CPSC 340:
Machine Learning and Data Mining

Outlier Detection

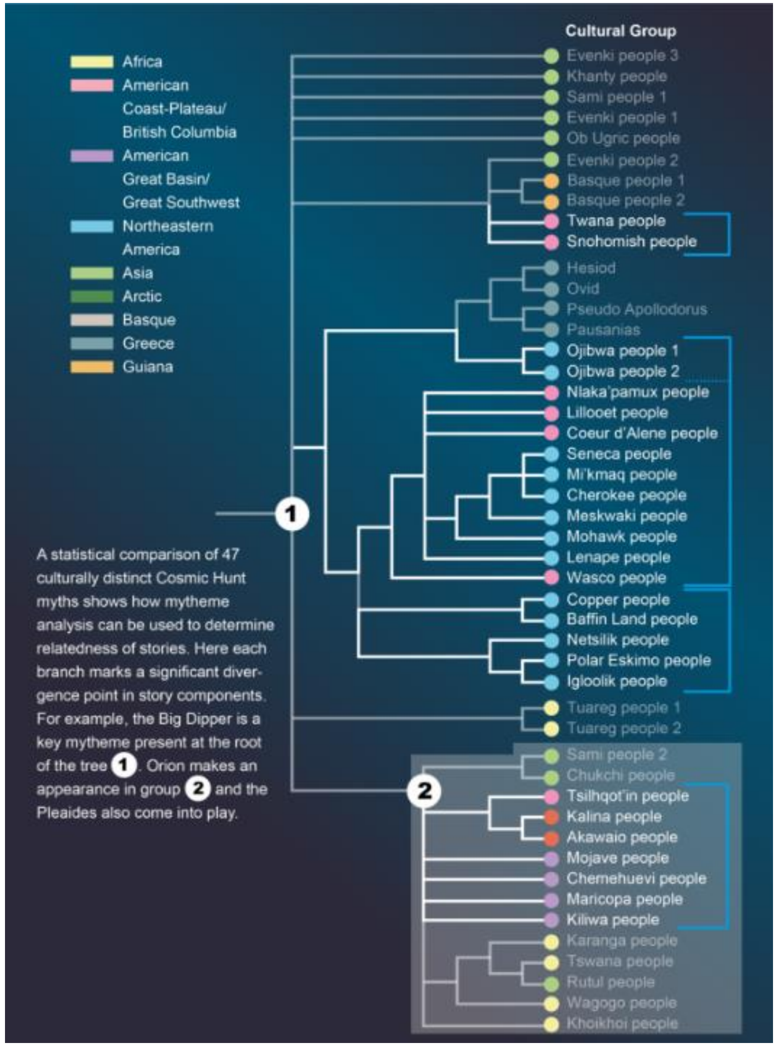
Fall 2016

Admin

- Assignment 1 solutions will be posted after class.
- Assignment 2 is out:
  - Due next Friday, but start early!
- Calculus and linear algebra terms to review for next week:
  - Vector addition and multiplication: $\alpha x + \beta y$.
  - Inner-product: $x^T y$.
  - Matrix multiplication: Xw.
  - Solving linear systems: $Ax = b$.
  - Matrix inverse: X^{-1}.
  - Norms: ||x||.
  - Gradient: $\nabla f(x)$.
  - Stationary points: $\nabla f(x) = 0$.
  - Convex functions: $f''(x) \geq 0$.

Last Time: Hierarchical Clustering

- We discussed hierarchical clustering:
  - Perform clustering at multiple scales.
  - Output is usually a tree diagram (“dendrogram”).
  - Reveals much more structure in data.
  - Usually non-parametric:
    - At finest scale, every point is its own clusters.

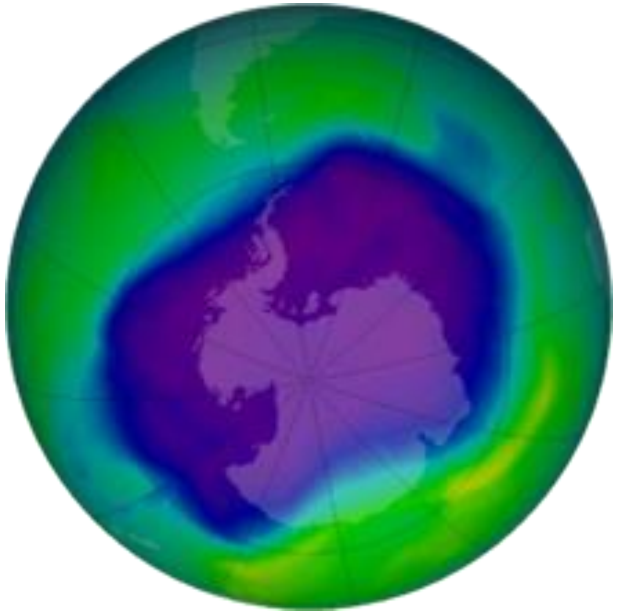


- Important application is phylogenetics.
  - Scientific American yesterday:
    - “Scientists Trace Society’s Myths to Primordial Origins”
    - “Cosmic Hunt”: Man hunts animal that becomes constellation.

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

Motivating Example: Finding Holes in Ozone Layer

- The huge Antarctic ozone hole was "discovered" in 1985.

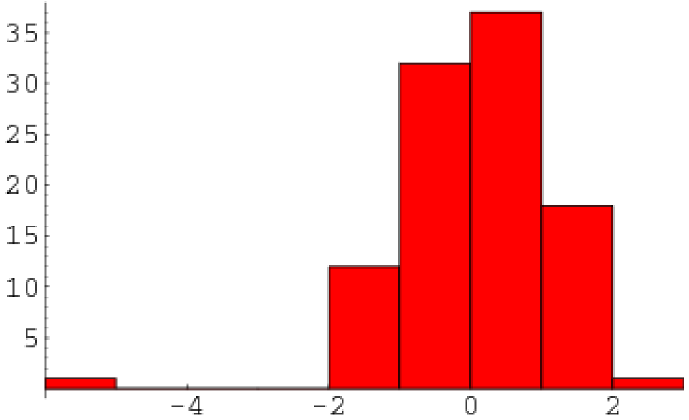


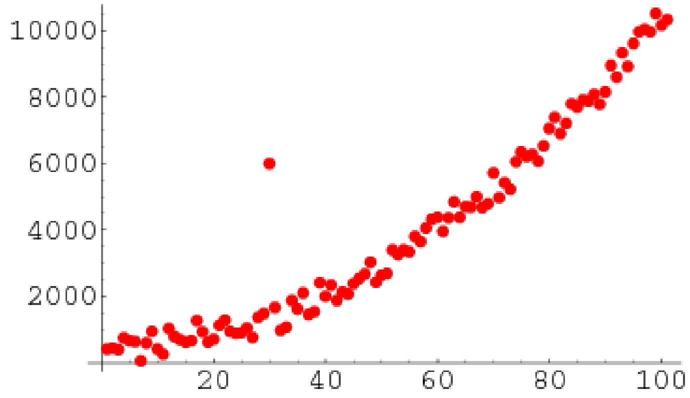
- It had been in satellite data since 1976:
  - But it was flagged and filtered out by quality-control algorithm.

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.





- 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).

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

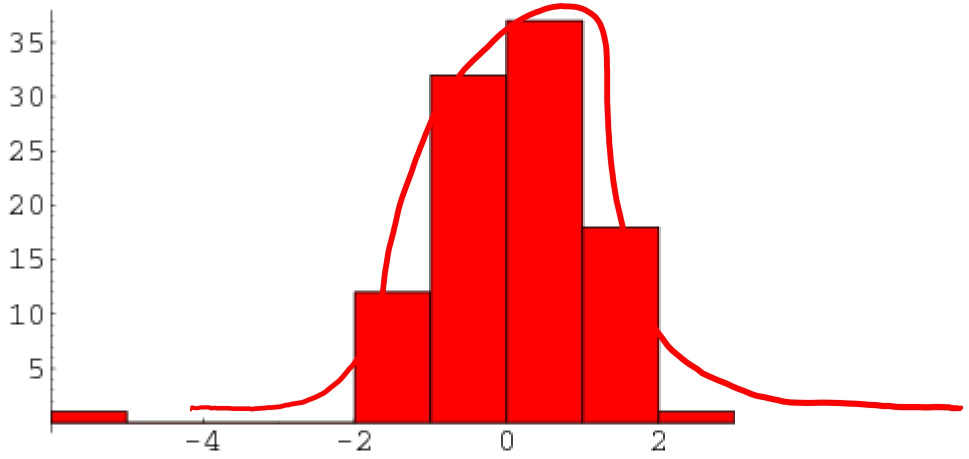
Classes of Methods for Outlier Detection

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”.
  – Next week we’ll get back to topics with more concrete solutions.

Model-Based Outlier Detection

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

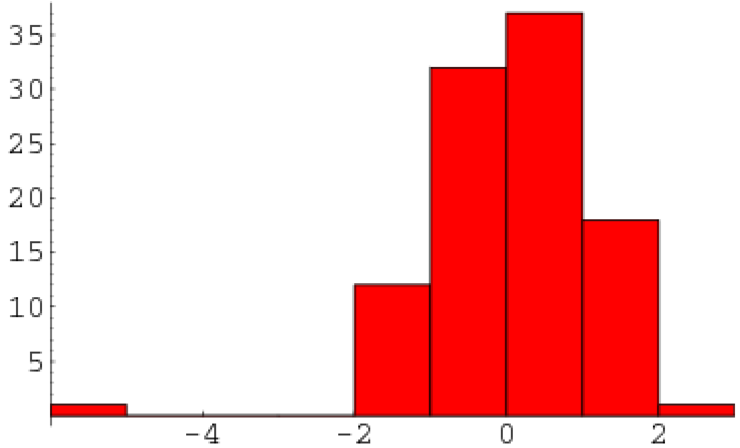


- Simplest approach is z-score:
  - If $z_i > 3$, 97% of data is larger than x_i?

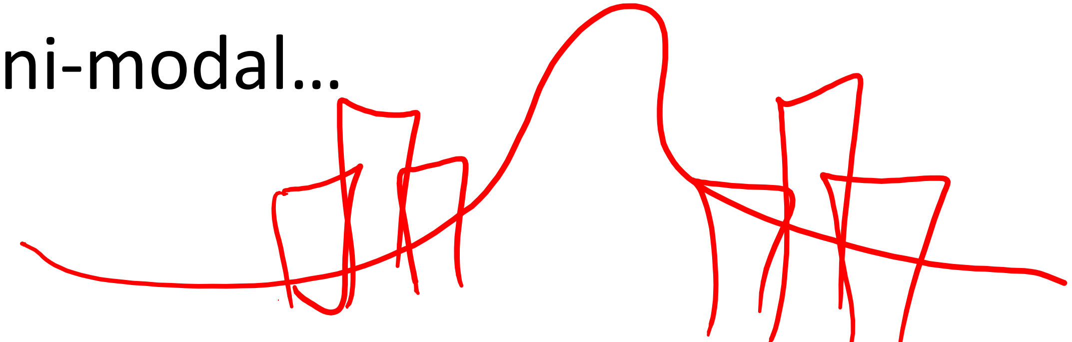
$$z_i = \frac{x_i - \mu}{\sigma}$$

Problems with Z-Score

- The z-score relies on mean and standard deviation:
  - These measure are sensitive to outliers.



  - Possible fixes: use quantiles, or sequentially remove worse outlier.
- The z-score also assumes that data is uni-modal…



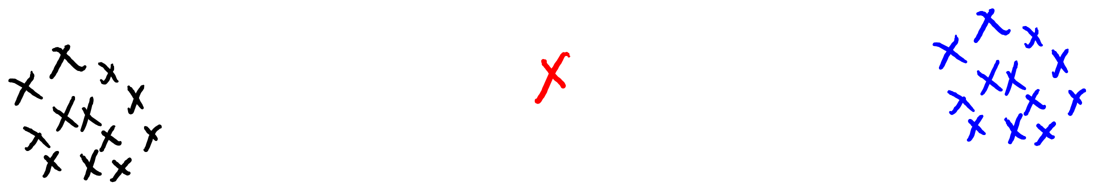
http://mathworld.wolfram.com/Outlier.html

Global vs. Local Outliers

- Is the red point an outlier?

Global vs. Local Outliers

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



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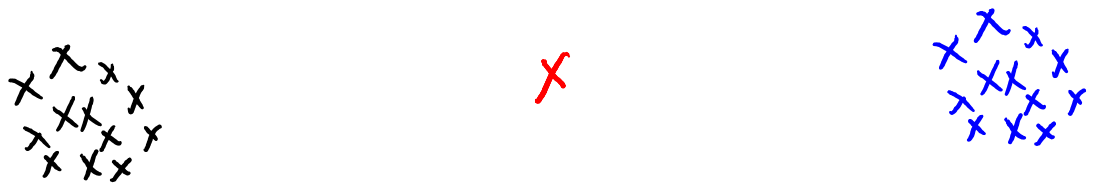

- Red point has the lowest z-score.
  - In the first case it was a “global” outlier.
  - In this second case it’s a “local” ouliter:
    - It’s within the range of the data, but is far away from other points.
- In general, hard to give precise definition of ‘outliers’.

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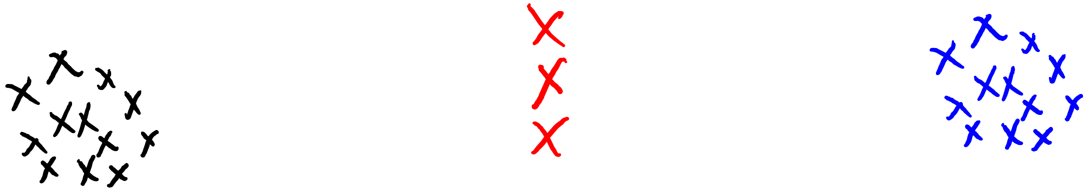

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  – Can we have outlier groups?

Global vs. Local Outliers

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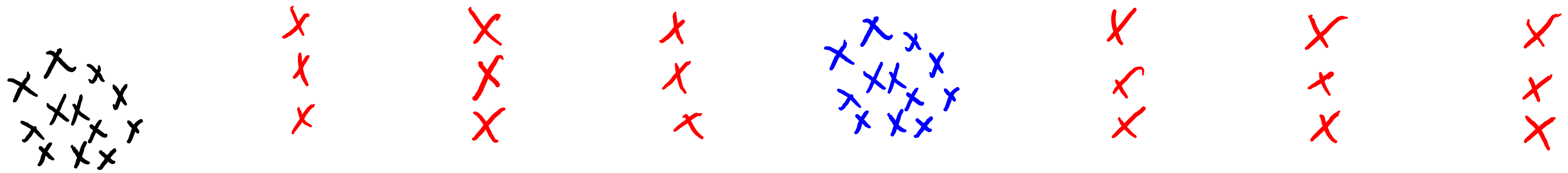

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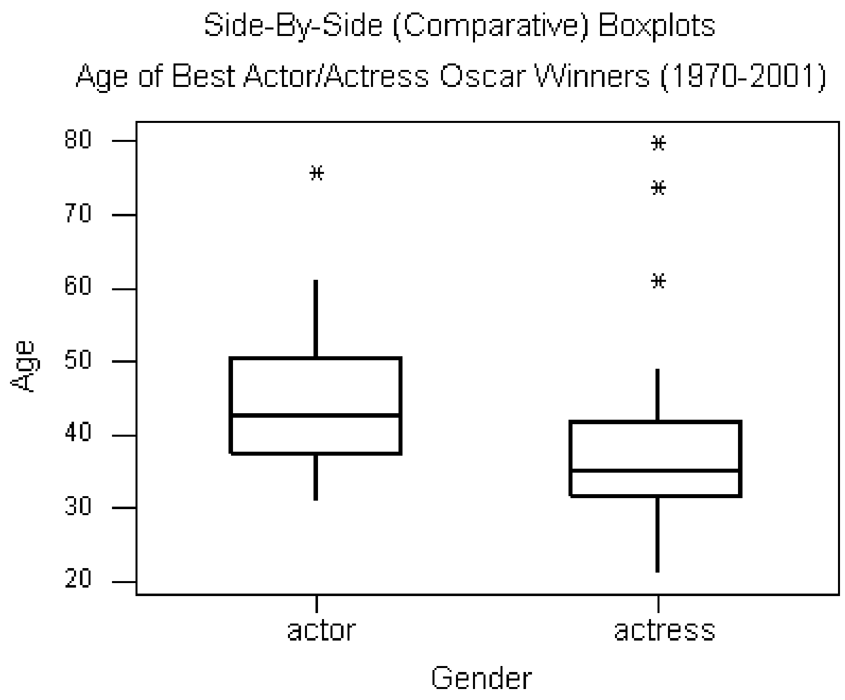
- In general, hard to give precise definition of ‘outliers’.
  - Can we have outlier groups?
  - What about repeating patterns?

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

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  1. Look at a plot of the data.
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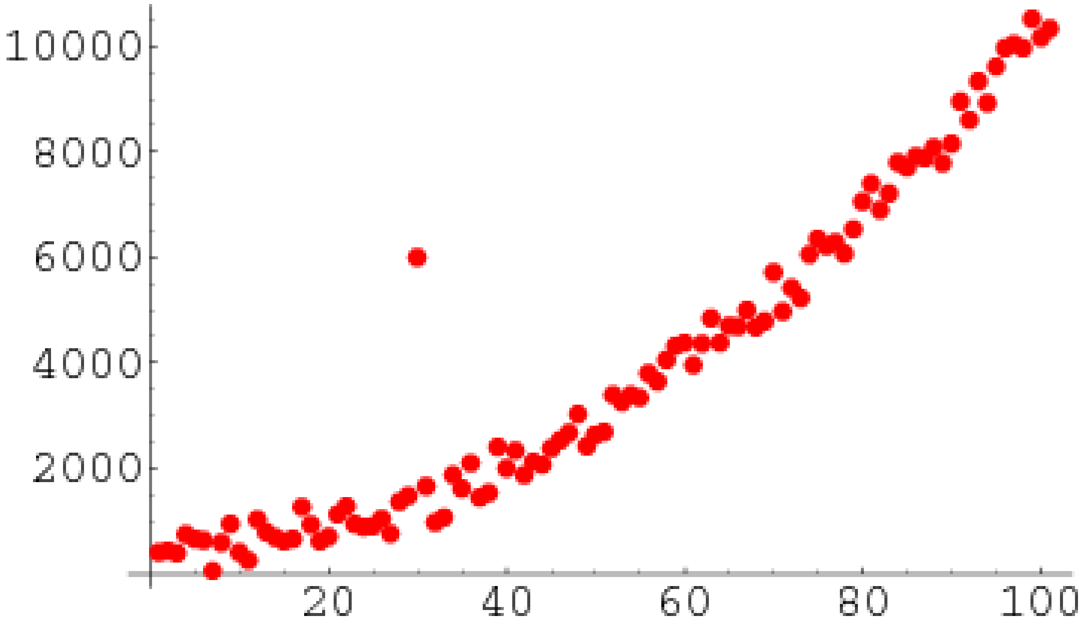
- Examples:
  1. Box plot.
  2. Scatterplot:
     - Can detect complex patterns.
     - Only 2 variables at a time.



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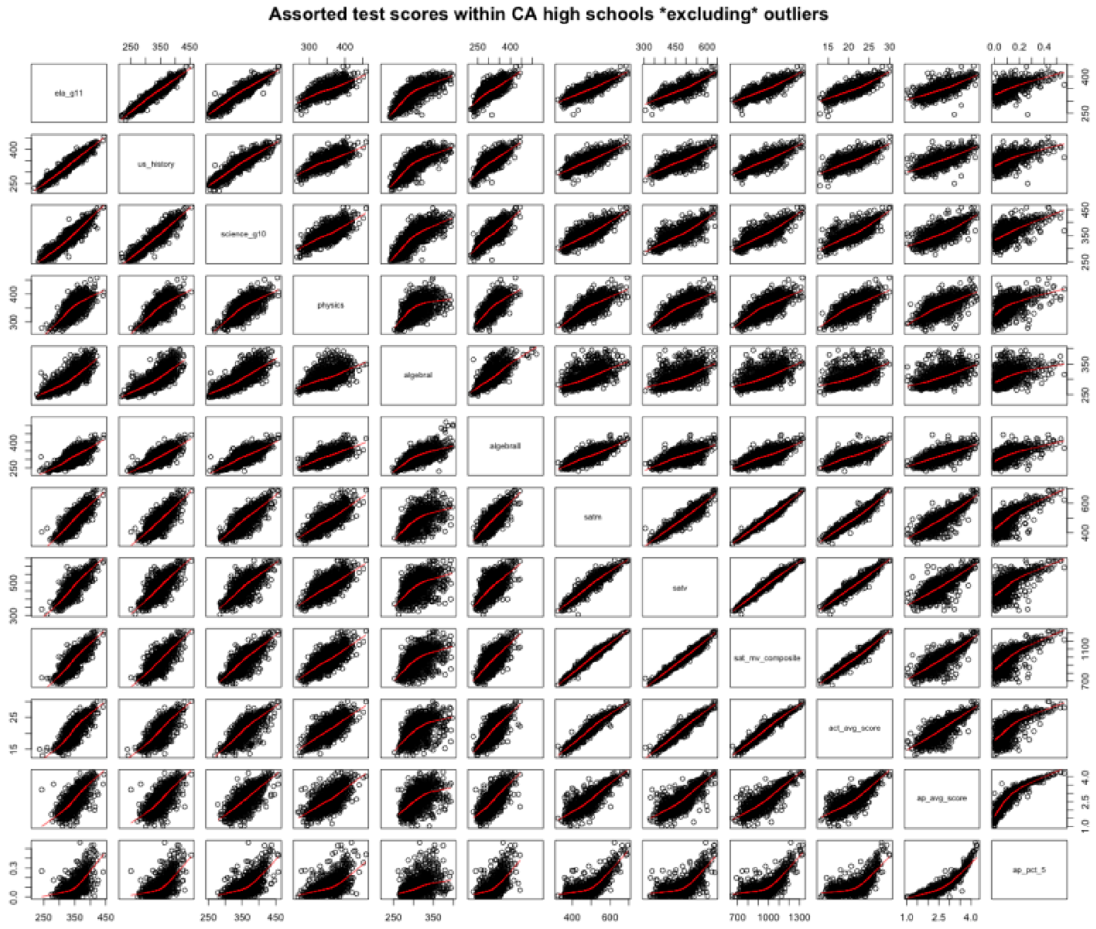
Graphical Outlier Detection

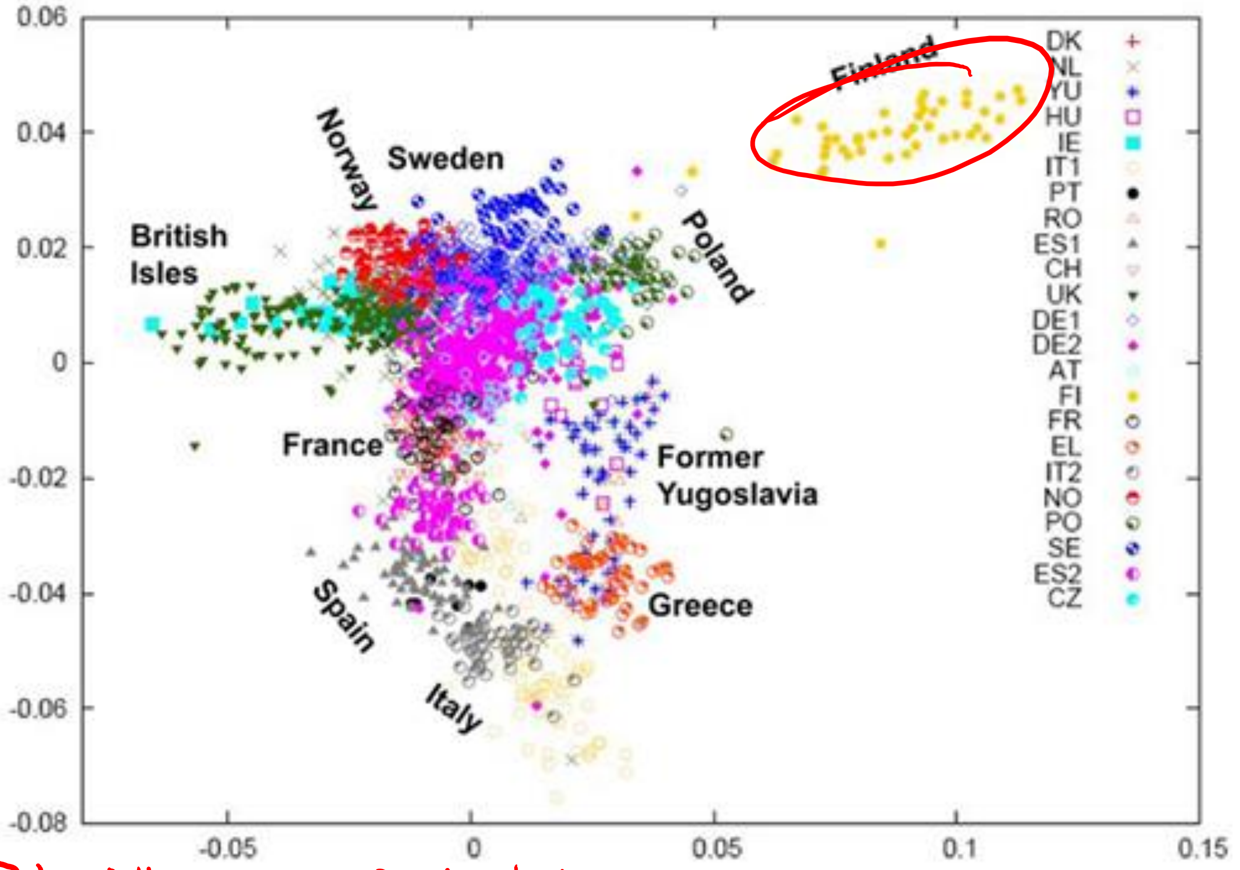
- Graphical approach to outlier detection:
  1. Look at a plot of the data.
  2. Human decides if data is an outlier.
- Examples:
  1. Box plot.
  2. Scatterplot.
  3. Scatterplot array:
     - Look at all combinations of variables.
     - But laborious in high-dimensions.
     - Still only 2 variables at a time.



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

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 PCA is sensitive to outliers.
     - There might be info in higher PCs.

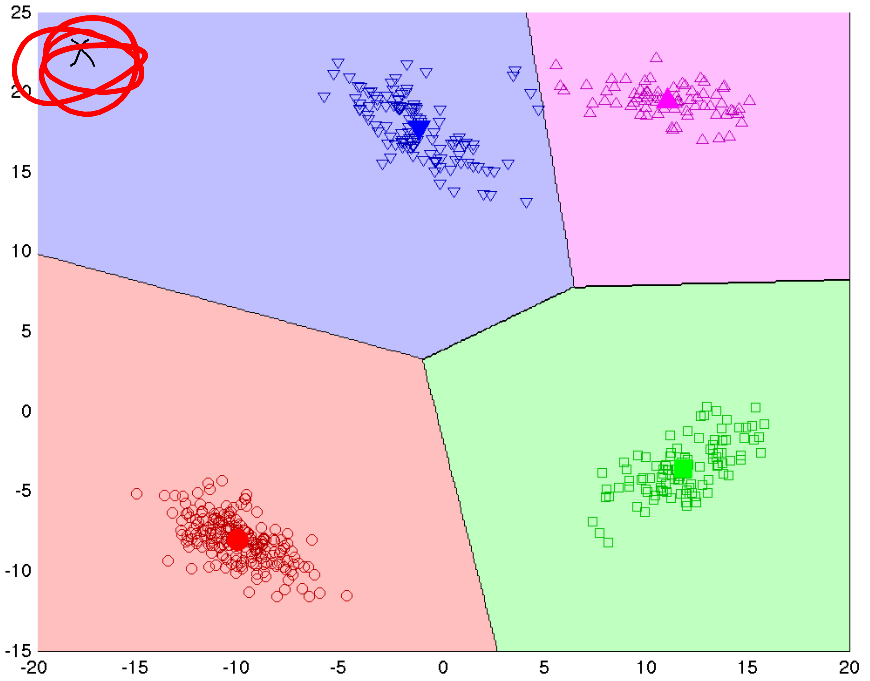


We'll cover PCA later in this course.

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

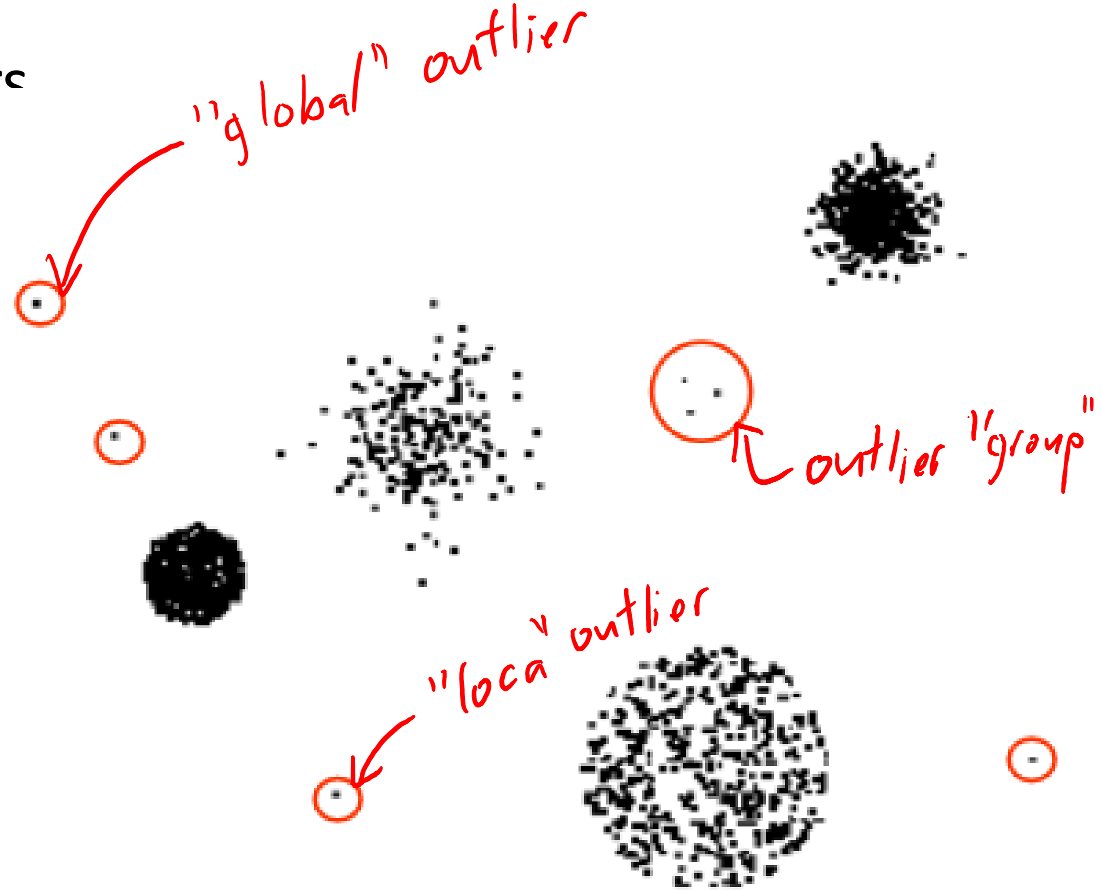
Cluster-Based Outlier Detection

- 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

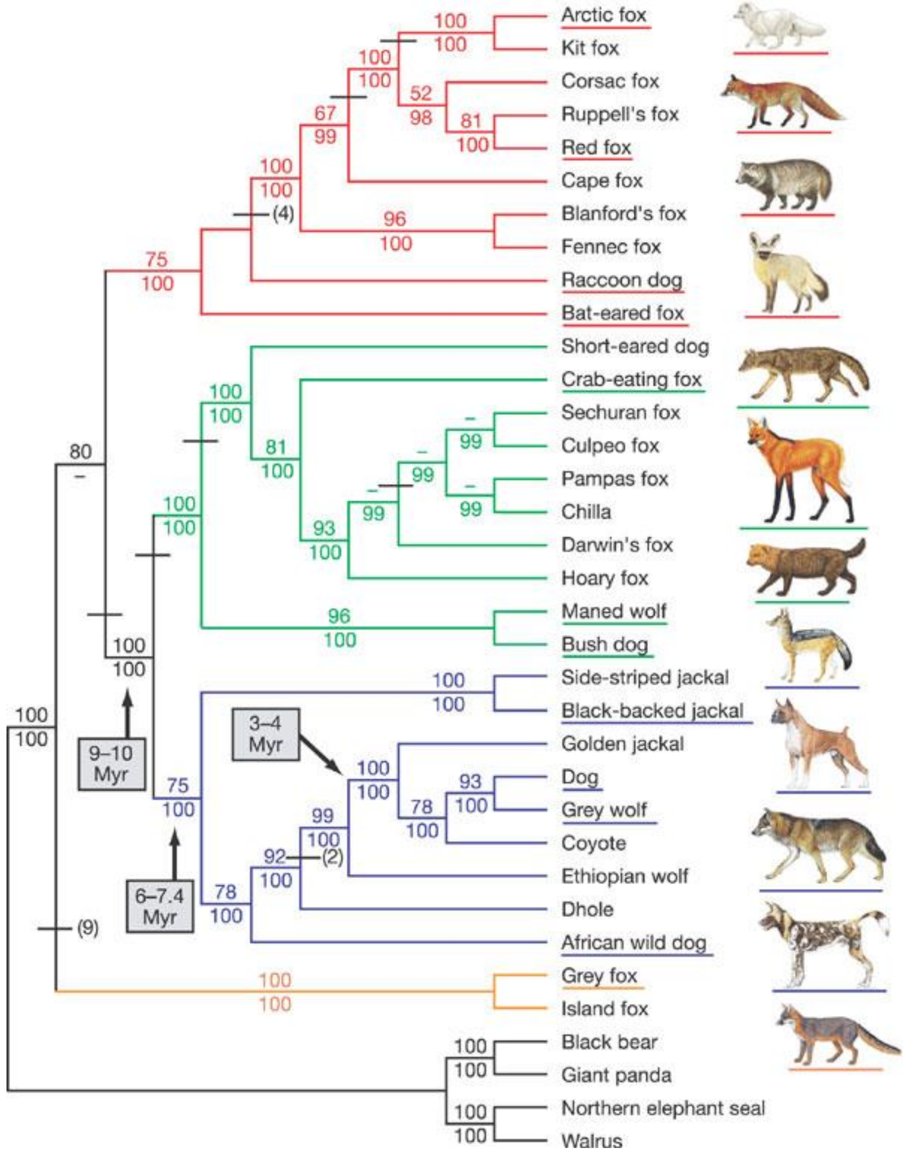
- Detect outliers based on clustering:
  1. Cluster the data.
  2. Find points that don’t belong to clusters
- Examples:
  1. K-means.
  2. Density-based clustering:
     - Outliers are points not assigned to cluster.



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

Distance-Based Outlier Detection

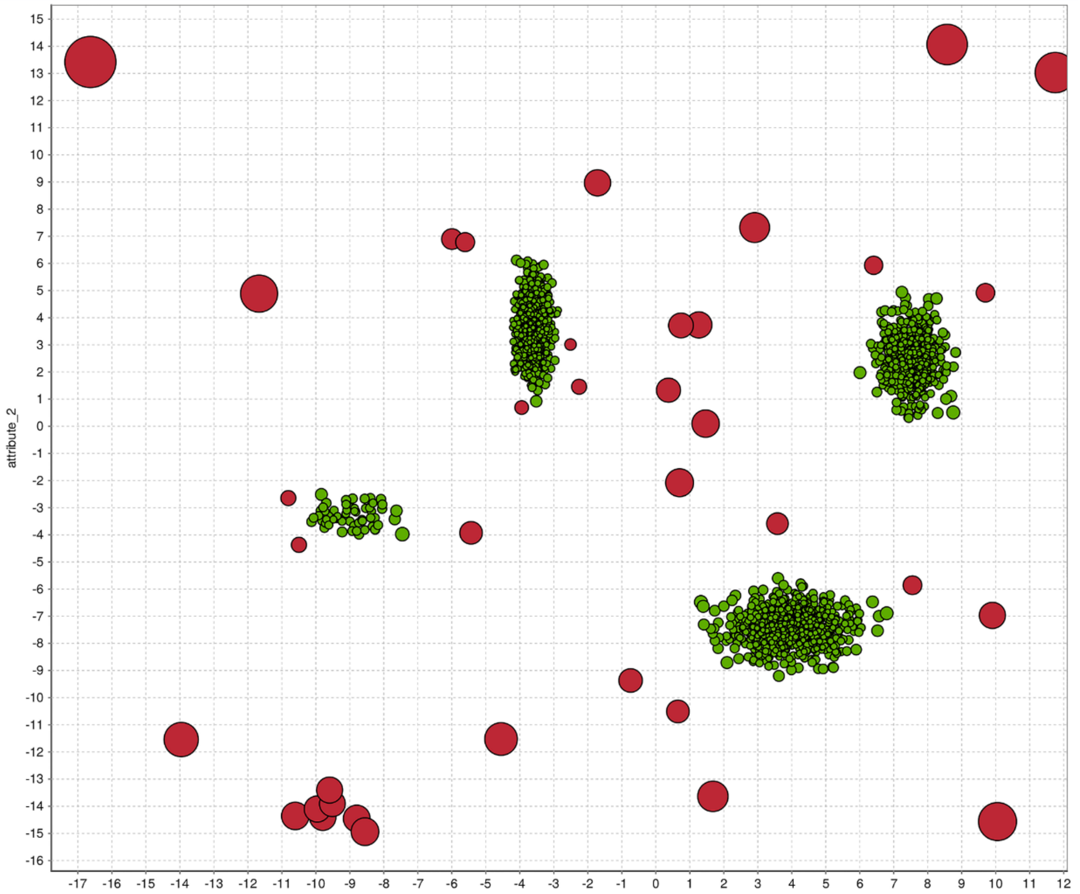
- Most of these approaches are based on distances.
- Can we skip the models/plot/clusters and directly use distances?
  - Directly measure of how close objects are to their neighbours.
- Examples:
  - How many points lie in a radius ‘r’?
  - What is distance to k^{th} nearest neighbour?

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

Global Distance-Based Outlier Detection: KNN

- KNN outlier detection:
  - For each point, compute the average distance to its KNN.
  - Sort these values.
  - Choose the biggest values as outliers.

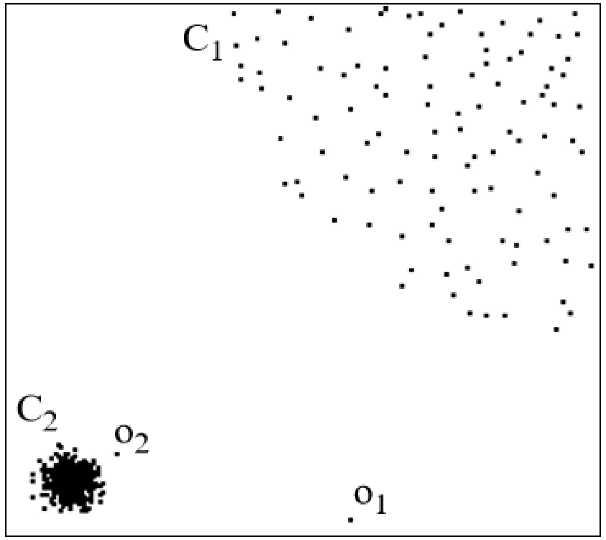
- Goldstein and Uchida [2016]:
  - Compared 19 methods on 10 datasets.
  - KNN best for finding "global" outliers.
  - "Local" outliers better detected by LOF…



http://journals.plos.org/plosone/article?id=10.1371%2Fjournal.pone.0152173

Local Distance-Based Outlier Detection

- As with density-based clustering, problem with differing densities:



- Outlier o_2 has similar density as elements of cluster C_1.
- Solution: "local outlier factor" (LOF) and variations like outlierness:
  - Is point "relatively" far away from its neighbours?

Outlierness

- Let $N_k(x_i)$ be the k-nearest neighbours of x_i.
- Let $D_k(x_i)$ be the average distance to k-nearest neighbours:

$$D_k(x_i) = \frac{1}{k}\sum_{j \in N_k(x_i)} \|x_i - x_j\|$$

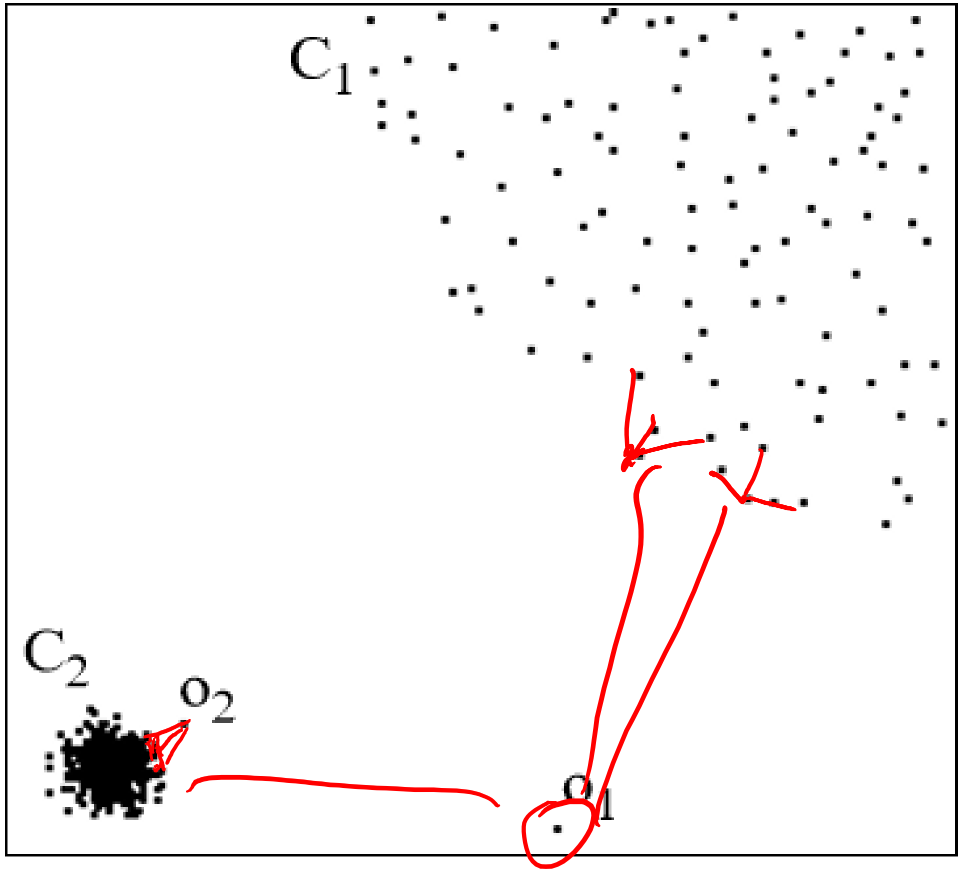
- Outlierness is ratio of $D_k(x_i)$ to average $D_k(x_j)$ for its neighbours 'j':

$$O_k(x_i) = \frac{D_k(x_i)}{\frac{1}{k}\sum_{j \in N_k(x_i)} D_k(x_j)}$$

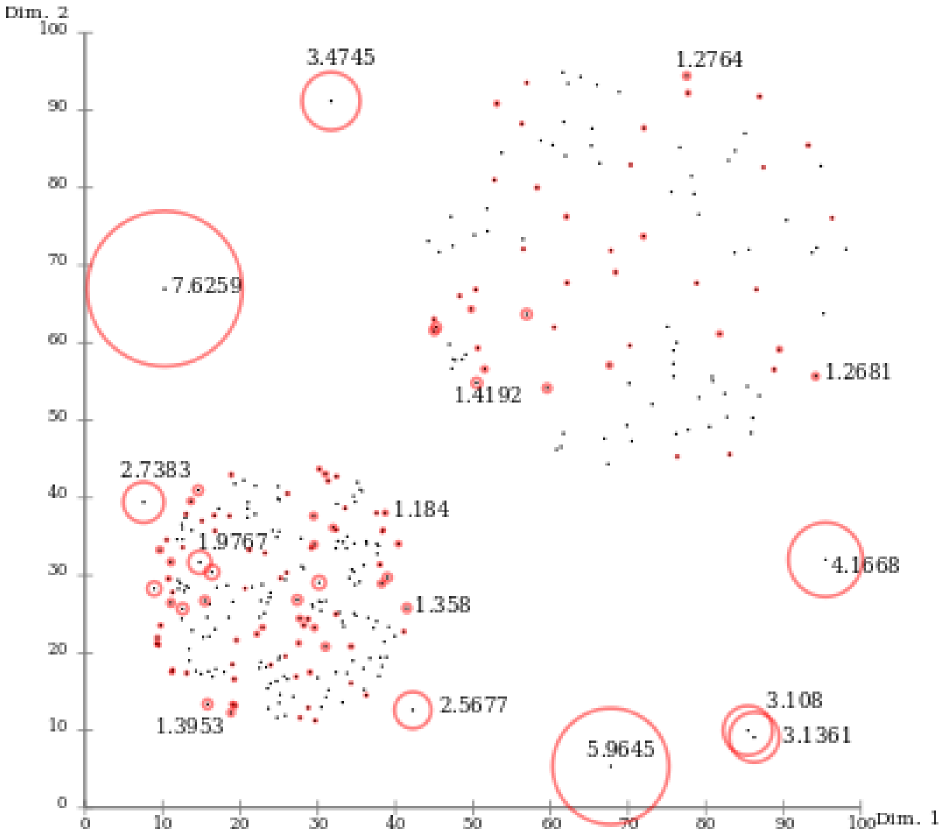
- If outlierness > 1, x_i is further away from neighbours than expected.

Outlierness Ratio

- Outlierness finds o_1 and o_2:



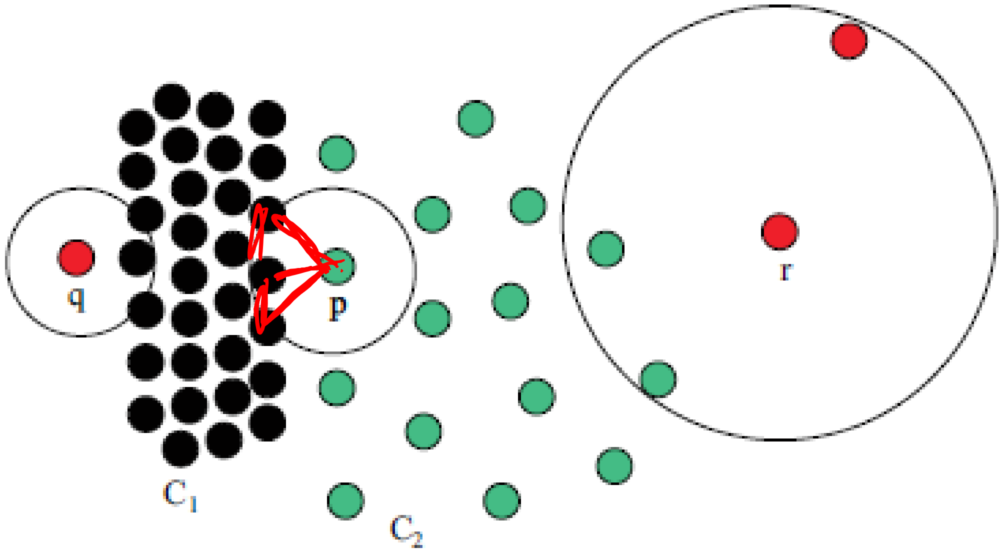
- More complicated data:



http://www.dbs.ifi.lmu.de/Publikationen/Papers/LOF.pdf
https://en.wikipedia.org/wiki/Local_outlier_factor

Outlierness with Close Clusters

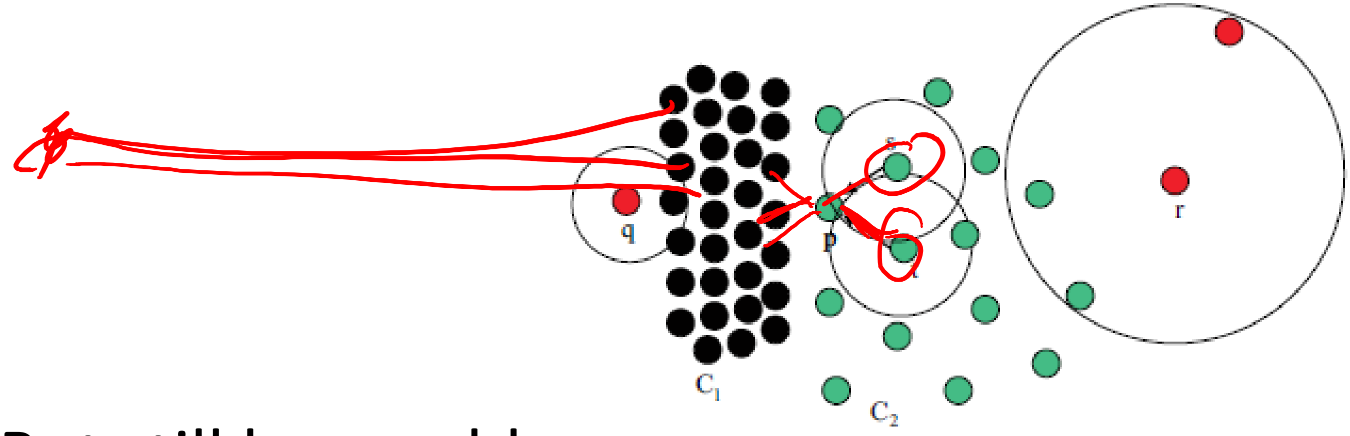
- If clusters are close, outlierness gives unintuitive results:



- In this example, ‘p’ has higher outlierness than ‘q’ and ‘r’:
  - The green points are not part of the KNN list of ‘p’ for small ‘k’.

Outlierness with Close Clusters

- ‘Influenced outlierness’ (INFLO) ratio:
  - Include in denominator the ‘reverse’ k-nearest neighbours:
    - Points that have ‘p’ in KNN list.
  - Adds ‘s’ and ‘t’ from bigger cluster that includes ‘p’:



- But still has problems:
  - Dealing with hierarchical clusters.
  - Yields many false positives if you have “global” outliers.
  - Goldstein and Uchida [2016] recommend just using KNN.

http://www.comp.nus.edu.sg/~atung/publication/pakdd06_outlier.pdf

Supervised Outlier Detection

- Final approach to outlier detection is to use supervised learning:
    - $y_i = 1$ if x_i is an outlier.
    - $y_i = 0$ if x_i is a regular point.

- Let’s us use our great methods for supervised learning:
  – We can find very complicated outlier patterns.

- But it needs supervision:
  – We need to know what outliers look like.
  – We may not detect new “types” of outliers.

Summary

- Outlier detection is task of finding unusually different object.
  - A concept that is very difficult to define.
- Model-based methods check if objects are unlikely in fitted model.
- Graphical methods plot data and use human to find outliers.
- Cluster-based methods check whether objects belong to clusters.
- Distance-based methods measure relative distance to neighbours.
- Supervised-learning methods just turn it into supervised learning.

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