Outlier Detection:

Extreme Values

Mining Massive Datasets

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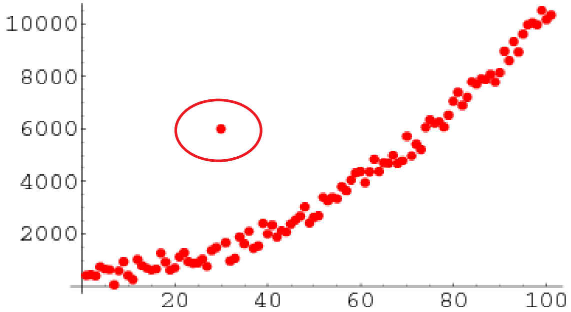
Sources

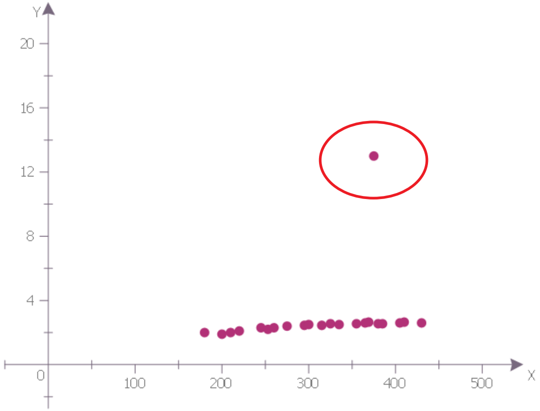
- Data Mining, The Textbook (2015) by Charu Aggarwal (chapter 8) – slides by Lijun Zhang

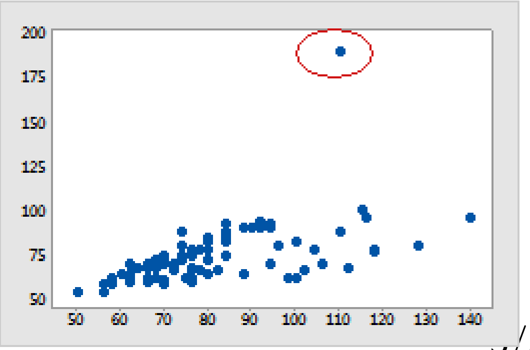
Outliers

Serena Williams

Sultan Kösen







What is an outlier?

- Informally, "An outlier is an observation which deviates so much from the other observations as to arouse suspicions that it was generated by a different mechanism."

Clustering groups points that are **similar**

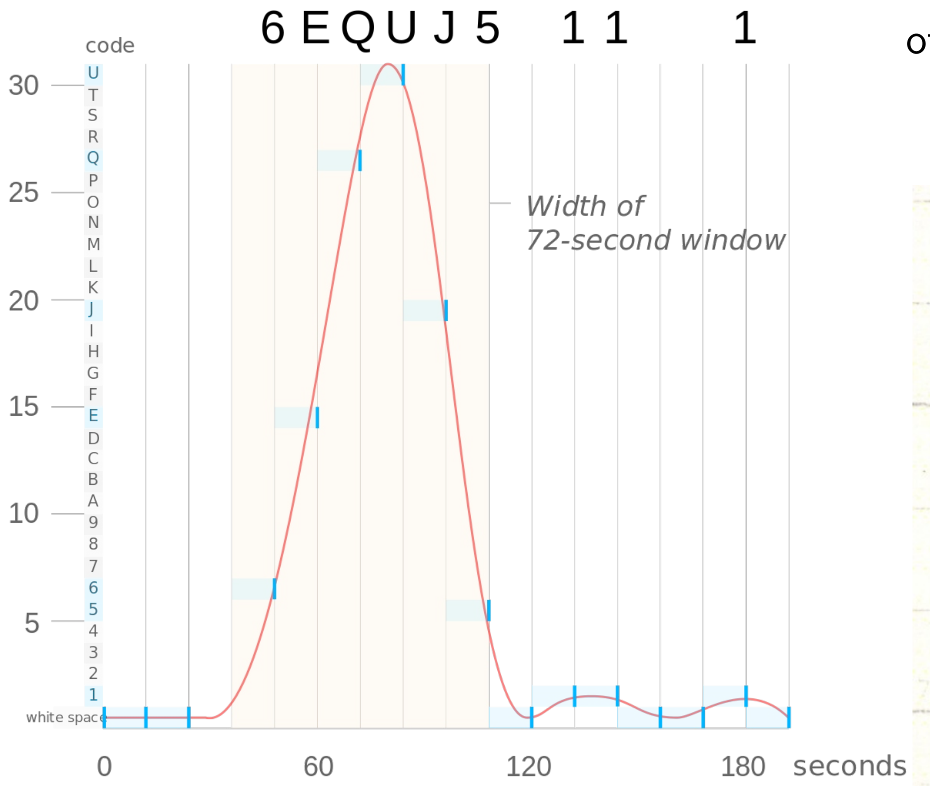
Outlier detection finds points that are **different**

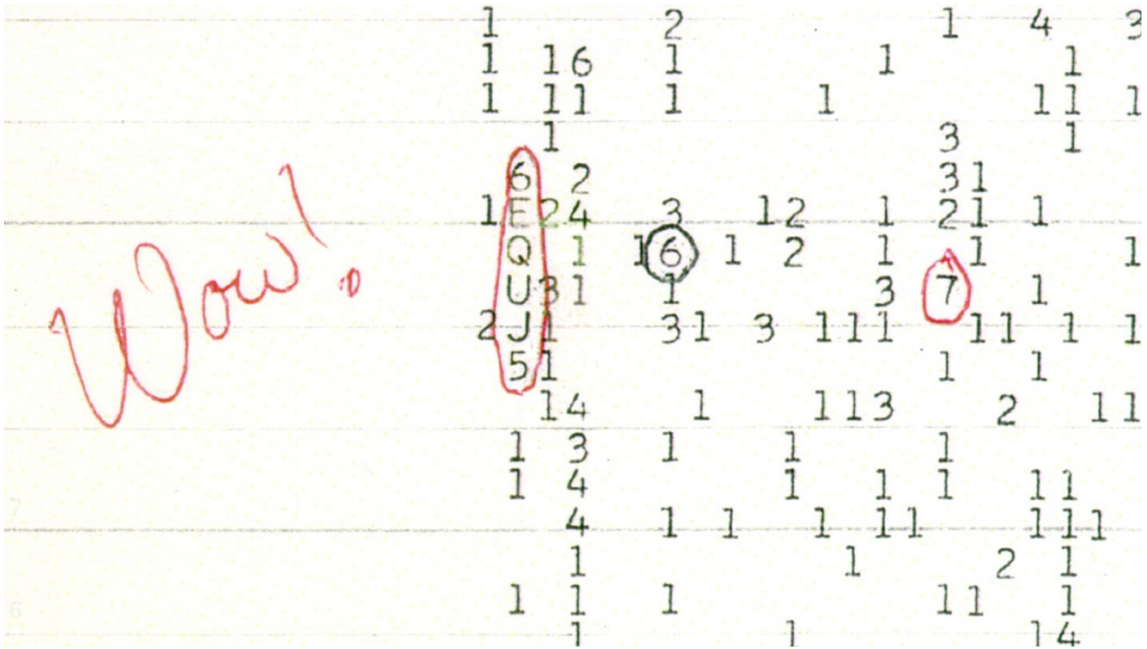
Outliers happen all the time

- Sensor malfunction
- Error in data transmission
- Transcription error
- Fraudulent behaviour
- Sample contamination
- Interesting natural occurrence

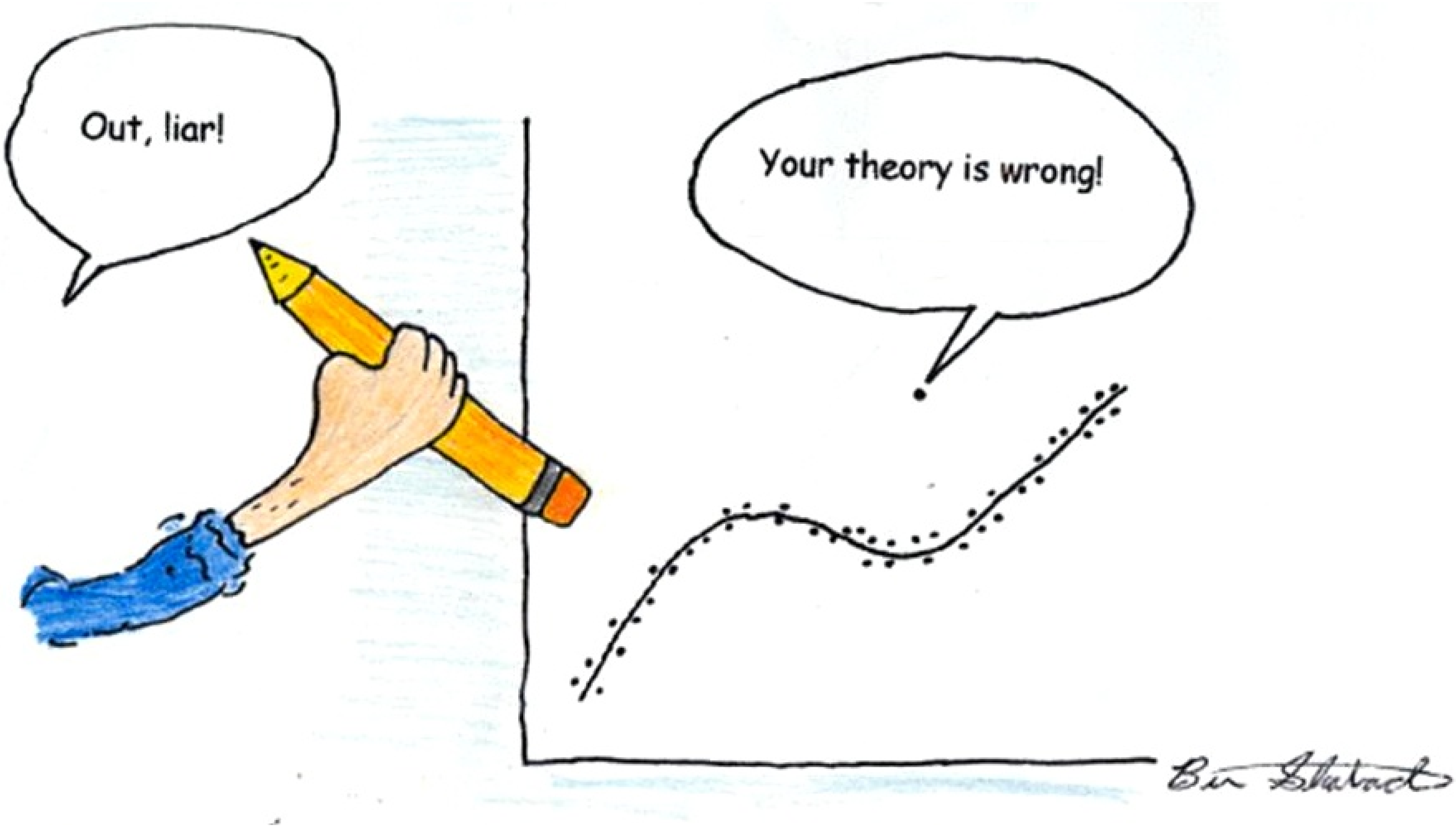
The Wow! Signal

Detected by a radio telescope in 1977, at its peak intensity it was 30 standard deviations above background noise in intensity (hence the letter “U” in the printout), and it remains unexplained until today. It is the strongest candidate for a signal of extraterrestrial origin, but it has never been observed again.





Wikipedia: Wow! Signal


Out, liar!
Your theory is wrong!

Some applications

- Remove noise
  - Find data that potentially has errors
- Credit card fraud
  - Find unusual patterns of credit card activity
- Network intrusion detection
  - Find unusual patterns or contents in network traffic

Outlier detection methods

- Key idea
  - Create a **model of normal patterns**
  - Outliers are data points that do not naturally fit within this normal model
  - The "*outlierness*" of a data point is quantified by a outlier score
- Outputs of Outlier Detection Algorithms
  - Real-valued outlier score
  - Binary label (outlier / not outlier)

Evaluation
(outlier validity)

Internal (unsupervised) criteria

- Rarely used in outlier analysis
- For any method, a measure can be created that will favor that method ($\sim$*overfit*)
- Solution space is small
  - Maybe there is just one outlier, finding it or missing it makes all the difference between perfect and useless performance

External (supervised) criteria

- **Known outliers** from a synthetic dataset or **rare items** (e.g., belonging to smallest class)
- Suppose D is the data, G are the real outliers, and S(t) are found when threshold t is used

$$TPR(t) = \text{Recall}(t) = 100 \cdot \frac{|S(t) \cap G|}{|G|}$$

$$FPR(t) = 100 \cdot \frac{|S(t) - G|}{|D - G|}$$

ROC curve = (FPR(t), TPR(t))$_t$

Rank of ground-truth outliers:

- Algorithm A

  1, 5, 8, 15, 20

- Algorithm B

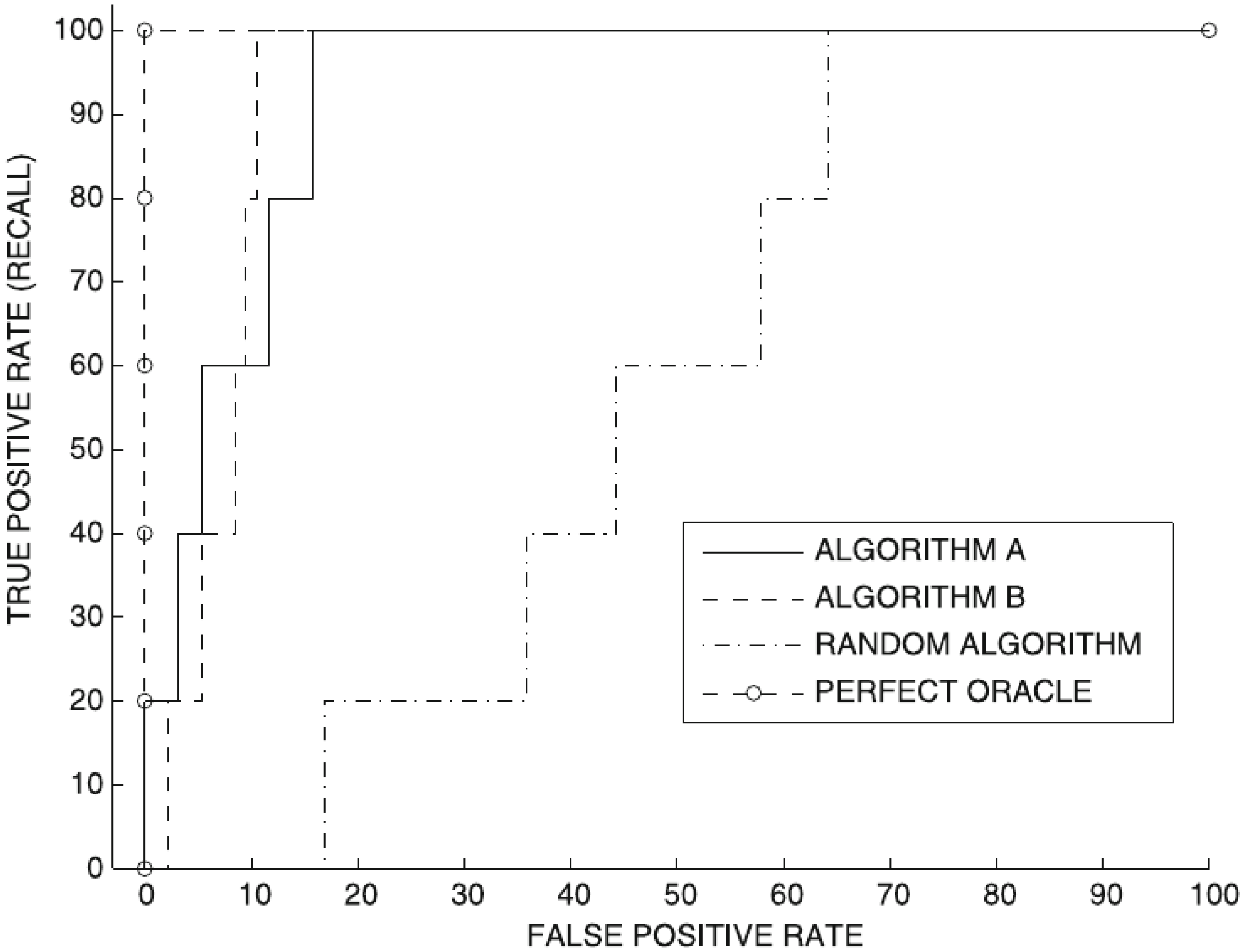
  3, 7, 11, 13, 15

- Random

  17, 36, 45, 59, 66

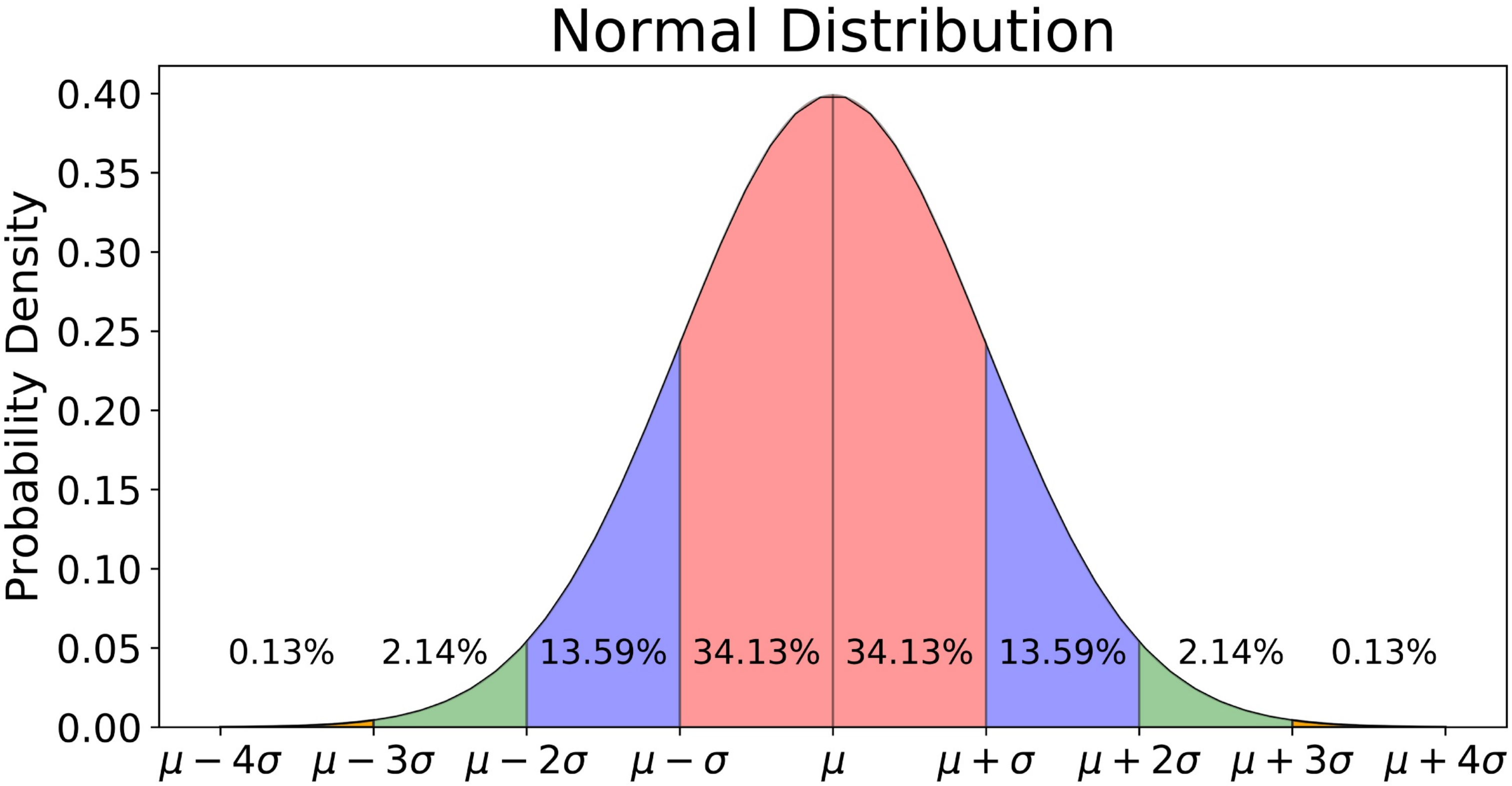
- Perfect oracle

  1, 2, 3, 4, 5



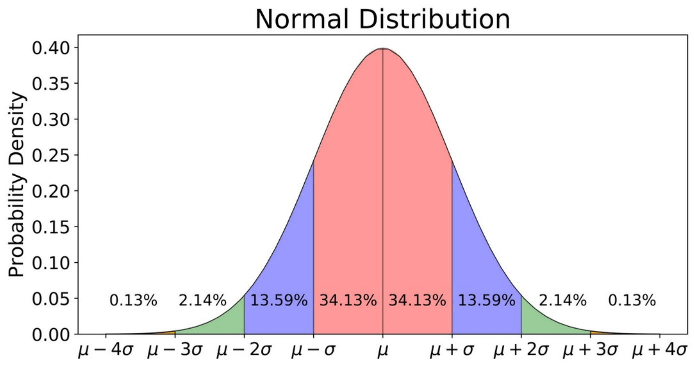
Extreme values analysis

Extreme value analysis: Statistical Tails



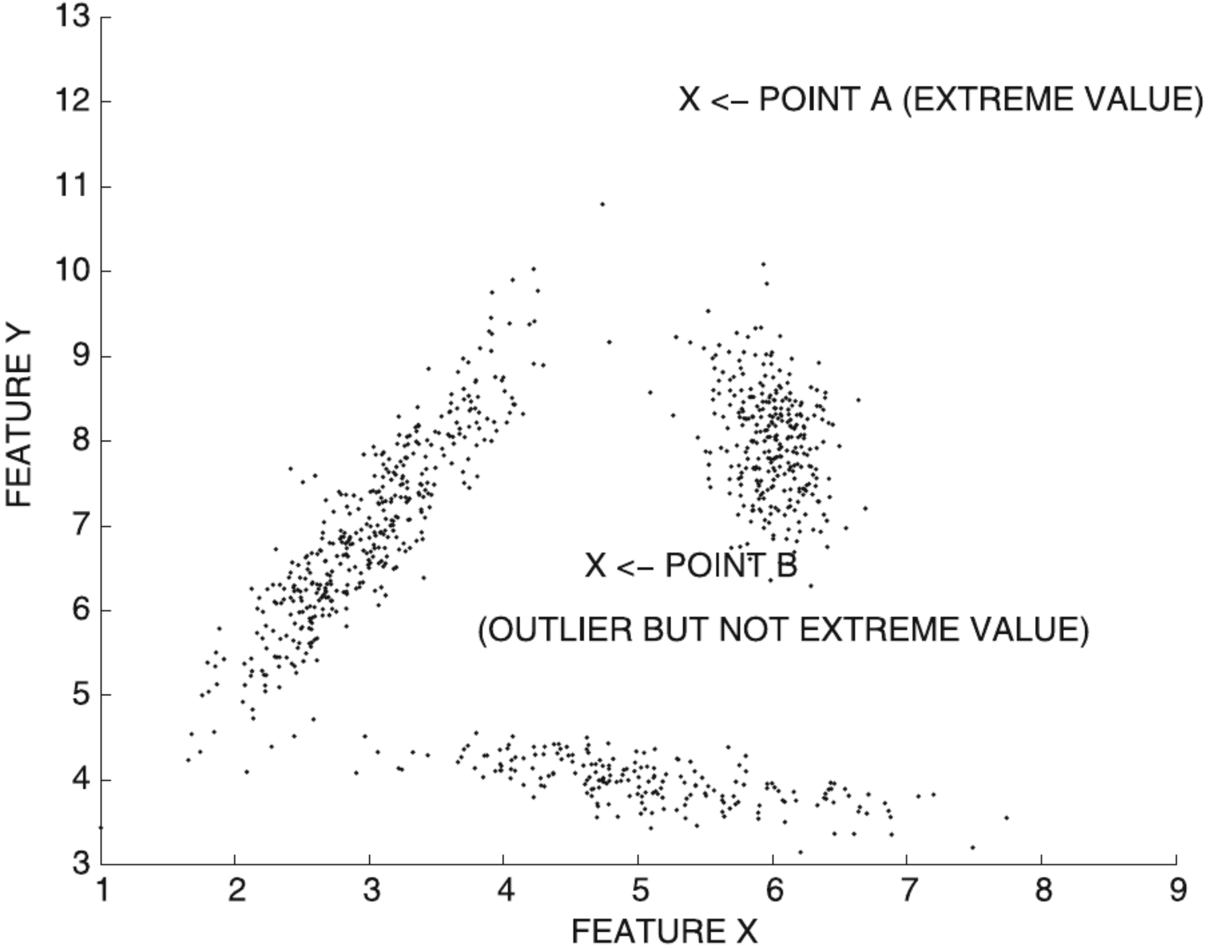
Extreme value analysis (cont.)

- Hypothesis: all extreme values are outliers
- However, outliers may not be extreme values:
  - $\{1,3,3,3,50,97,97,100\}$
  - 1 and 100 are extreme values
  - 50 is an outlier but no an extreme value



Extreme value analysis (cont.)

- Point A is an extreme value (hence, an outlier)
- Point B is an outlier but not an extreme value



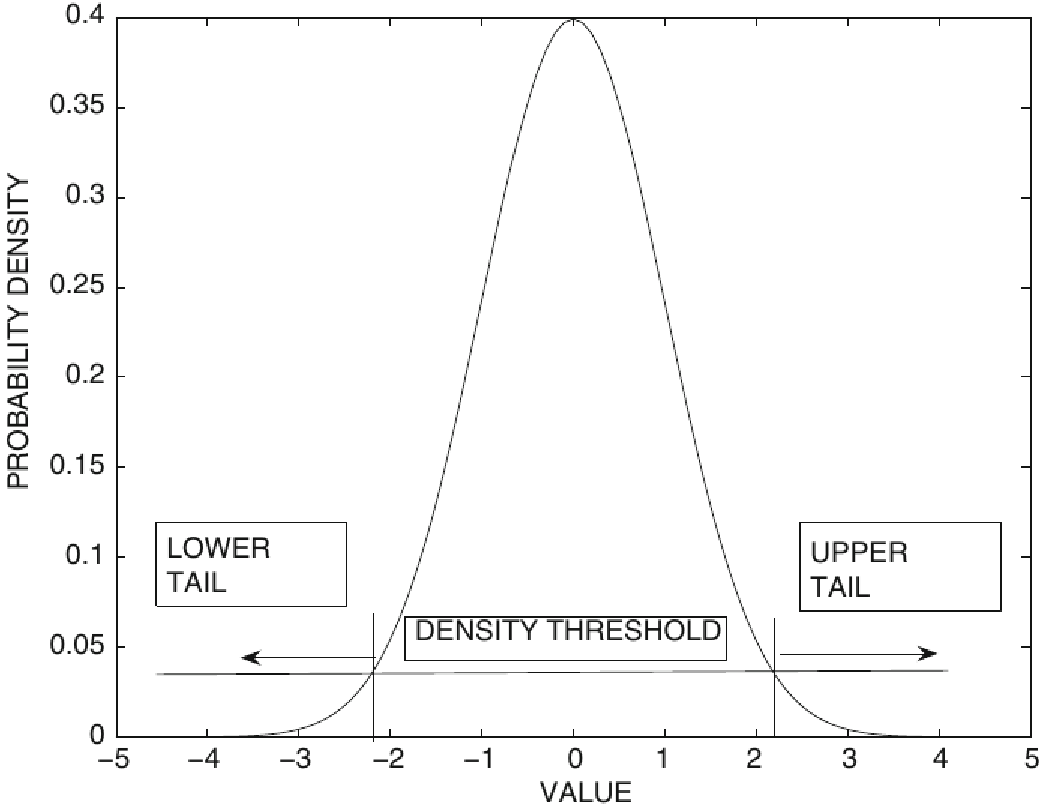
Univariate extreme value analysis

- Statistical tail confidence test
  - Let density be $f_X(x)$
  - Tails are **extreme** regions s.t. $f_X(x) \leq \theta$

Univariate extreme value analysis (cont.)

Let density be $f_X(x)$; tails are extreme regions s.t. $f_X(x) \leq \theta$

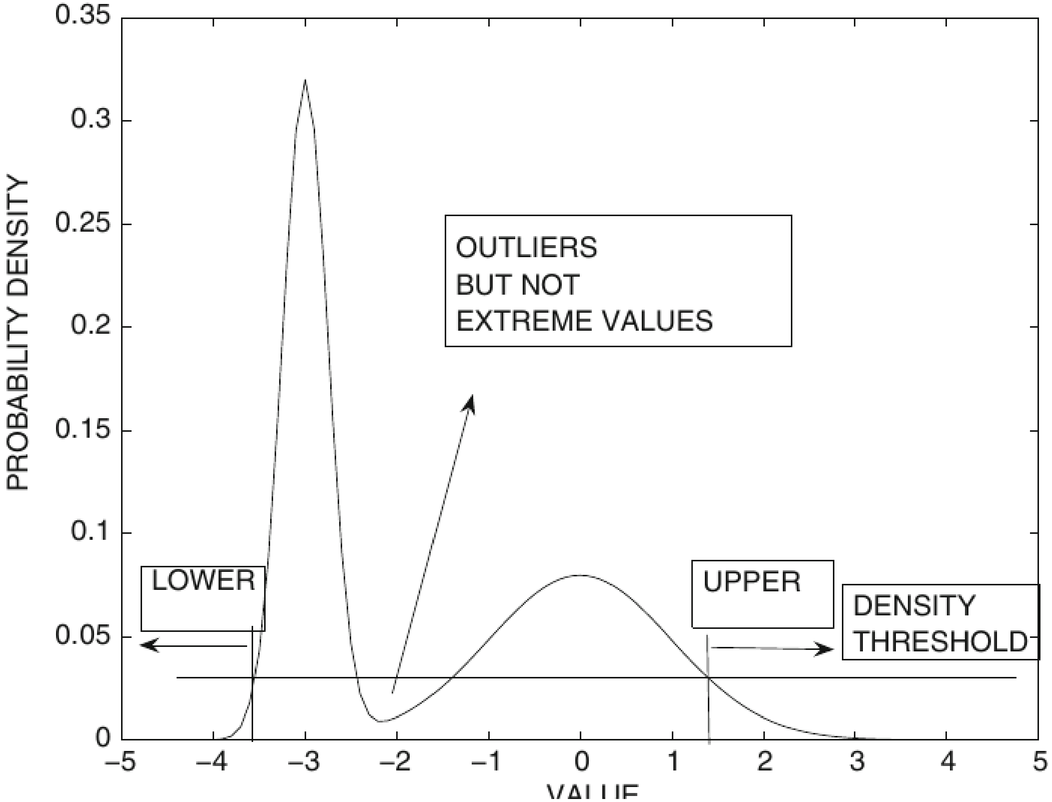
- Symmetric distribution
  - Two symmetric tails
  - Areas inside tails represent cumulative distribution



Univariate extreme value analysis (cont.)

Let density be $f_X(x)$; tails are extreme regions s.t. $f_X(x) \leq \theta$

- Asymmetric distribution
  - Areas in two tails are different
  - Regions in the interior are not tails



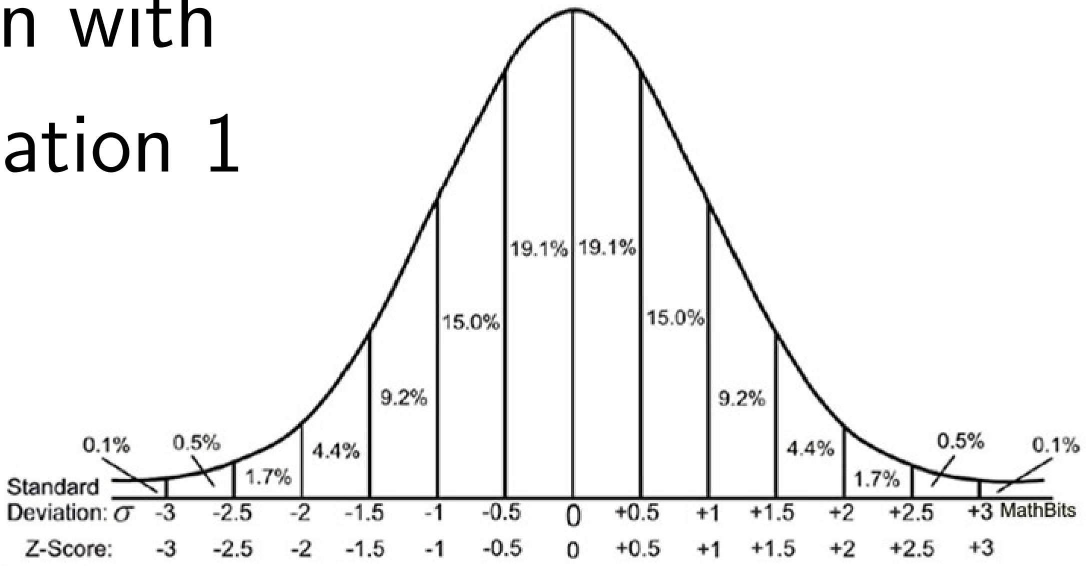
Standardization for univariate outlier analysis

- Normal distribution assumed $$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$
- Parameters
  - From prior knowledge
  - Estimated from data

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \hat{\mu})^2$$

Standardization for univariate outlier analysis (cont.)

- *z-value* $z_i = \dfrac{x_i - \mu}{\sigma}$
- Follows normal distribution with mean 0 and standard deviation 1
  - Large z-value: upper tail
  - Small z-value: lower tail



Exercise: outliers through extreme values

- Find the absolute z-score of each feature in the electrical scooters dataset
- Compute max z-score across features as an outlier metric
- Indicate which are the #1 and #2 most unusual electric scooters in this list and why

Spreadsheet links: https://upfbarcelona.padlet.org/chato/hogch321o6pws1fd

Multivariate extreme values

- Probability density function of a Multivariate Gaussian distribution in d dimensions

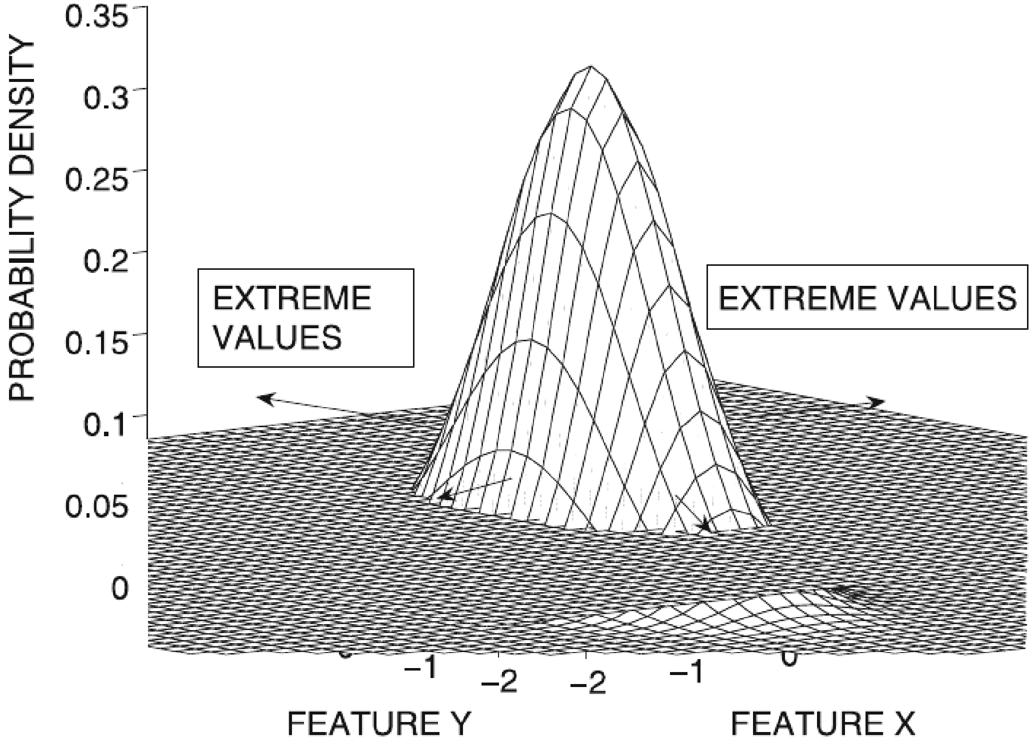
$$f(\overline{X}) = \frac{1}{\sqrt{|\Sigma|} \cdot (2 \cdot \pi)^{(d/2)}} \cdot e^{-\frac{1}{2} \cdot (\overline{X} - \overline{\mu}) \Sigma^{-1} (\overline{X} - \overline{\mu})^T}$$

$$= \frac{1}{\sqrt{|\Sigma|} \cdot (2 \cdot \pi)^{(d/2)}} \cdot e^{-\frac{1}{2} \cdot Maha(\overline{X}, \overline{\mu}, \Sigma)^2}$$

- $Maha(\overline{X}, \bar{\mu}, \Sigma)$ is the Mahalanobis distance
- $|\Sigma|$ is the determinant of the covariances matrix

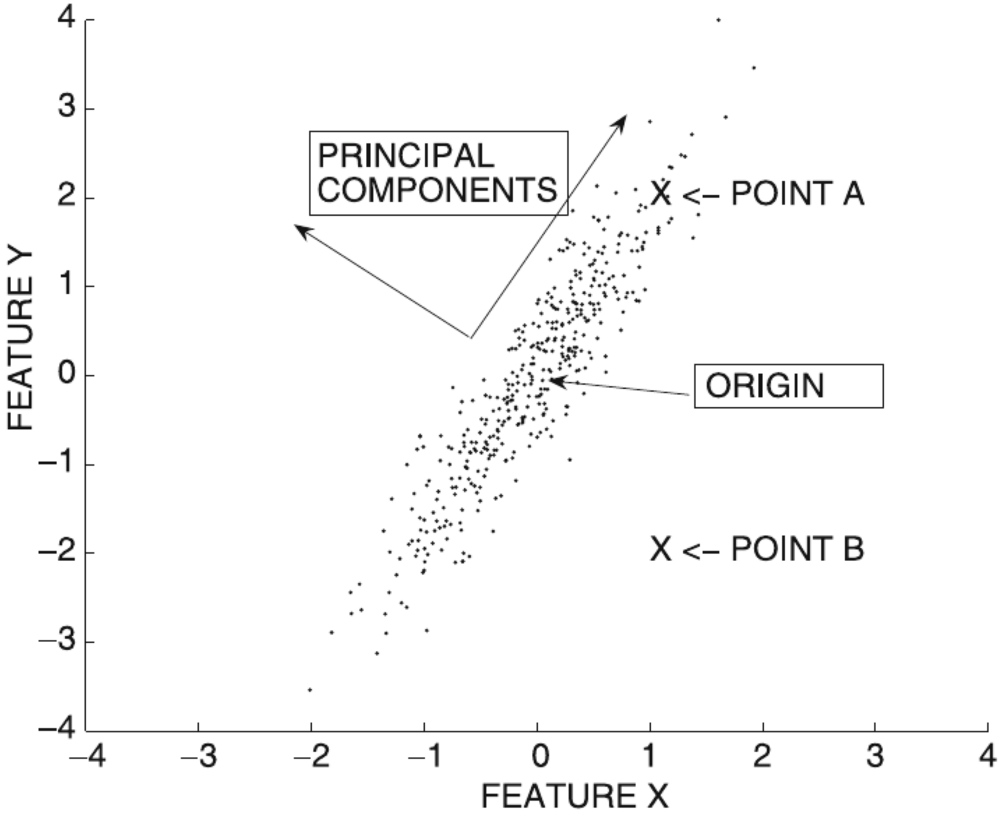
Multivariate extreme values (cont.)

- Extreme value score of $\overline{X}$
  - $Maha(\overline{X}, \overline{\mu}, \Sigma)$
  - Mahalanobis distance to the mean of the data
  - Larger values imply more extreme behavior



Multivariate extreme values (cont.)

- Extreme value score of $\overline{X}$
  - $Maha(\overline{X}, \bar{\mu}, \Sigma)$
  - Mahalanobis distance to the mean of the data
  - Larger values imply more extreme behavior
  - The Mahalanobis distance is the Euclidean distance in a transformed (axes-rotated) data set after dividing each of the transformed coordinate values by the standard deviation along its direction



Summary

Things to remember

- Extreme value analysis
  - Univariate, multivariate, depth based
- Outlier evaluation/validity

Exercises for TT19-TT21

- Data Mining, The Textbook (2015) by Charu Aggarwal
  - Exercises 8.11 $\rightarrow$ all except 10, 15, 16, 17

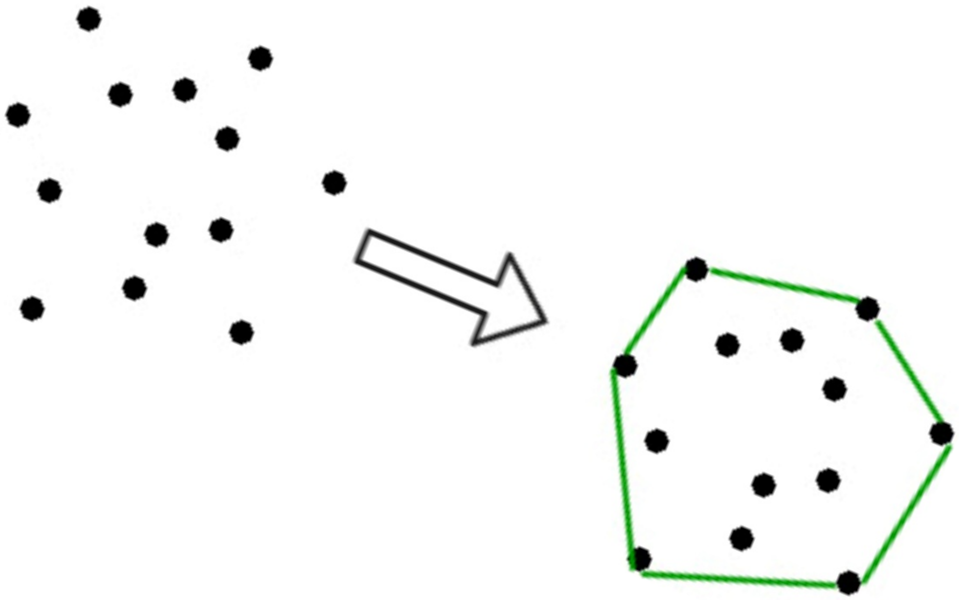
Additional contents
(not included in exams)

Depth-based methods

Key concept: convex hull

The convex hull of a set C is the set of
all convex combinations of points in C

$$
\begin{aligned}
\text{conv } C = \{\theta_1 x_i + \cdots + \theta_k x_k |\\
x_i \in C,\\
\theta_i \geq 0,\\
\theta_1 + \cdots + \theta_k = 1\}
\end{aligned}
$$



Algorithm

Algorithm *FindDepthOutliers*(Data Set: $\mathcal{D}$, Score Threshold: r)
begin
  $k = 1$;
  repeat
    Find set S of corners of convex hull of $\mathcal{D}$;
    Assign depth k to points in S;
    $\mathcal{D} = \mathcal{D} - S$;
    $k = k + 1$;
  until(D is empty);
  Report points with depth at most r as outliers;
end

Explanation: peeling layers

Algorithm *FindDepthOutliers*(Data Set: $\mathcal{D}$, Score Threshold: r)
begin
  $k = 1$;
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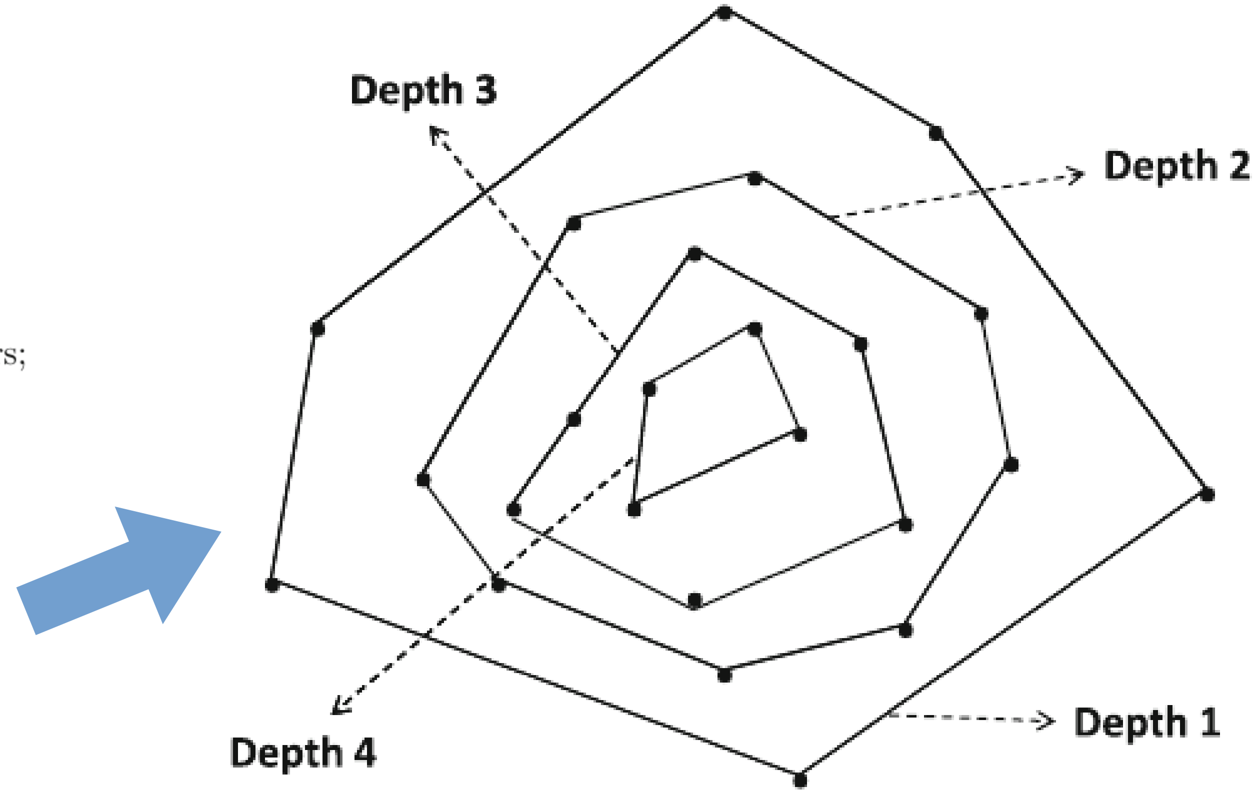

Limitations of this method

- No normalization
- Computational complexity increases significantly with dimensionality
- Many data points are indistinguishable