Outlier Analysis

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Outline

- **Introduction**
- Extreme Value Analysis
- Probabilistic Models
- Clustering for Outlier Detection
- Distance-Based Outlier Detection
- Density-Based Methods
- Information-Theoretic Models
- Outlier Validity
- Summary

Introduction (1)

A Quote

> "You are unique, and if that is not fulfilled, then something has been lost."—Martha Graham

An Informal Definition

"*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.*"

A Complementary Concept to Clustering

- Clustering attempts to determine groups of data points that are similar
- Outliers are individual data points that are different from the remaining data

Introduction (2)

Applications

- Data cleaning
  - ✓ Remove noise in data
- Credit card fraud
  - ✓ Unusual patterns of credit card activity
- Network intrusion detection
  - ✓ Unusual records/changes in network traffic

Introduction (3)

- The 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

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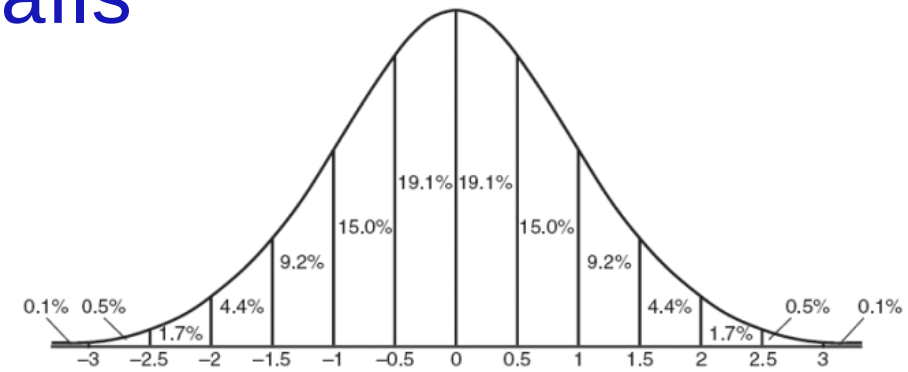
Extreme Value Analysis (1)

- Statistical Tails

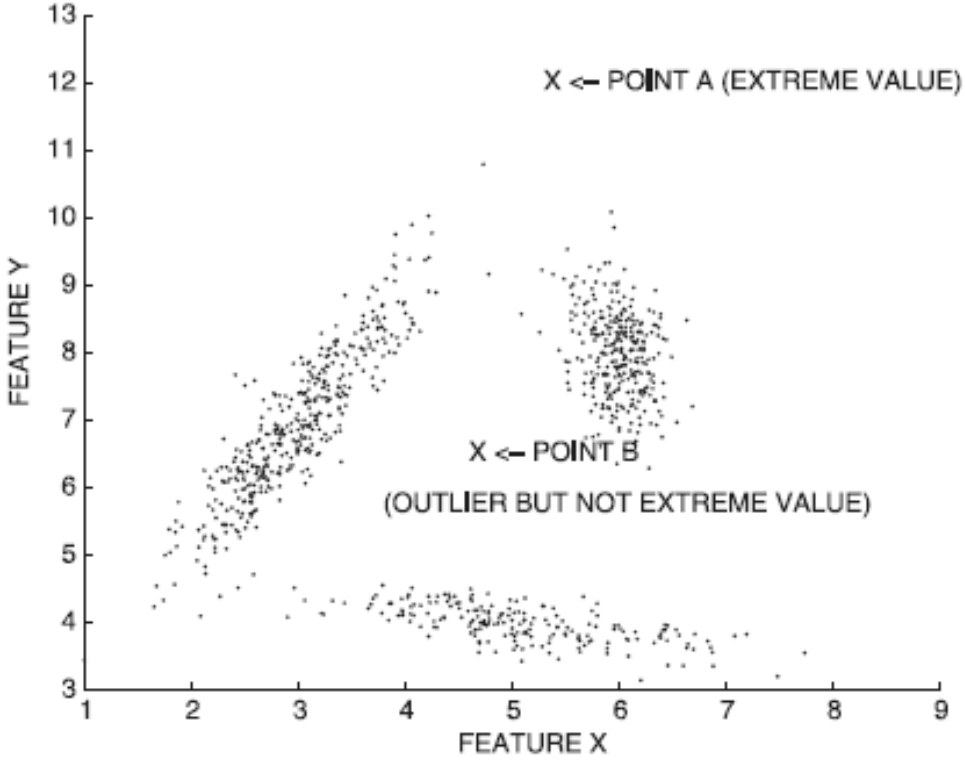
http://www.regentsprep.org/regents/math/algtrig/ats2/normallesson.htm



- All extreme values are outliers
- Outliers may not be extreme values
  - {1,3,3,3,50,97,97,97,100}
  - 1 and 100 are extreme values
  - 50 is an outlier but not extreme value

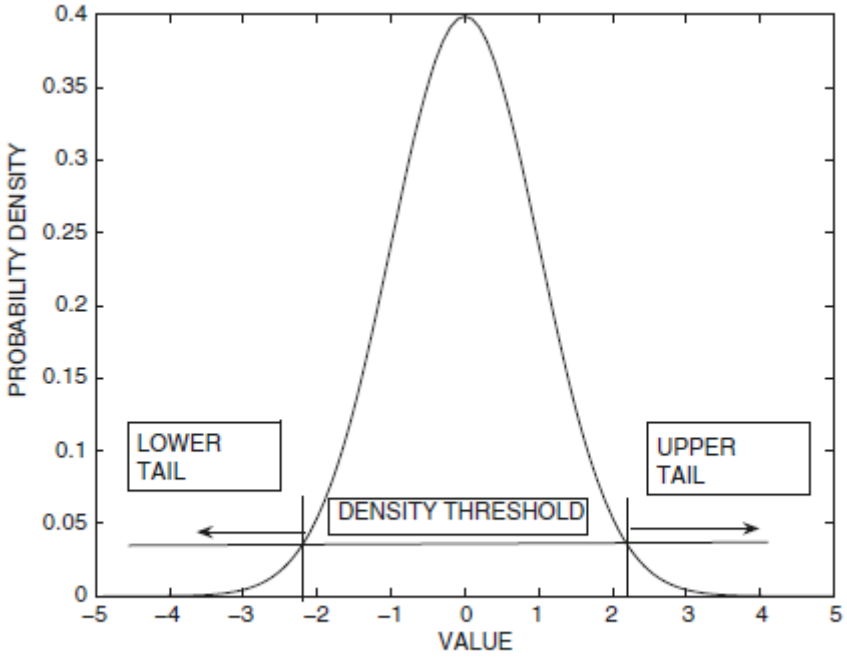
Extreme Value Analysis (2)

- All extreme values are outlies
- Outlies may not be extreme values



Univariate Extreme Value Analysis (1)

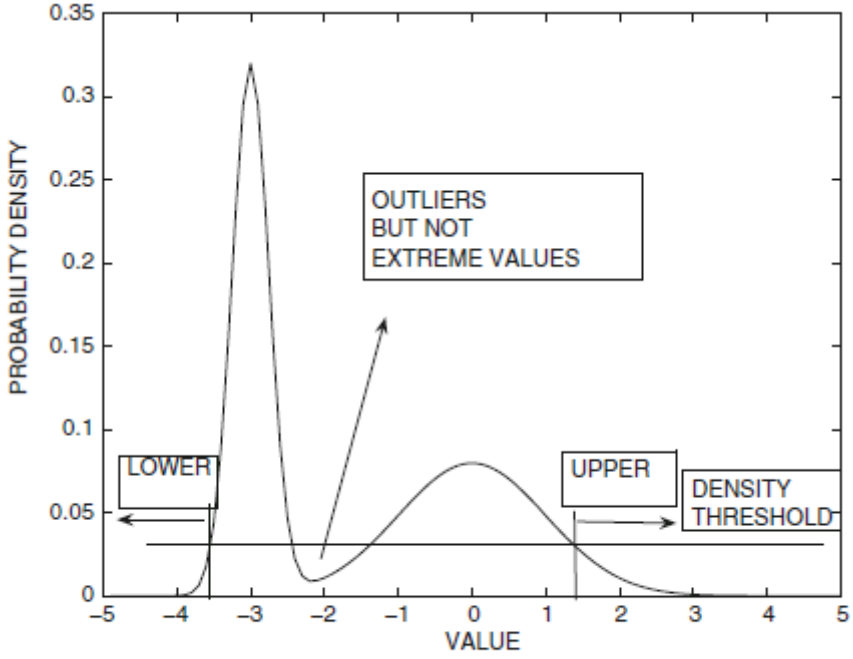
- Statistical Tail Confidence Tests
  - Suppose the density distribution is $f_X(x)$
  - Tails are extreme regions s.t. $f_X(x) \leq \theta$
- Symmetric Distribution
  - Two symmetric tails
  - The areas inside tails represent the cumulative probability



(a) Symmetric distribution

Univariate Extreme Value Analysis (2)

- Statistical Tail Confidence Tests
  - Suppose the density distribution is $f_X(x)$
  - 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



(b) Asymmetric distribution

The Procedure (1)

- A model distribution is selected
  - Normal Distribution with mean μ and standard deviation σ

$$f_X(x) = \frac{1}{\sigma \cdot \sqrt{2 \cdot \pi}} \cdot e^{\frac{-(x-\mu)^2}{2 \cdot \sigma^2}}$$

- Parameter Selection
  - Prior domain knowledge
  - Estimate from data

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

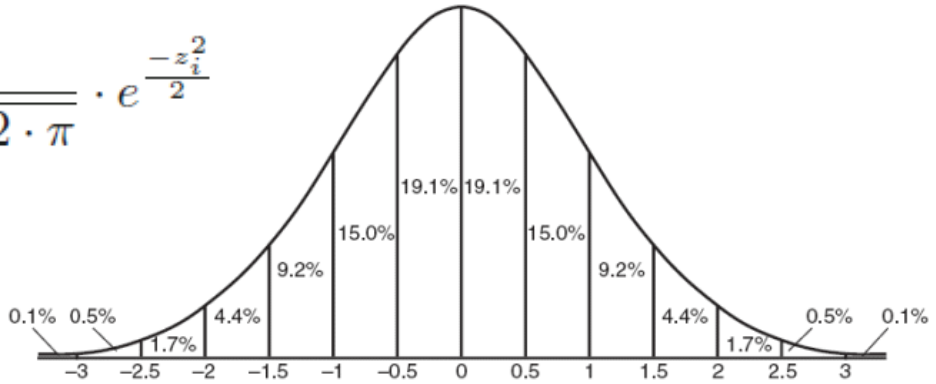
The Procedure (2)

- Z-value of a random variable

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

  - Large positive values of z_i correspond to the upper tail
  - Large negative values of z_i correspond to the lower tail
  - z_i follows the standard normal distribution

$$f_X(z_i) = \frac{1}{\sigma \cdot \sqrt{2 \cdot \pi}} \cdot e^{\frac{-z_i^2}{2}}$$



- Extreme values
  - $|z_i| \geq \tau$

Multivariate Extreme Values (1)

- Unimodal probability distributions with a single peak
  - Suppose the density distribution is $f_X(x)$
  - Tails are extreme regions s.t. $f_X(x) \leq \theta$
- Multivariate Gaussian Distribution

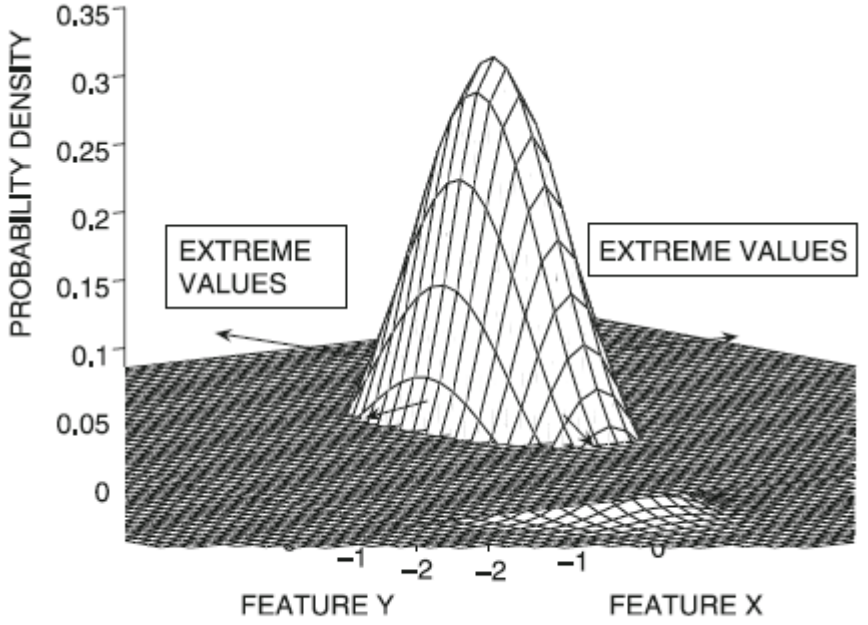
$$f(\overline{X}) = \frac{1}{\sqrt{|\Sigma|} \cdot (2 \cdot \pi)^{(d/2)}} \cdot e^{-\frac{1}{2} \cdot (\overline{X} - \overline{\mu}) \Sigma^{-1} (\overline{X} - \overline{\mu})^T}$$

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

where $Maha(\bar{X}, \bar{\mu}, \Sigma)$ is the Mahalanobis distance between $\bar{X}$ and $\bar{\mu}$

Multivariate Extreme Values (2)

- Extreme-value Score of $\bar{X}$
  - $Maha(\bar{X}, \bar{\mu}, \Sigma)$
  - Larger values imply more extreme behavior



(b) Multivariate extreme values

Multivariate Extreme Values (2)

- Extreme-value Score of $\bar{X}$
  - $Maha(\bar{X}, \bar{\mu}, \Sigma)$
  - Larger values imply more extreme behavior
- Extreme-value Probability of $\bar{X}$
  - Let $\mathcal{R}$ be the region

    $$\mathcal{R} = \{\bar{Y} | Maha(\bar{Y}, \bar{\mu}, \Sigma) \geq Maha(\bar{X}, \bar{\mu}, \Sigma)\}$$

  - Cumulative probability of $\mathcal{R}$
  - Cumulative Probability of χ^2 distribution for which the value is larger than $Maha(\bar{X}, \bar{\mu}, \Sigma)$

Why χ^2 distribution?

The Mahalanobis distance

- Let Σ be the covariance matrix

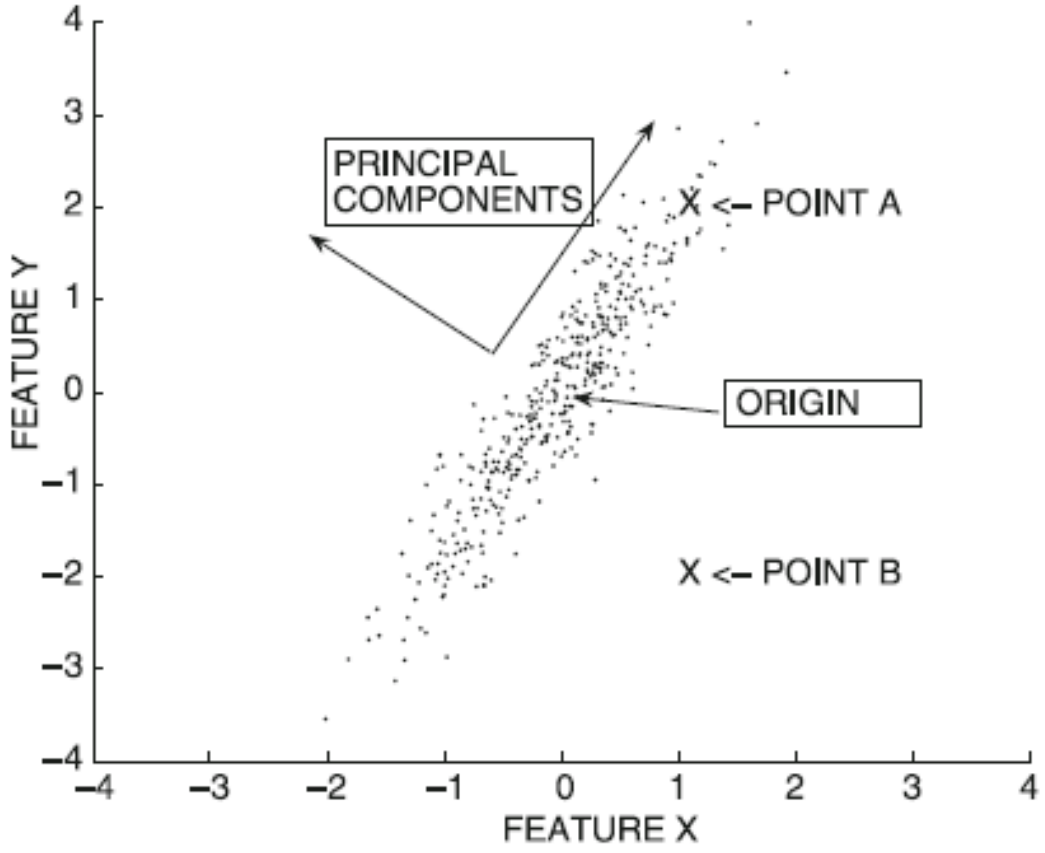
$$Maha(\bar{Y}, \bar{\mu}, \Sigma) = \sqrt{(\bar{Y} - \bar{\mu})\Sigma^{-1}(\bar{Y} - \bar{\mu})^{\mathsf{T}}}$$

- Projection+Normalization
  - ✓ Let $\Sigma = U\Lambda U^{\mathsf{T}} = \sum_{i=1}^{d} \sigma_i^2 \mathbf{u}_i \mathbf{u}_i^{\mathsf{T}}$
  - ✓ Then, $\Sigma^{-1} = U\Lambda^{-1}U^{\mathsf{T}} = \sum_{i=1}^{d} \sigma_i^{-2} \mathbf{u}_i \mathbf{u}_i^{\mathsf{T}}$

$$Maha(\bar{Y}, \bar{\mu}, \Sigma) = \sqrt{(\bar{Y} - \bar{\mu})\left(\sum_{i=1}^{d} \sigma_i^{-2} \mathbf{u}_i \mathbf{u}_i^{\mathsf{T}}\right)(\bar{Y} - \bar{\mu})^{\mathsf{T}}} = \sqrt{\sum_{i=1}^{d} \left(\frac{\mathbf{u}_i (\bar{Y} - \bar{\mu})^{\mathsf{T}}}{\sigma_i}\right)^2}$$

Adaptive to the Shape

- B is an extreme value



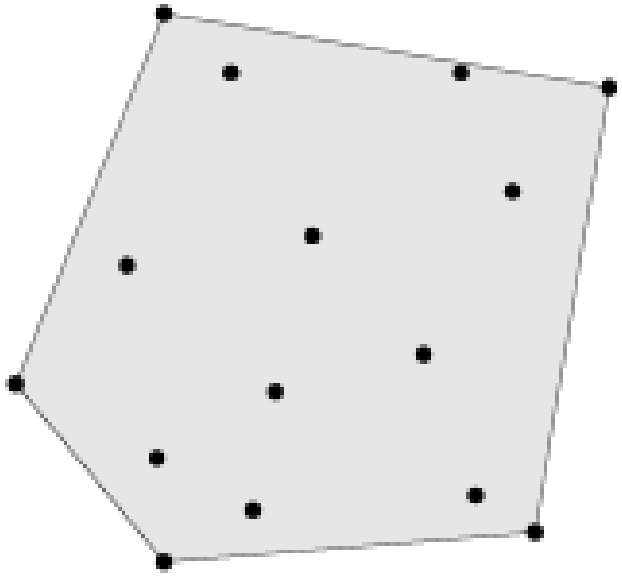
Depth-Based Methods

Convex Hull

The *convex hull* of a set C, denoted $\mathbf{conv}\, C$, is the set of all convex combinations of points in C:

$$\mathbf{conv}\, C = \{\theta_1 x_1 + \cdots + \theta_k x_k \mid x_i \in C,\ \theta_i \geq 0,\ i = 1, \ldots, k,\ \theta_1 + \cdots + \theta_k = 1\}.$$

- Corners



The Procedure

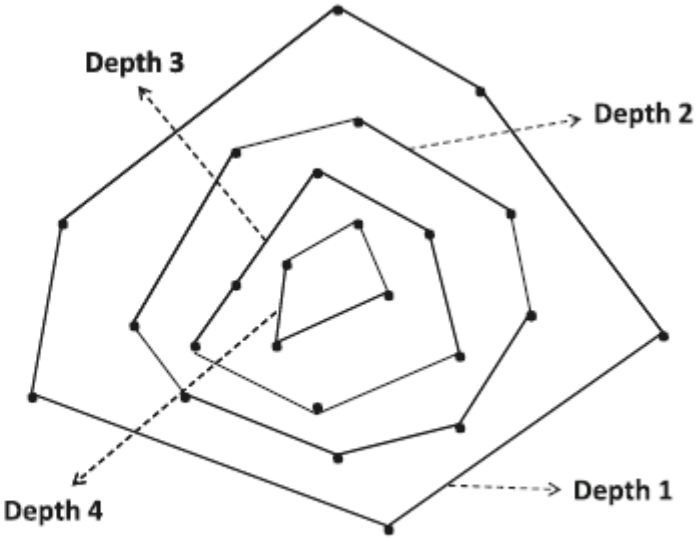
- The index k is the outlier score
  - Smaller values indicate a grate tendency

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

An Example

- Peeling Layers of an Onion

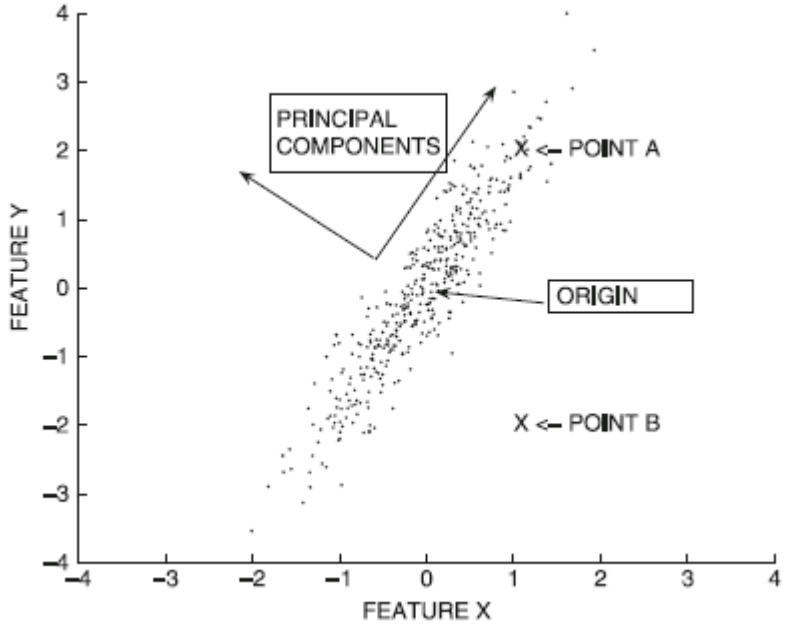
(a)



(b)

Limitations

- No Normalization



- Many data points are indistinguishable
- The computational complexity increases significantly with dimensionality

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Probabilistic Models

- Related to Probabilistic Model-Based Clustering
- The Key Idea
  - Assume data is generated from a mixture-based generative model
  - Learn the parameter of the model from data
    - ✓ EM algorithm
  - Evaluate the probability of each data point being generated by the model
    - ✓ Points with low values are outliers

Mixture-based Generative Model

- Data was generated from a mixture of k distributions with probability distribution $\mathcal{G}_1, \ldots, \mathcal{G}_k$
- $\mathcal{G}_i$ represents a cluster/mixture component
- Each point $\bar{X}$ is generated as follows
  - Select a mixture component with probability $\alpha_i = P(\mathcal{G}_i),\ i = 1, \ldots, k$
  - Assume the r-th component is selected
  - Generate a data point from G_r

Learning Parameter from Data

- The probability that $\overline{X_j}$ generated by the mixture model $\mathcal{M}$ is given by

$$f^{point}(\overline{X_j}|\mathcal{M}) = \sum_{i=1}^{k} P(\mathcal{G}_i, \overline{X_j}) = \sum_{i=1}^{k} P(\mathcal{G}_i)P(\overline{X_j}|\mathcal{G}_i) = \sum_{i=1}^{k} \alpha_i \cdot f^i(\overline{X_j})$$

- The probability of the data set $\mathcal{D} = \{\overline{X_1}, \ldots, \overline{X_n}\}$ generated by $\mathcal{M}$

$$f^{data}(\mathcal{D}|\mathcal{M}) = \prod_{j=1}^{n} f^{point}(\overline{X_j}|\mathcal{M}).$$

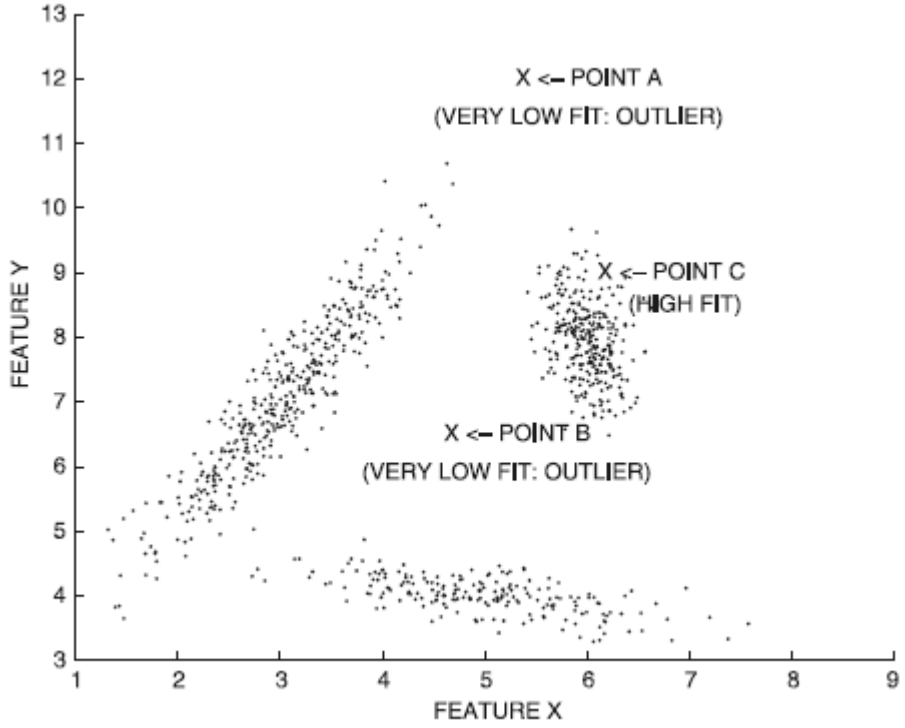
- Learning parameters that maximize

$$\mathcal{L}(\mathcal{D}|\mathcal{M}) = \log(\prod_{j=1}^{n} f^{point}(\overline{X_j}|\mathcal{M})) = \sum_{j=1}^{n} \log(\sum_{i=1}^{k} \alpha_i f^i(\overline{X_j}))$$

Identify Outliers

- Outlier Score is defined as

$$f^{point}(\bar{X}_j|\mathcal{M}) = \sum_{i=1}^{k} P(\mathcal{G}_i, \bar{X}_j) = \sum_{i=1}^{k} P(\mathcal{G}_i)P(\bar{X}_j|\mathcal{G}_i) = \sum_{i=1}^{k} \alpha_i \cdot f^i(\bar{X}_j)$$



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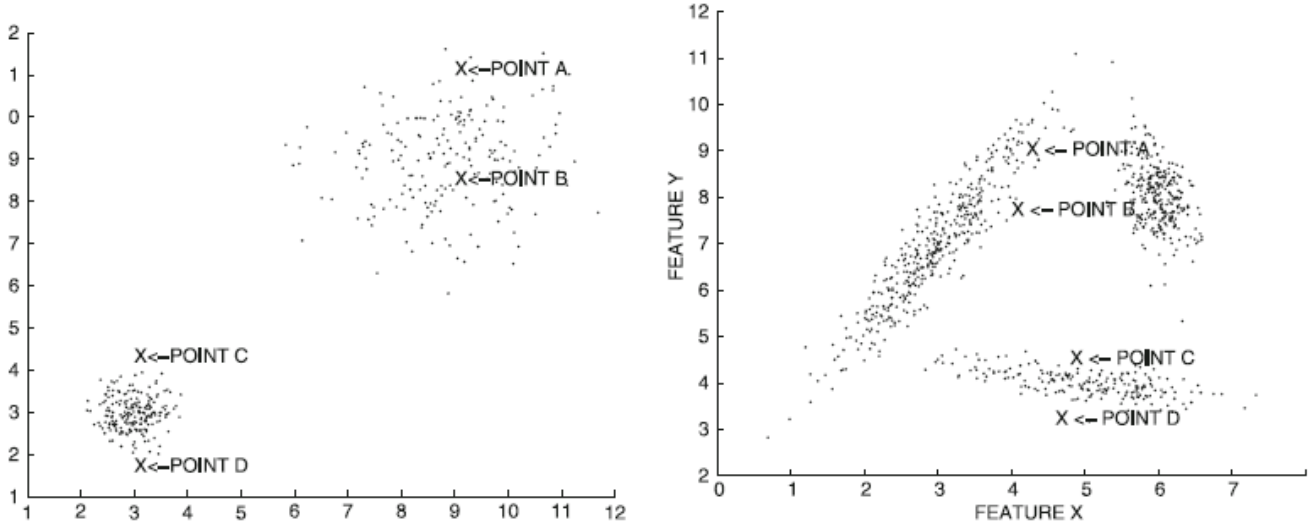
Clustering for Outlier Detection

- Outlier Analysis v.s. Clustering
  - Clustering is about finding “crowds” of data points
  - Outlier analysis is about finding data points that are far away from these crowds
- Every data point is
  - Either a member of a cluster
  - Or an outlier
- Some clustering algorithms also detect outliers
  - DBSCAN, DENCLUE

The Procedure (1)

- A Simple Way
  1. Cluster the data
  2. Define the outlier score as the distance of the data point to its cluster centroid



(a) local density variation (b) local orientation variation

The Procedure (2)

A Better Approach

1. Cluster the data
2. Define the outlier score as the local Mahalanobis distance
   - ✓ Suppose $\bar{X}$ belongs to cluster r

$$Maha(\overline{X}, \overline{\mu_r}, \Sigma_r) = \sqrt{(\overline{X} - \overline{\mu_r})\Sigma_r^{-1}(\overline{X} - \overline{\mu_r})^T}.$$

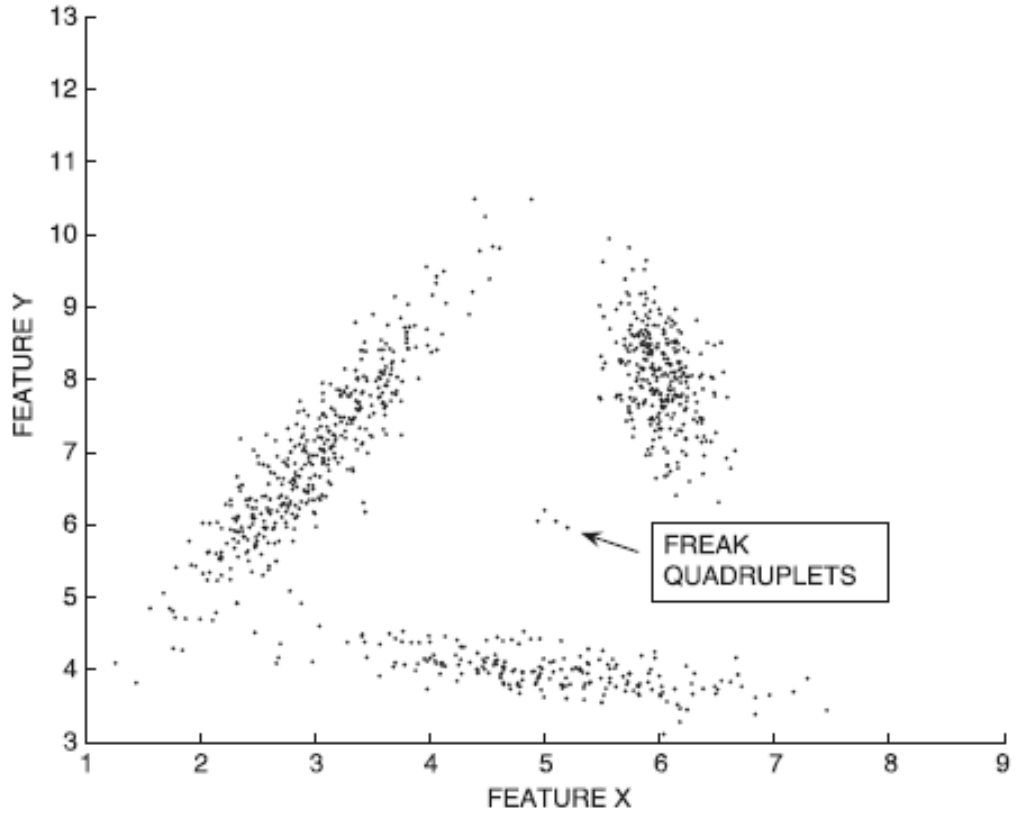
   - ✓ $\overline{\mu_r}$ is the mean vector of the r-th cluster
   - ✓ Σ_r is the covariance matrix of the r-th cluster

Multivariate Extreme Value Analysis

- Global Mahalanobis distance

A Post-processing Step

- Remove Small-Size Clusters



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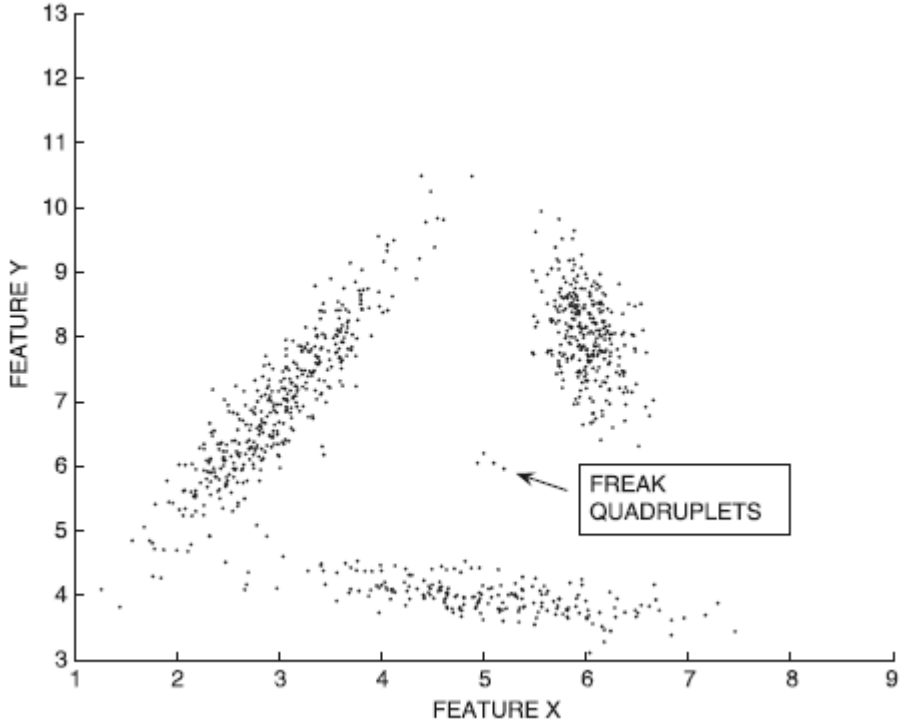
Distance-Based Outlier Detection

An *Instance-Specific* Definition

- The distance-based outlier score of an object O is its distance to its k-th nearest neighbor

$k > 3$

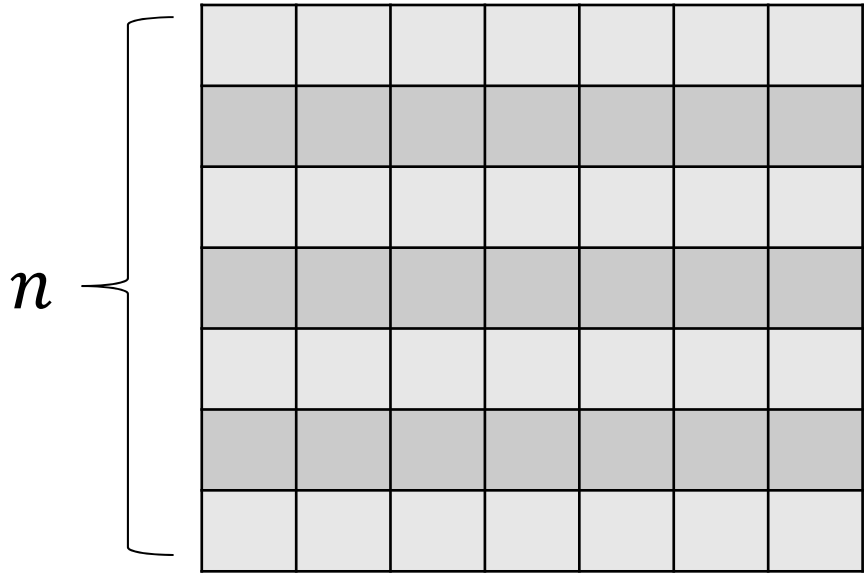


Distance-Based Outlier Detection

- An *Instance-Specific* Definition
  - The distance-based outlier score of an object O is its distance to its k-th nearest neighbor
  - Sometimes, average distance is used
- High-computational Cost $O(n^2)$
  - Index structure
    - ✓ Effective when the dimensionality is low
  - Pruning tricks
    - ✓ Designed for the case that only the top-r outliers are needed

The Naïve Approach for Finding Top r-Outliers

1. Evaluate the $n \times n$ distance matrix



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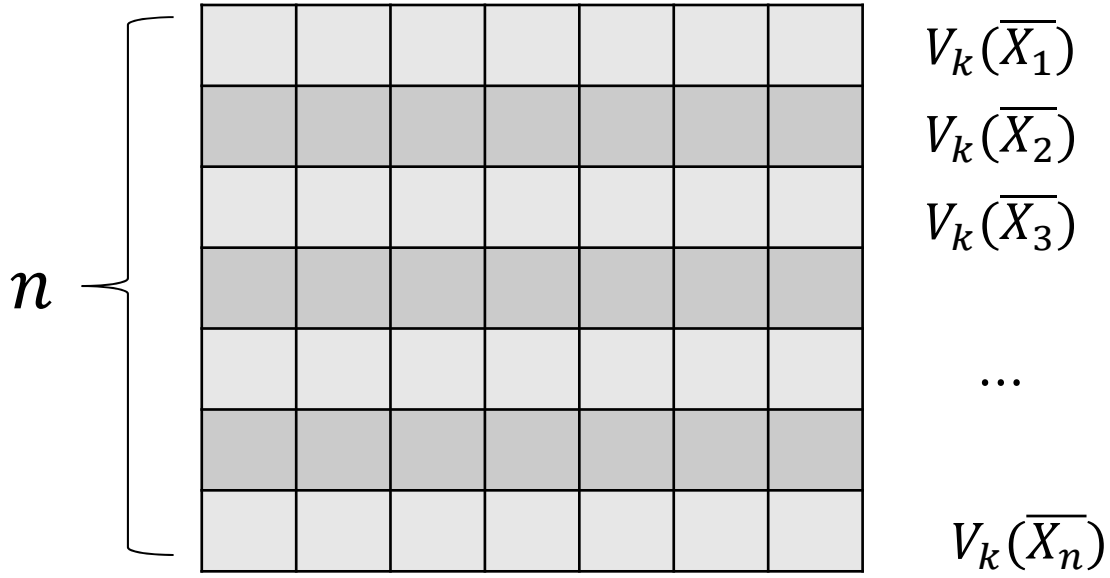

2. Find the k-th smallest value in each row

The Naïve Approach for Finding Top r-Outliers

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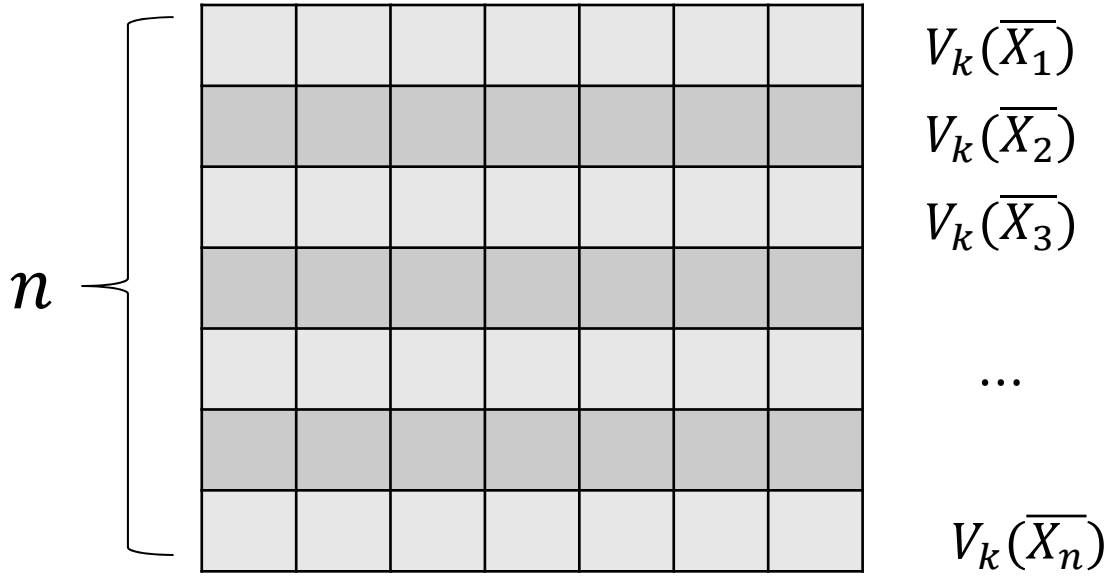
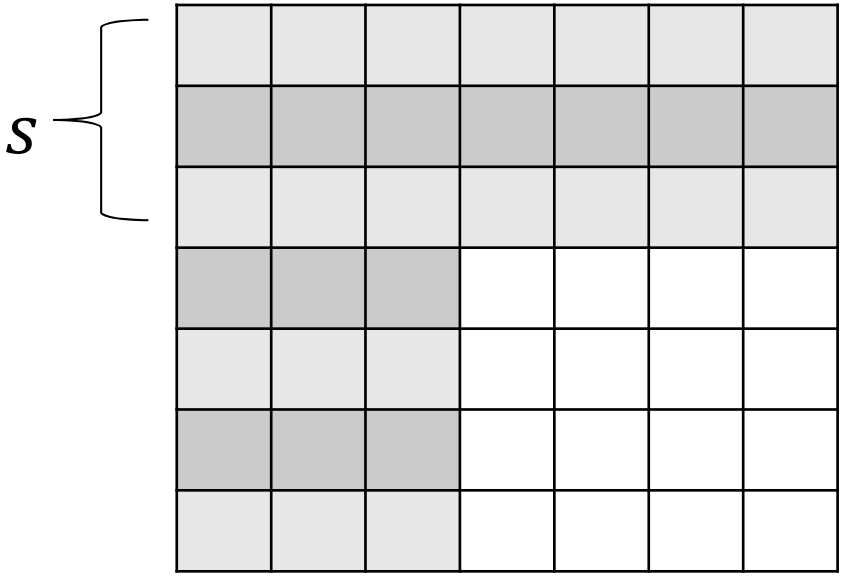


2. Find the k-th smallest value in each row

3. Choose r data points with largest $V_k(\cdot)$

Pruning Methods—Sampling

1. Evaluate a $s \times n$ distance matrix



Pruning Methods—Sampling

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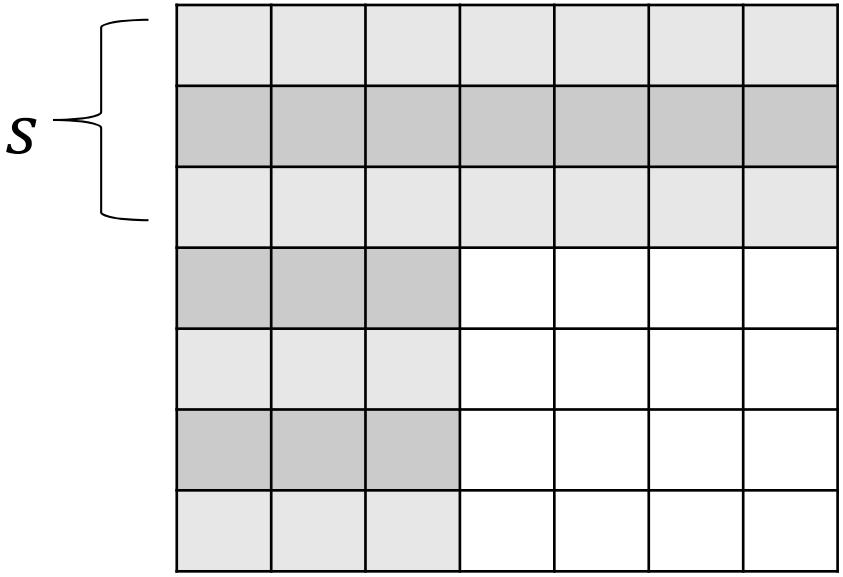


$V_k(\overline{X_1})$

…

$V_k(\overline{X_s})$

$\widehat{V_k}(\overline{X_{s+1}}) \geq V_k(\overline{X_{s+1}})$

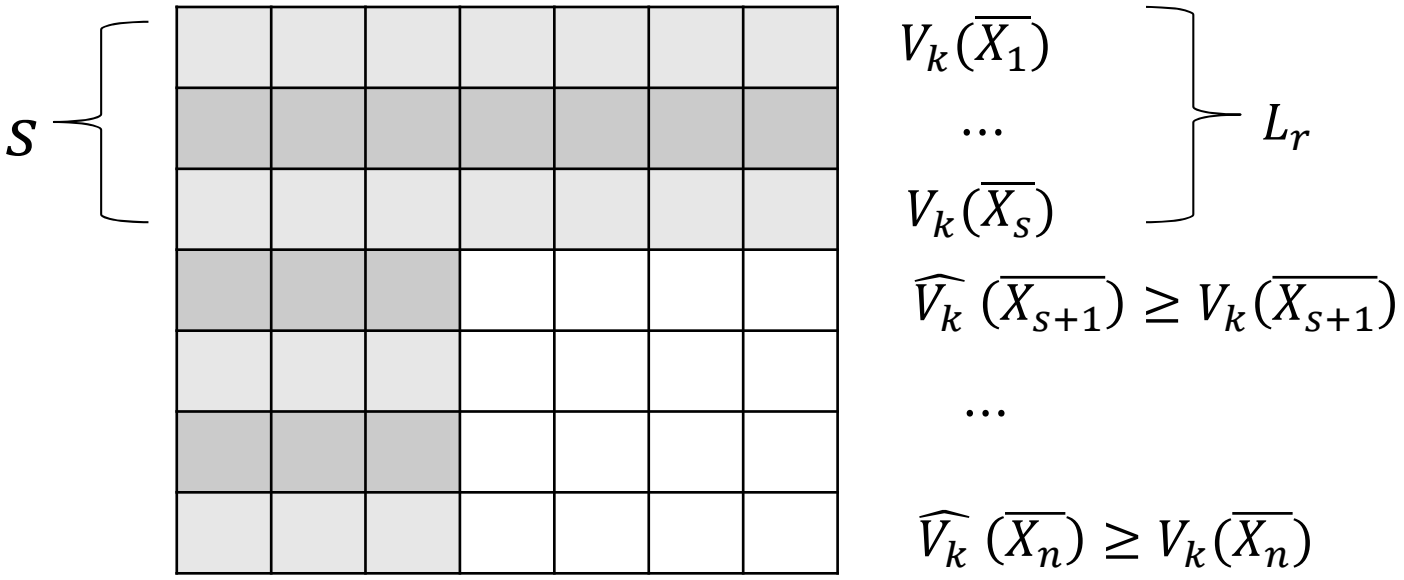
…

$\widehat{V_k}(\overline{X_n}) \geq V_k(\overline{X_n})$

2. Find the k-th smallest value in each row

Pruning Methods—Sampling

1. Evaluate a $s \times n$ distance matrix

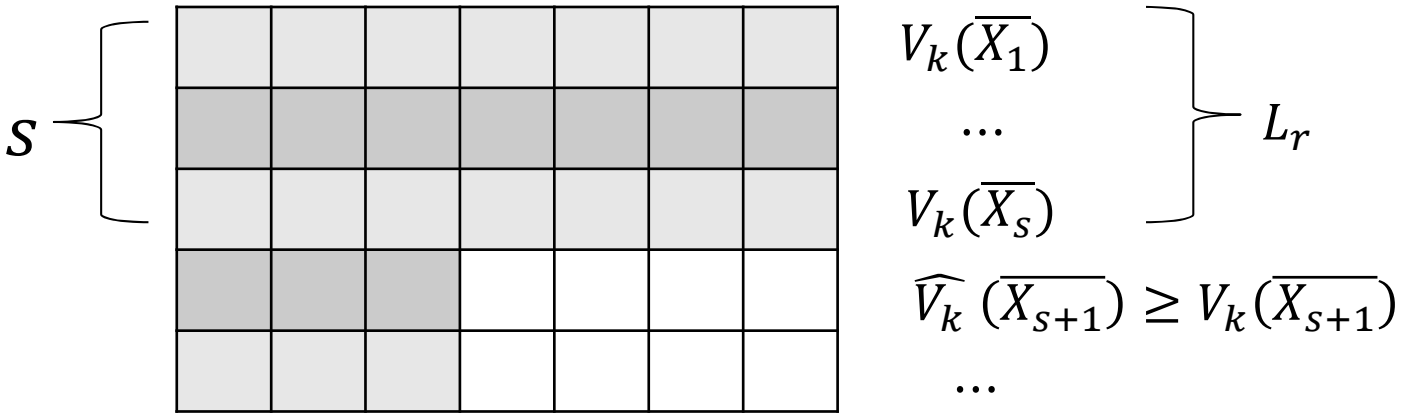


2. Find the k-th smallest value in each row

3. Identify the r-th score in top s-rows

Pruning Methods—Sampling

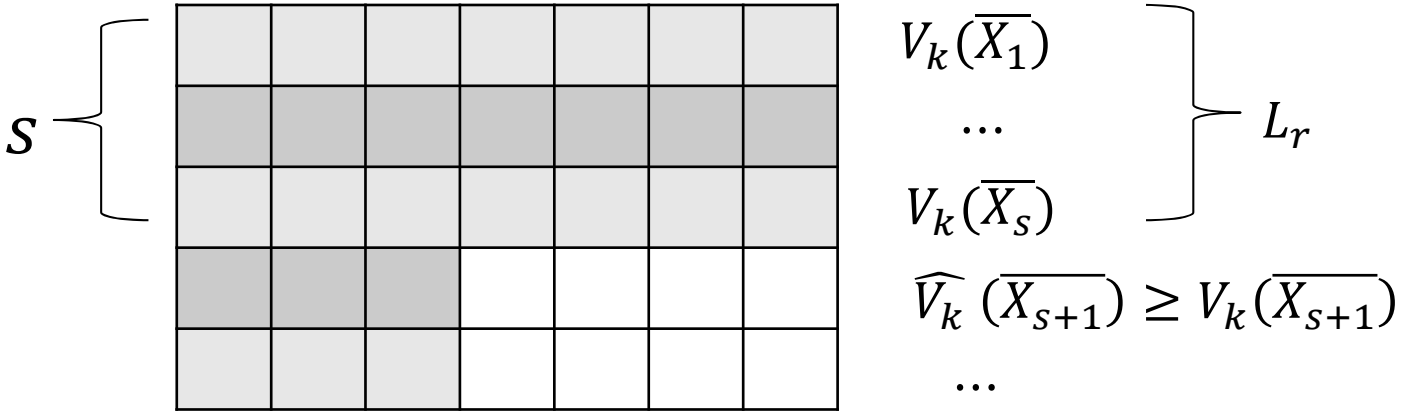
1. Evaluate a $s \times n$ distance matrix



2. Find the k-th smallest value in each row
3. Identify the r-th score in top s-rows
4. Remove points with $\widehat{V_k}(\cdot) \leq L_r$

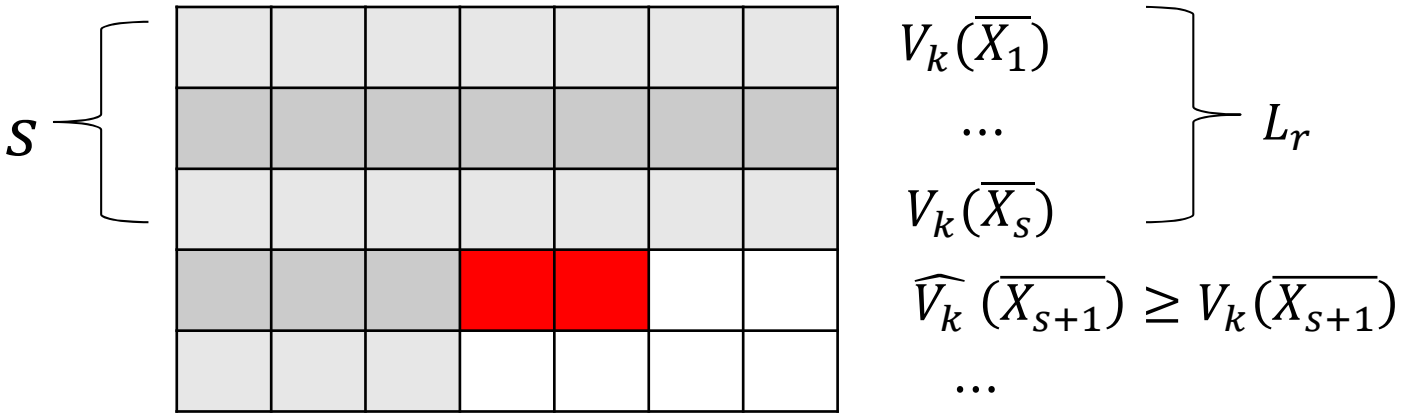
Pruning Methods—Early Termination

- When completing the empty area



Pruning Methods—Early Termination

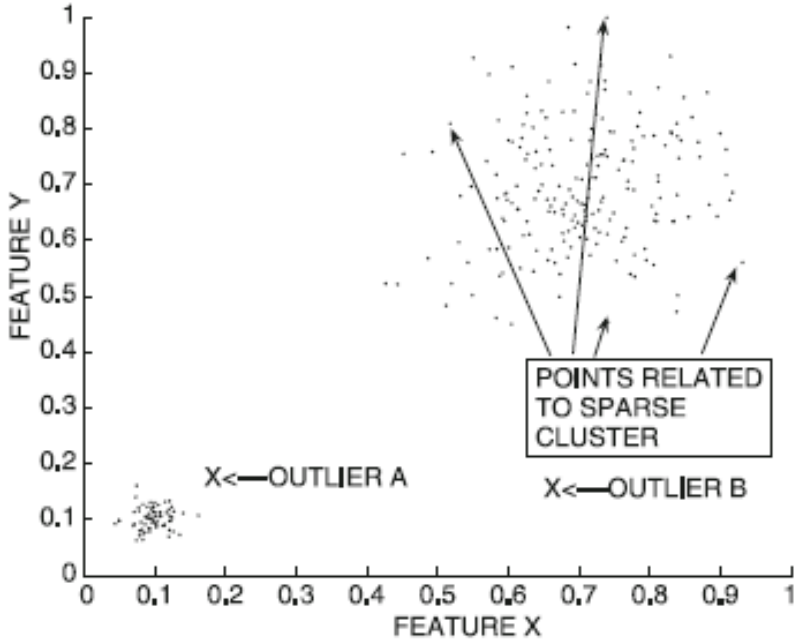
- When completing the empty area



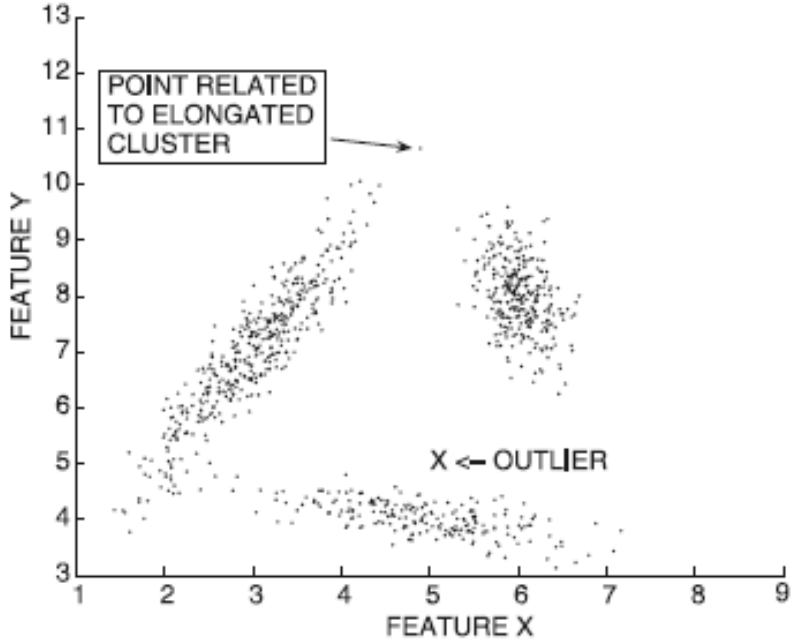
- Update $\widehat{V_k}(\cdot)$ when more distances are known
- Stop if $\widehat{V_k}(\cdot) \leq L_r$
- Update L_r if necessary

Local Distance Correction Methods

Impact of Local Variations



(a) Varying cluster density



(b) Varying cluster shape

Local Outlier Factor (LOF)

- Let $V^k(\bar{X})$ be the distance of $\bar{X}$ to its k-nearest neighbor
- Let $L_k(\bar{X})$ be the set of points within the k-nearest neighbor distance of $\bar{X}$
- Reachability Distance

$$R_k(\overline{X}, \overline{Y}) = \max\{Dist(\overline{X}, \overline{Y}), V^k(\overline{Y})\}$$

  - Not symmetric between $\bar{X}$ and $\bar{Y}$
  - If $Dist(\bar{X}, \bar{Y})$ is large, $R_k(\bar{X}, \bar{Y}) = Dist(\bar{X}, \bar{Y})$
  - Otherwise, $R_k(\bar{X}, \bar{Y}) = V^k(\bar{Y})$
    - ✓ Smoothed out by $V^k(\bar{Y})$, more stable

Local Outlier Factor (LOF)

- Average Reachability Distance

$$AR_k(\overline{X}) = \text{MEAN}_{\overline{Y} \in L_k(\overline{X})} R_k(\overline{X}, \overline{Y})$$

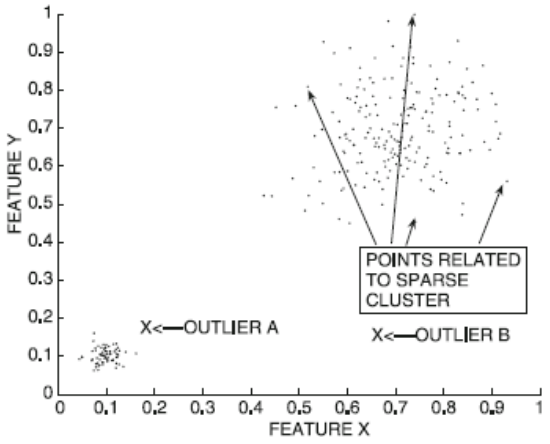
- Local Outlier Factor

$$LOF_k(\overline{X}) = \text{MEAN}_{\overline{Y} \in L_k(\overline{X})} \frac{AR_k(\overline{X})}{AR_k(\overline{Y})}$$

  - Larger for Outliers
  - Close to 1 for Others

- Outlier Score

$$\max_k LOF_k(\bar{X})$$



(a) Varying cluster density

Instance-Specific Mahalanobis Distance (1)

- Define a local Mahalanobis distance for each point
  - Based on the covariance structure of the neighborhood of a data point
- The Challenge
  - Neighborhood of a data point is hard to define with the Euclidean distance
  - Euclidean distance is biased toward capturing the circular region around that point

Instance-Specific Mahalanobis Distance (2)

- An agglomerative approach for neighborhood construction
  - Add $\bar{X}$ to $L^k(\bar{X})$
  - Data points are iteratively added to $L^k(\bar{X})$ that have the smallest distance to $L^k(\bar{X})$

$$\text{argmin}_{\bar{Y}\in\mathcal{D}} \min_{\bar{Z}\in L^k(\bar{X})} dist(\bar{Y}-\bar{Z})$$

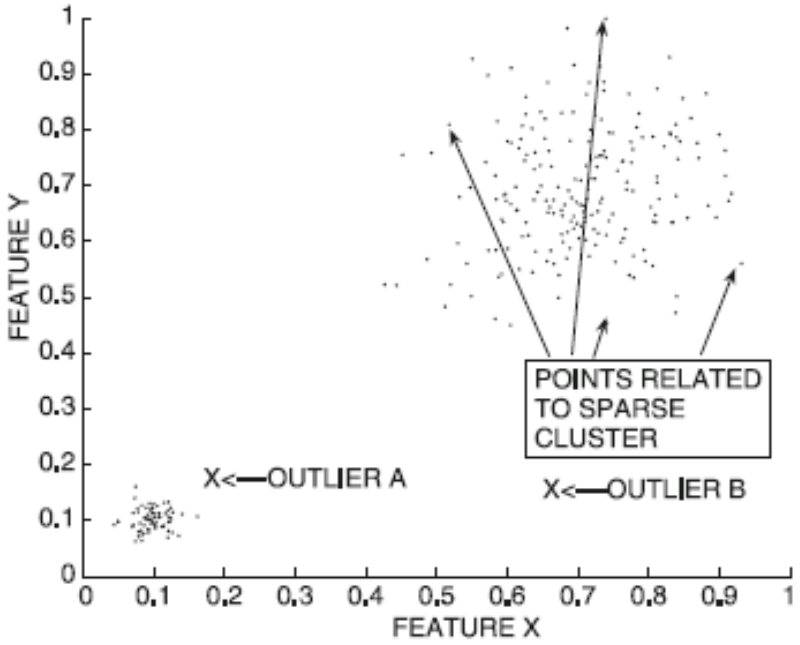
- Instance-specific Mahalanobis score

$$LMaha_k(\overline{X}) = Maha(\overline{X}, \overline{\mu_k(X)}, \Sigma_k(\overline{X}))$$

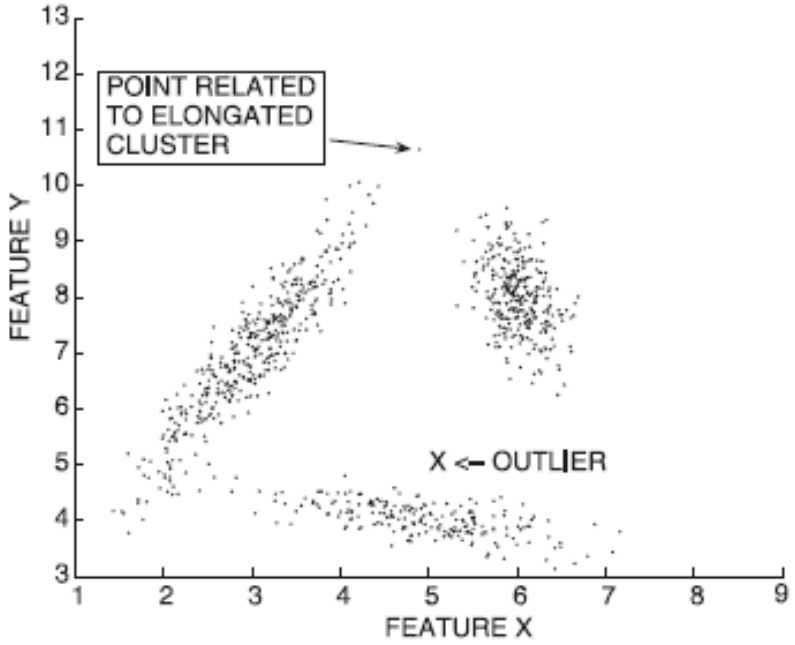
- Outlier score $\max_k LMaha_k(\bar{X})$

Instance-Specific Mahalanobis Distance (3)

- Can be applied to both cases



(a) Varying cluster density



(b) Varying cluster shape

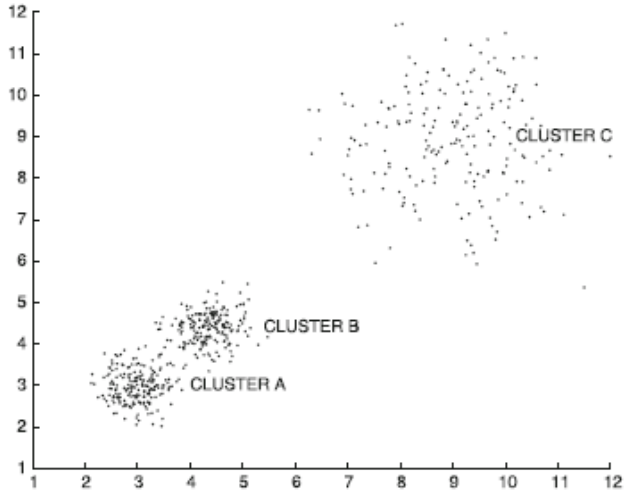
- Relation to clustering-based approaches

Outline

- Introduction
- Extreme Value Analysis
- Probabilistic Models
- Clustering for Outlier Detection
- Distance-Based Outlier Detection
- **Density-Based Methods**
- Information-Theoretic Models
- Outlier Validity
- Summary

Density-Based Methods

- The Key Idea
  - Determine sparse regions in the underlying data
- Limitations
  - Cannot handle variations of density

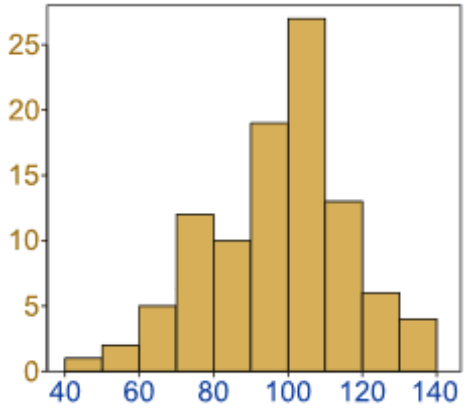


Histogram- and Grid-Based Techniques

Histogram for 1-dimensional data

- Data points that lie in bins with very low frequency are reported as outliers

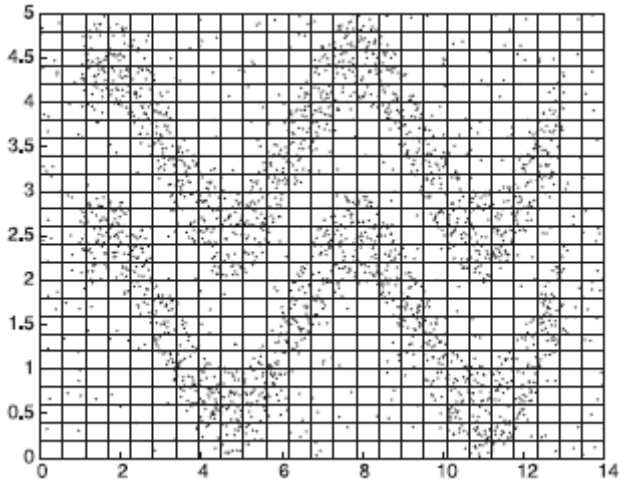
https://www.mathsisfun.com/data/histograms.html



Grid for high-dimensional data

Challenges

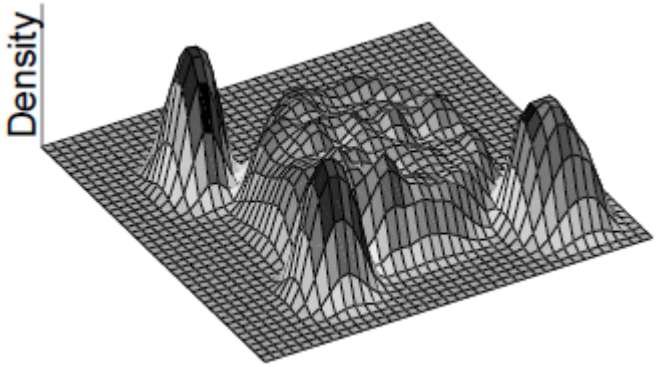
- Size of grid
- Too local
- Sparsity



Kernel Density Estimation

- Given n data points $\overline{X_1}, \ldots, \overline{X_n}$

$$f(\overline{X}) = \frac{1}{n}\sum_{i=1}^{n} K(\overline{X} - \overline{X_i}).$$



  - $K(\cdot)$ is a kernel function

$$K(\overline{X} - \overline{X_i}) = \left(\frac{1}{h\sqrt{2\pi}}\right)^{d} e^{-\frac{||\overline{X} - \overline{X_i}}{2 \cdot h^2}}$$

- The density at each data point
  - Computed without including the point itself in the density computation
  - Low values of the density indicate greater tendency to be an outlier

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Information-Theoretic Models

- An Example

  ABABABABABABABABABABABABABABAB

  ABABACABABABABABABABABABABABAB

  - The 1st One: “AB 17 times”
  - C in 2nd string increases its minimum description length
- Conventional Methods
  - Fix model, then calculate the deviation
- Information-Theoretic Models
  - Fix the deviation, then learn the model
  - Outlier score of $\bar{X}$: increase of the model size when $\bar{X}$ is present

Probabilistic Models

- The Conventional Method
  - Learn the parameters of generative model with a fixed size
  - Use the fit of each data point as the outlier score
- Information-Theoretic Method
  - Fix a maximum allowed deviation (a minimum value of fit)
  - Learn the size and values of parameters
  - Increase of size is used as the outlier score

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Outlier Validity

- Methodological Challenges
  - Internal criteria are rarely used in outlier analysis
  - A particular validity measure will favor an algorithm using a similar objective function criterion
  - Magnified because of the small sample solution space
- External Measures
  - The known outlier labels from a synthetic data set
  - The rare class labels from a real data set

Receiver Operating Characteristic (ROC) curve

- $\mathcal{G}$ is the set of outliers (ground-truth)
- An algorithm outputs a outlier score
- Given a threshold t, we denote the set of outliers by $\mathcal{S}(t)$
  - True-positive rate (recall)

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

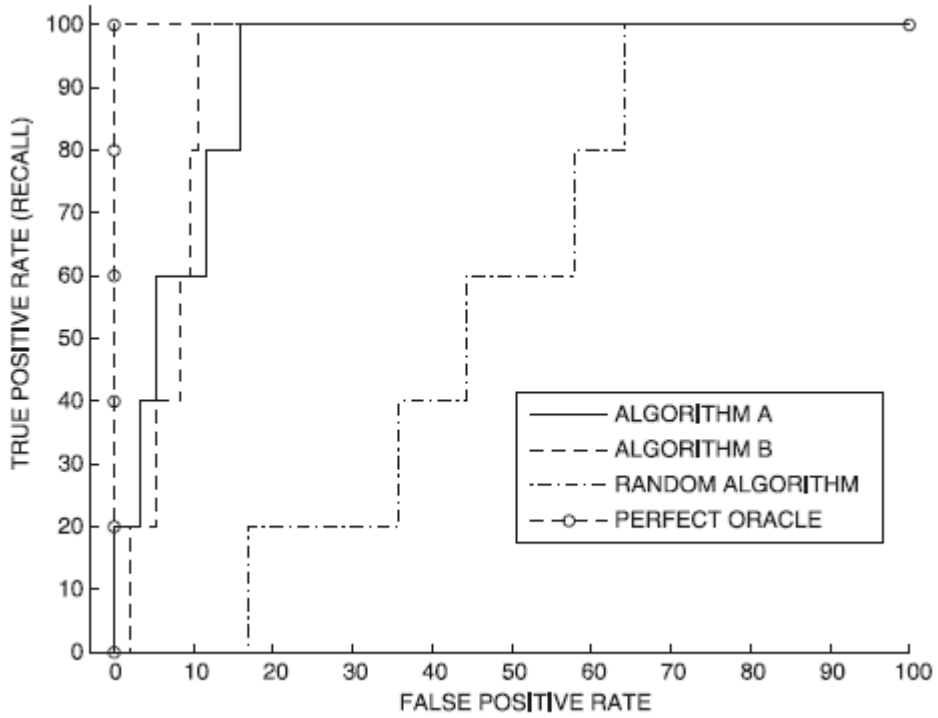
  - The false positive rate

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

- ROC Curve
  - Plot $TPR(t)$ versus $FPR(t)$

An Example

Algorithm	Rank of ground-truth outliers
Algorithm A	1, 5, 8, 15, 20
Algorithm B	3, 7, 11, 13, 15
Random Algorithm	17, 36, 45, 59, 66
Perfect Oracle	1, 2, 3, 4, 5



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Summary

- Extreme Value Analysis
  - Univariate, Multivariate, Depth-Based
- Probabilistic Models
- Clustering for Outlier Detection
- Distance-Based Outlier Detection
  - Pruning, LOF, Instance-Specific
- Density-Based Methods
  - Histogram- and Grid-Based, Kernel Density
- Information-Theoretic Models
- Outlier Validity
  - ROC curve