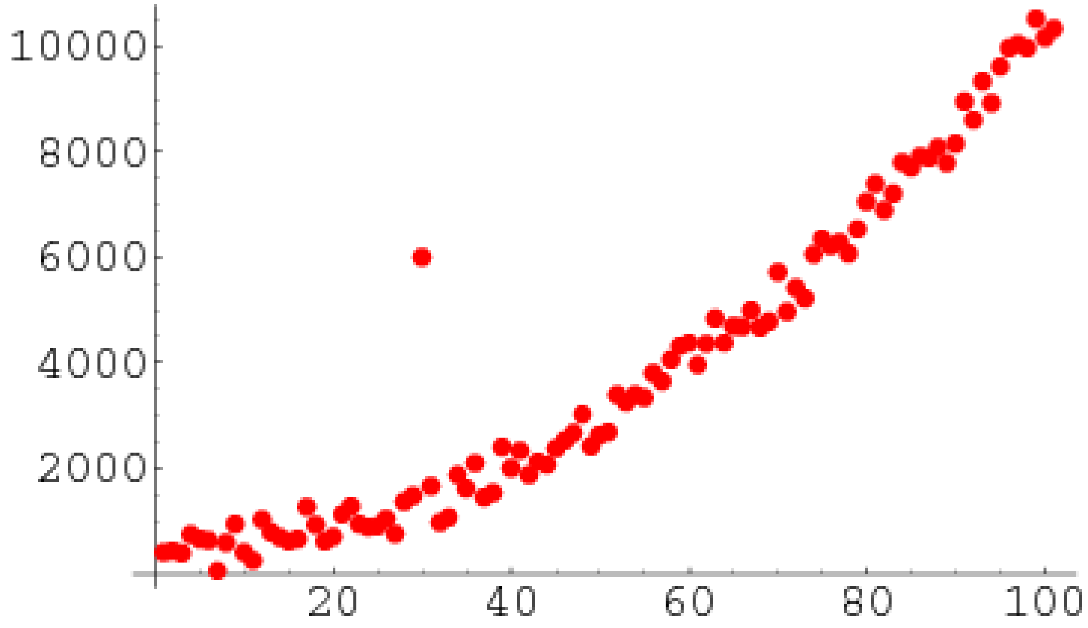
- Graphical approach to outlier detection:
  1. Look at a plot of the data.
  2. Human decides if data is an outlier.
- Examples:
  1. Box plot:
     - Visualization of quantiles/outliers.
     - Only 1 variable at a time.



http://bolt.mph.ufl.edu/6050-6052/unit-1/one-quantitative-variable-introduction/boxplot/

Graphical Outlier Detection

- Graphical approach to outlier detection:
  1. Look at a plot of the data.
  2. Human decides if data is an outlier.
- Examples:
  1. Box plot.
  2. Scatterplot:
     - Can detect complex patterns.
     - Only 2 variables at a time.



http://mathworld.wolfram.com/Outlier.html

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  1. Look at a plot of the data.
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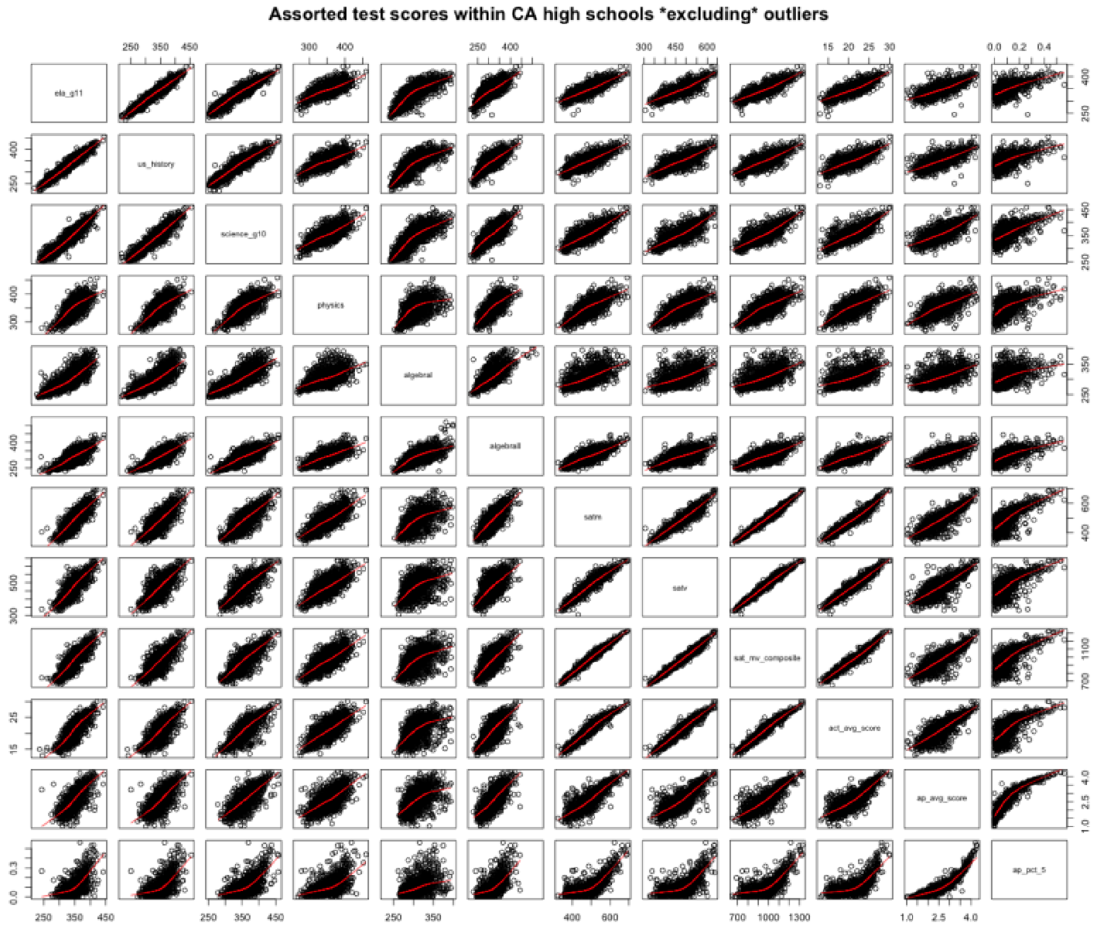
- Examples:
  1. Box plot.
  2. Scatterplot.
  3. Scatterplot array:
     - Look at all combinations of variables.
     - But laborious in high-dimensions.
     - Still only 2 variables at a time.



https://randomcriticalanalysis.wordpress.com/2015/05/25/standardized-tests-correlations-within-and-between-california-public-schools/

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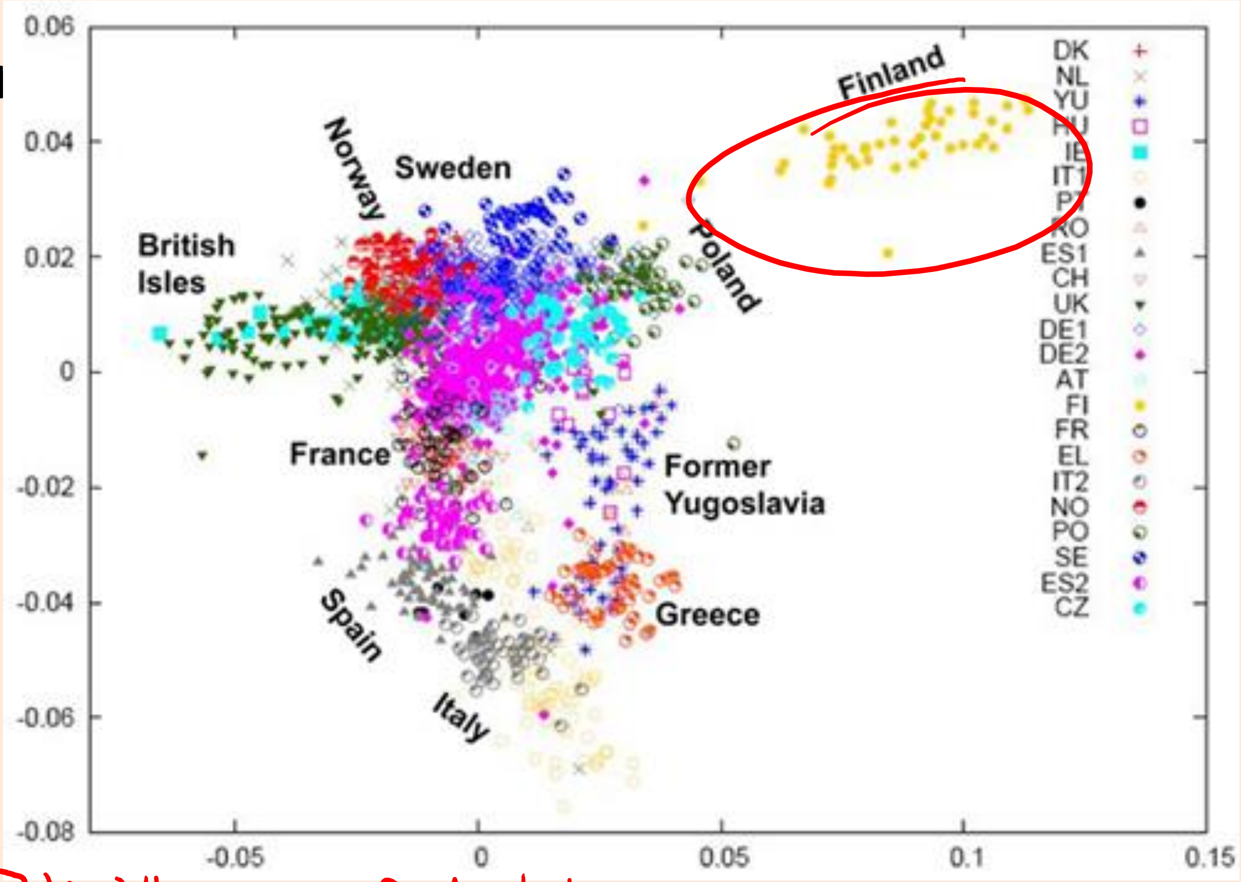
- Examples:
  1. Box plot.
  2. Scatterplot.
  3. Scatterplot array.
  4. Scatterplot of 2-dimensional PCA:
     - 'See' high-dimensional structure.
     - But loses information and sensitive to outliers.

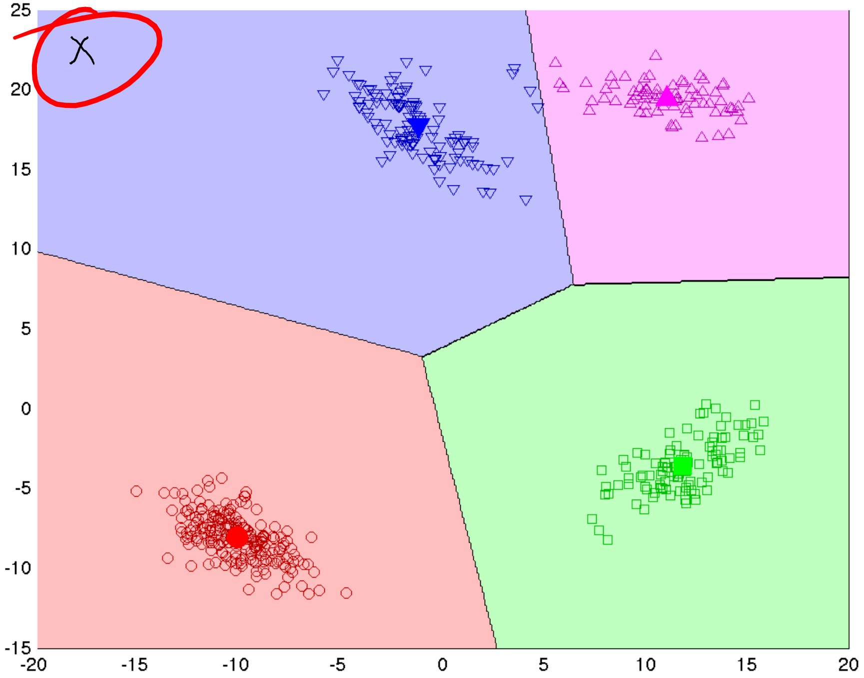


We'll cover PCA later in this course.

http://scienceblogs.com/gnxp/2008/08/14/the-genetic-map-of-europe/

Cluster-Based Outlier Detection

- Detect outliers based on clustering:
  1. Cluster the data.
  2. Find points that don’t belong to clusters.
- Examples:
  1. K-means:
     - Find points that are far away from any mean.
     - Find clusters with a small number of points.



Cluster-Based Outlier Detection

- Detect outliers based on clustering:
  1. Cluster the data.
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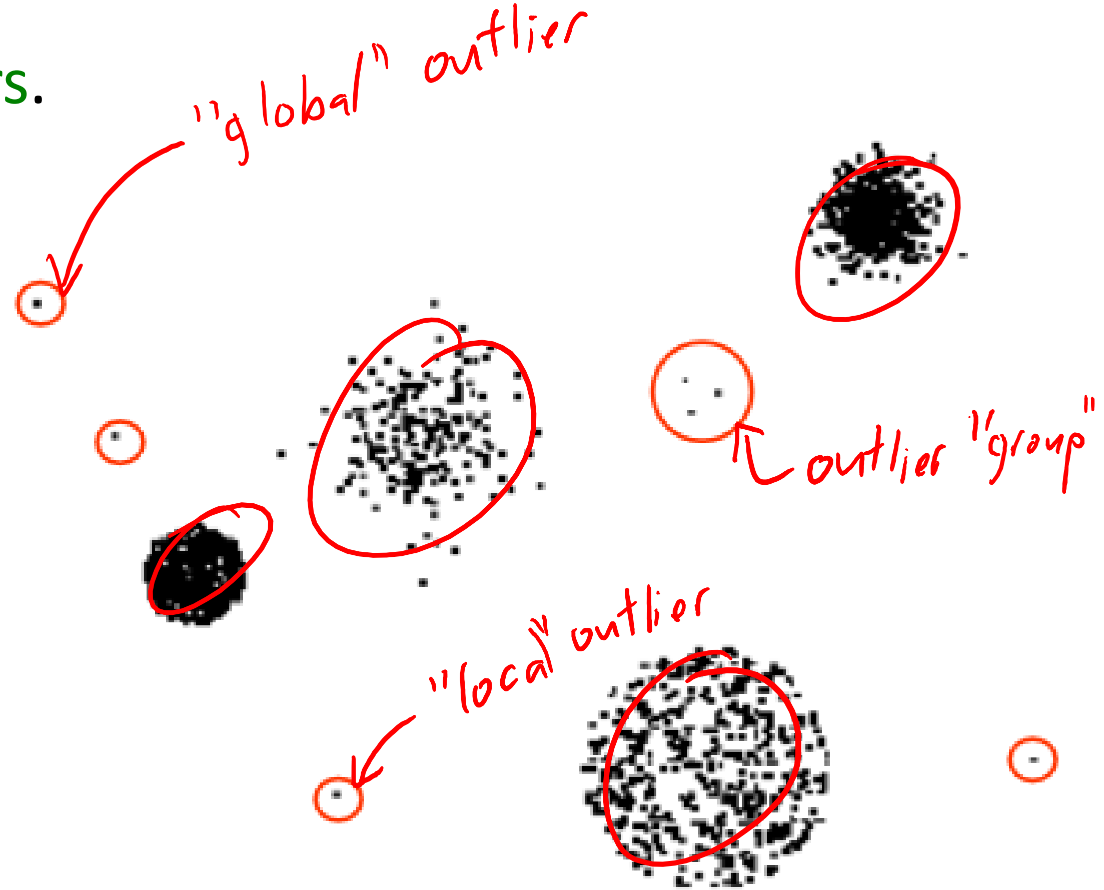
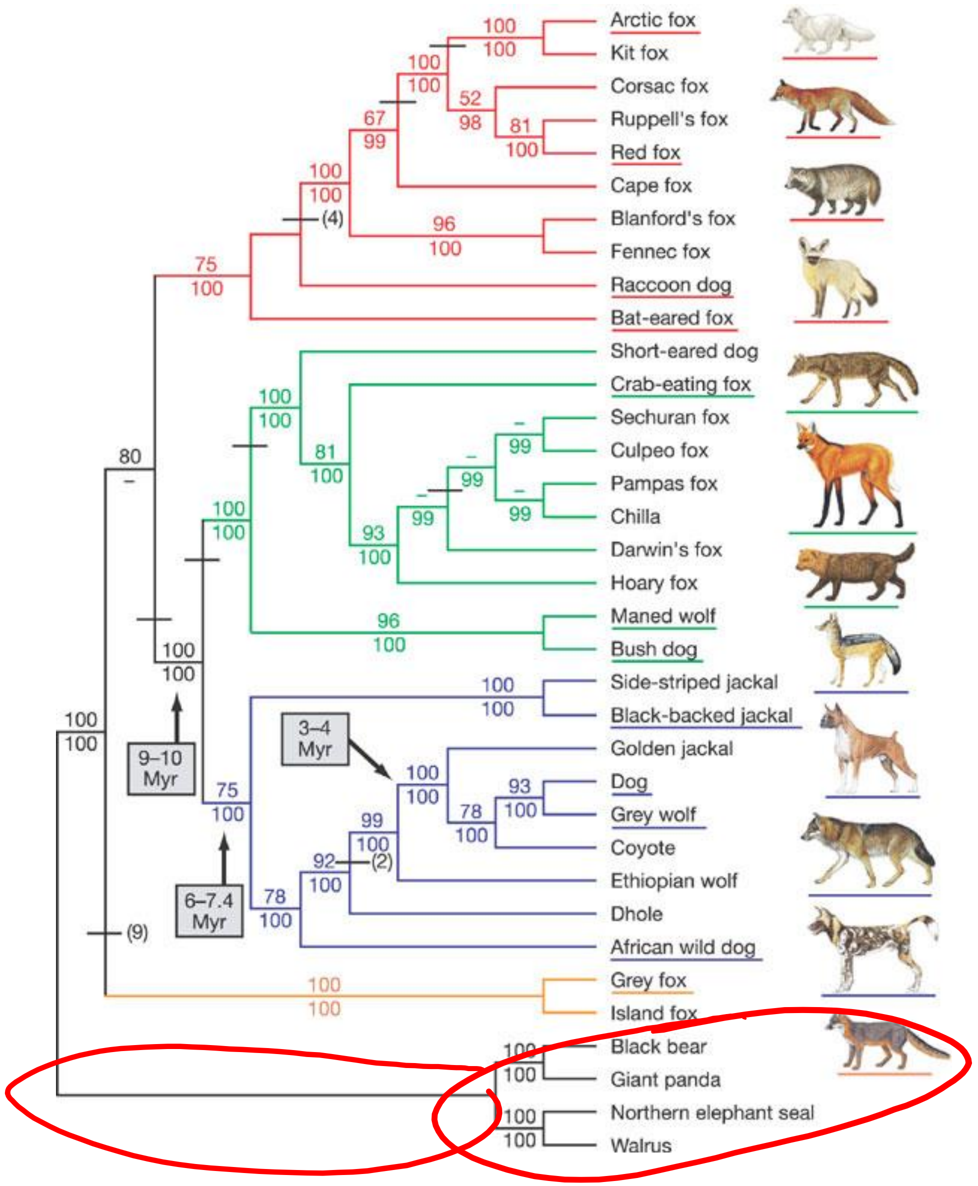
- Examples:
  1. K-means.
  2. Density-based clustering:
     - Outliers are points not assigned to cluster.



http://www-users.cs.umn.edu/~kumar/dmbook/dmslides/chap10_anomaly_detection.pdf

Cluster-Based Outlier Detection

- Detect outliers based on clustering:
  1. Cluster the data.
  2. Find points that don't belong to clusters.
- Examples:
  1. K-means.
  2. Density-based clustering.
  3. Hierarchical clustering:
     - Outliers take longer to join other groups.
     - Also good for outlier groups.



http://www.nature.com/nature/journal/v438/n7069/fig_tab/nature04338_F10.html

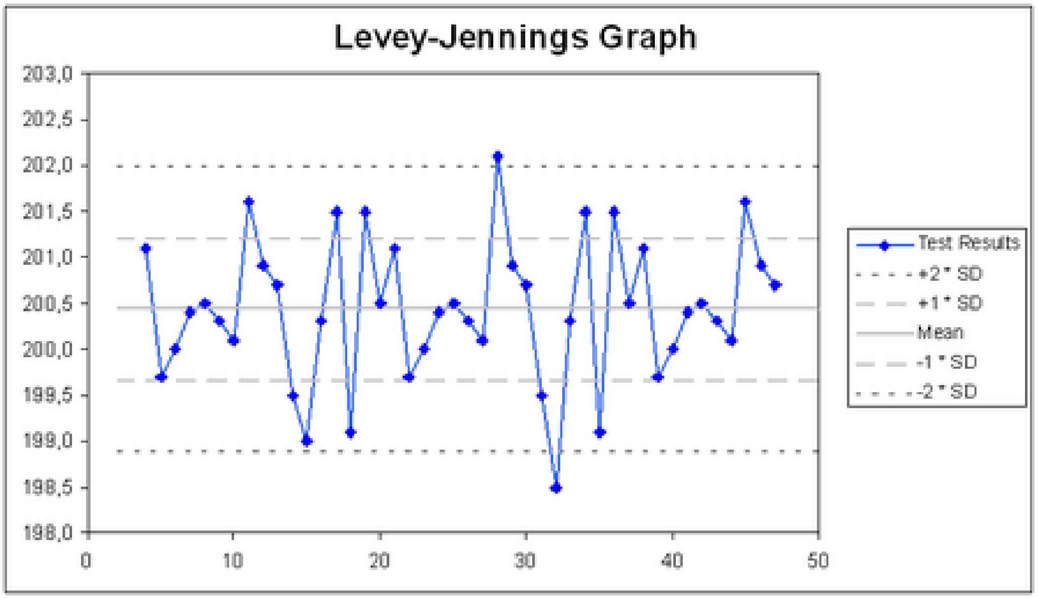
Summary

- Hierarchical clustering: more informative than fixed clustering.
- Agglomerative clustering: standard hierarchical clustering method.
  – Each point starts as a cluster, sequentially merge clusters.
- Outlier detection is task of finding unusually different object.
  – A concept that is very difficult to define.
  – Model-based find unlikely objects given a model of the data.
  – Graphical methods plot data and use human to find outliers.
  – Cluster-based methods check whether objects belong to clusters.

- Next time: "customers who bought this item also bought".

“Quality Control”: Outlier Detection in Time-Series

- A field primarily focusing on outlier detection is quality control.
- One of the main tools is plotting z-score thresholds over time:



- Usually don’t do tests like “$|z_i| > 3$”, since this happens normally.
- Instead, identify problems with tests like “$|z_i| > 2$ twice in a row”.

https://en.wikipedia.org/wiki/Laboratory_quality_control

Distances between Clusters

- Other choices of the distance between two clusters:
  - "Single-link": minimum distance between points in clusters.
  - "Average-link": average distance between points in clusters.
  - "Complete-link": maximum distance between points in clusters.
  - Ward's method: minimize within-cluster variance.
  - "Centroid-link": distance between a representative point in the cluster.
    - Useful for distance measures on non-Euclidean spaces (like Jaccard similarity).
    - "Centroid" often defined as point in cluster minimizing average distance to other points.

Cost of Agglomerative Clustering

- One step of agglomerative clustering costs $O(n^2d)$:
  - We need to do the $O(d)$ distance calculation between up to $O(n^2)$ points.
  - This is assuming the standard distance functions.
- We do at most $O(n)$ steps:
  - Starting with 'n' clusters and merging 2 clusters on each step, after $O(n)$ steps we'll only have 1 cluster left (though typically it will be much smaller).
- This gives a total cost of $O(n^3d)$.

- This can be reduced to $O(n^2d \log n)$ with a priority queue:
  - Store distances in a sorted order, only update the distances that change.
- For single- and complete-linkage, you can get it down to $O(n^2d)$.
  - "SLINK" and "CLINK" algorithms.

Bonus Slide: Divisive (Top-Down) Clustering

- Start with all objects in one cluster, then start dividing.
- E.g., run k-means on a cluster, then run again on resulting clusters.
  - A clustering analogue of decision tree learning.