

CPSC 340: Machine Learning and Data Mining

Hierarchical Clustering

and

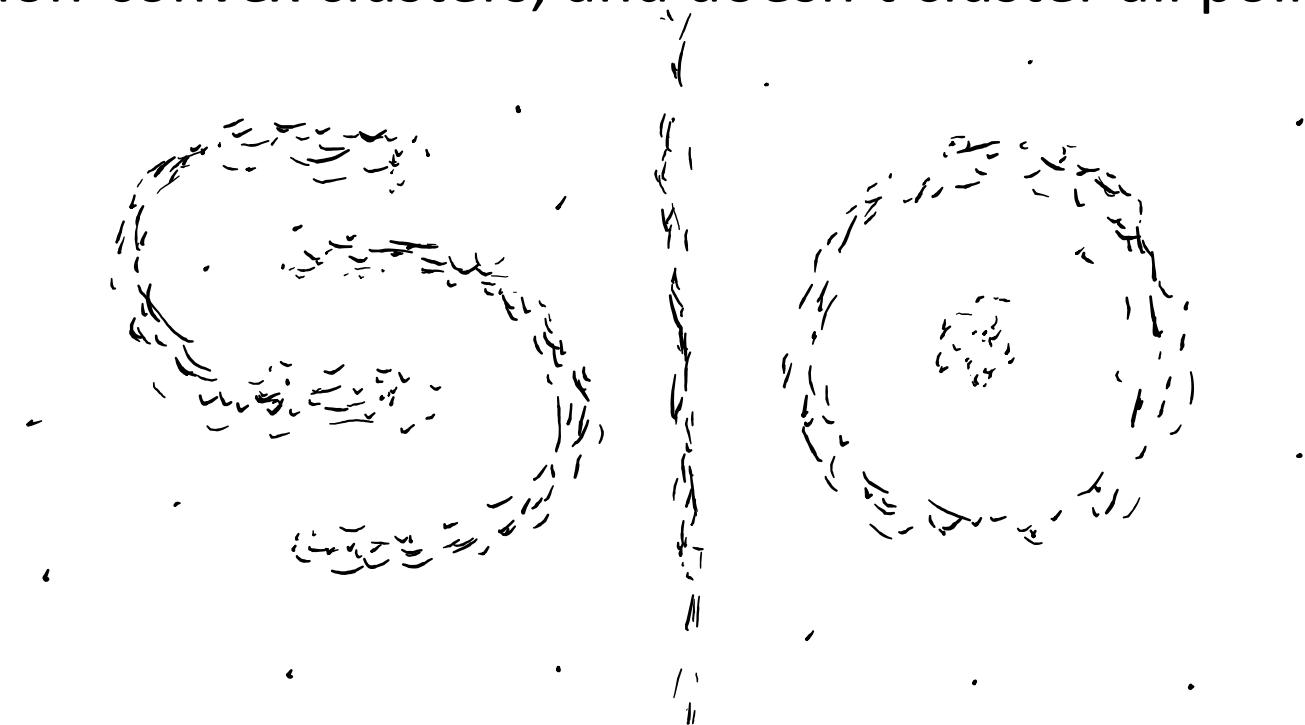
Outlier Detection

Admin

- Assignment 2 is due Friday.
- UBC ML club: first meeting this Thursday 5-6pm in ICCS 246
- Seeking a software developer for the summer
 - To work on GitHub course development system

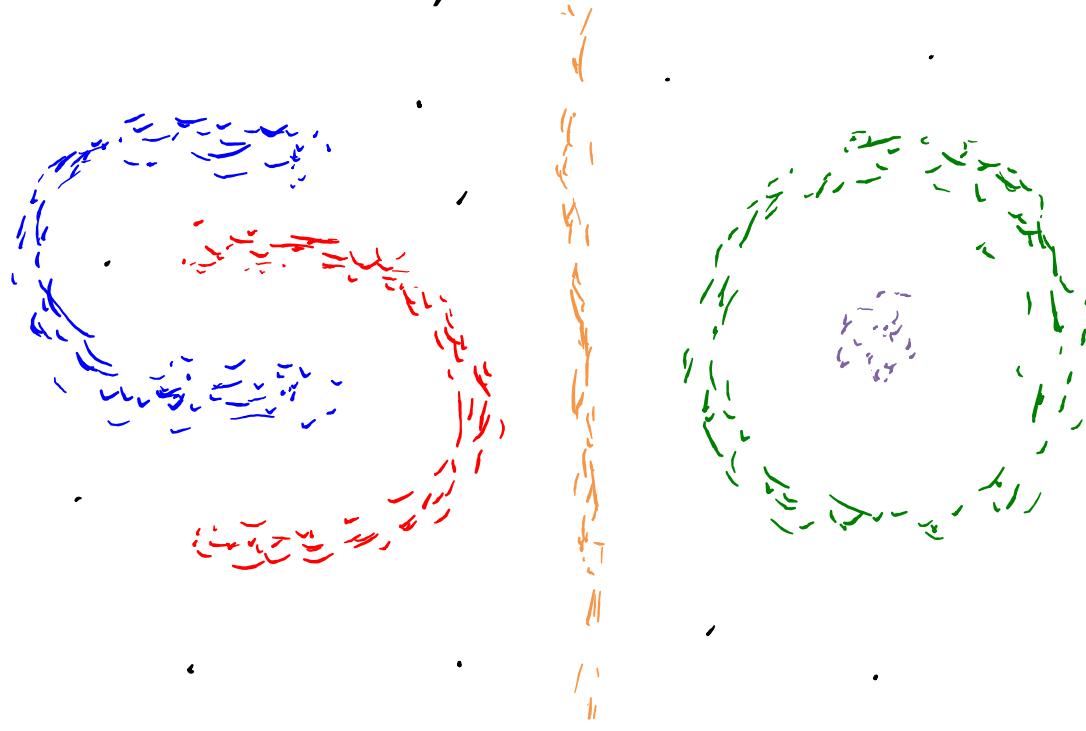
Last Time: Density-Based Clustering

- 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.



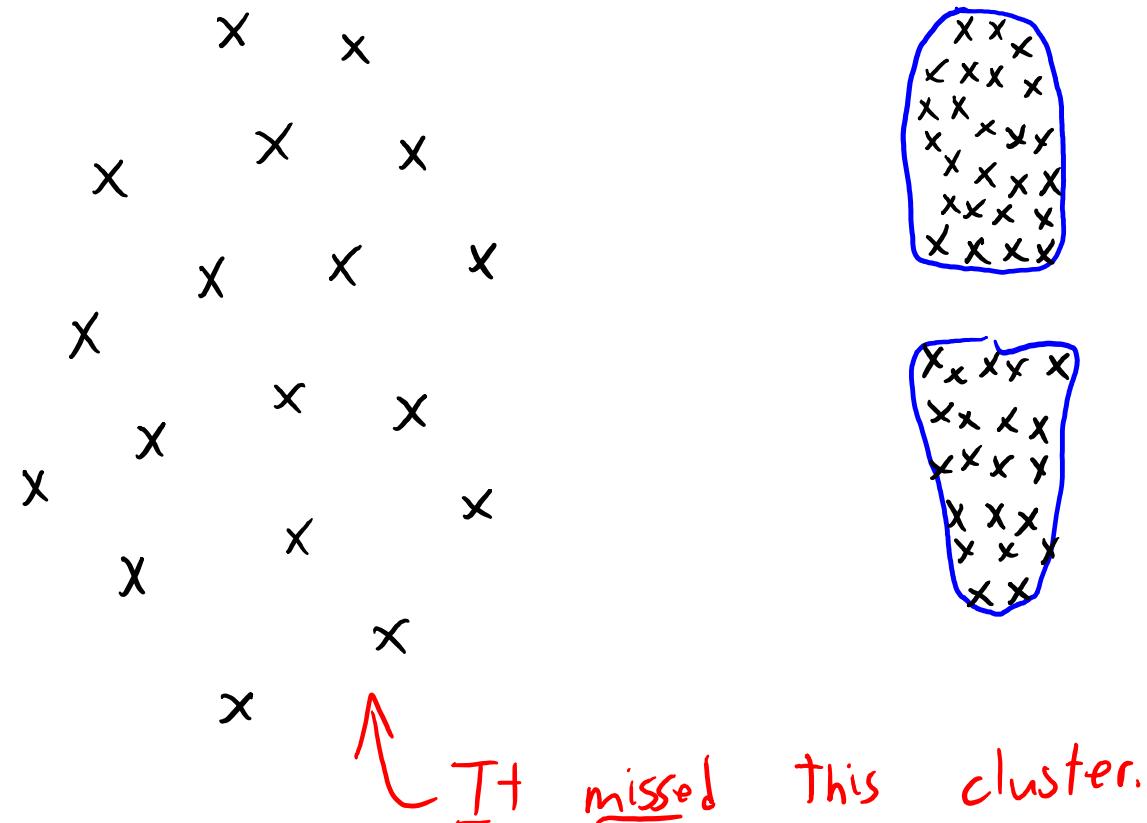
Last Time: Density-Based Clustering

- 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.



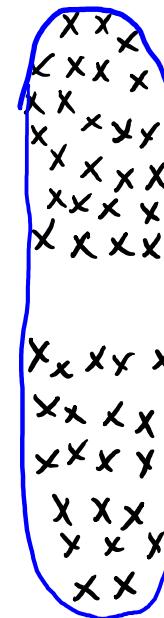
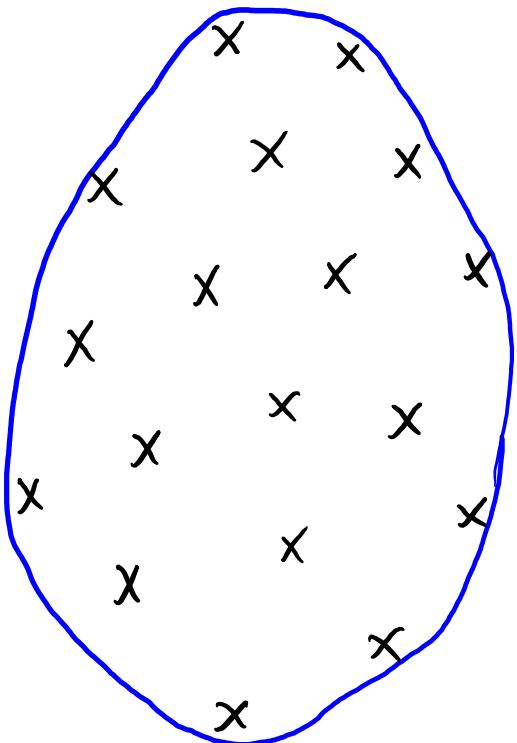
Differing Densities

- Consider density-based clustering on this data:



Differing Densities

- Increase epsilon and run it again:

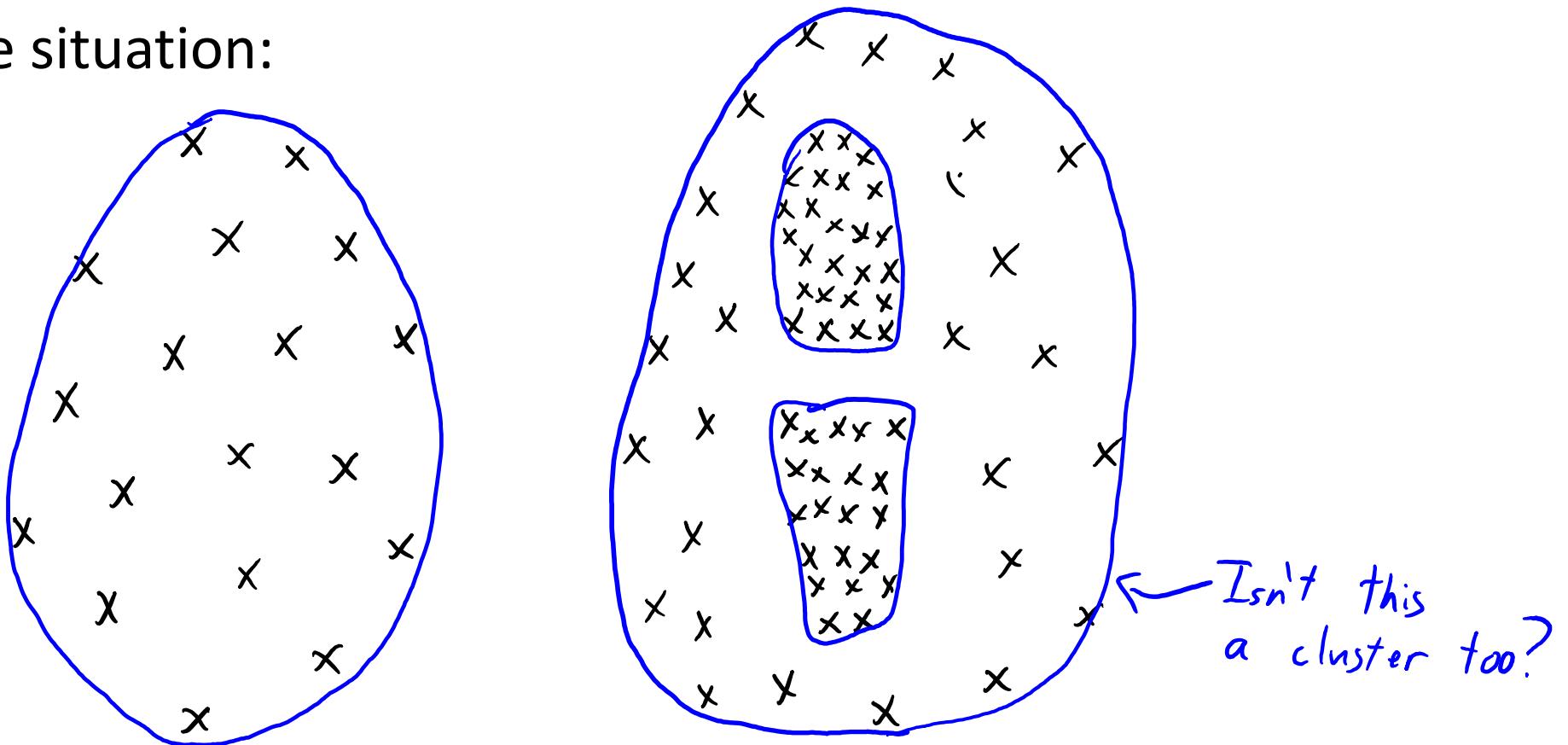


These 2 clusters
are now "close."

- There may be no density-level that gives you 3 clusters.
- See Jupyter notebook demo for previous lecture.

Differing Densities

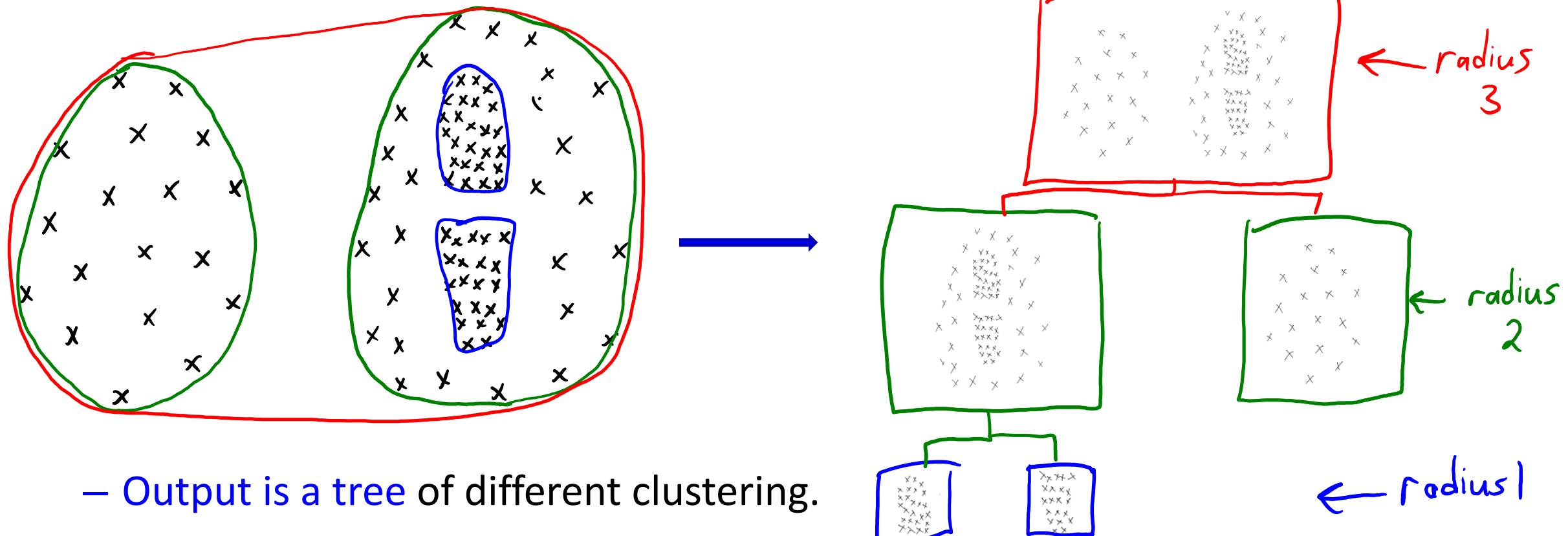
- Here is a worse situation:



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

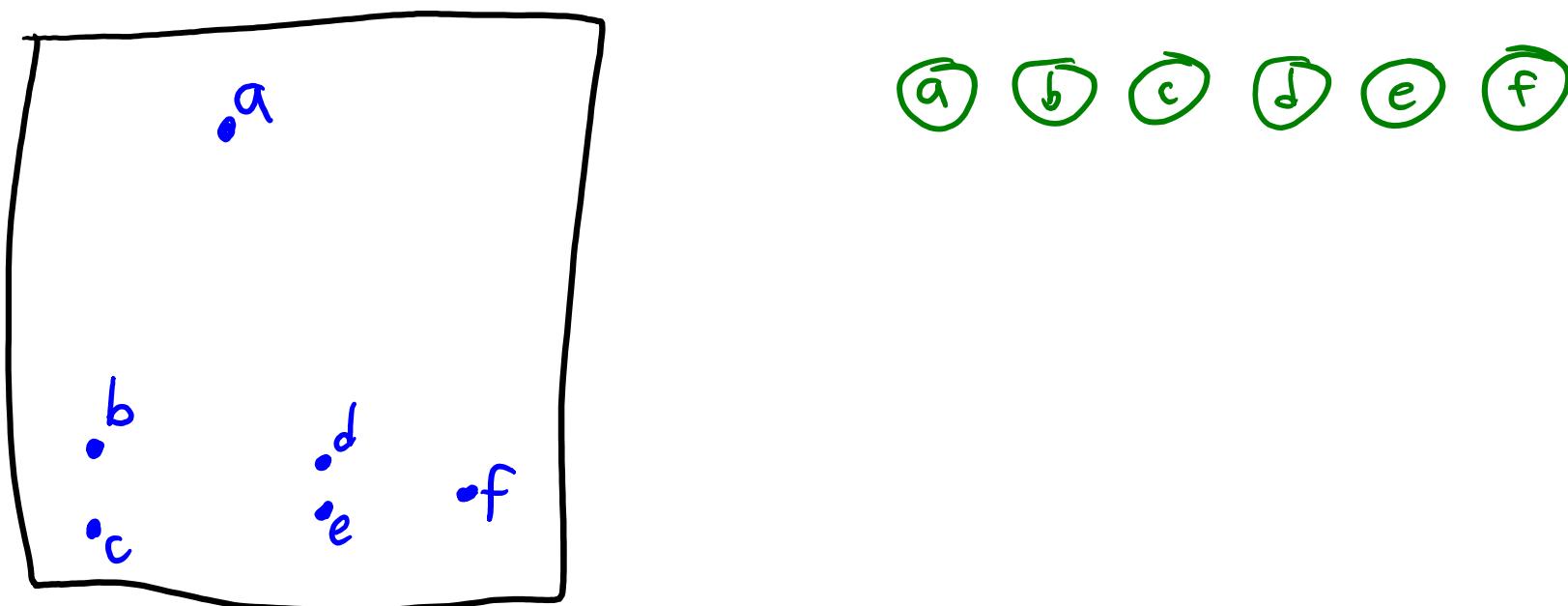
Density-Based Hierarchical Clustering

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



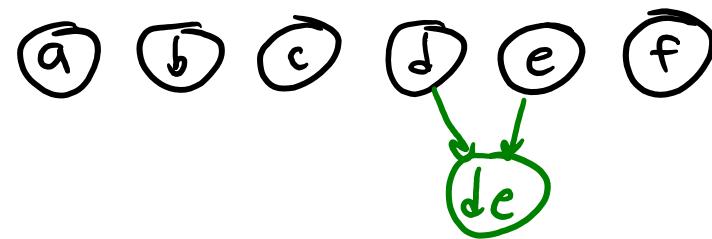
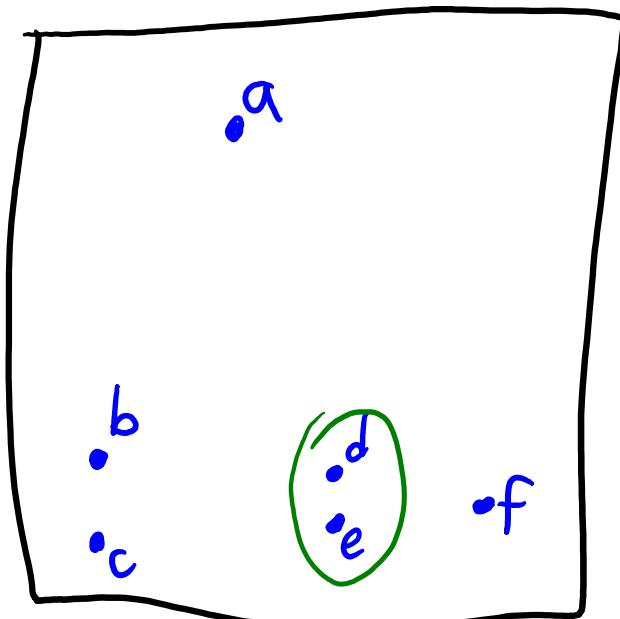
Agglomerative (Bottom-Up) Clustering

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



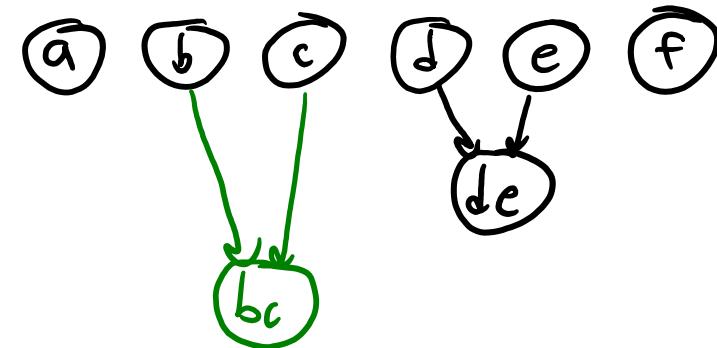
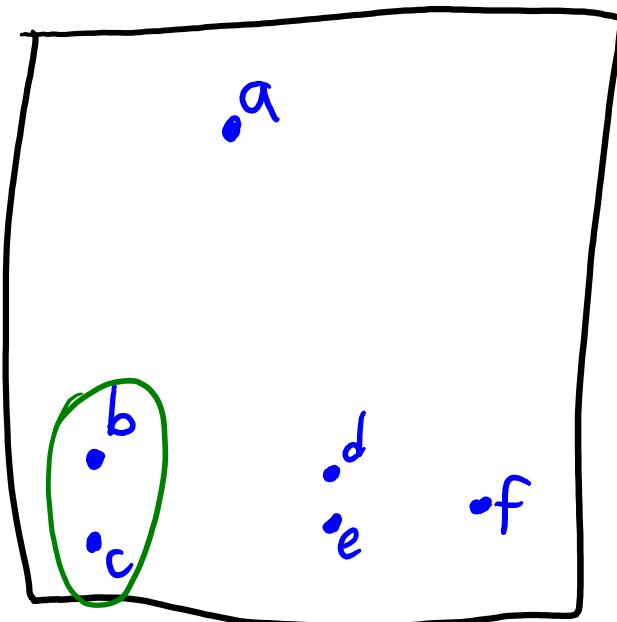
Agglomerative (Bottom-Up) Clustering

- More common hierarchical method: **agglomerative clustering**.
 1. Starts with each point in its own cluster.
 2. Each step merges the two “closest” clusters.



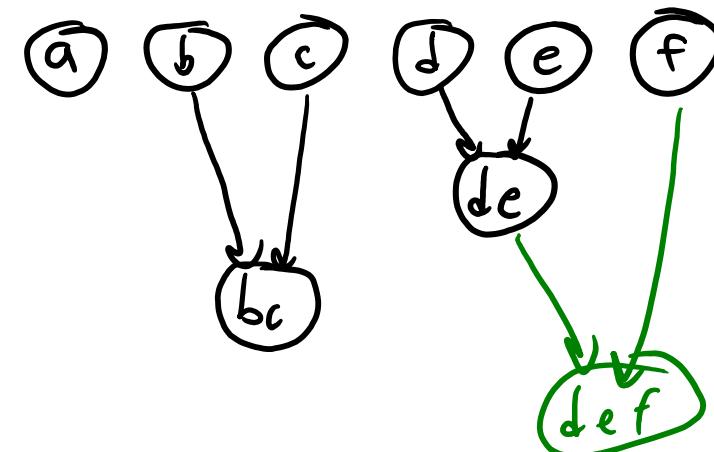
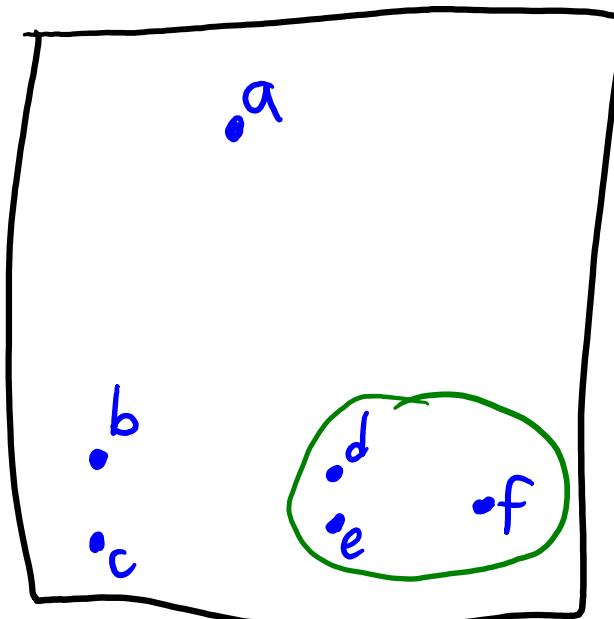
Agglomerative (Bottom-Up) Clustering

- More common hierarchical method: **agglomerative clustering**.
 1. Starts with each point in its own cluster.
 2. Each step merges the two “closest” clusters.



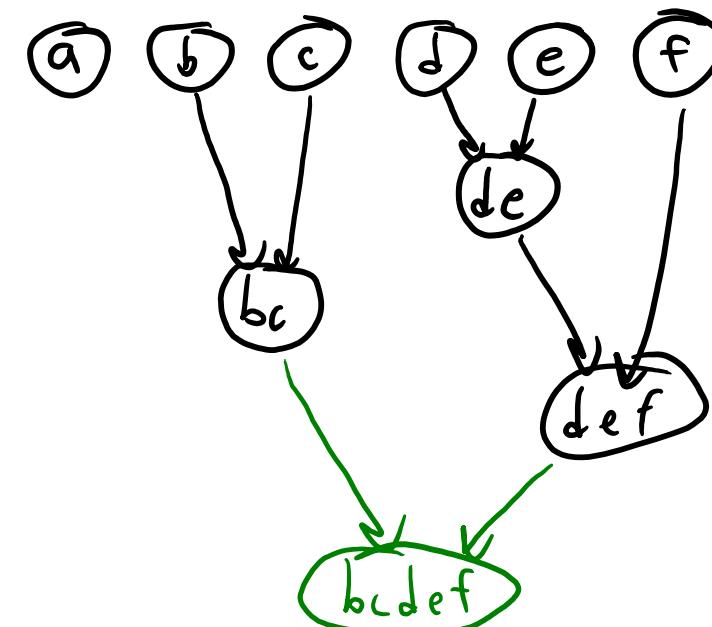
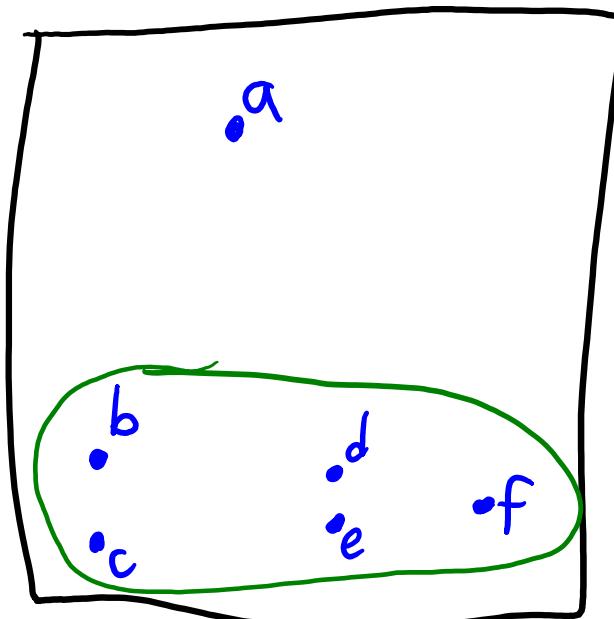
Agglomerative (Bottom-Up) Clustering

- More common hierarchical method: **agglomerative clustering**.
 1. Starts with each point in its own cluster.
 2. Each step merges the two “closest” clusters.



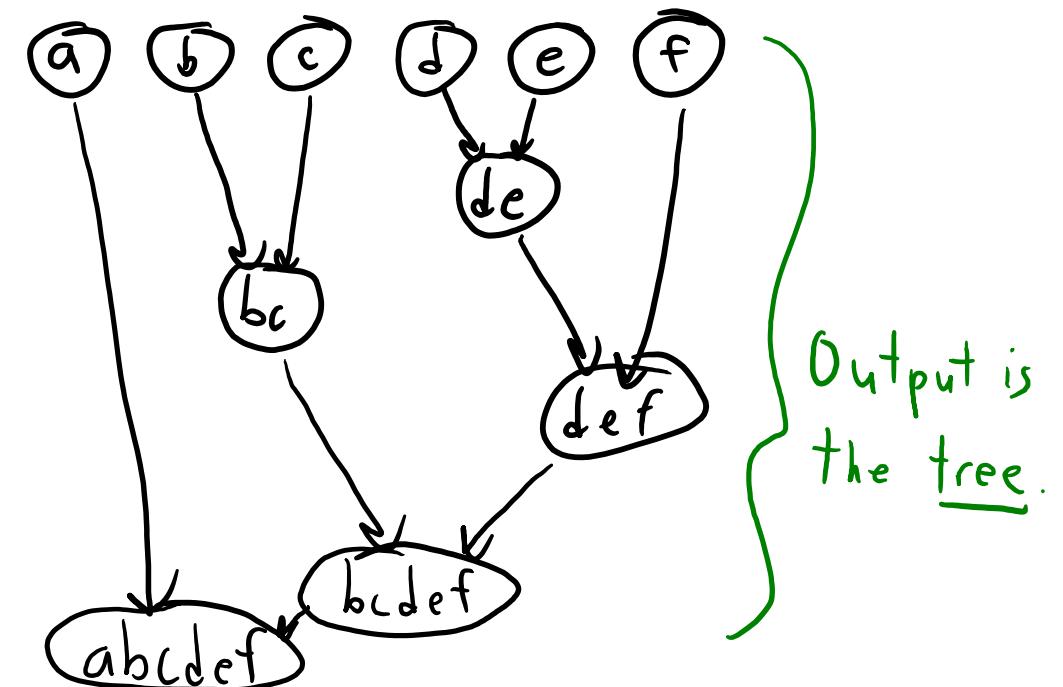
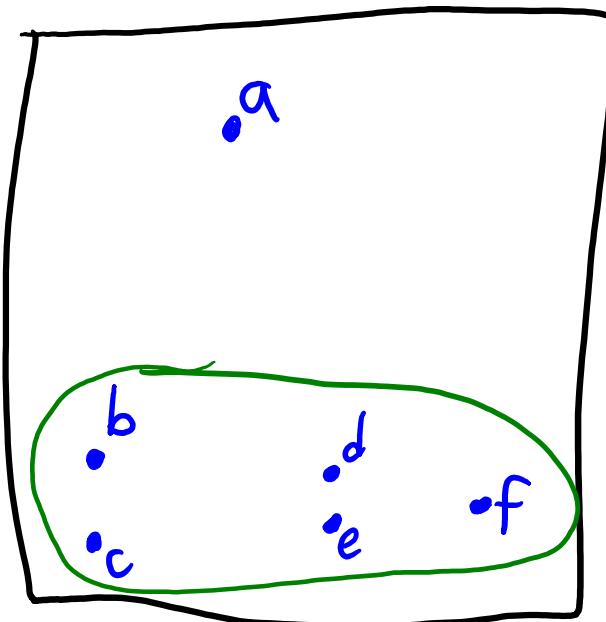
Agglomerative (Bottom-Up) Clustering

- More common hierarchical method: **agglomerative clustering**.
 1. Starts with each point in its own cluster.
 2. Each step merges the two “closest” clusters.



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.



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.

(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.

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 (e.g., security).
- Some sources of outliers:
 - Measurement errors.
 - Data entry errors.
 - Contamination of data from different sources.
 - Rare events.

Applications of Outlier Detection

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

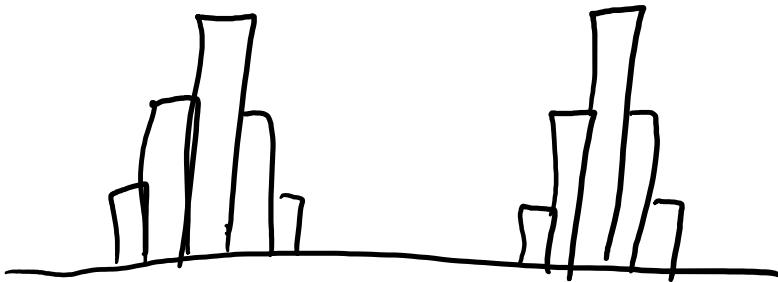
- Example:
 - Assume data follows normal distribution.
 - The z-score for 1D data is given by:

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

- “Number of standard deviations away from the mean”.
- Say “outlier” is $|z| > 4$, or some other threshold.

Problems with Z-Score

- Unfortunately, the mean and variance are sensitive to outliers.
 - Possible fixes: use quantiles, or sequentially remove worst outlier.
- The z-score also assumes that data is “uni-modal”.
 - Data is concentrated around the mean.



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

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



- 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

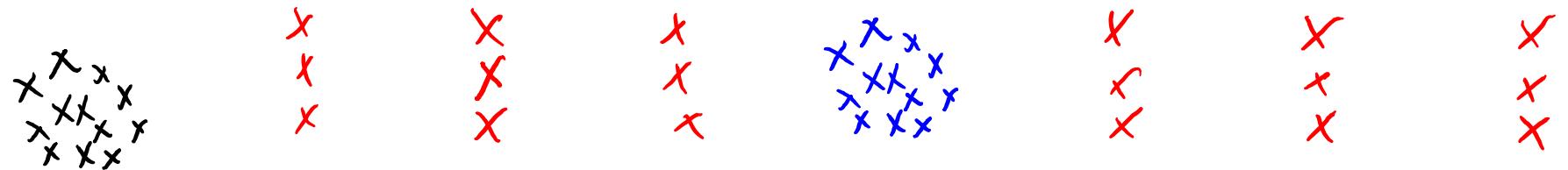
- Is the **red point** an outlier? What if we add the **blue points**?



- 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”.
 - Can we have **outlier groups**?

Global vs. Local Outliers

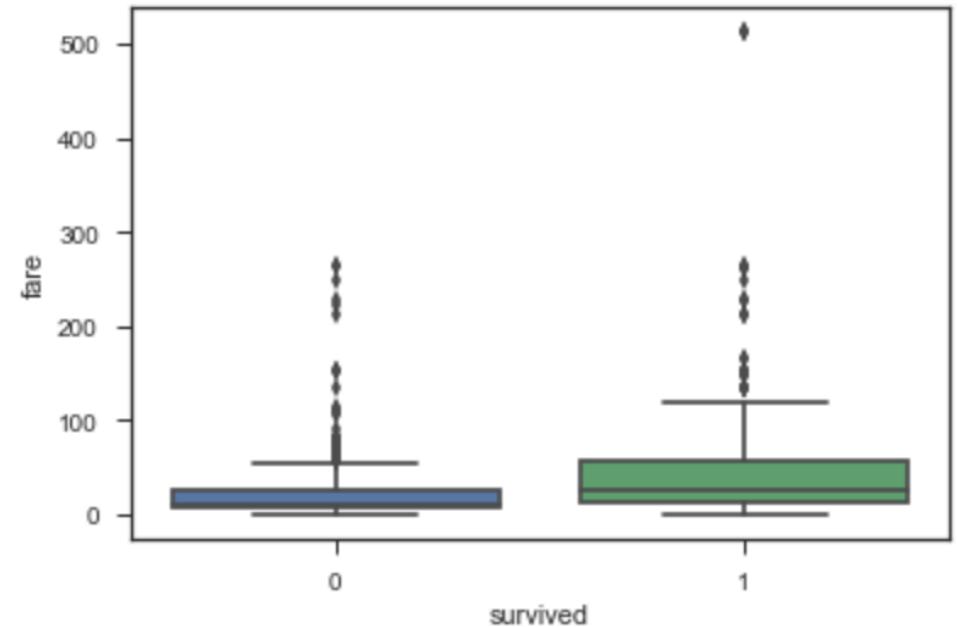
- Is the **red point** an outlier? What if we add the **blue points**?



- 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”.
 - Can we have **outlier groups**? What about repeating patterns?

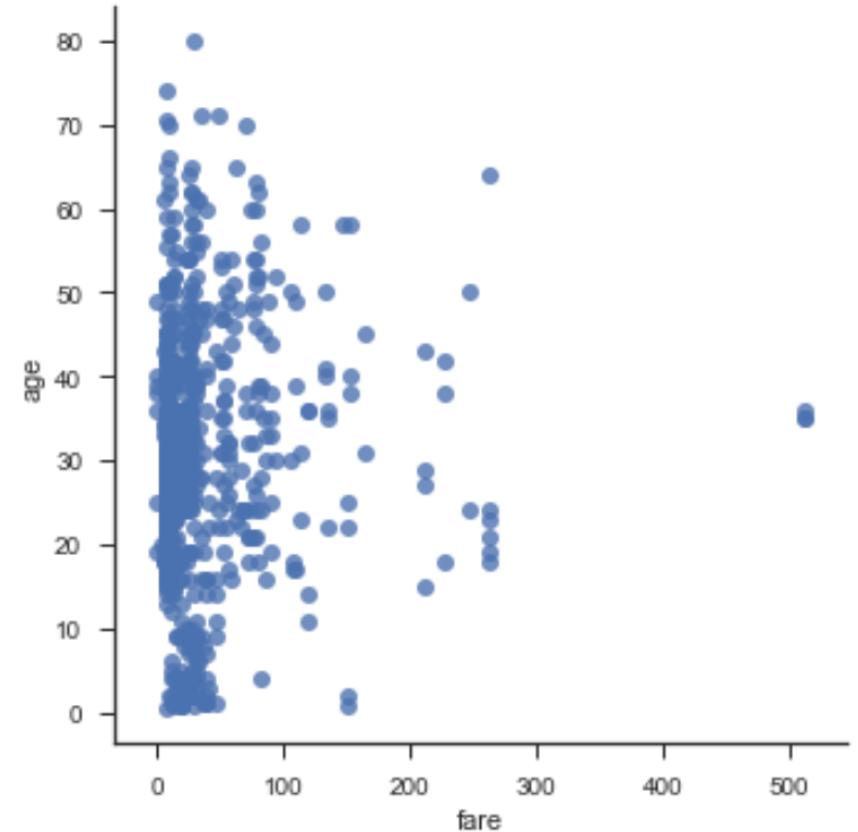
Graphical Outlier Detection

- 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.



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.

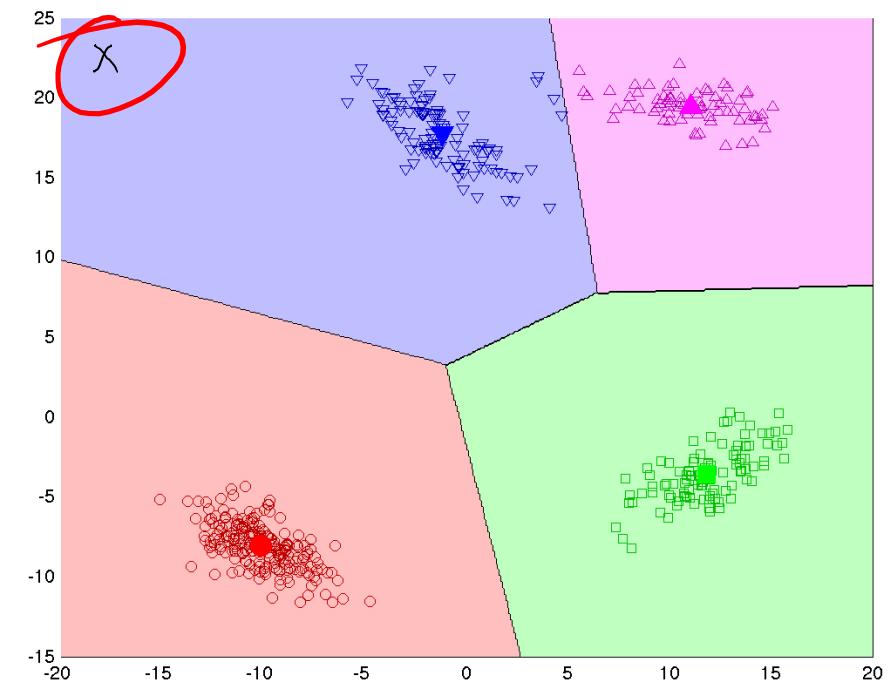


Graphical Outlier Detection

- 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.
 3. Scatterplot array:
 - Look at all combinations of variables.
 - But laborious in high-dimensions.
 - Still only 2 variables at a time.

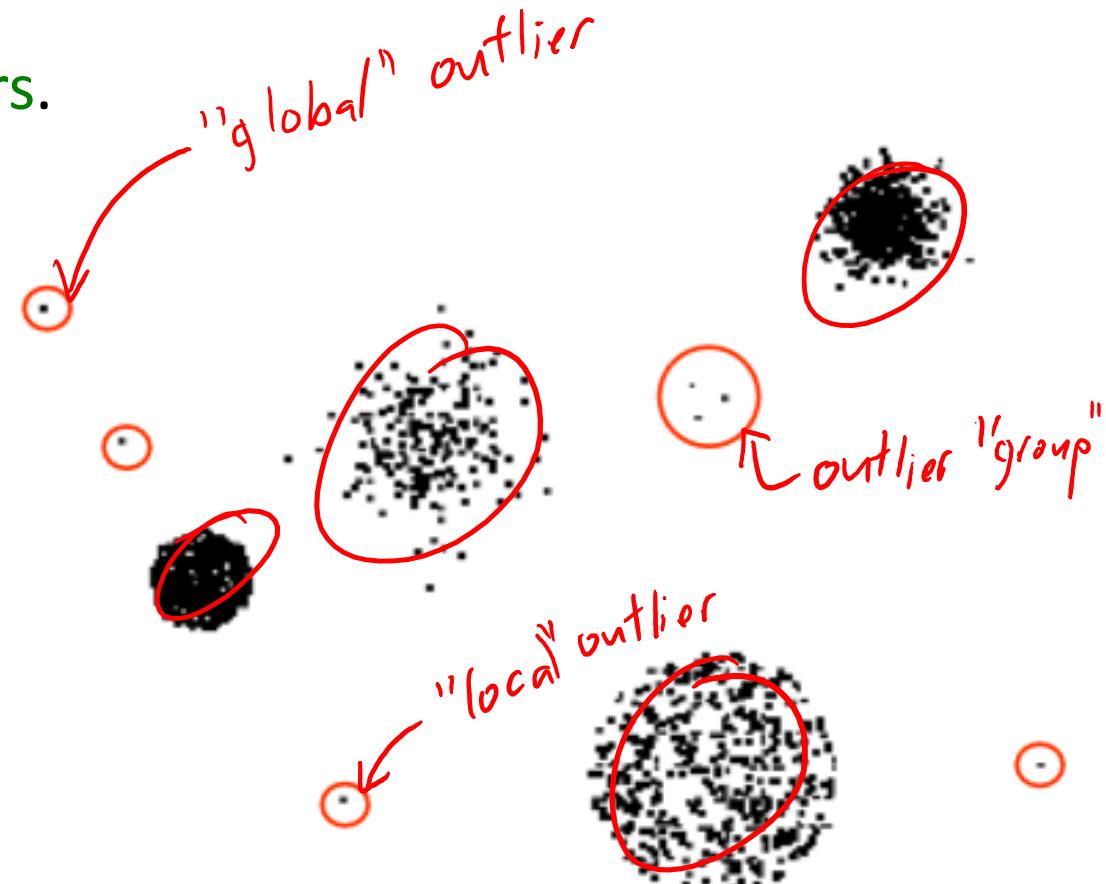
Cluster-Based Outlier Detection

- 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.
 2. Find points that don't belong to clusters.
- Examples:
 1. K-means.
 2. Density-based clustering:
 - Outliers are points not assigned to cluster.



Cluster-Based Outlier Detection

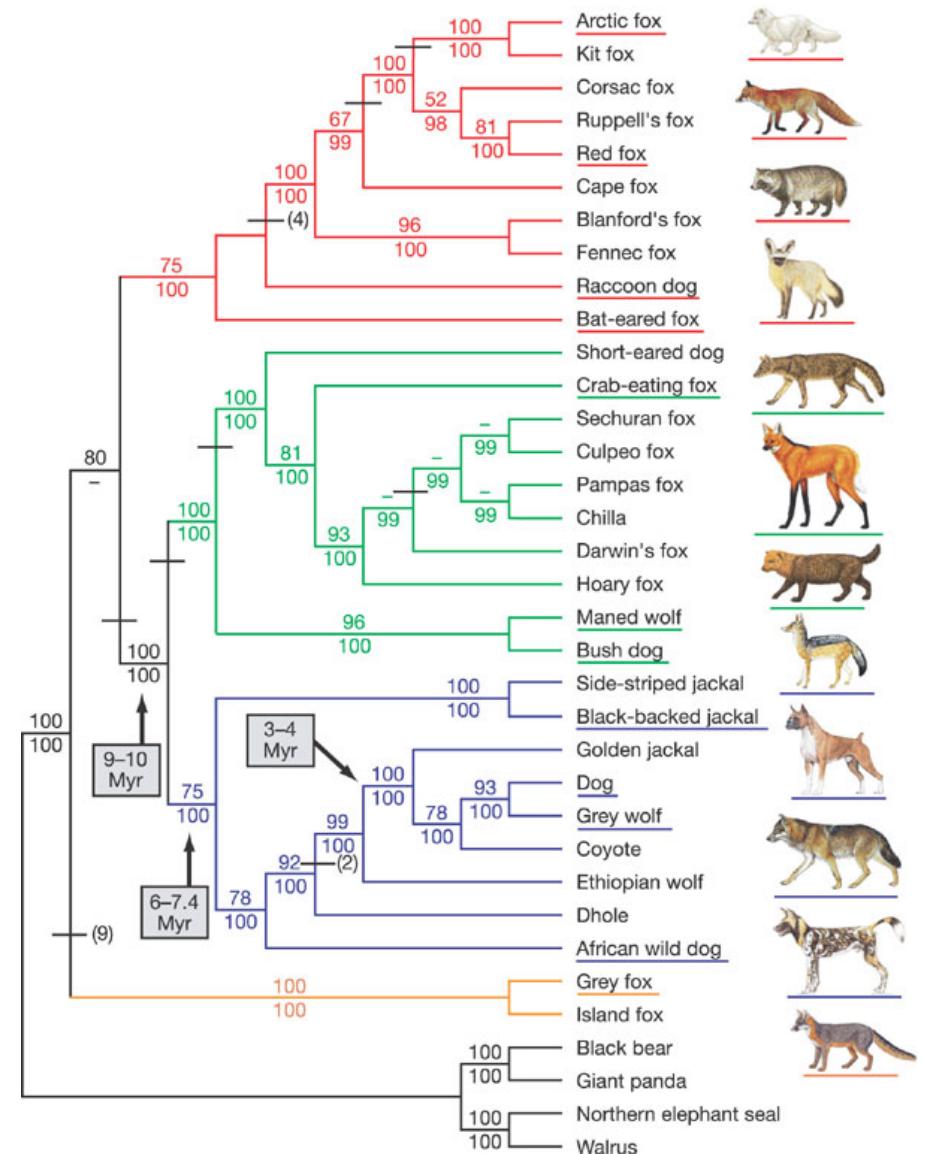
- Detect outliers based on clustering:
 1. Cluster the data.
 2. Find points that don't belong to clusters.
- Examples:
 1. K-means.
 2. Density-based clustering.
 3. Hierarchical clustering:
 - Outliers take longer to join other groups.
 - Also good for outlier groups.

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.

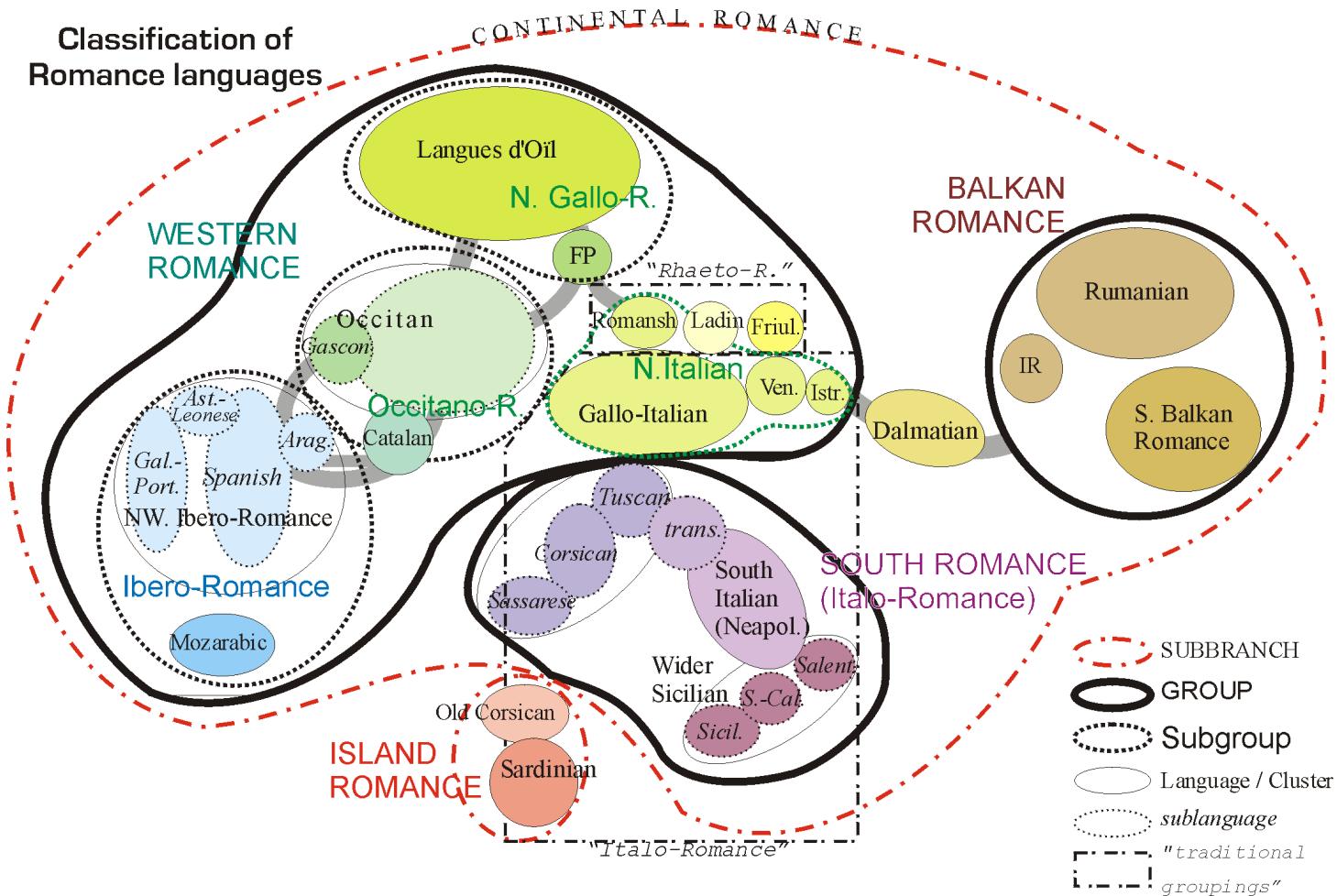
Application: Phylogenetics

- 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.



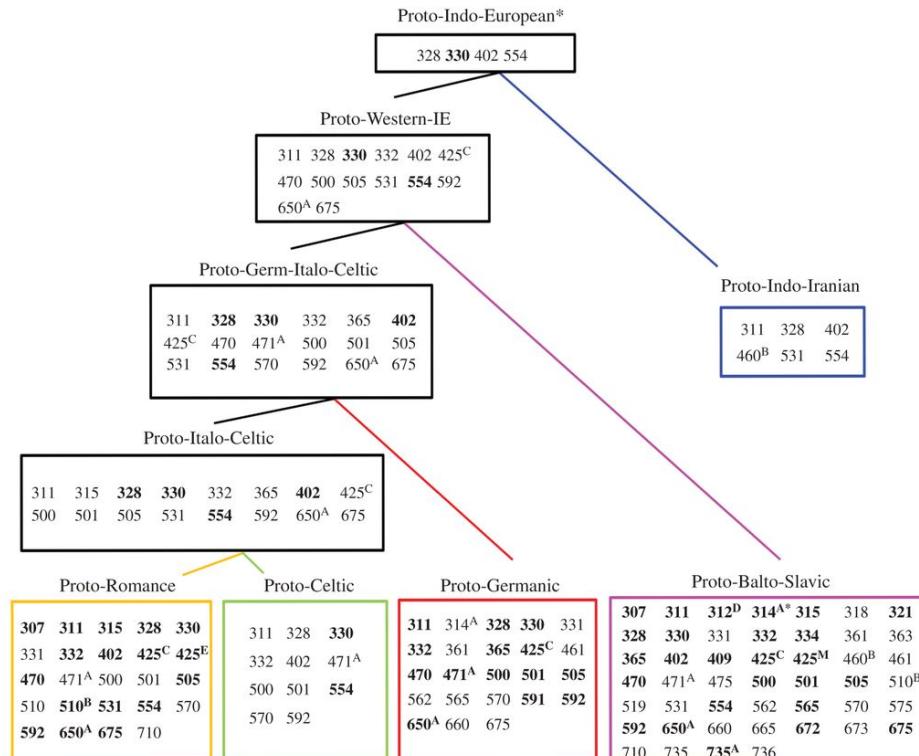
Application: Phylogenetics

- Comparative method in linguistics studies evolution of languages:



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.

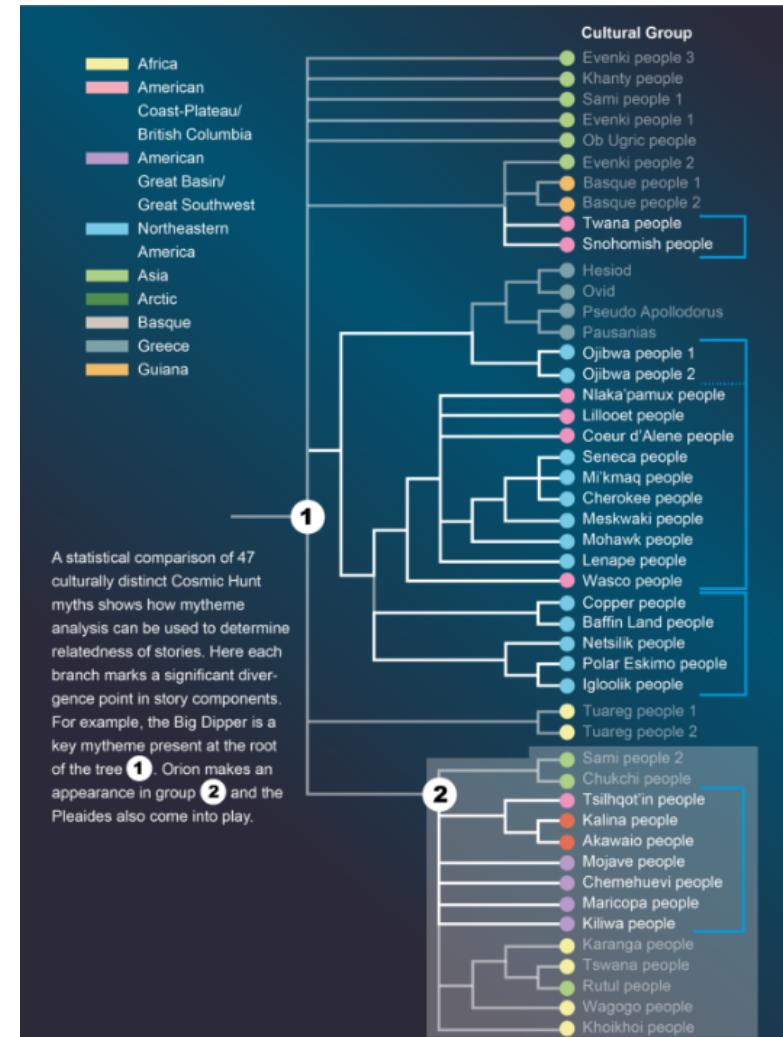


International tale types

307	The Princess in the Coffin	409	The Girl as Wolf	562	The Spirit in the Blue Light
311	Rescue by Sister	425C	Beauty and the Beast	565	The Magic Mill
312D	Rescue by the Brother	425E	The Enchanted Husband	570	The Rabbit-Herd
314A	The Shepherd and the Giants	425M	The Snake Bridegroom	575	The Prince's Wings
314A*	Animal Helper in the Flight	460B	The Journey	591	The Thieving Pot
315	The Faithless Sister	461	Three Hairs	592	The Dance Among Thorns
318	The Faithless Wife	470	Friends in Life and Death	650A	Strong John
321	Eyes Recovered from Witch	471A	The Monk and the Bird	660	The Three Doctors
328	The Boy Steals Ogre's Treasure	475	The Man as the Heater	665	The Man who Flew and Swam
330	The Smith and the Devil	500	Supernatural Helper	672	The Serpent's Crown
331	The Spirit in the Bottle	501	The Three Old Spinning Women	673	The White Serpent's Flesh
332	Godfather Death	505	The Grateful Dead	675	The Lazy Boy
334	Household of the Witch	510	Cinderella and Peau d'Âne	710	Our Lady's Child
361	Bear Skin	510B	Peau d'Âne	735	The Rich and the Poor Man
363	The Corpse-Eater	519	The Strong Woman as Bride	735A	Bad Luck Imprisoned
365	The Dead Bridegroom	531	The Clever Horse	736	Luck and Wealth
402	The Animal Bride	554	The Grateful Animals		

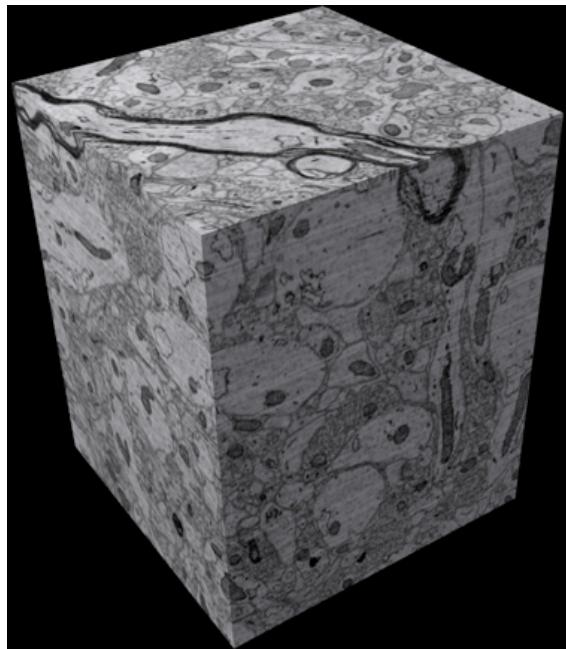
Application: Phylogenetics

- 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.

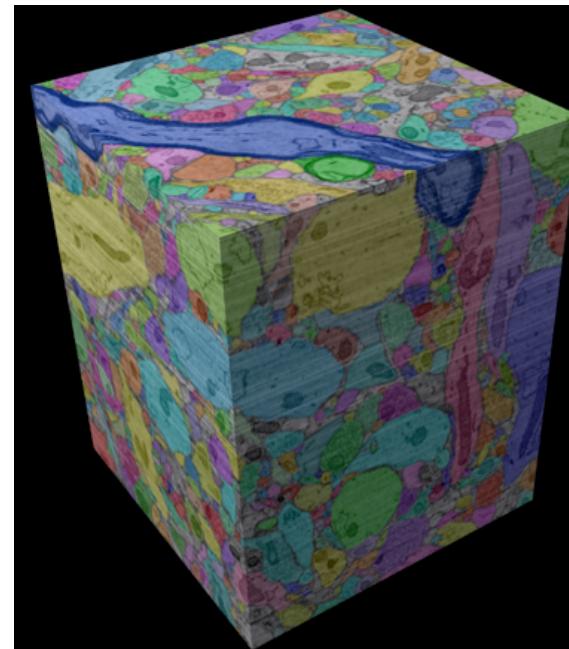


Supervised learning for clustering

- An important application is **image segmentation**, which means clustering pixels (or voxels) in an image.
- Some image segmentation methods use supervised learning
 - This is tricky because of label switching and other issues – but possible!



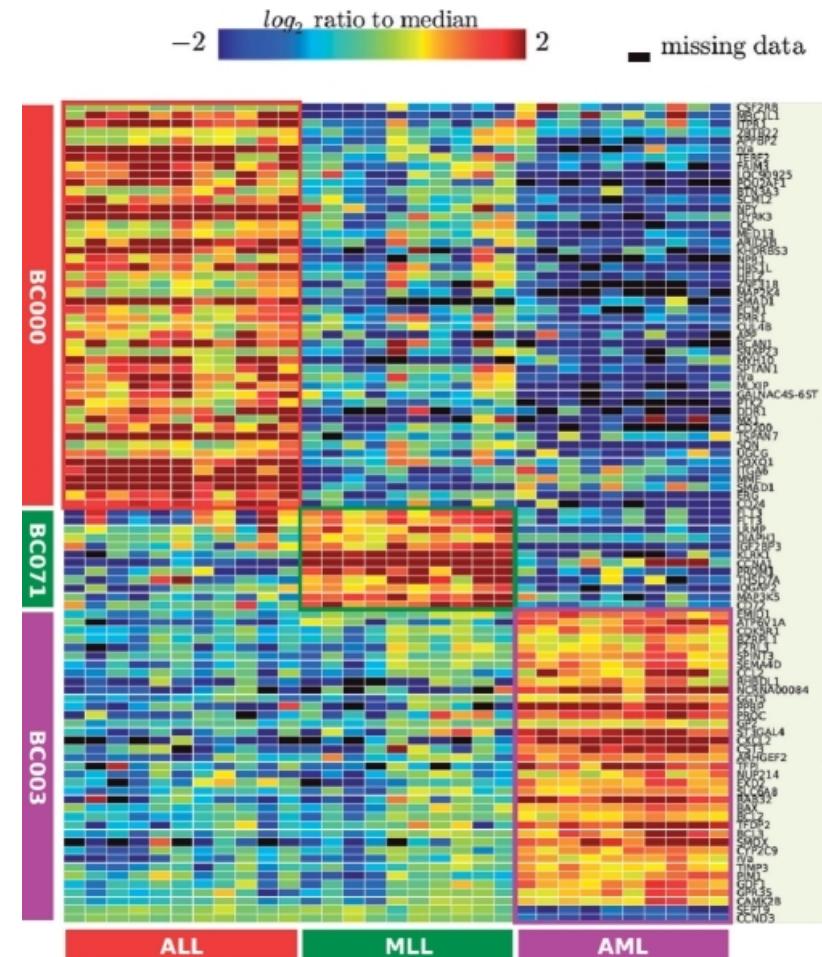
supervised learning



Images from conectomethebook.com

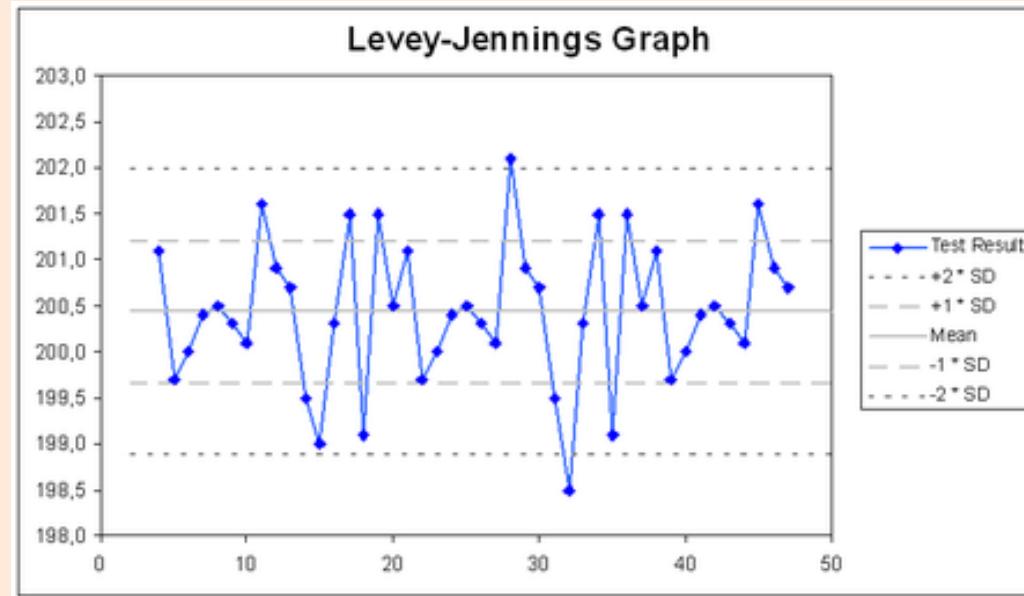
Other Clustering Methods

- 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.
- Bioclustering:
 - Simultaneously cluster objects and features.
- Spectral clustering and graph-based clustering:
 - Clustering of data described by graphs.



“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".

Distances between Clusters

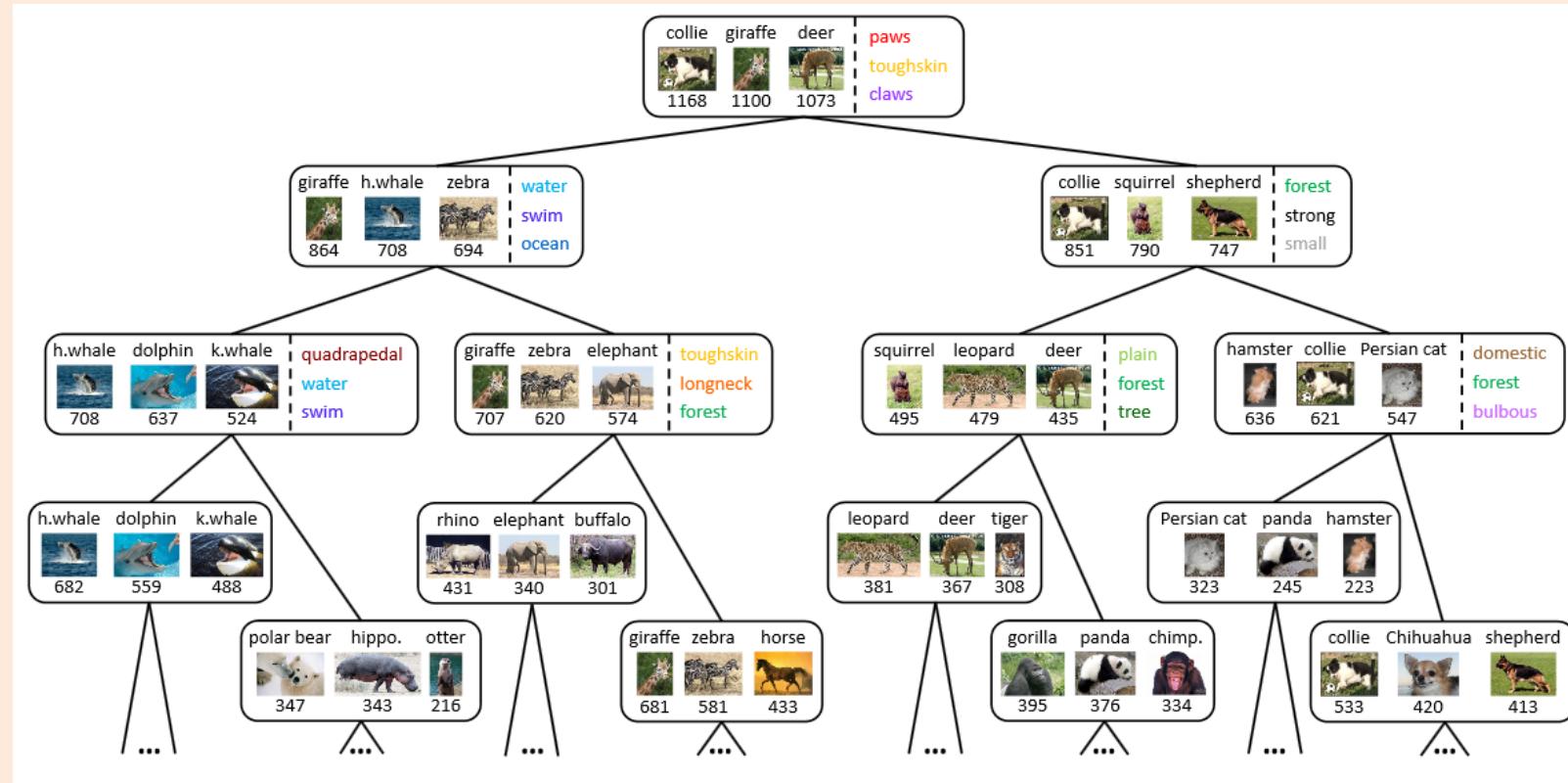
- Other choices of the distance between two clusters:
 - “Single-link”: minimum distance between points in clusters.
 - “Average-link”: average distance between points in clusters.
 - “Complete-link”: maximum distance between points in clusters.
 - Ward’s method: minimize within-cluster variance.
 - “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.



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.
3. Scatterplot array.
4. Scatterplot of 2-dimensional PCA:
 - ‘See’ high-dimensional structure.
 - But loses information and sensitive to outliers.

