

Heiko Paulheim

Anomaly Detection

- Also known as "Outlier Detection"
- Automatically identify data points that are somehow different from the rest
- Working assumption:
 - There are considerably more "normal" observations than "abnormal" observations (outliers/anomalies) in the data
- Challenges
 - How many outliers are there in the data?
 - What do they look like?
 - Method is unsupervised
 - Validation can be quite challenging (just like for clustering)

Recap: Errors in Data

Sources

- malfunctioning sensors
- errors in manual data processing (e.g., twisted digits)
- storage/transmission errors
- encoding problems, misinterpreted file formats
- bugs in processing code
- **—** ...



Image: http://www.flickr.com/photos/16854395@N05/3032208925/

Recap: Errors in Data

- Simple remedy
 - remove data points outside a given interval
 - this requires some domain knowledge
- Advanced remedies
 - automatically find suspicious data points

```
cond = df['temp'].between(30,100)
df_filtered = df.drop(df[~cond].index)
```

Applications: Data Preprocessing

- Data preprocessing
 - removing erroneous data
 - removing true, but useless deviations
- Example: tracking people down using their GPS data
 - GPS values might be wrong
 - person may be on holidays in Hawaii
 - what would be the result of a kNN classifier?

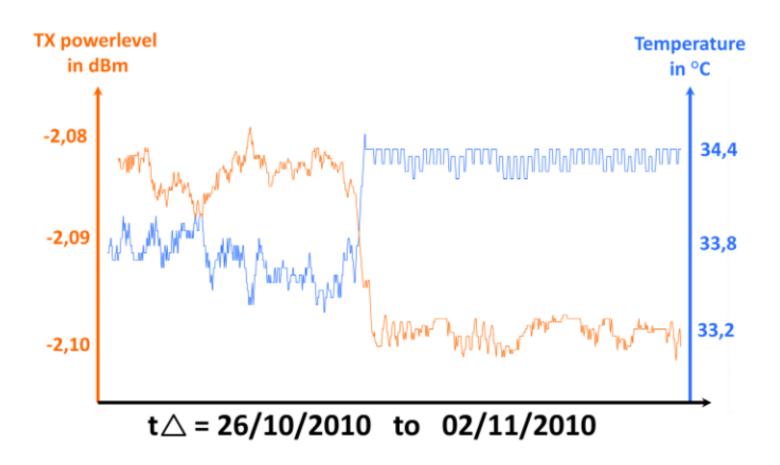


Applications: Credit Card Fraud Detection

- Data: transactions for one customer
 - €15.10 Amazon
 - €12.30 Deutsche Bahn tickets, Mannheim central station
 - €18.28 Edeka Mannheim
 - \$500.00 Cash withdrawal. Dubai Intl. Airport
 - €48.51 Gas station Heidelberg
 - €21.50 Book store Mannheim
- Goal: identify unusual transactions
 - possible attributes: location, amount, currency, ...



Applications: Hardware Failure Detection

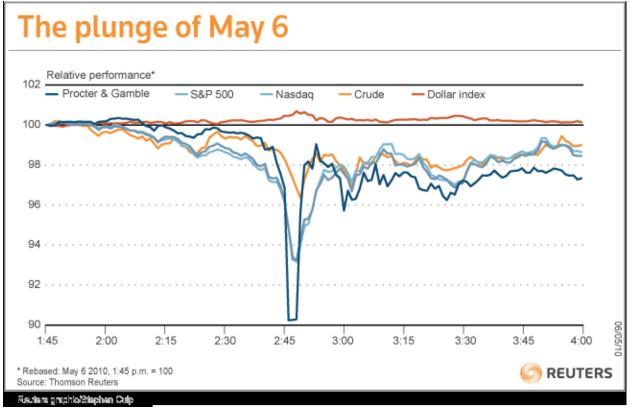


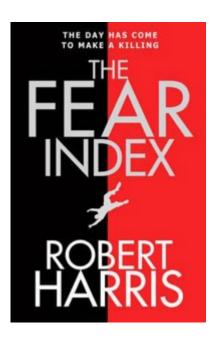
collected data from one 10Gig Ethernet SR interface @ man-da

Thomas Weible: An Optic's Life (2010).

Applications: Stock Monitoring

- Stock market prediction
- Computer trading



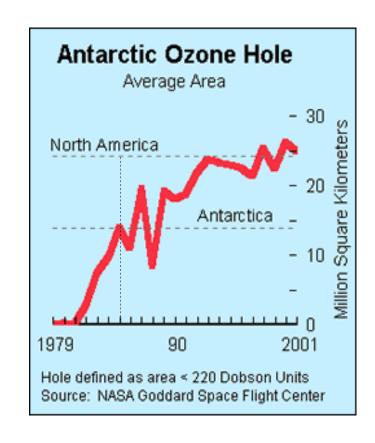


http://blogs.reuters.com/reuters-investigates/2010/10/15/flash-crash-fallout/

Errors vs. Natural Outliers

Ozone Depletion History

- In 1985 three researchers (Farman, Gardinar and Shanklin) were puzzled by data gathered by the British Antarctic Survey showing that ozone levels for Antarctica had dropped 10% below normal levels
- Why did the Nimbus 7 satellite, which had instruments aboard for recording ozone levels, not record similarly low ozone concentrations?
- The ozone concentrations recorded by the satellite were so low they were being treated as outliers by a computer program and discarded!



Sources:

http://exploringdata.cqu.edu.au/ozone.html http://www.epa.gov/ozone/science/hole/size.html

Errors, Outliers, Anomalies, Novelties...

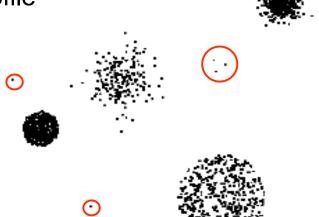
- What are we looking for?
 - Wrong data values (errors)
 - Unusual observations (outliers or anomalies)
 - Observations not in line with previous observations (novelties)
- Unsupervised Setting:
 - Data contains both normal and outlier points
 - Task: compute outlier score for each data point
- Supervised setting:
 - Training data is considered normal
 - Train a model to identify outliers in test dataset

Methods for Anomaly Detection

- Graphical
 - Look at data, identify suspicious observations
- Statistic
 - Identify statistical characteristics of the data
 - e.g., mean, standard deviation
 - Find data points which do not follow those characteristics
- Density-based
 - Consider distributions of data
 - Dense regions are considered the "normal" behavior
- Model-based
 - Fit an explicit model to the data
 - Identify points which do not behave according to that model

Anomaly Detection Schemes

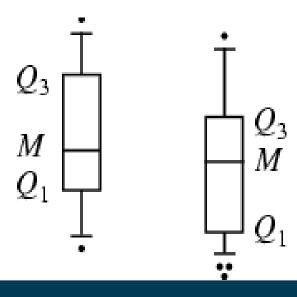
- General Steps
 - Build a profile of the "normal" behavior
 - Profile can be patterns or summary statistics for the overall population
 - Use the "normal" profile to detect anomalies
 - Anomalies are observations whose characteristics differ significantly from the normal profile
- Types of anomaly detection schemes
 - Graphical & Statistical-based
 - Distance-based
 - Model-based

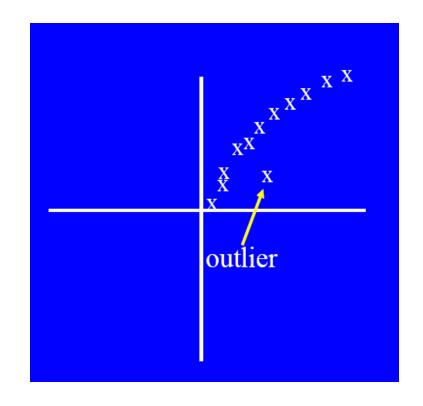


Graphical Approaches

Boxplot (1-D), Scatter plot (2-D), Spin plot (3-D)

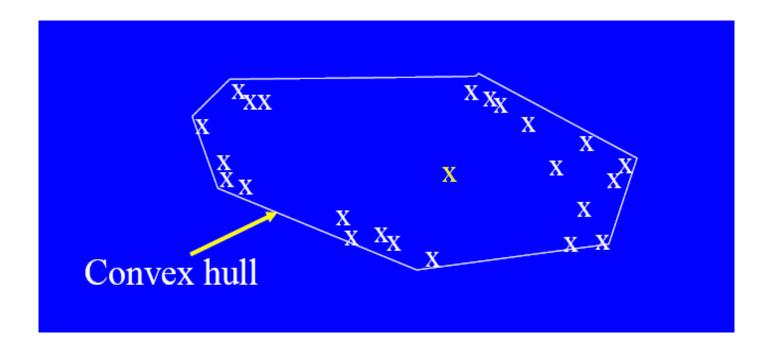
- Limitations
 - Time consuming
 - Subjective





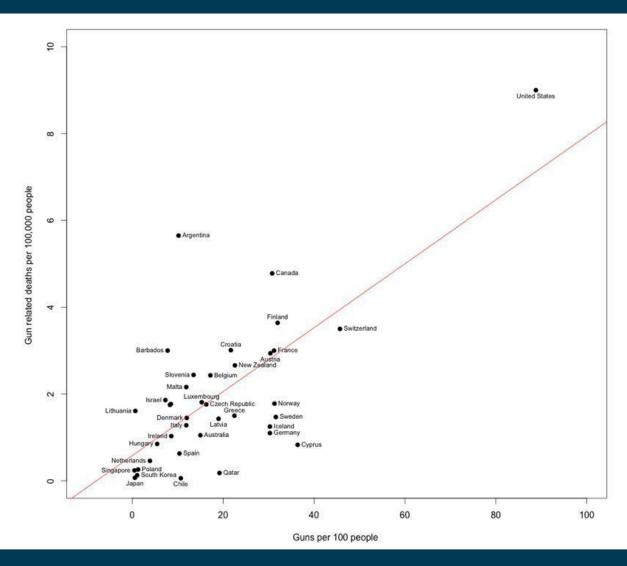
Convex Hull Method

- Extreme points are assumed to be outliers
- Use convex hull method to detect extreme values



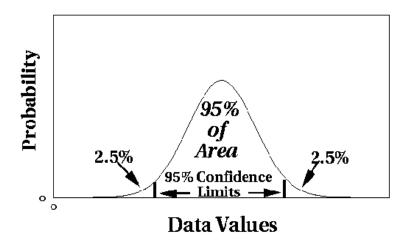
What if the outlier occurs in the middle of the data?

Interpretation: What is an Outlier?



Statistical Approaches

- Assume a parametric model describing the distribution of the data (e.g., normal distribution)
- Apply a statistical test that depends on
 - Data distribution
 - Parameter of distribution (e.g., mean, variance)
 - Number of expected outliers (confidence limit)

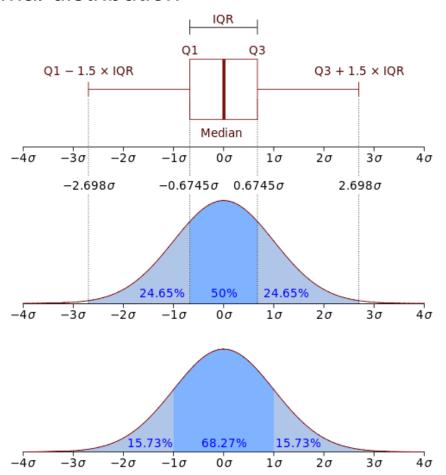


Interquartile Range

- Divides data in quartiles
- Definitions:
 - Q1: $x \ge Q1$ holds for 75% of all x
 - Q3: $x \ge Q3$ holds for 25% of all x
 - IQR = Q3-Q1
- Outlier detection:
 - All values outside [median-1.5*IQR; median+1.5*IQR]
- Example:
 - 0,1,1,3,3,5,7,42 \rightarrow median=3, Q1=1, Q3=7 \rightarrow IQR = 6
 - Allowed interval: [3-1.5*6; 3+1.5*6] = [-6; 12]
 - Thus, 42 is an outlier

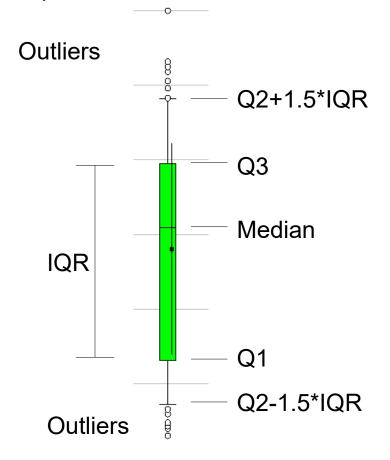
Interquartile Range

Assumes a normal distribution



Interquartile Range

Visualization in box plot



Median Absolute Deviation (MAD)

MAD is the median deviation from the median of a sample, i.e.

$$MAD := median_i(X_i - median_j(X_j))$$

- MAD can be used for outlier detection
 - all values that are k*MAD away from the median are considered to be outliers
 - e.g., k=3
- Example:
 - 0,1,1,3,5,7,42 \rightarrow median = 3
 - deviations: 3,2,2,0,2,4,39 → MAD = 2
 - allowed interval: [3-3*2; 3+3*2] = [-3;9]
 - therefore, 42 is an outlier

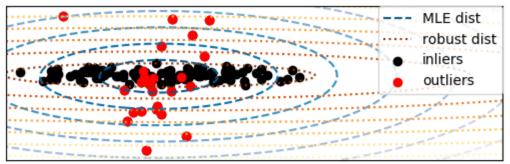


Carl Friedrich Gauss, 1777-1855

Fitting Elliptic Curves

- Multi-dimensional datasets
 - can be seen as following a normal distribution on each dimension
 - the intervals in one-dimensional cases become elliptic curves
- In Python: covariance. Elliptic Envelope

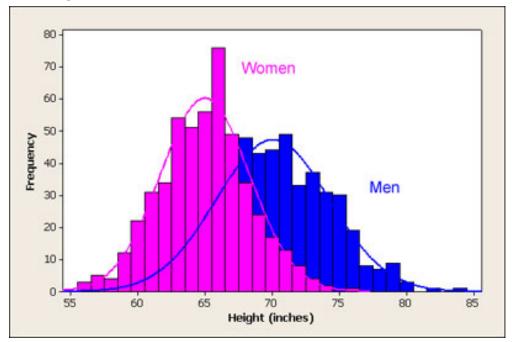
Mahalanobis distances of a contaminated data set:



Limitations of Statistical Approaches

- Most of the tests are for a single attribute (called: univariate)
- For high dimensional data, it may be difficult to estimate the true distribution
- In many cases, the data distribution may not be known
 - e.g., IQR Test: assumes Gaussian distribution

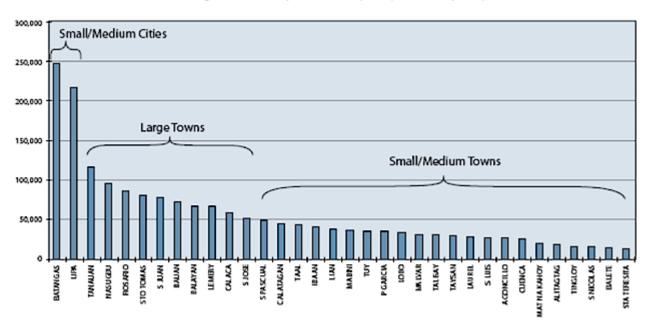
- Normal (gaussian) distribution
 - e.g., people's height



http://www.usablestats.com/images/men_women_height_histogram.jpg

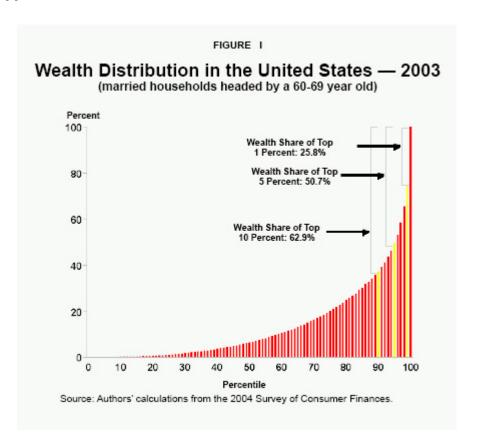
- Power law distribution
 - e.g., city population

Batangas 2000 Population, by City/Municipality



http://www.jmc2007compendium.com/V2-ATAPE-P-12.php

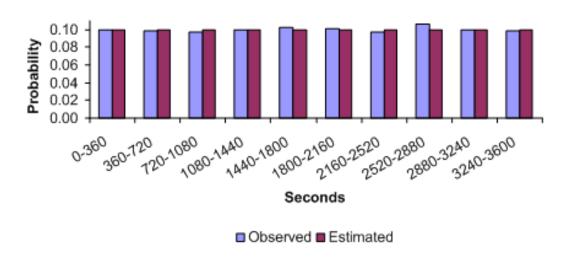
- Pareto distribution
 - e.g., wealth



http://www.ncpa.org/pub/st289?pg=3

- Uniform distribution
 - e.g., distribution of web server requests across an hour

Arrival Time of HTTP Requests Within Hour



http://www.brighton-webs.co.uk/distributions/uniformc.aspx

Outliers vs. Extreme Values

- So far, we have looked at extreme values only
 - But outliers can occur as non-extremes
 - In that case, methods like IQR fail

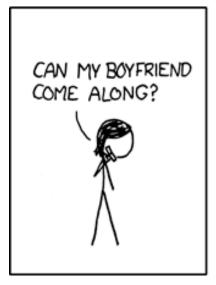


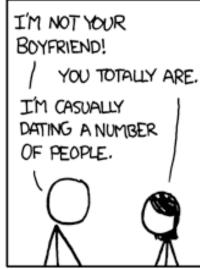
Outliers vs. Extreme Values

- IQR on the example below:
 - Q2 (Median) is 0
 - Q1 is -1, Q3 is 1
 - \rightarrow IQR = 2
 - \rightarrow everything outside [-3,+3] is an outlier
 - → there are no outliers in this example

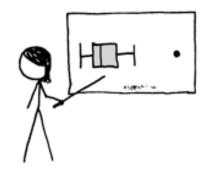


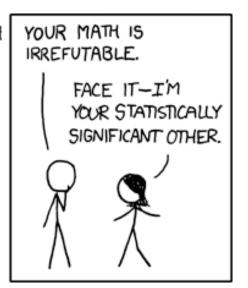
Time for a Short Break





BUT YOU SPEND TWICE AS MUCH TIME WITH ME AS WITH ANYONE ELSE. I'M A CLEAR OUTUER.





http://xkcd.com/539/

Distance-based Approaches

- Data is represented as a vector of features
- Various approaches
 - Nearest-neighbor based
 - Density based
 - Clustering based
 - Model based

Nearest-Neighbor Based Approach

Approach:

- Compute the distance between every pair of data points
- There are various ways to define outliers:
 - ◆ Data points for which there are fewer than *p* neighboring points within a distance *D*
 - The top n data points whose distance to the kth nearest neighbor is
 greatest

 RapidMiner

The top n data points whose average distance to the k nearest neighbors is greatest

Package PyOD

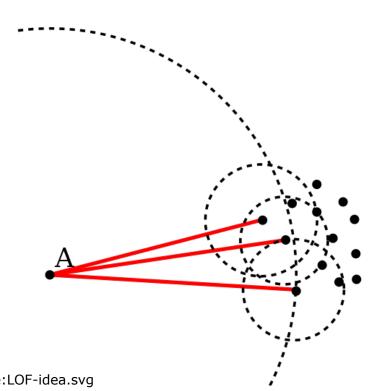
```
from pyod.models.knn import KNN
detector = KNN(contamination=0.1, n_neighbors=10)
detector.fit(data)
```

Density-based: LOF approach

- For each point, compute the density of its local neighborhood
 - if that density is higher than the average density,
 the point is in a cluster
 - if that density is lower than the average density,
 the point is an outlier
- Compute local outlier factor (LOF) of a point A
 - ratio of average density of A's neighbors to density of point A
- Outliers are points with large LOF value
 - typical: larger than 1

LOF: Illustration

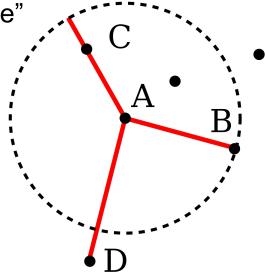
- Using 3 nearest neighbors
- We compute
 - the average density of A
 - the average density of A's neighbors
- If the density of A is lower than the neighbors' density
 - A might be an outlier



http://commons.wikimedia.org/wiki/File:LOF-idea.svg

LOF: Defining Density

- LOF uses a concept called "reachability distance"
- All points within the k-neighborhood have the same k-distance
 - in the example: $d_3(A,B) = d_3(A,C)$
- Reachability distance rd_k(A,B):
 - distance of A,B, lower bound by d_k(B)
 - $rd_k(A,B) = max(d_k(B),distance(A,B))$
- In the example:
 - $rd_k(D,A) = d(D,A)$, but
 - $rd_k(C,A) = k-distance(A)$
- Rationale: all sufficiently close points are regarded as equally close
 - lessens the impact of small variations



https://commons.wikimedia.org/wiki/File:Reachability-distance.svg

LOF: Defining Density

Average reachability distance

-
$$avgrd_k(A) = \frac{\sum\limits_{P:k \, nearest \, neighbors \, of \, A} rd_k(A, P)}{|N_k(A)|}$$

no. of k nearest neighbors of A, usually =k

- Density is defined as the inverse
 - idea: the larger the avg. reachability distance,
 the sparser the region in which the data point lies
 - local reachability density $lrb_k(A) = 1/avgrd_k(A)$
- Local outlier factor: relation of density of A's neighbors to A's density:

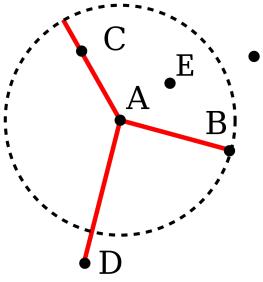
$$LOF_{k}(A) = \frac{\sum\limits_{P: k \text{ nearest neighbors of } A} \frac{lrb_{k}(P)}{lrb_{k}(A)}}{|N_{k}(A)|} = \frac{\sum\limits_{P: k \text{ nearest neighbors of } A} lrb_{k}(P)}{|N_{k}(A)| \cdot lrb_{k}(A)}$$

LOF: Example

- d(A,B)=1, d(A,C)=0.75, d(A,D) $\rightarrow rd_k(A,B)=rd_k(A,C)=rd_k(A,E)=1$, $rd_k(A,D)=1.2$
- Average reachability:

$$avgrd_{k}(A) = \frac{\sum_{P:k \text{ nearest neighbors of } A} rd_{k}(A, P)}{|N_{k}(A)|} = \frac{1+1+1}{3} = 1$$

Density Irb_k(A) = 1/avgrd_k(A) = 1



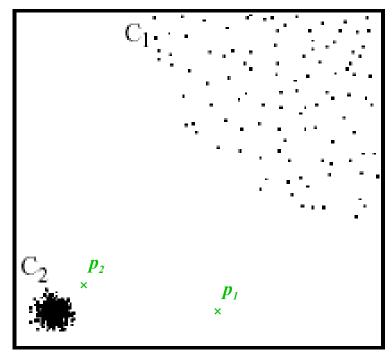
- Let's assume: avgrd_k(B)=0.8, avgrd_k(C)=1.2, avgrd_k(E)=0.6
 - \rightarrow Irb_k(B)=1.25, Irb_k(C)=0.83, Irb_k(E)=1.67

 $>1 \rightarrow$ outlier

Local outlier factor of A: $LOF_k(A) = \frac{\sum\limits_{P:k \, nearest \, neighbors \, of \, A} lrb_k(P)}{|N_k(A)| \cdot lrb_k(A)} = \frac{1.25 + 0.86 + 1.67}{3 \cdot 1} = 1.26$

Nearest-Neighbor vs. LOF

- With kNN, only p₁ is found as an outlier
 - there are enough near neighbors for p₂ in cluster C₂
- With LOF, both p₁ and p₂ are found as outliers

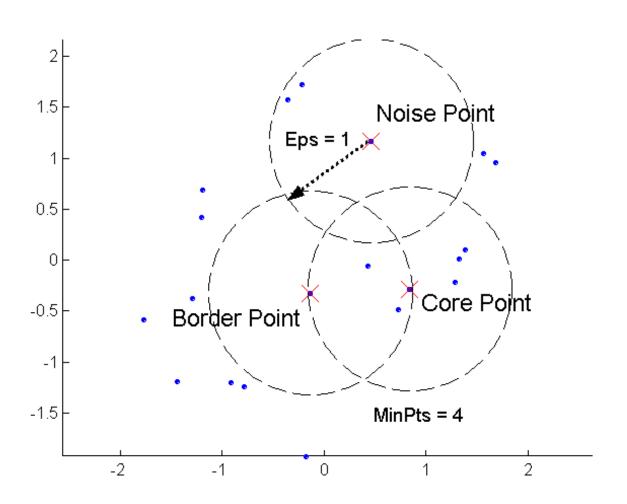


sklearn.neighbors.LocalOutlierFactor

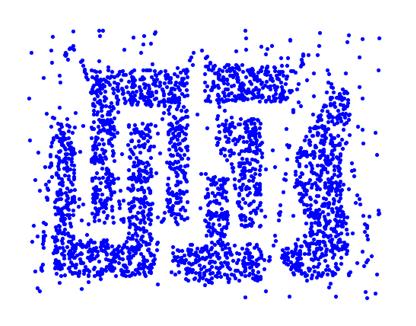
Recap: DBSCAN

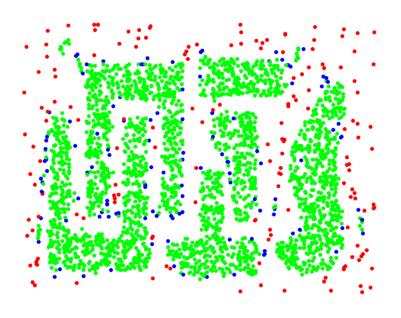
- DBSCAN is a density-based algorithm
 - Density = number of points within a specified radius (Eps)
- Divides data points in three classes:
 - A point is a core point if it has more than a specified number of points (MinPts) within Eps
 - These are points that are at the interior of a cluster
 - A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point
 - A noise point is any point that is not a core point or a border point

Recap: DBSCAN



Recap: DBSCAN





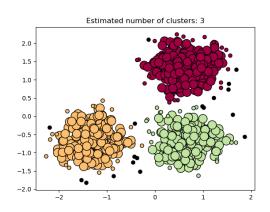
Original Points

Point types: core, border and noise

Eps = 10, MinPts = 4

DBSCAN for Outlier Detection

- DBSCAN directly identifies noise points
 - these are outliers not belonging to any cluster
 - in RapidMiner: assigned to cluster 0
 - in scikit-learn: label -1
 - allows for performing outlier detection directly



```
# Apply DBSCAN with eps=0.5 and min_samples=5
dbscan = DBSCAN(eps=0.1, min_samples=5)
dbscan.fit(X)

# Identify the noise points
noise_mask = dbscan.labels_ == -1
print(noise_mask)

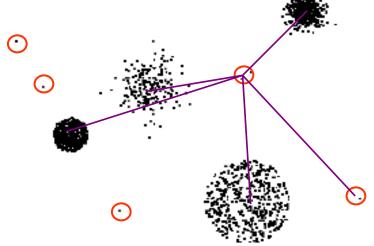
# Remove the noise points from the dataframe
X = X[~noise_mask]
```

Clustering-based Outlier Detection

Basic idea:

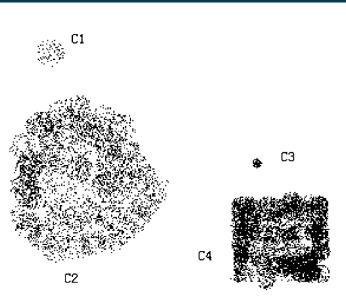
- Cluster the data into groups of different density
- Choose points in small cluster as candidate outliers
- Compute the distance between candidate points and non-candidate clusters

 If candidate points are far from all other non-candidate points, they are outliers



Clustering-based Local Outlier Factor

- Idea: anomalies are data points that are
 - in a very small cluster or
 - far away from other clusters
- CBLOF is run on clustered data
- Assigns a score based on
 - the size of the cluster a data point is in
 - the distance of the data point to the next large cluster



Clustering-based Local Outlier Factor

- General process:
 - first, run a clustering algorithm (of your choice)
 - then, apply CBLOF

Package PyOD

Result: data points with outlier score

```
from sklearn.cluster import KMeans
from pyod.models.cblof import CBLOF

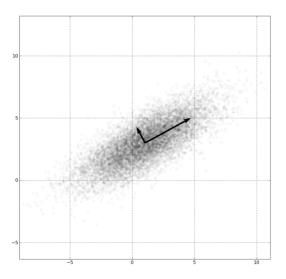
# clustering
clust = KMeans()

# outlier detection
detector = CBLOF(n_clusters=8, clustering_estimator=clust)
detector.fit(X)

# removal
noise_mask =detector.predict(X) == 1
X = X[~noise_mask]
```

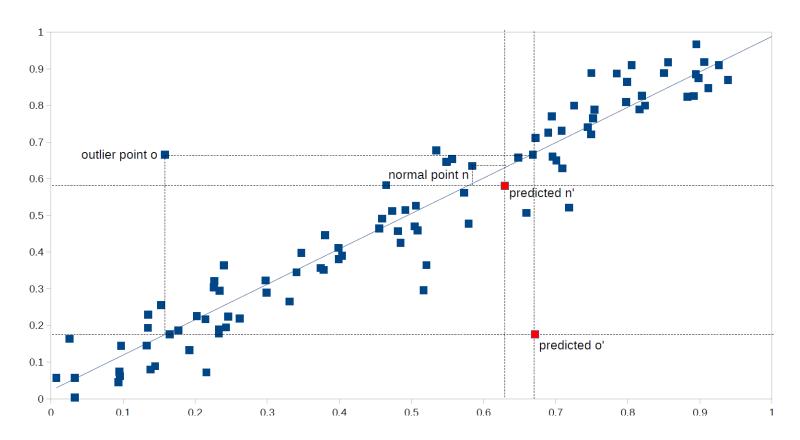
PCA and Reconstruction Error

- Recap: PCA tries to capture most dominant variations in the data
 - those can be seen as the "normal" behavior
- Reconstruct original data point by inversing PCA
 - close to original: normally behaving data point
 - far from original: unnormally behaving data point



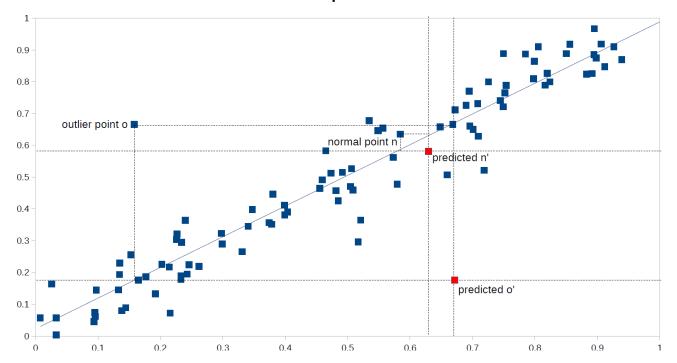
Model-based Outlier Detection (ALSO)

- Idea: there is a model underlying the data
 - Data points deviating from the model are outliers

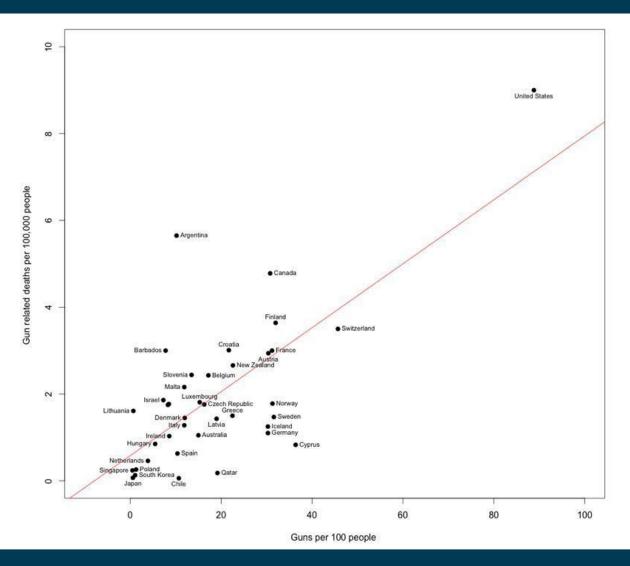


Model-based Outlier Detection (ALSO)

- ALSO (Attribute-wise Learning for Scoring Outliers)
 - Learn a model for each attribute given all other attributes
 - Use model to predict expected value
 - Deviation between actual and predicted value → outlier



Interpretation: What is an Outlier? (recap)



Model-based Outlier Detection (ALSO)

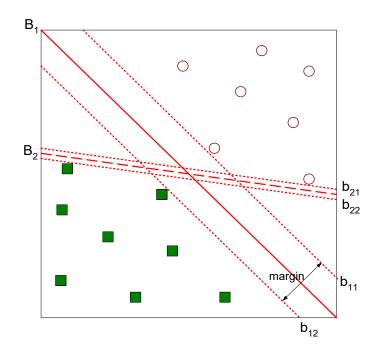
- For each data point i, compute vector of predictions i'
- Outlier score: Euclidean distance of i and i'
 - in z-transformed space $o_{unweighted}(i) := \sqrt{\sum_{l=1}^{n}{(i_k i_k')^2}}$
- Refinement: assign weights to attributes
 - given the strength of the pattern learned
 - measure: RRSE

$$o(i) := \sqrt{\frac{1}{\sum_{k=1}^{n} w_k} \sum_{k=1}^{n} w_k \cdot (i_k - i'_k)^2},$$

- Rationale:
 - ignores deviations on unpredictable attributes (e.g., database IDs)
 - for an outlier, require both a strong pattern and a strong deviation

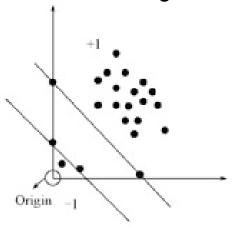
One-Class Support Vector Machines

- Recap: Support Vector Machines
 - Find a maximum margin hyperplane to separate two classes
 - Use a transformation of the vector space
 - Thus, non-linear boundaries can be found



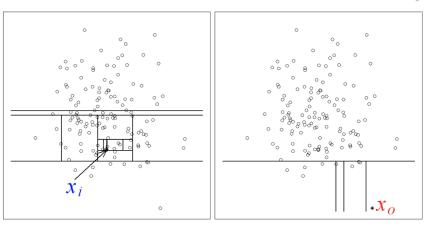
One-Class Support Vector Machines

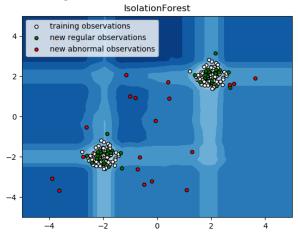
- One-Class Support Vector Machines
 - Find best hyperplane that separates the origin from the rest of the data
 - Maximize margin
 - Minimize errors
 - Points on the same side as the origin are outliers



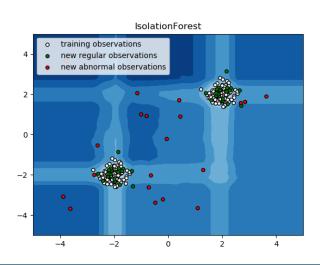
- Recap: SVMs require extensive parameter tunining
 - Difficult to automatize for anomaly detection, since we have no training data

- Isolation tree:
 - a decision tree that has only leaves with one example each
- Isolation forests:
 - train a set of random isolation trees
- Idea:
 - path to outliers in a tree is shorter than path to normal points
 - across a set of random trees, average path length is an outlier score

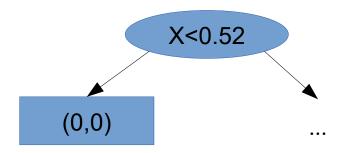


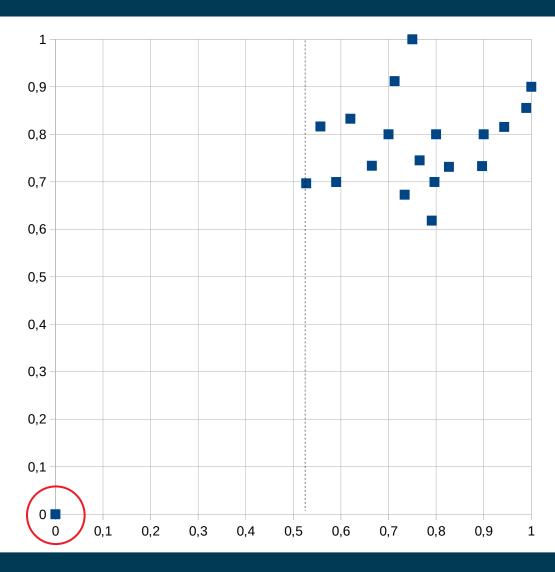


- Training a single isolation tree
 - for each leaf node w/ more than one data point
 - pick an attribute Att and a value V at random
 - create inner node with test Att<V
 - train isolation tree for each subtree
- Output
 - A tree with just one instance per node
 - Usually, an upper limit on height is used

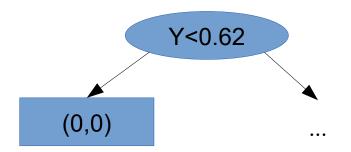


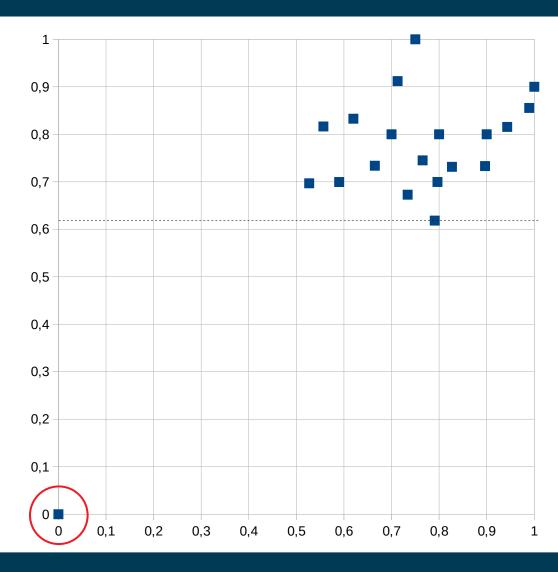
- Probability of (0,0) ending in a leaf at height 1
 - pick Att X, pick V<0.52





- Probability of (0,0) ending in a leaf at height 1
 - pick Att Y, pick V<0.62



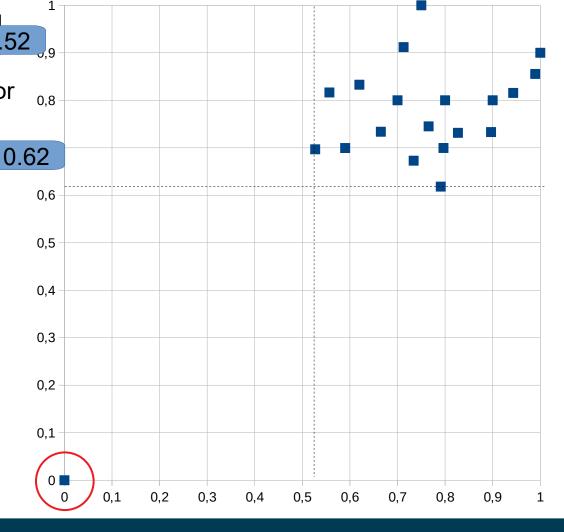


Probability of (0,0) ending in a leaf at height 1

pick Att X, pick V<0.52, or

pick Att Y, pick V<0.62

• 0.5*0.52 + 0.5*0.62 $\rightarrow 0.57$

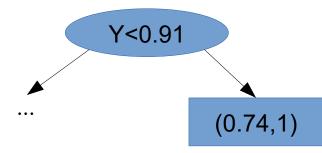


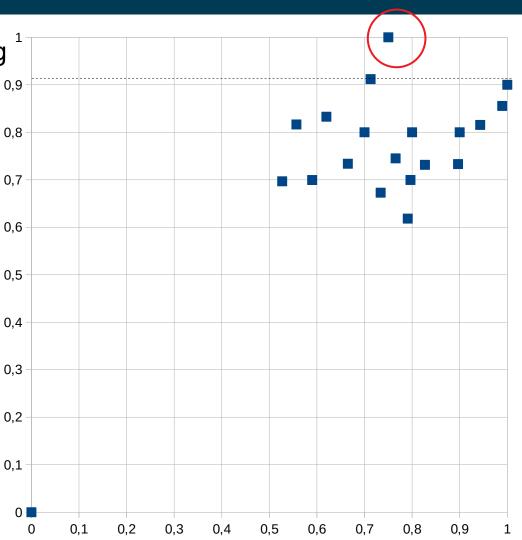
Probability of (0.74,1) ending in a leaf at height 1

- pick Att Y, pick V>0.91

• 0.5 * 0.09

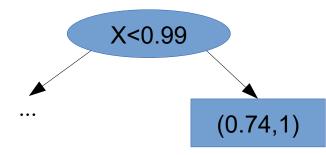
 $\to 0.045$

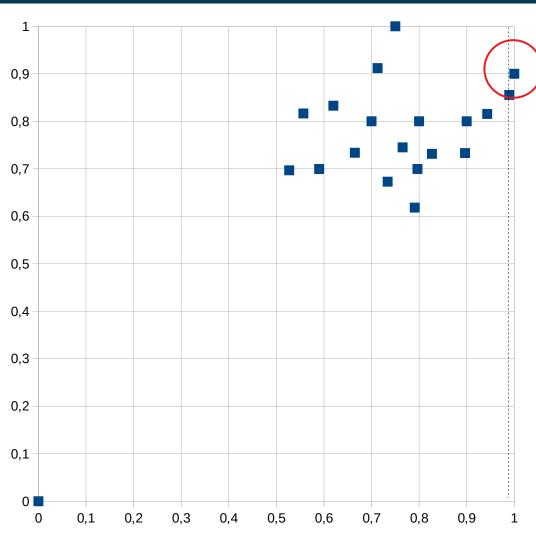




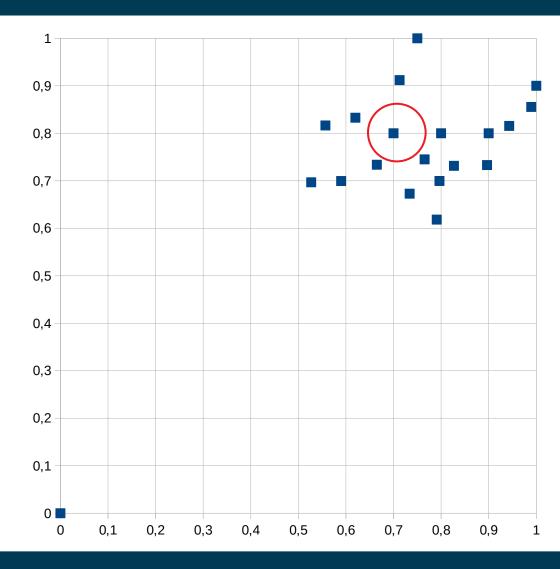
- Probability of (1,0.9) ending in a leaf at height 1
 - pick Att X, pick V>0.98
- 0.5 * 0.02

 $\rightarrow 0.01$

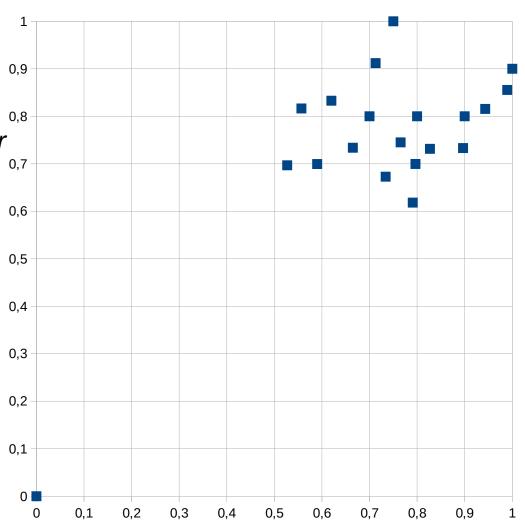




- Probability of any other data point ending in a leaf at height 1
 - this is not possible!
 - at least two tests are necessary



- Observations
 - data points in dense areas need more tests
 - i.e., they end up deeper in the trees
 - data points far away from the rest have a higher probability to be isolated earlier
 - i.e., they end up *higher* in the trees



- A large number of attributes may cause problems
 - many anomaly detection approaches use distance measures
 - those get problematic for very high-dimensional spaces
 - meaningless attributes obscure the distances
- Practical hint:
 - perform dimensionality reduction first
 - i.e., feature subset selection, PCA
 - note: anomaly detection is unsupervised
 - thus, supervised selection (like forward/backward selection) does not work

- Recap: attributes may have different scales
 - Hence, different attributes may have different contributions to outlier scores
- Compare the following two datasets:
- Baden-Württemberg
 - population = 10,569,111
 - area = 35,751.65 km²
- Bavaria
 - population = 12,519,571
 - area = 70,549.44 km²
- ..

- Baden-Württemberg
 - population = 10,569,111
 - area = 35,751,650,000 m²
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 - population = 12,519,571
 - area = 70,549,440,000 m²
- ...
- In the second set, outliers in the population are unlikely to be discovered
 - Even if we change the population of Bavaria by a factor of 100,
 the Euclidean distance does not change much
- Thus, outliers in the population are masked by the area attribute

- Solution:
 - Normalization!
- Advised:
 - z-Transformation
 - More robust w.r.t. outliers than simple projection to [0;1]

$$x' = \frac{|x - \mu|}{\Omega}$$

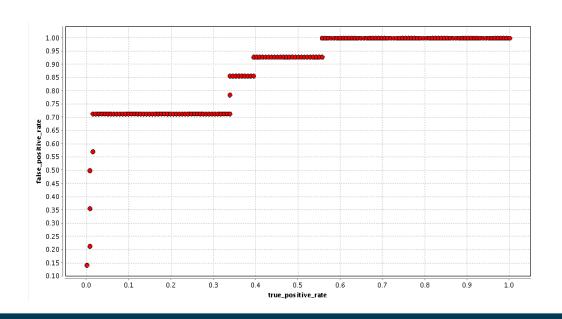
X = StandardScaler().fit_transform(X)

Evaluation Measures

- Anomaly Detection is an unsupervised task
- Evaluation: usually on a labeled subsample
- Evaluation Measures:
 - F-measure on outliers
 - Area under ROC curve

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 - Plots false positives against true positives



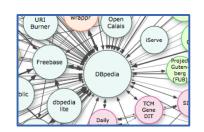
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Semi-Supervised Anomaly Detection

- All approaches discussed so far are unsupervised
 - they run fully automatic
 - without human intelligence
- Semi-supervised anomaly detection
 - experts manually label some data points as being outliers or not
 - → anomaly detection becomes similar to a classification task
 - the class label being outlier/non-outlier
 - Challenges:
 - Outliers are scarce → unbalanced dataset
 - Outliers are not a class

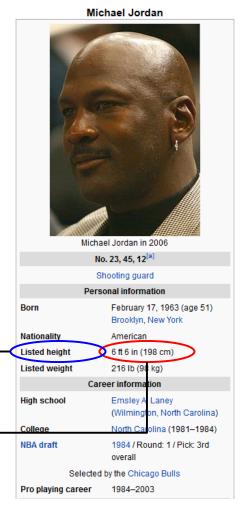




- DBpedia
 - extracts data from infoboxes in Wikipedia
 - based on crowd-sourced mappings to an ontology
- Example
 - Wikipedia page on Michael Jordan

```
dbpedia:Michael_Jordan
  dbpedia-owl:height
"1.981200"^^xsd:double .
```

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- DBpedia is based on heuristic extraction
- Several things can go wrong
 - wrong data in Wikipedia
 - unexpected number/date formats
 - errors in the extraction code
 - **–** ...
- Can we use anomaly detection to remedy the problem?

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- Challenge
 - Wikipedia is made for humans, not machines
 - Input format in Wikipedia is not constrained
- The following are all valid representations of the same height value (and perfectly understandable by humans)

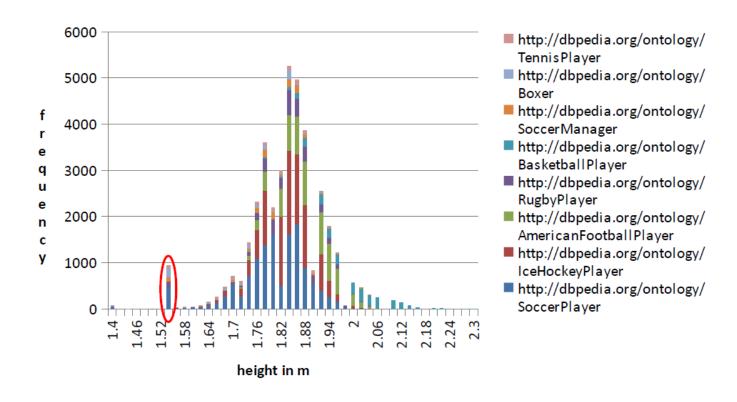
```
- 6 ft 6 in, 6ft 6in, 6'6'', 6'6", 6'6', ...
- 1.98m, 1,98m, 1m 98, 1m 98cm, 198cm, 198 cm, ...
- 6 ft 6 in (198 cm), 6ft 6in (1.98m), 6'6'' (1.98 m), ...
- 6 ft 6 in<sup>[1]</sup>, 6 ft 6 in <sup>[citation needed]</sup>, ...
```

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- Preprocessing: split data for different types
 - height is used for persons or buildings
 - population is used for villages, cities, countries, and continents
 - **–** ...
- Separate into single distributions
 - makes anomaly detection better
- Result
 - errors are identified at ~90% precision
 - systematic errors in the extraction code can be found

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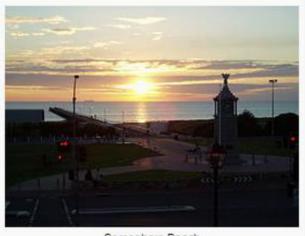
Footprint of a systematic error



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- Typical error sources
 - unit conversions gone wrong (e.g., imperial/metric)
 - misinterpretation of numbers
- e.g., village Semaphore in Australia
 - population: 28,322,006(all of Australia: 23,379,555!)
 - a clear outlier among villages

Semaphore Adelaide, South Australia



Semaphore Beach

Population: 2,832 2006 Census [1]

Established: 1849 Postcode: 5019

Location: 14 km (9 mi) from CBD

LGA: City of Port Adelaide

Enfield

Lee

State/territory electorate(s):

Federal Division(s):

Port Adelaide

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Errors vs. Natural Outliers

- Hard task for a machine
- e.g., an adult person 58cm high
- e.g., a 7.4m high vehicle



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Wrap-up

- Anomaly Detection is useful for
 - data preprocessing and cleansing
 - finding suspect data (e.g., network intrusion, credit card fraud)
- Methods
 - visual/manual
 - statistics based
 - density based
 - model based

Questions?

