CPSC 340:
Machine Learning and Data Mining

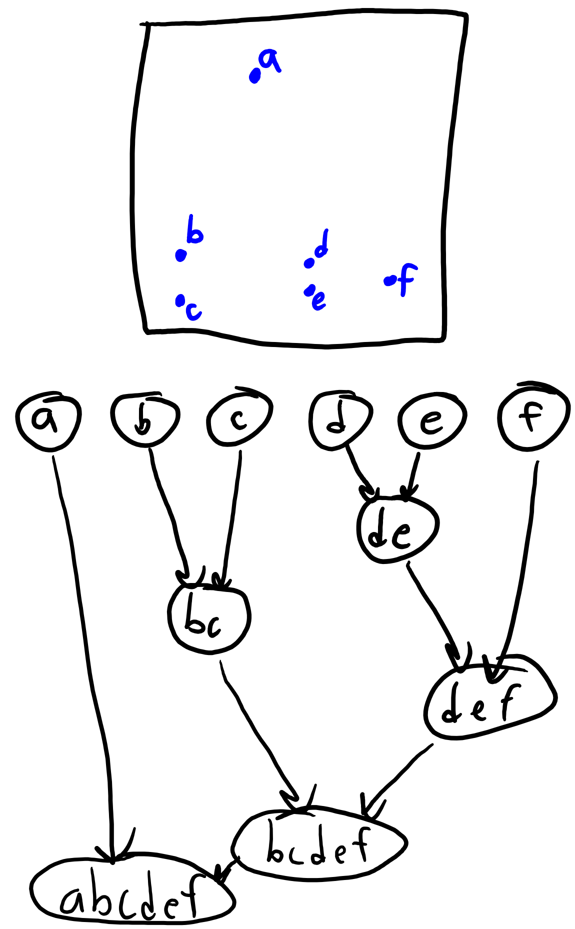
Outlier Detection

Fall 2020

Last Time: Hierarchical Clustering

- We discussed hierarchical clustering:
  - Performs 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.

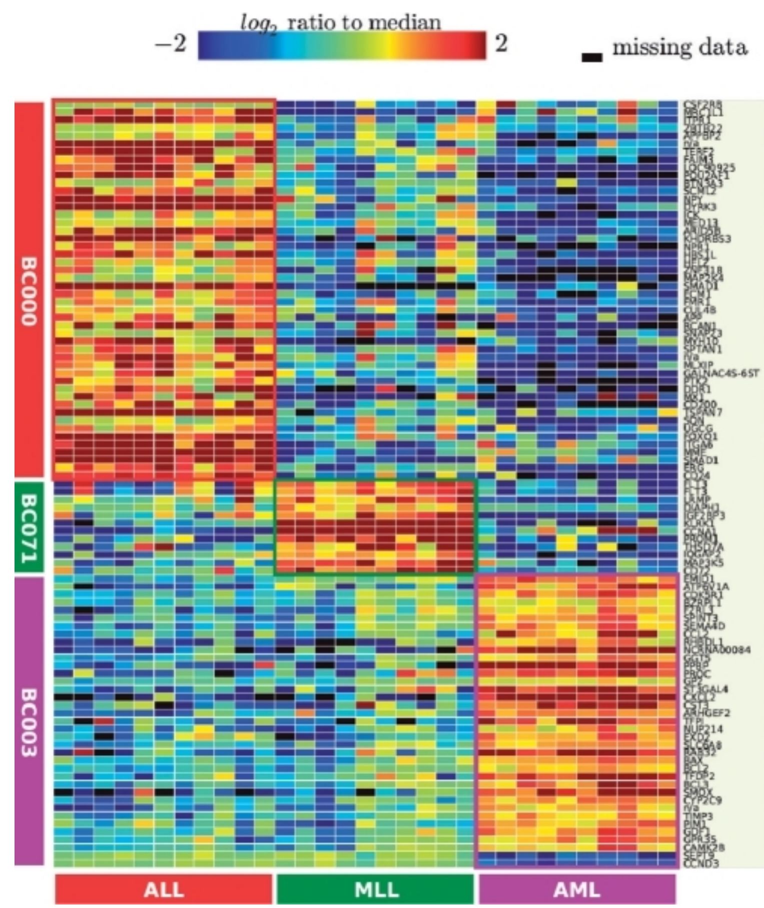
- We discussed some application areas:
  - Animals (phylogenetics).
  - Languages.
  - Stories.
  - Fashion.



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

Biclustering

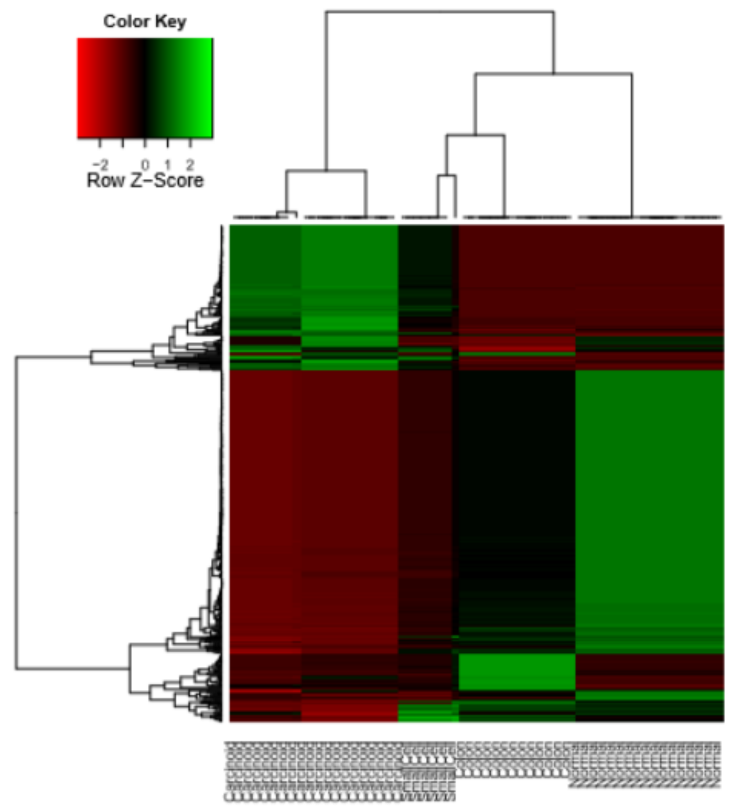
- Biclustering:
  - Cluster the training examples and features.
  - Also gives feature relationship information.
- Simplest and most popular method:
  - Run clustering method on 'X' (examples).
  - Run clustering method on 'X^T' (features).
- Often plotted with 'X' as a heatmap.
  - Where rows/columns arranged by clusters.
  - Helps you 'see' why things are clustered.



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

Biclustering

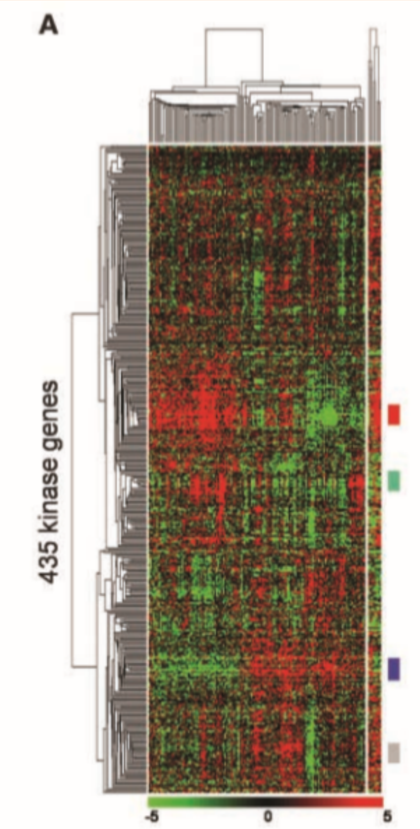
- Visualization: hierarchical biclustering + heatmap + dendrograms.
  - Popular in biology/medicine.



https://arxiv.org/pdf/1408.0856v1.pdf

Application: Medical data

- Hierarchical clustering is very common in medical data analysis.
  - Biclustering different samples of breast cancer:



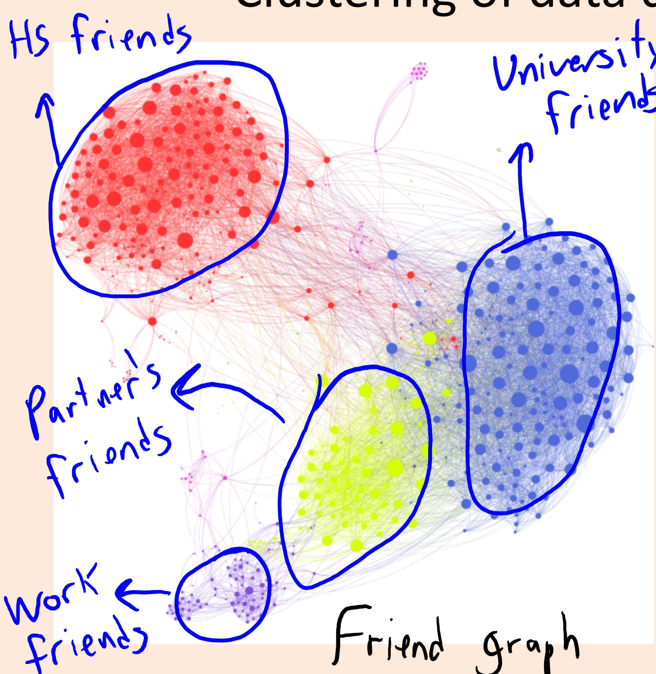
http://members.cbio.mines-paristech.fr/~jvert/svn/bibli/local/Finetti2008Sixteen-kinase.pdf

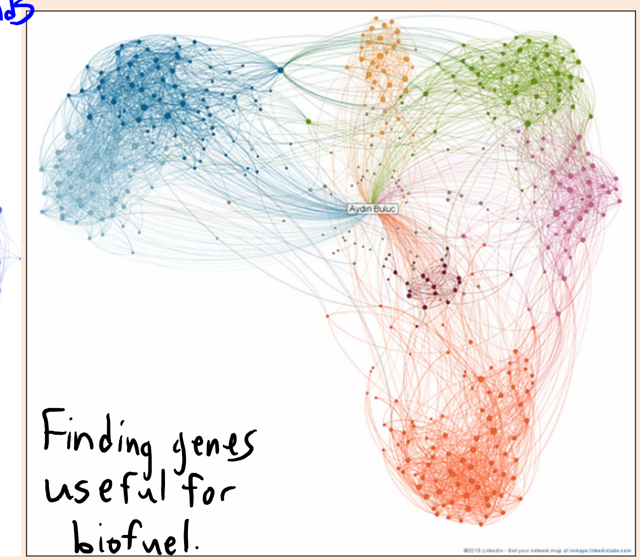
Other Clustering Methods

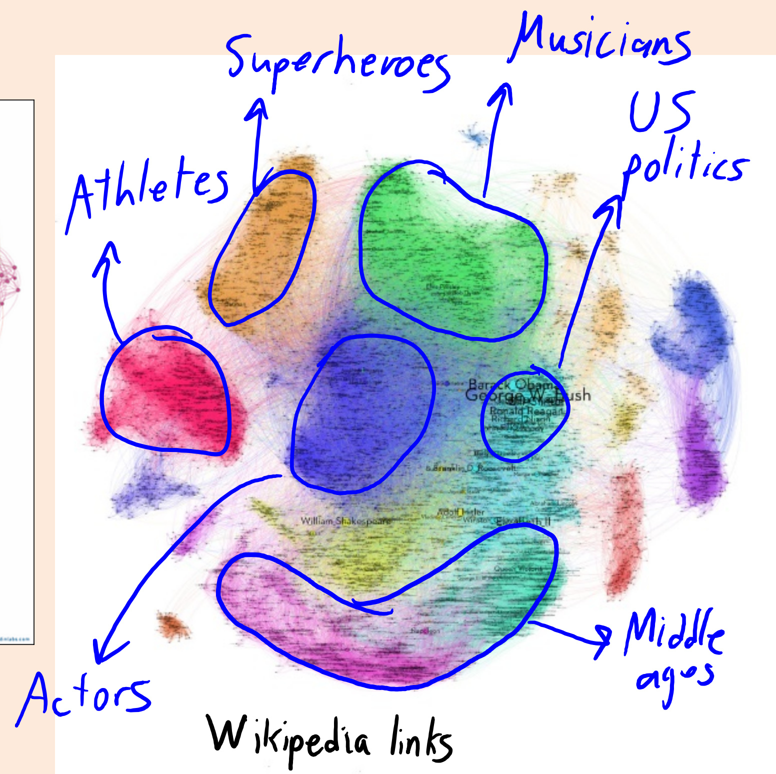
- Mixture models:
  - Probabilistic clustering.
- Mean-shift clustering:
  - Finds local “modes” in density of points.
  - Alternative approach to vector quantization.
- Bayesian clustering:
  - A variant on ensemble methods.
  - Averages over models/clusterings,
    weighted by “prior” belief in the model/clustering.

Graph-Based Clustering

- Spectral clustering and graph-based clustering:
  - Clustering of data described by graphs.





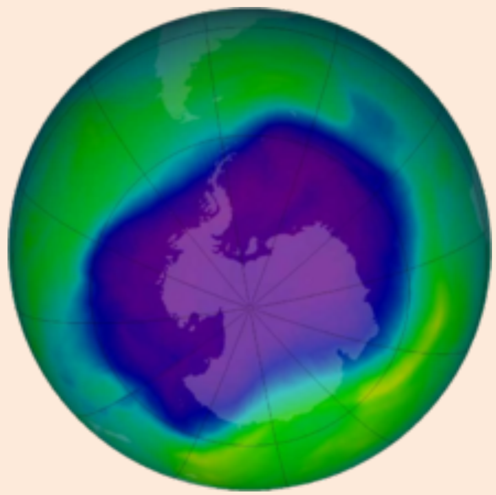


https://griffsgraphs.wordpress.com/tag/clustering/
http://ascr-discovery.science.doe.gov/2013/09/sifting-genomes/
https://www.hackdiary.com/2012/04/05/extracting-a-social-graph-from-wikipedia-people-pages/

(pause)

Motivating Example: Finding Holes in Ozone Layer

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

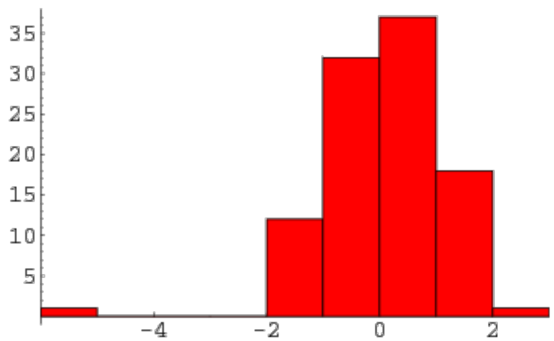


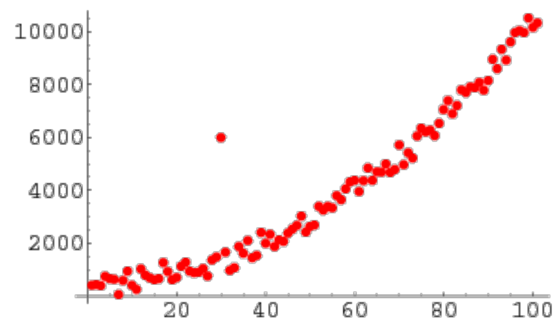
- It had been in satellite data since 1976:
  - But it was flagged and filtered out by a quality-control algorithm.

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…

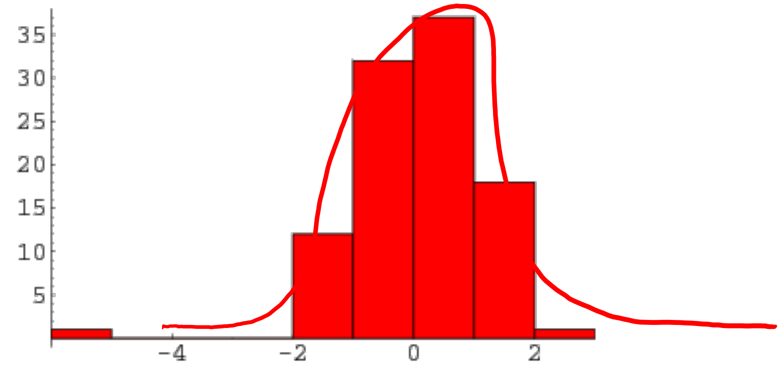
- Usually it's good to do some basic sanity checking…

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	2
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:

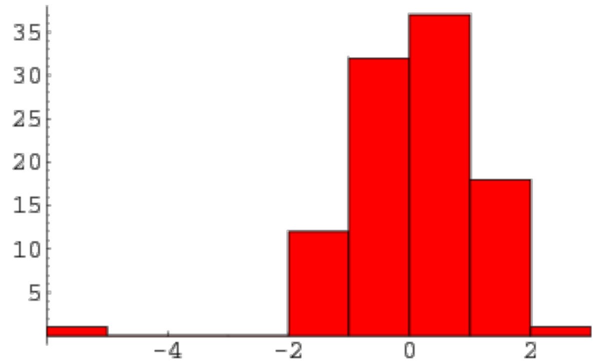
$$z_i = \frac{x_i - \mu}{\sigma} \quad \text{where } \mu = \frac{1}{n}\sum_{i=1}^{n} x_i \quad \text{and } \sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2}$$

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

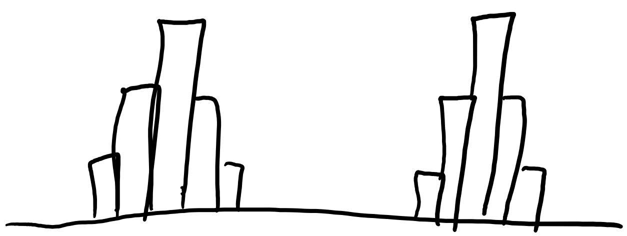
http://mathworld.wolfram.com/Outlier.html

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.

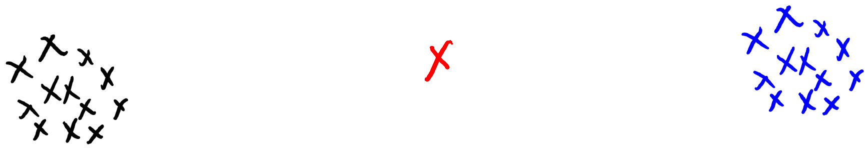


Global vs. Local Outliers

- 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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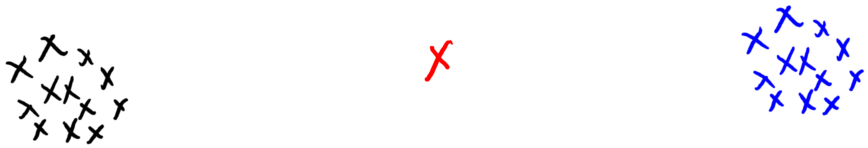

- Red point has the lowest z-score.
  - In the first case it was a "global" outlier.
  - In this second case it's a "local" outlier:
    - Within normal data range, but far from other points.
- It's hard to precisely define "outliers".

Global vs. Local Outliers

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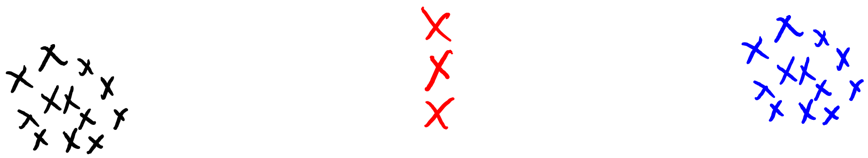

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  - Can we have outlier groups?

Global vs. Local Outliers

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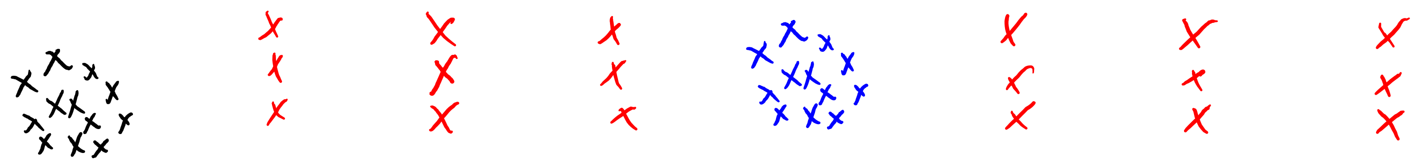

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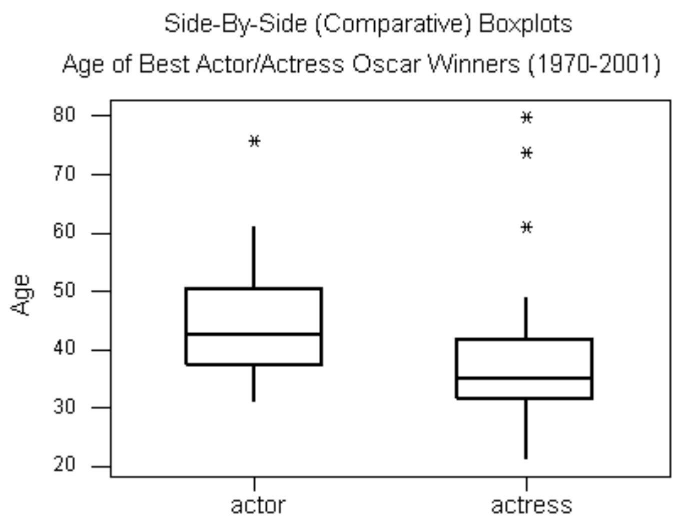
  - In the first case it was a "global" outlier.
  - In this second case it's a "local" outlier:
    - Within normal data range, but far from other points.
- It's hard to precisely define "outliers".
  - Can we have outlier groups? What about repeating patterns?

Graphical Outlier Detection

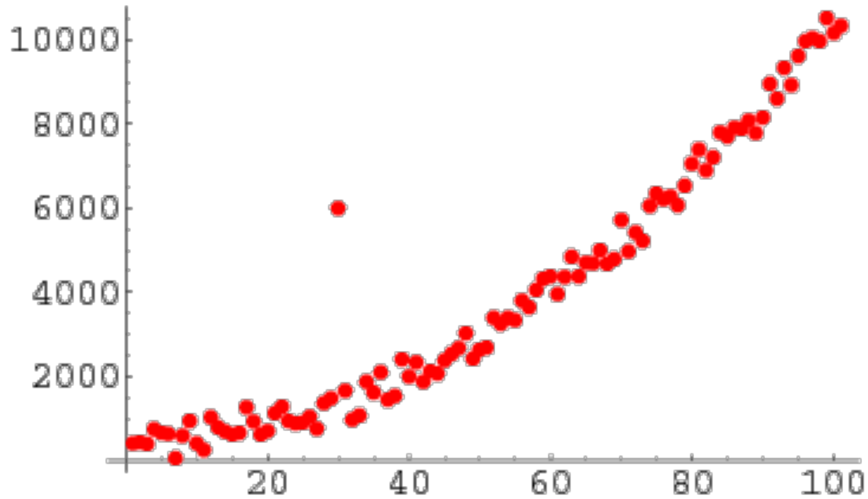
- Graphical approach to outlier detection:
  1. Look at a plot of the data.
  2. Human decides if data is an outlier.
- Examples:
  1. Box plot:
     - Visualization of quantiles/outliers.
     - Only 1 variable at a time.



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

Graphical Outlier Detection

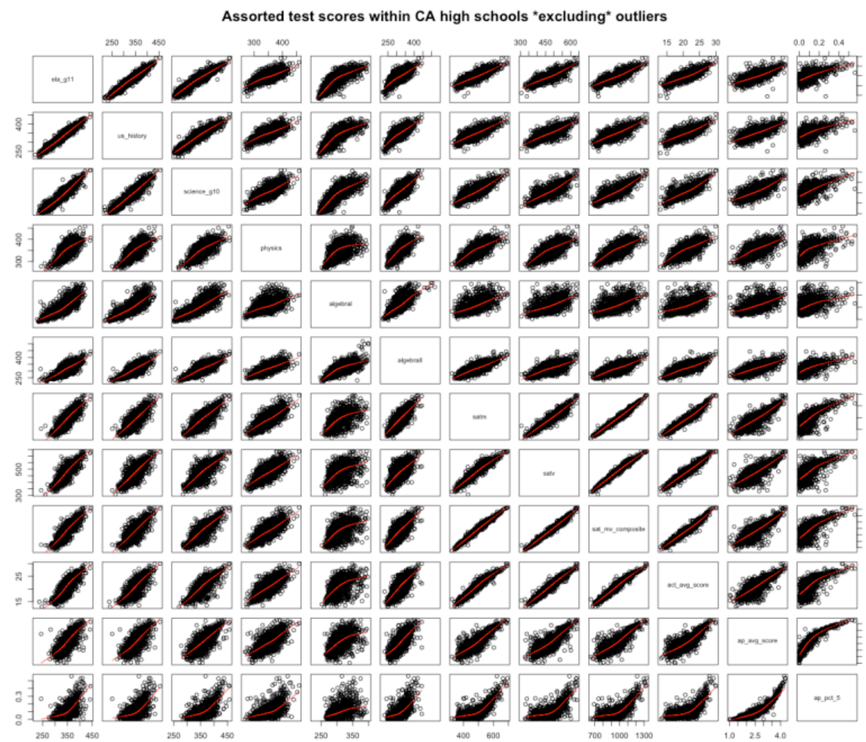
- Graphical approach to outlier detection:
  1. Look at a plot of the data.
  2. Human decides if data is an outlier.
- Examples:
  1. Box plot.
  2. Scatterplot:
     - Can detect complex patterns.
     - Only 2 variables at a time.



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

Graphical Outlier Detection

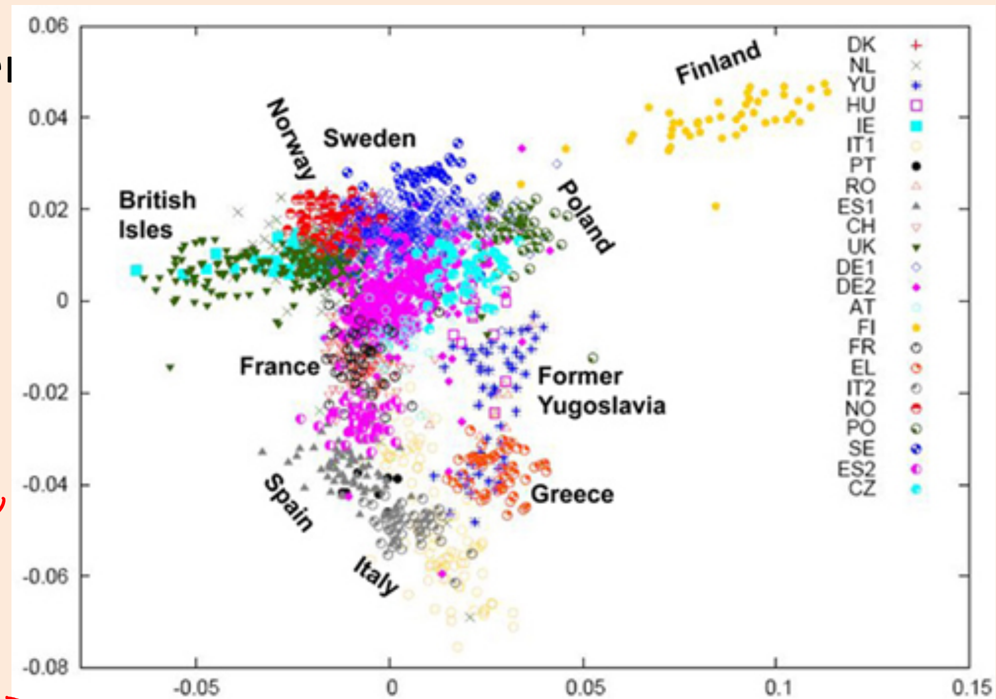
- Graphical approach to outlier detection:
  1. Look at a plot of the data.
  2. Human decides if data is an outlier.
- Examples:
  1. Box plot.
  2. Scatterplot.
  3. Scatterplot array:
     - Look at all combinations of variables.
     - But laborious in high-dimensions.
     - Still only 2 variables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

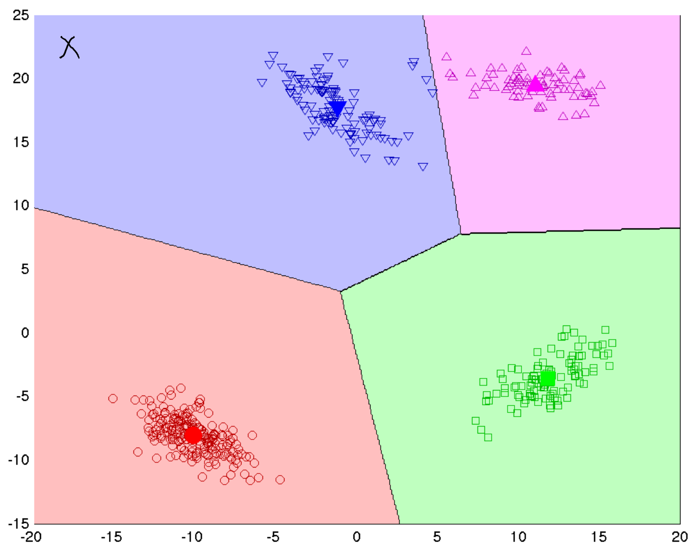


We'll cover PCA later in this course.

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

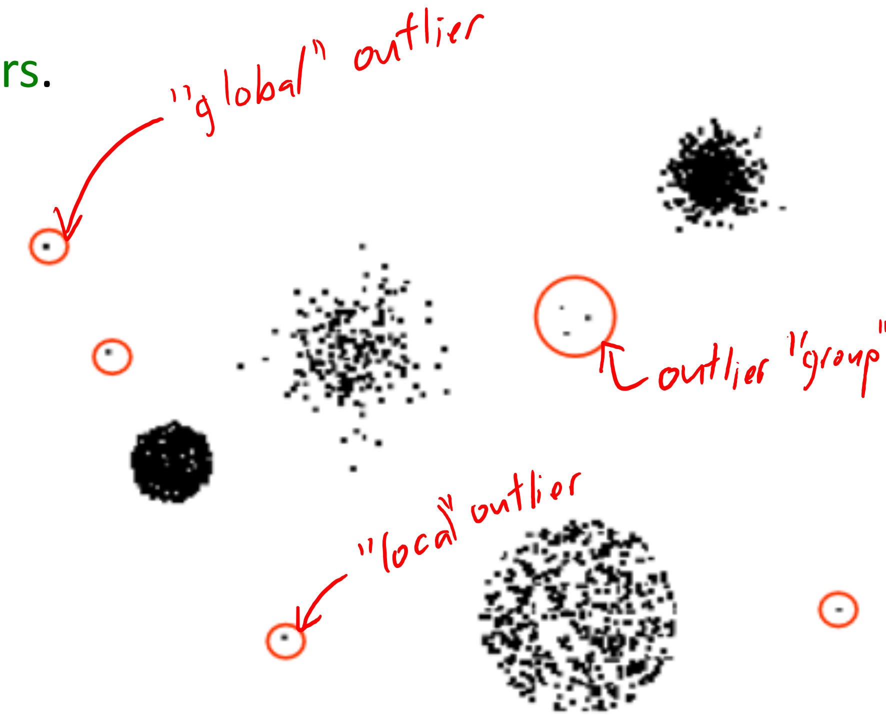
Cluster-Based Outlier Detection

- 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

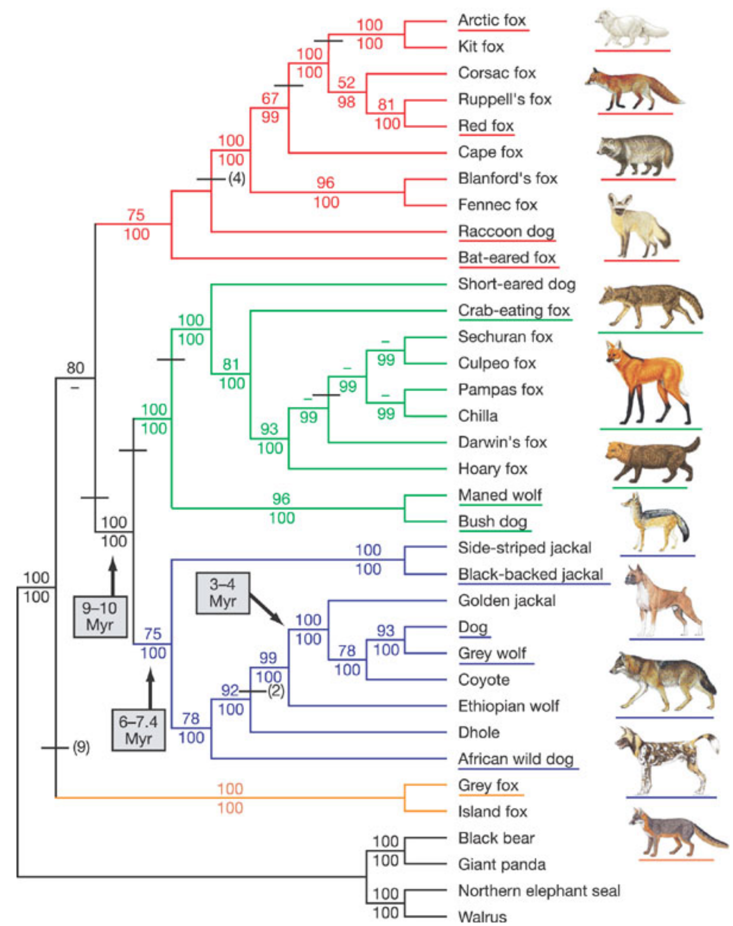
- Detect outliers based on clustering:
  1. Cluster the data.
  2. Find points that don't belong to clusters.
- Examples:
  1. K-means.
  2. Density-based clustering:
     - Outliers are points not assigned to cluster.



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 outlier detection approaches are based on distances.
- Can we skip the model/plot/clustering and just measure distances?
  - How many points lie in a radius 'epsilon'?
  - What is distance to k^{th} nearest neighbour?

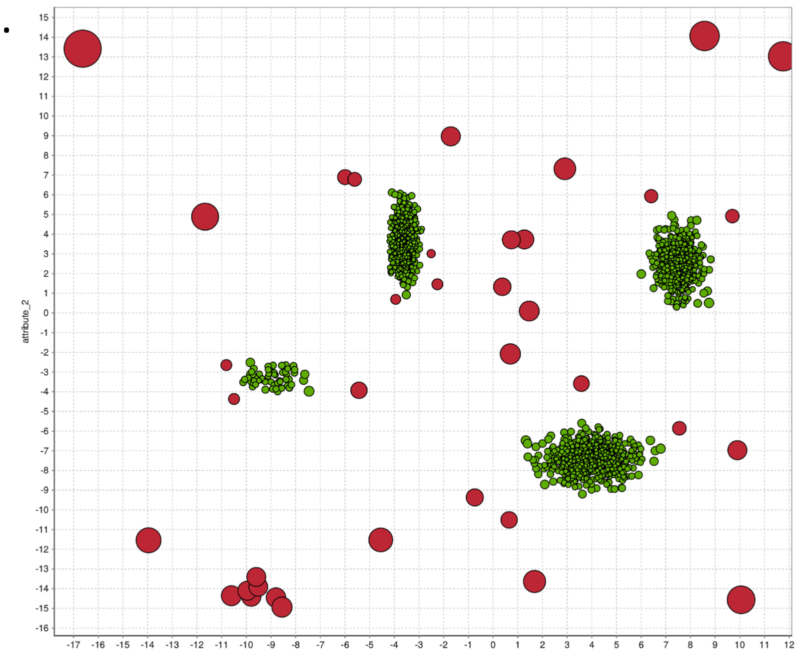
- UBC connection (first paper on this topic):

Algorithms for Mining Distance-Based Outliers in Large Datasets

Edwin M. Knorr and Raymond T. Ng
Department of Computer Science
University of British Columbia

Global Distance-Based Outlier Detection: KNN

- KNN outlier detection:
  - For each point, compute the average distance to its KNN.
  - Choose points with biggest values (or values above a threshold) as outliers.
    - "Outliers" are points that are far from their KNNs.

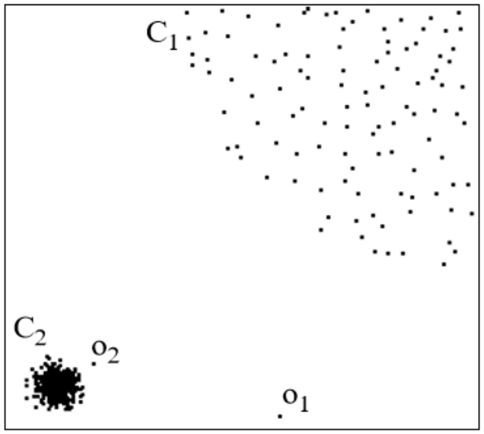


- Goldstein and Uchida [2016]:
  - Compared 19 methods on 10 datasets.
  - KNN best for finding "global" outliers.
  - "Local" outliers best found with local distance-based methods…

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.
- Basic idea behind local distance-based methods:
  – Outlier o_2 is "relatively" far compared to its neighbours.

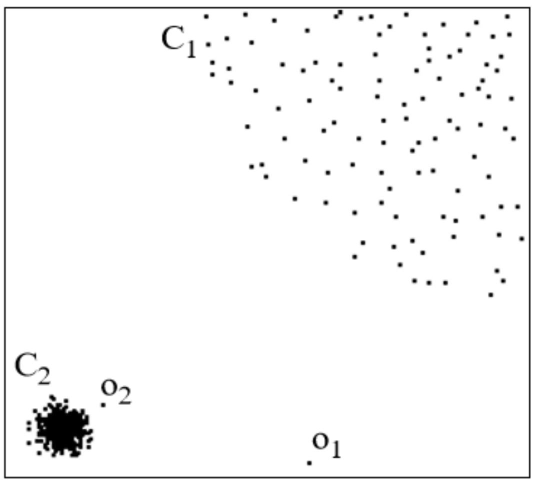
http://www.dbs.ifi.lmu.de/Publikationen/Papers/LOF.pdf

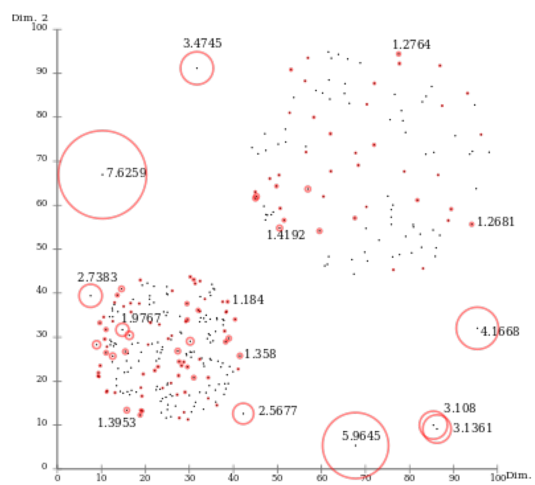
Local Distance-Based Outlier Detection

- "Outlierness" ratio of example 'i':

$$\frac{\text{average distance of 'i' to its KNNs}}{\text{average distance of neighbours of 'i' to their KNNs}}$$

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



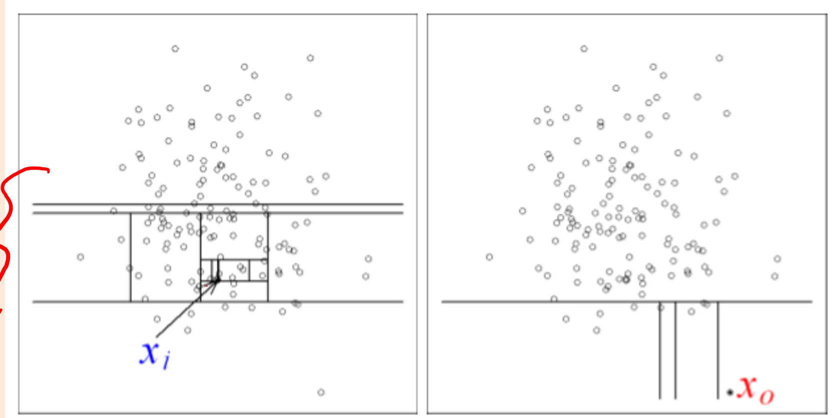


http://www.dbs.ifi.lmu.de/Publikationen/Papers/LOF.pdf
https://en.wikipedia.org/wiki/Local_outlier_factor

Isolation Forests

- Recent method based on random trees is isolation forests.
  - Grow a tree where each stump uses a random feature and random split.
  - Stop when each example is "isolated" (each leaf has one example).
  - The "isolation score" is the depth before example gets isolated.
    - Outliers should be isolated quickly, inliers should need lots of rules to isolate.

Depth 12:
- needed 12 rules to isolate
so may be inlier



(a) Isolating x_i (b) Isolating x_o

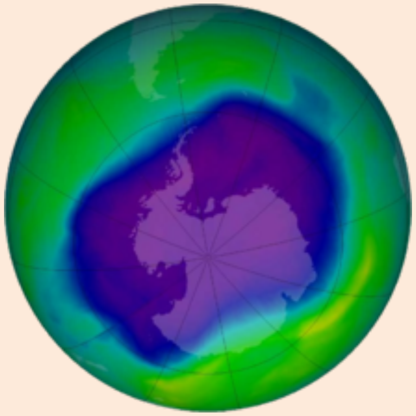
depth 4
so more likely to be outlier

  - Repeat for different random trees, take average score.

https://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/icdm08b.pdf

Problem with Unsupervised Outlier Detection

- Why wasn't the hole in the ozone layer discovered for 9 years?



- Can be hard to decide when to report an outler:
  - If you report too many non-outliers, users will turn you off.
  - Most antivirus programs do not use ML methods (see "base-rate fallacy")

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

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.

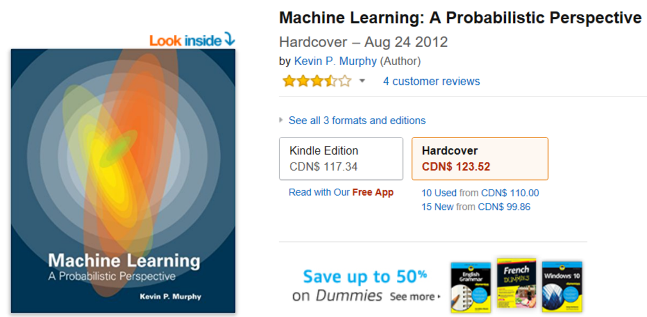
- We can use our methods for supervised learning:
  – We can find very complicated outlier patterns.
  – Classic credit card fraud detection methods used decision trees.

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

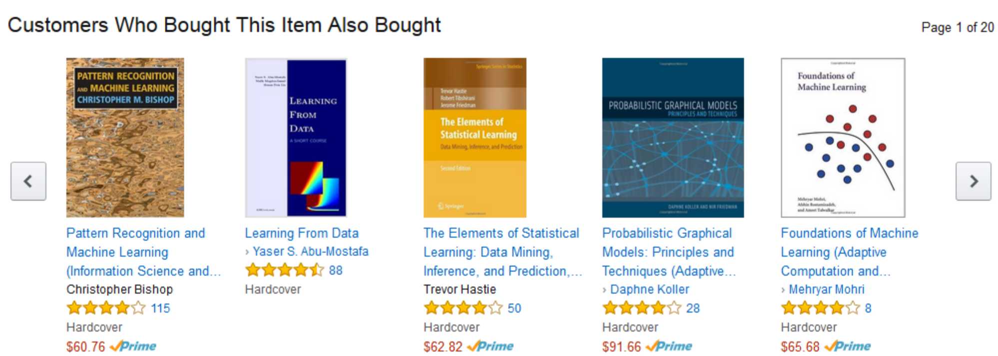
(pause)

Motivation: Product Recommendation

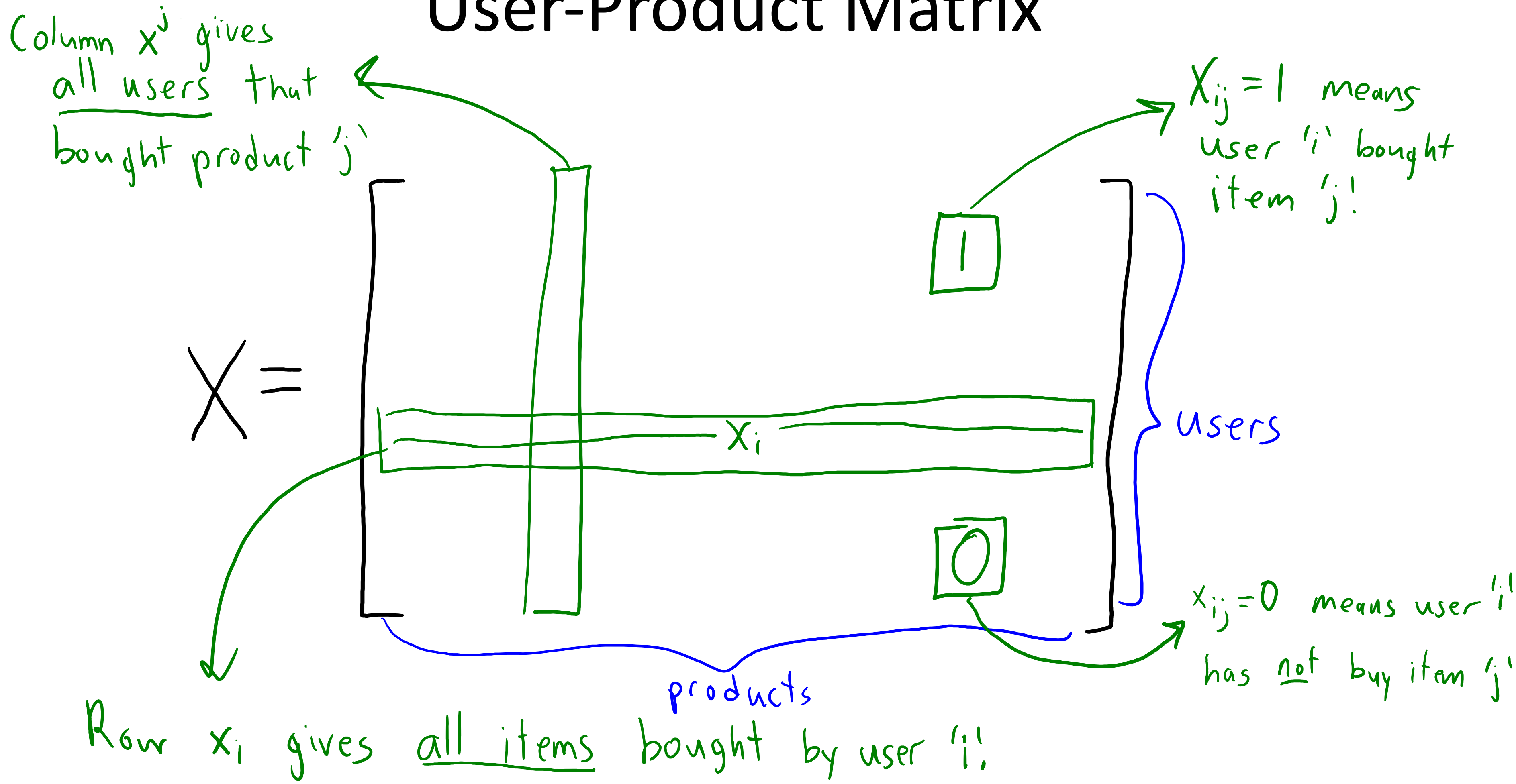
- A customer comes to your website looking to buy an item:



- You want to find similar items that they might also buy:

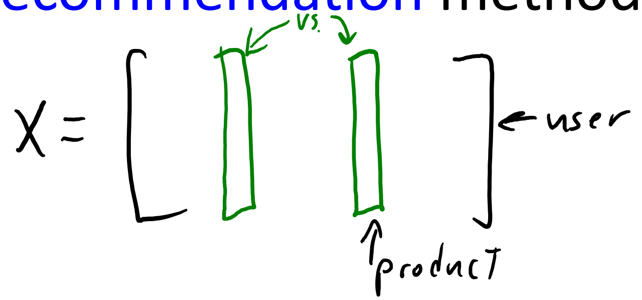


User-Product Matrix



Amazon Product Recommendation

- Amazon product recommendation method:



- Return the KNNs across columns.
  - Find 'j' values minimizing $||x^i - x^j||$.
  - Products that were bought by similar sets of users.

- But first divide each column by its norm, $x^i/||x^i||$.
  - This is called normalization.
  - Reflects whether product is bought by many people or few people.

End of Part 2: Key Concepts

- We focused on 3 unsupervised learning tasks:
  - Clustering.
    - Partitioning (k-means) vs. density-based.
    - "Flat" vs. hierarachial (agglomerative).
    - Vector quantization.
    - Label switching.
  - Outlier Detection.
    - Surveyed common approaches (and said that problem is ill-defined).

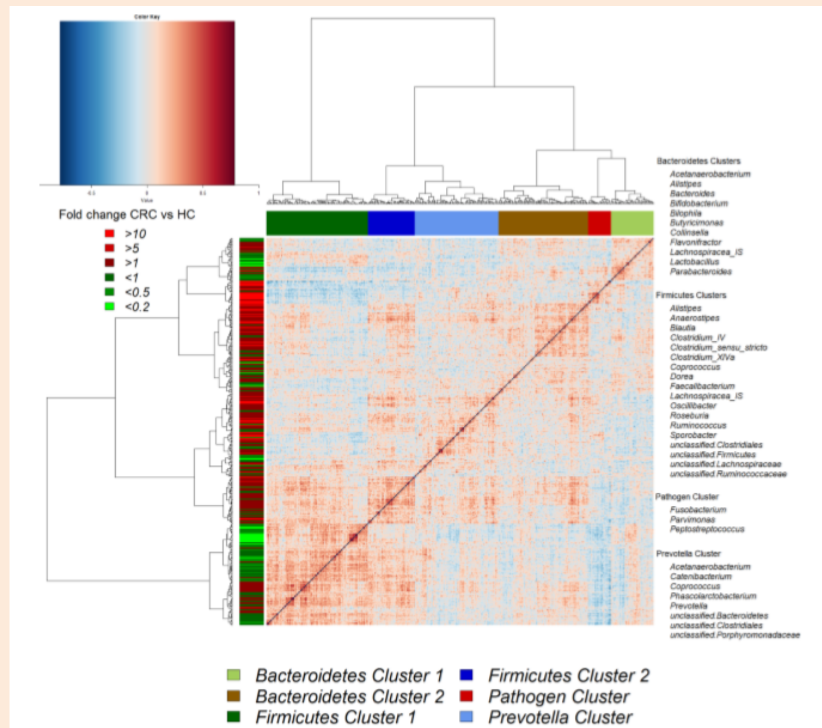
Summary

- Biclustering: clustering of the examples *and* the features.
- Outlier detection is task of finding unusually different example.
  - A concept that is very difficult to define.
  - Model-based find unlikely examples given a model of the data.
  - Graphical methods plot data and use human to find outliers.
  - Cluster-based methods check whether examples belong to clusters.
  - Distance-based outlier detection: measure (relative) distance to neighbours.
  - Supervised-learning for outlier detection: turns task into supervised learning.

- Next time: supervised learning with continuous labels.

Application: Medical data

- Hierarchical clustering is very common in medical data analysis.
  - Clustering different samples of colorectoral cancer:

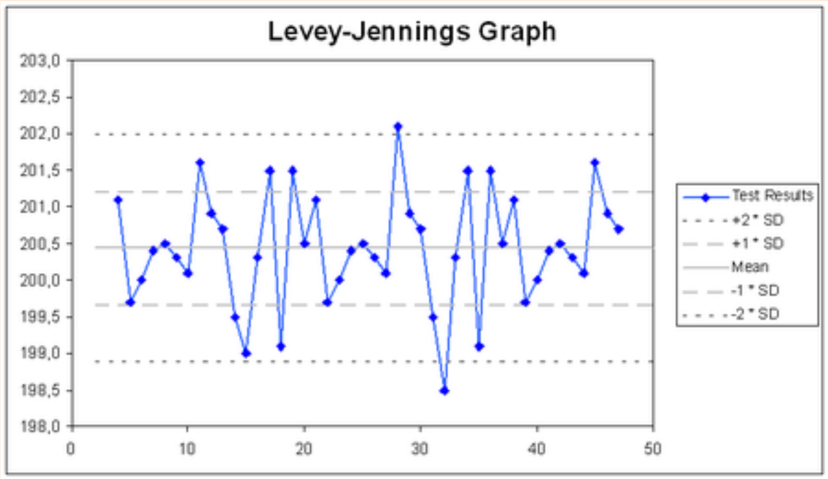


  - This plot is different, it's not a biclustering:
    - The matrix is 'n' by 'n'.
    - Each matrix element gives correlation.
    - Clusters should look like "blocks" on diagonal.
    - Order of examples is reversed in columns.
      - This is why diagonal goes from bottom-to-top.
      - Please don't do this reversal, it's confusing to me.

https://gut.bmj.com/content/gutjnl/66/4/633.full.pdf

“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

Outlierness (Symbol Definition)

- 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:

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

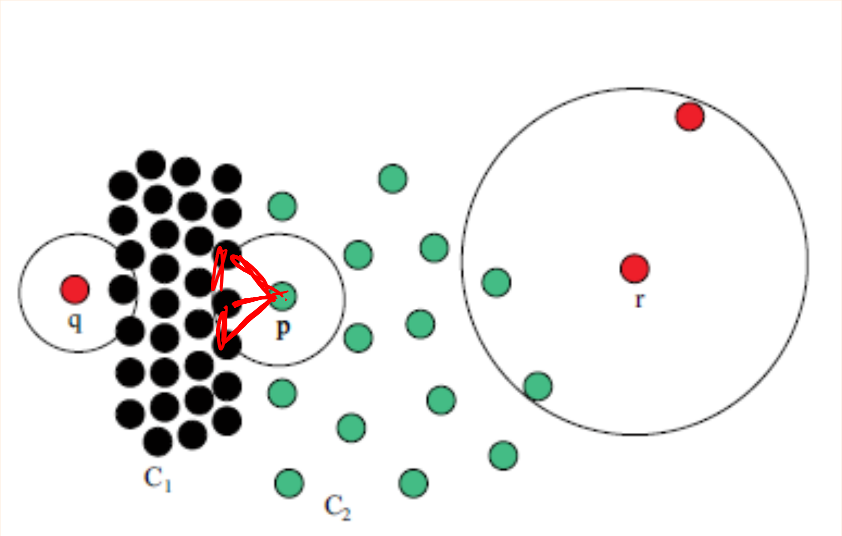
- Outlierness is ratio of $D_k(x_i)$ to average $D_k(x_j)$ for its neighbours 'j':

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

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

Outlierness with Close Clusters

- If clusters are close, outlierness gives unintuitive results:

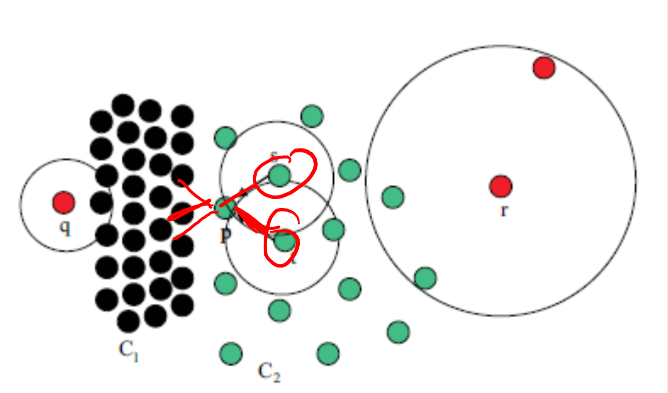


- In this example, ‘p’ has higher outlierness than ‘q’ and ‘r’:
  - The green points are not part of the KNN list of ‘p’ for small ‘k’.

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

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

Training/Validation/Testing (Supervised)

- A typical supervised learning setup:
  - Train parameters on dataset D_1.
  - Validate hyper-parameters on dataset D_2.
  - Test error evaluated on dataset D_3.
- What should we choose for D_1, D_2, and D_3?
- Usual answer: should all be IID samples from data distribution D_s.

Training/Validation/Testing (Outlier Detection)

- A typical outlier detection setup:
  - Train parameters on dataset D_1 (there may be no "training" to do).
    - For example, find z-scores.
  - Validate hyper-parameters on dataset D_2 (for outlier detection).
    - For example, see which z-score threshold separates D_1 and D_2.
  - Test error evaluated on dataset D_3 (for outlier detection).
    - For example, check whether z-score recognizes D_3 as outliers.

- D_1 will still be samples from D_s (data distribution).
- D_2 could use IID samples from another distribution D_m.
  - D_m represents the "none" or "outlier" class.
  - Tune parameters so that D_m samples are outliers and D_s samples aren't.
    - Could just fit a binary classifier here.

Training/Validation/Testing (Outlier Detection)

- A typical outlier detection setup:
  - Train parameters on dataset D_1 (there may be no “training” to do).
    - For example, find z-scores.
  - Validate hyper-parameters on dataset D_2 (for outlier detection).
    - For example, see which z-score threshold separates D_1 and D_2.
  - Test error evaluated on dataset D_3 (for outlier detection).
    - For example, check whether z-score recognizes D_3 as outliers.

- D_1 will still be samples from D_s (data distribution).
- D_2 could use IID samples from another distribution D_m.
- D_3 could use IID samples from D_m.
  - How well do you do at recognizing “data” samples from “none” samples?

Training/Validation/Testing (Outlier Detection)

- Seems like a reasonable setup:
  - D_1 will still be samples from D_s (data distribution).
  - D_2 could use IID samples from another distribution D_m.
  - D_3 could use IID samples from D_m.

- What can go wrong?

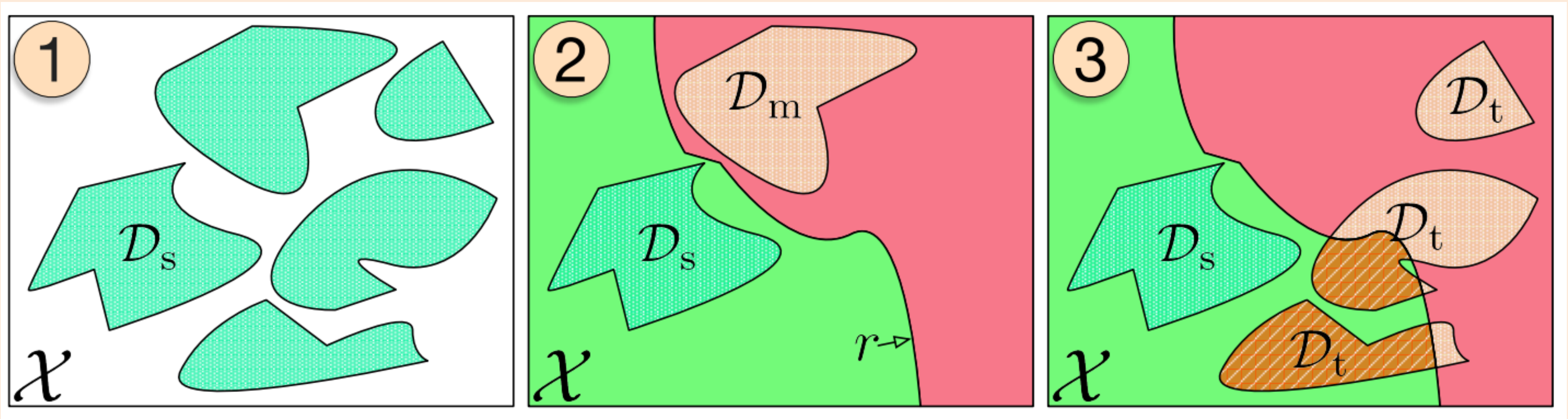
- You needed to pick a distribution D_m to represent “none”.
  - But in the wild, your outliers might follow another “none” distribution.
  - This procedure can overfit to your D_m.
    - You can overestimate your ability to detect outliers.

OD-Test: a better way to evaluate outlier detections

- A reasonable setup:
  - D_1 will still be samples from D_s (data distribution).
  - D_2 could use IID samples from another distribution D_m.
  - ~~D_3 could use IID samples from D_m.~~
  - D_3 could use IID samples from yet-another distribution D_t.

- "How do you perform at detecting different types of outliers?"
  - Seems like a harder problem, but arguably closer to reality.

OD-Test: a better way to evaluate outlier detections



- "How do you perform at detecting different types of outliers?"

https://arxiv.org/pdf/1809.04729.pdf