



**Università
degli Studi
di Palermo**



Outlier Analysis

CORSO DI BIG DATA – MODULO ANALISI PER I BIG DATA
a.a. 2022/2023

Prof. Roberto Pirrone



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



Outline

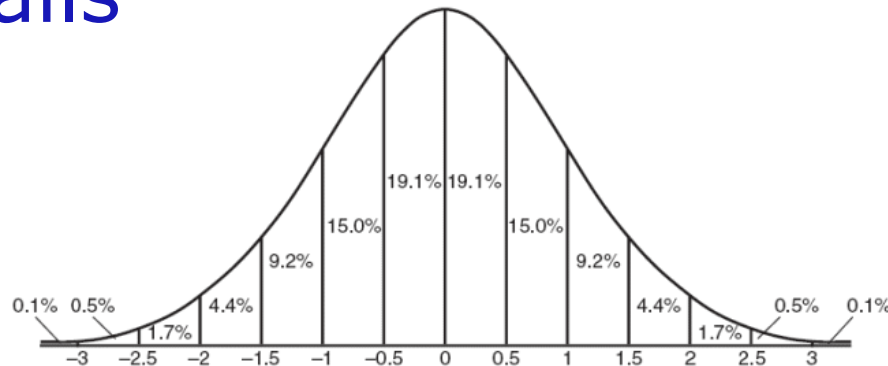
- ☐ Introduction
- ☐ **Extreme Value Analysis**
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Extreme Value Analysis (1)

□ Statistical Tails

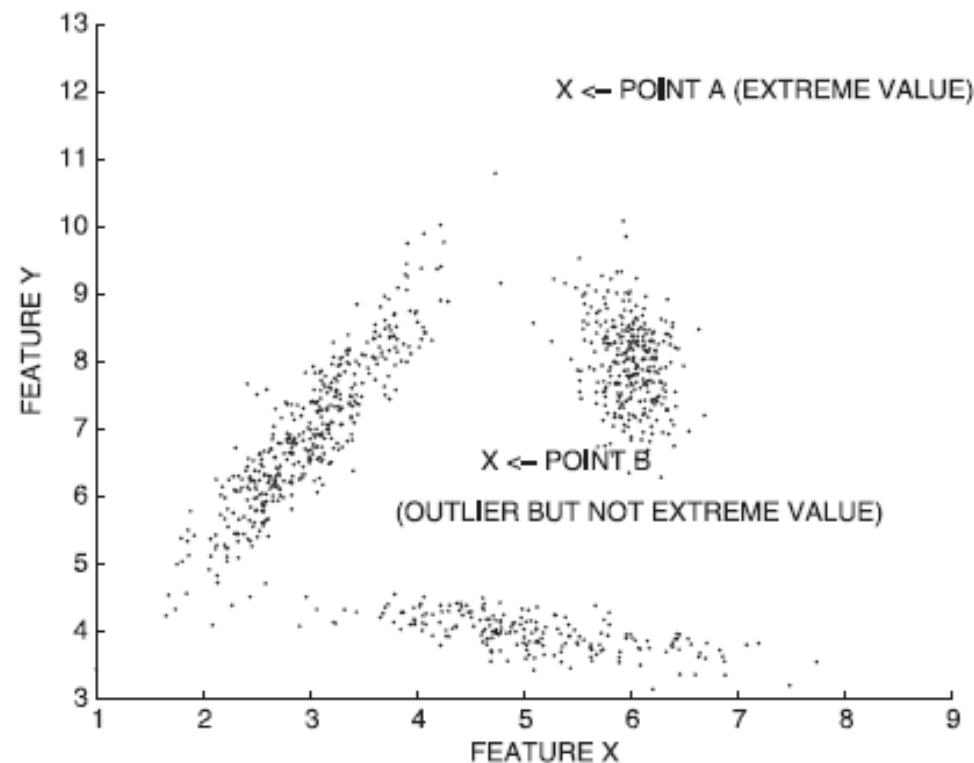
<http://www.regentsprep.org/regents/math/algtrig/ats2/normallesson.htm>



- 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 outliers
- ❑ Outliers may not be extreme values



Univariate Extreme Value Analysis (1)

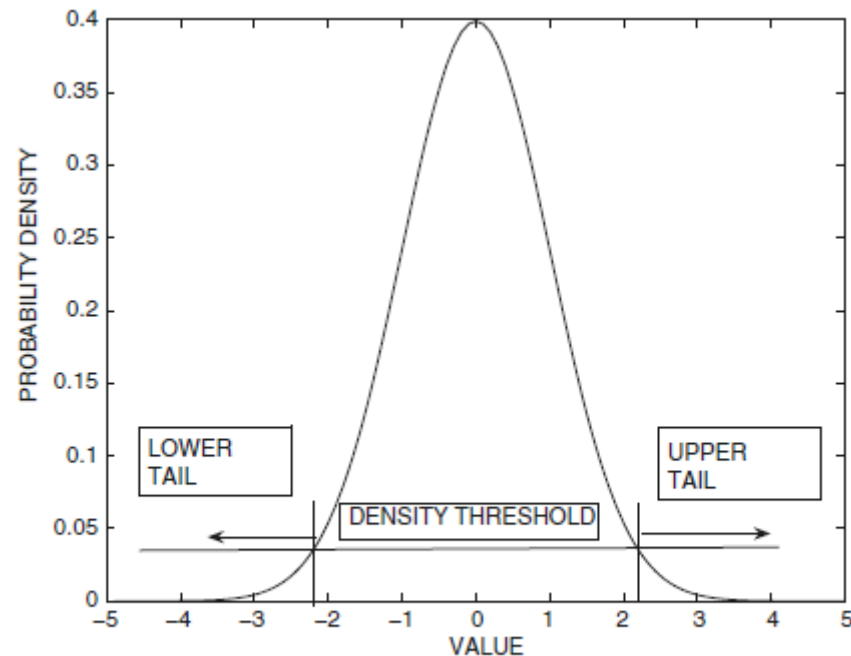


□ Statistical Tail Confidence Tests

- 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)



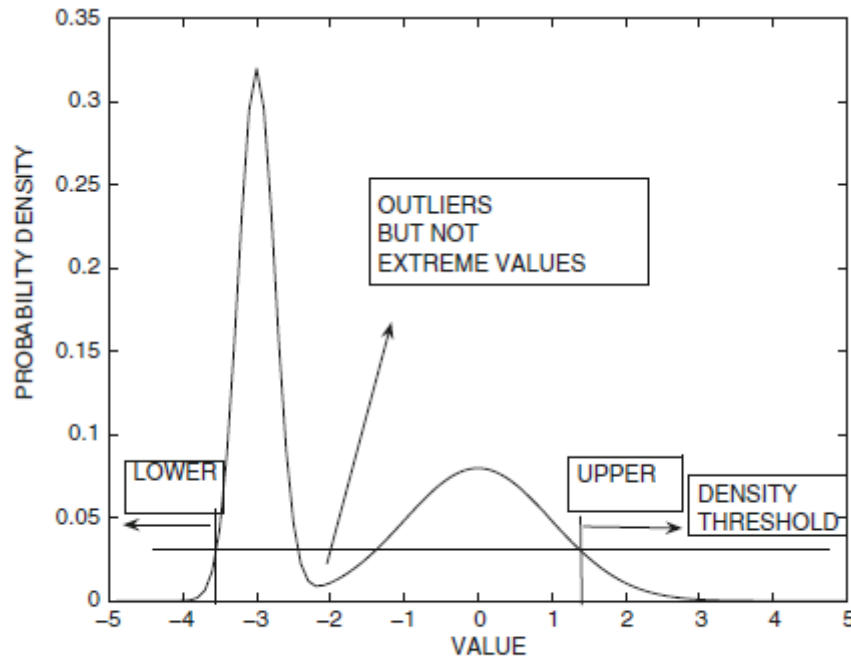
□ Statistical Tail Confidence Tests

- Suppose the density distribution is $f_X(x)$
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□ Asymmetric Distribution

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

E' necessario trovare un modello per quantificare la probabilità delle code



(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

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

The Procedure (2)

□ Z-value of a random variable

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

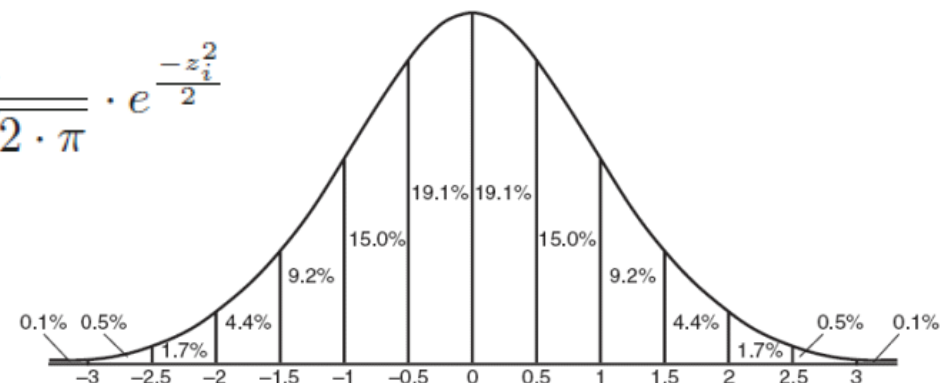
- Large positive values of z_i correspond to the upper tail
- Large negative values of z_i correspond to the lower tail
- z_i follows the **standard** normal distribution

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

□ Extreme values

- $|z_i| \geq \tau$

|z_i| ≥ 3 garantisce che i punti selezionati siano outliers





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

$$\begin{aligned} f(\bar{X}) &= \frac{1}{\sqrt{|\Sigma|} \cdot (2 \cdot \pi)^{(d/2)}} \cdot e^{-\frac{1}{2} \cdot (\bar{X} - \bar{\mu}) \Sigma^{-1} (\bar{X} - \bar{\mu})^T} \\ &= \frac{1}{\sqrt{|\Sigma|} \cdot (2 \cdot \pi)^{(d/2)}} \cdot e^{-\frac{1}{2} \cdot Maha(\bar{X}, \bar{\mu}, \Sigma)^2} \end{aligned}$$

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

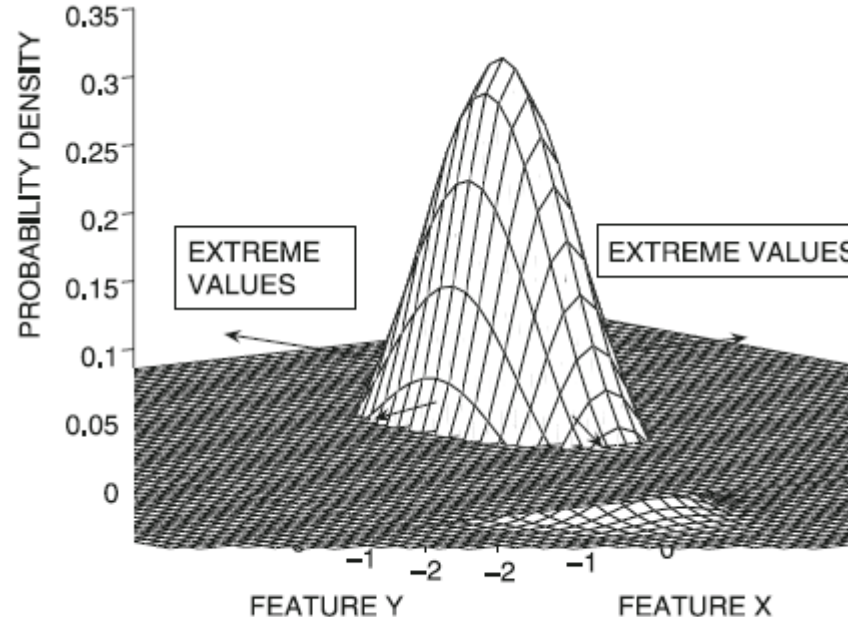
Multivariate Extreme Values (2)

□ Extreme-value Score of \bar{X}

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

La distanza di Mahalanobis diventa quella Euclidea se il data set è riferito alle sue componenti principali

Lungo ogni componente principale si può riproporre l'analisi svolta per la gaussiana unidimensionale



(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

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

- Projection+Normalization

- ✓ Let $\Sigma = U\Lambda U^\top = \sum_{i=1}^d \sigma_i^2 \mathbf{u}_i \mathbf{u}_i^\top$

- ✓ Then, $\Sigma^{-1} = U\Lambda^{-1}U^\top = \sum_{i=1}^d \sigma_i^{-2} \mathbf{u}_i \mathbf{u}_i^\top$

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■ Projection+Normalization

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z-score delle singole componenti di \bar{Y} lungo le direzioni degli autovettori di Σ



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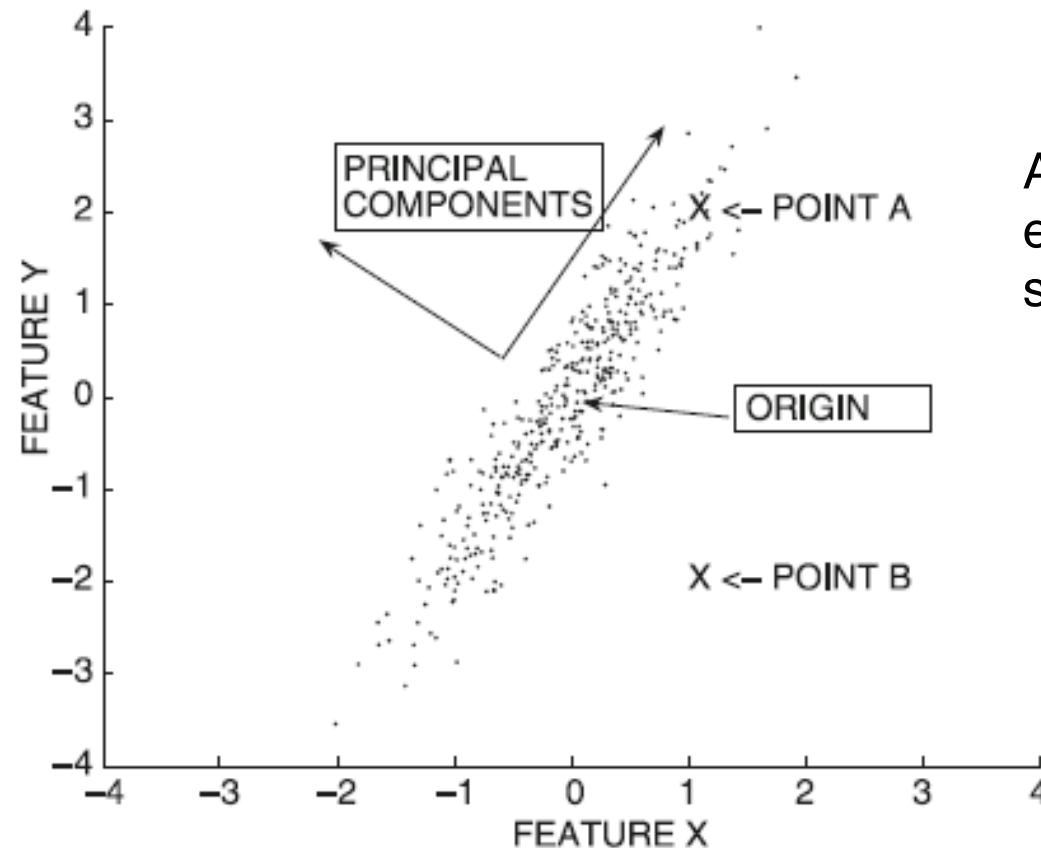
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Per definizione la distribuzione chi-square con d gradi di libertà è quella che assume la somma dei quadrati di d variabili con distribuzione normale standard ($\mu=0, \sigma=1$)

z-score delle singole componenti di \bar{Y} lungo le direzioni degli autovettori di Σ

Adaptive to the Shape

□ B is an extreme value



A sembra essere un punto estremo, ma non lo è nel senso di Mahalanobis.

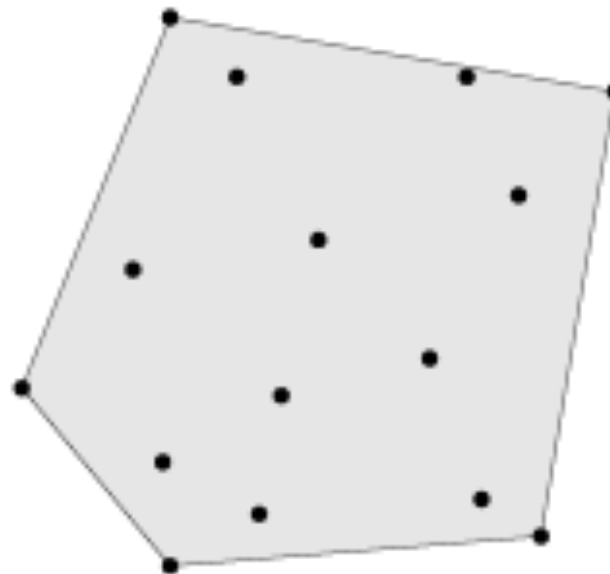
Depth-Based Methods

□ Convex Hull

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

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

■ Corners





The Procedure

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

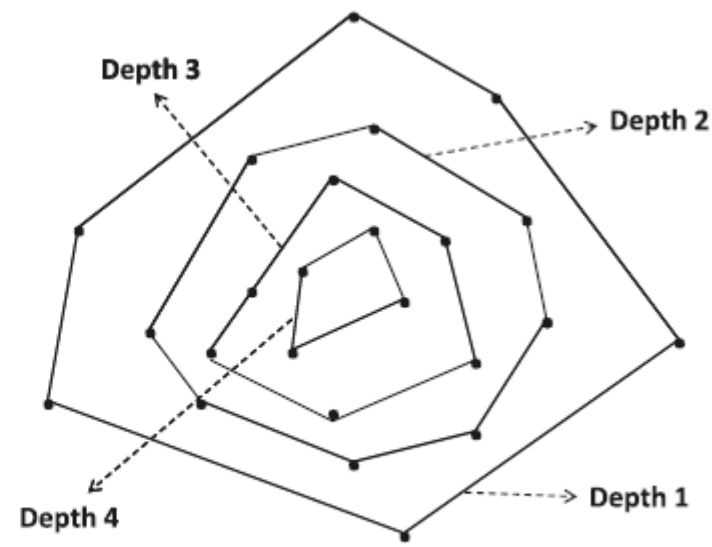
Algorithm *FindDepthOutliers*(Data Set: \mathcal{D} , Score Threshold: r)
begin
 $k = 1$;
 repeat
 Find set S of corners of convex hull of \mathcal{D} ;
 Assign depth k to points in S ;
 $\mathcal{D} = \mathcal{D} - S$;
 $k = k + 1$;
 until(\mathcal{D} is empty);
 Report points with depth at most r as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

An Example

□ Peeling Layers of an Onion



(a)

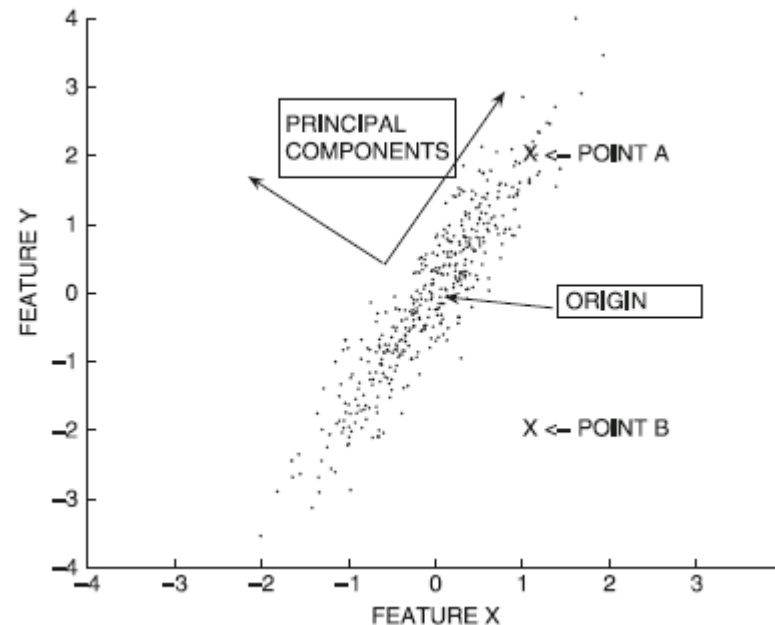


(b)

Saranno davvero tutti outlier? Non c'è distinzione!!!

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



Learning Parameter from Data

- The probability that \bar{X}_j generated by the mixture model \mathcal{M} is given by

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

- The probability of the data set $\mathcal{D} = \{\bar{X}_1, \dots, \bar{X}_n\}$ generated by \mathcal{M}

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

- Learning parameters that maximize

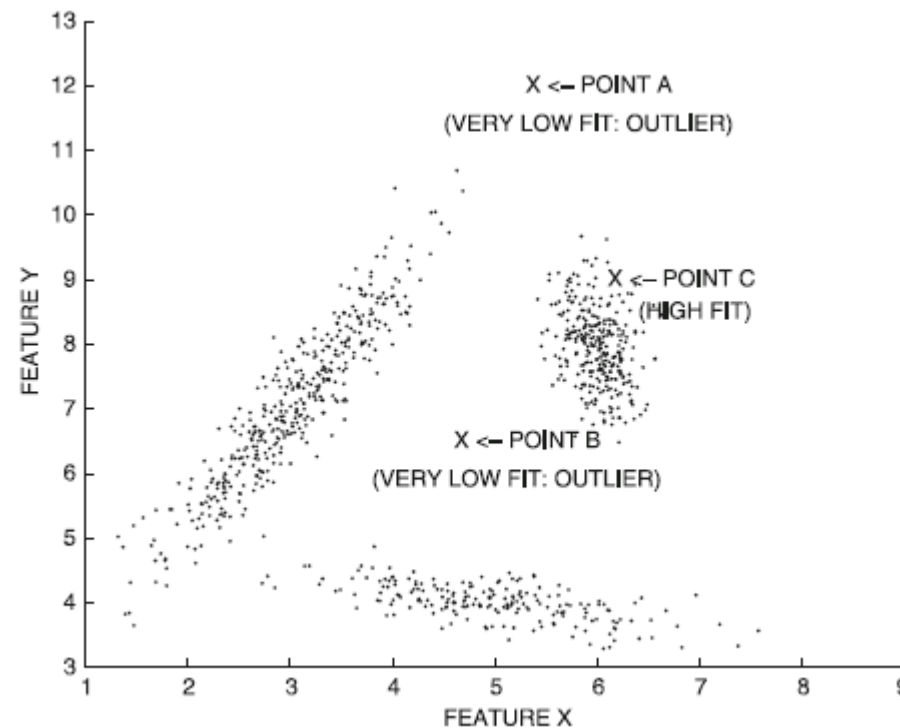
$$\mathcal{L}(\mathcal{D}|\mathcal{M}) = \log\left(\prod_{j=1}^n f^{point}(\bar{X}_j|\mathcal{M})\right) = \sum_{j=1}^n \log\left(\sum_{i=1}^k \alpha_i f^i(\bar{X}_j)\right)$$



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**

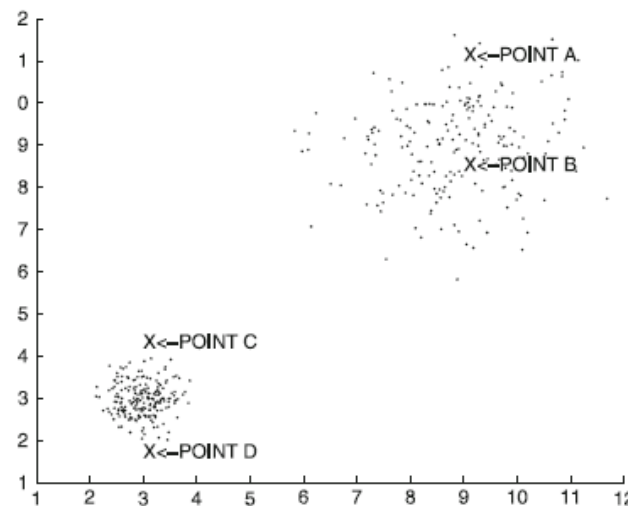
Algoritmo di clustering basato sul concetto di “Kernel density estimation”

Si fa una stima della densità di funzioni kernel $K(\cdot)$ che si sostituiscono ai punti del data set e si ottiene una stima “dolce” dei contorni dei cluster.

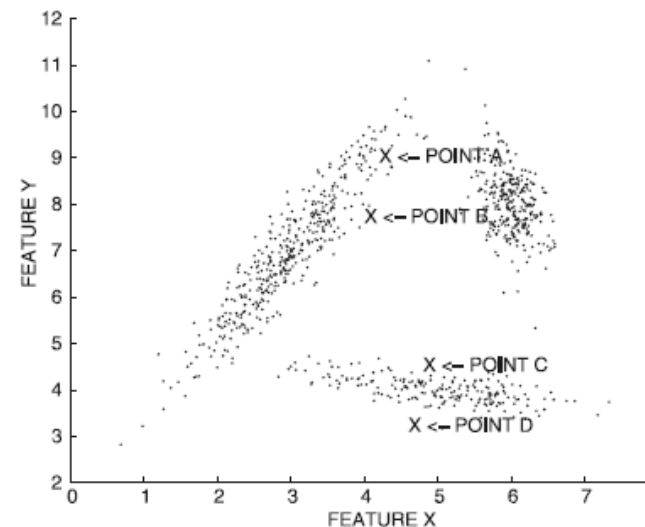
The Procedure (1)

□ 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

La struttura locale di ogni cluster può inficiare la validità di uno score basato su distanze dirette dai centroidi



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

$$Maha(\bar{X}, \bar{\mu}_r, \Sigma_r) = \sqrt{(\bar{X} - \bar{\mu}_r) \Sigma_r^{-1} (\bar{X} - \bar{\mu}_r)^T}.$$

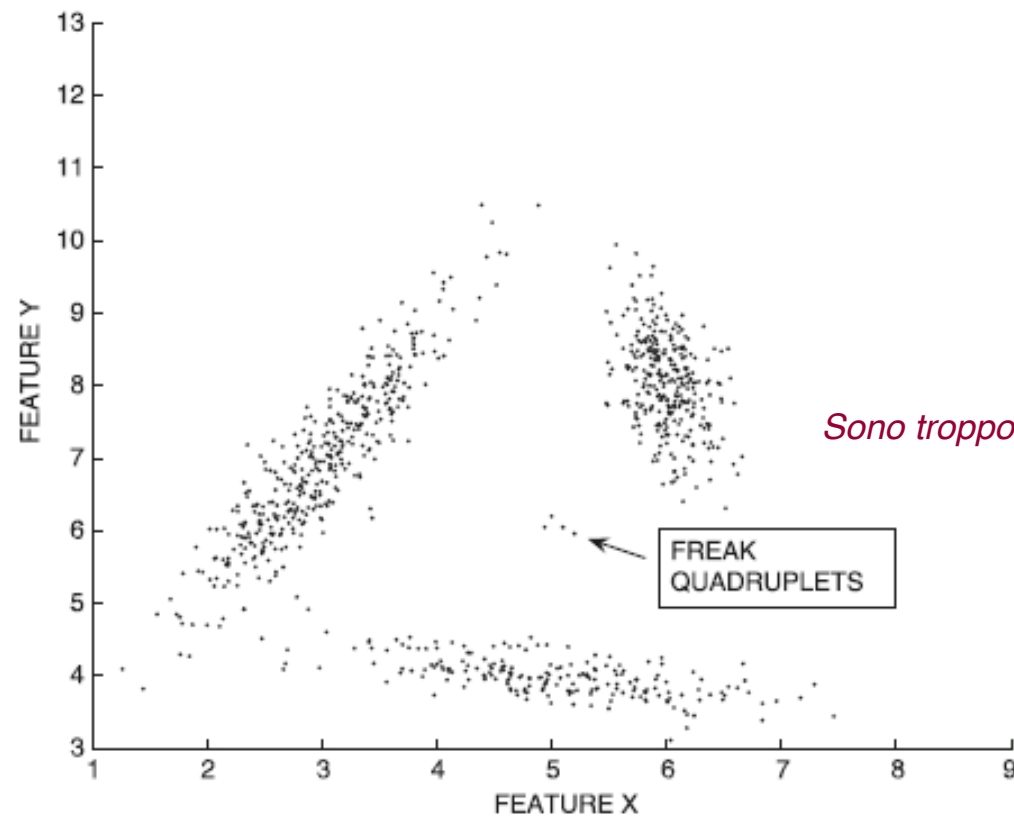
- ✓ $\bar{\mu}_r$ is the mean vector of the r -th cluster
- ✓ Σ_r is the covariance matrix of the r -th cluster

□ Multivariate Extreme Value Analysis

- **Global Mahalanobis distance**

A Post-processing Step

□ Remove Small-Size Clusters





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Distance-Based Outlier Detection

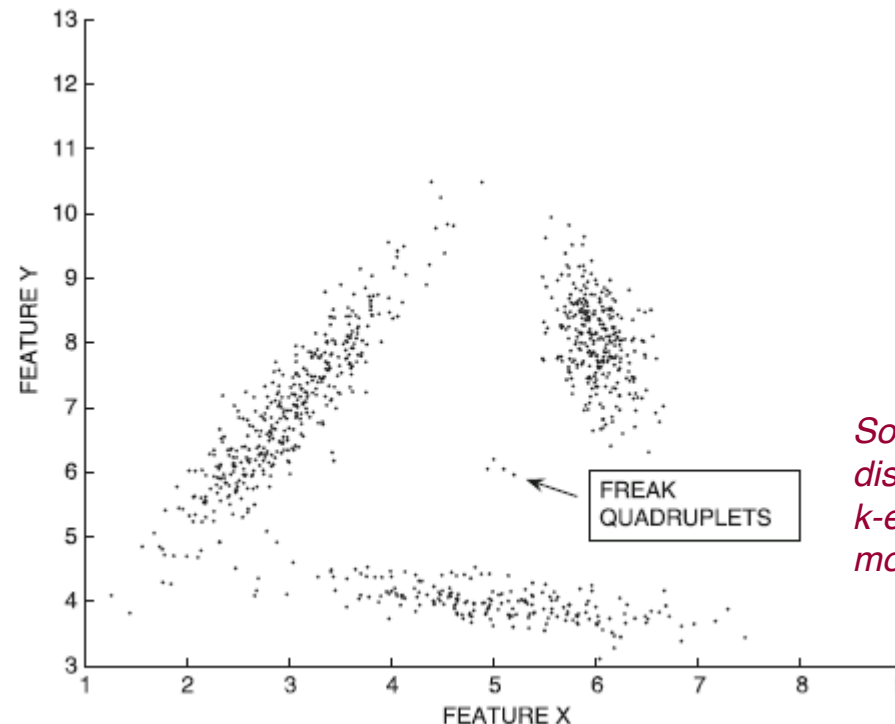


□ *An Instance-Specific Definition*

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

k è un parametro
scelto dall'utente

$$k > 3$$



*Sono tutti outlier perché la
distanza $V^k(X)$ dal
 k -esimo vicino è sempre
molto elevata*

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

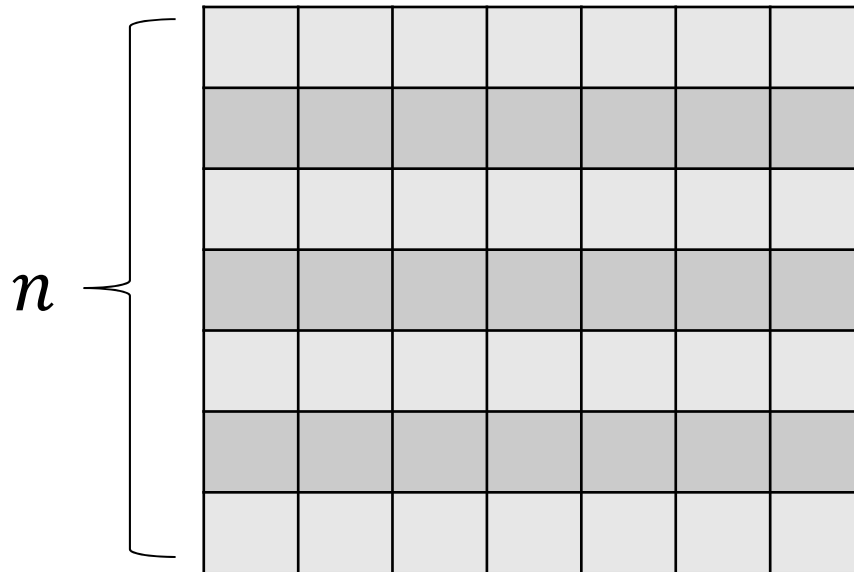
□ *High-computational Cost $O(n^2)$*

- 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



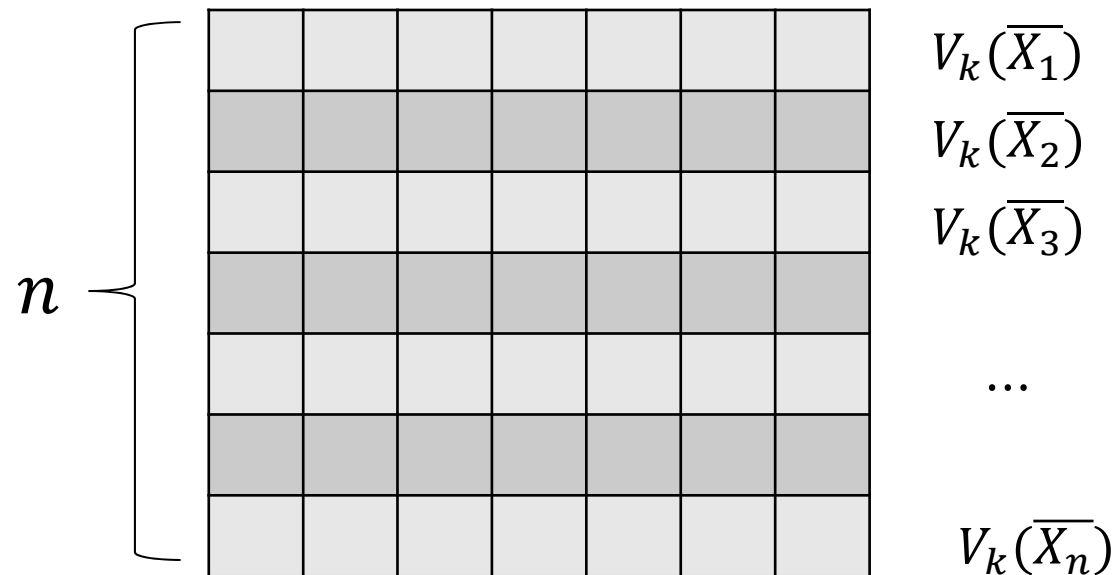
1. Evaluate the $n \times n$ distance matrix



The Naïve Approach for Finding Top r -Outliers



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

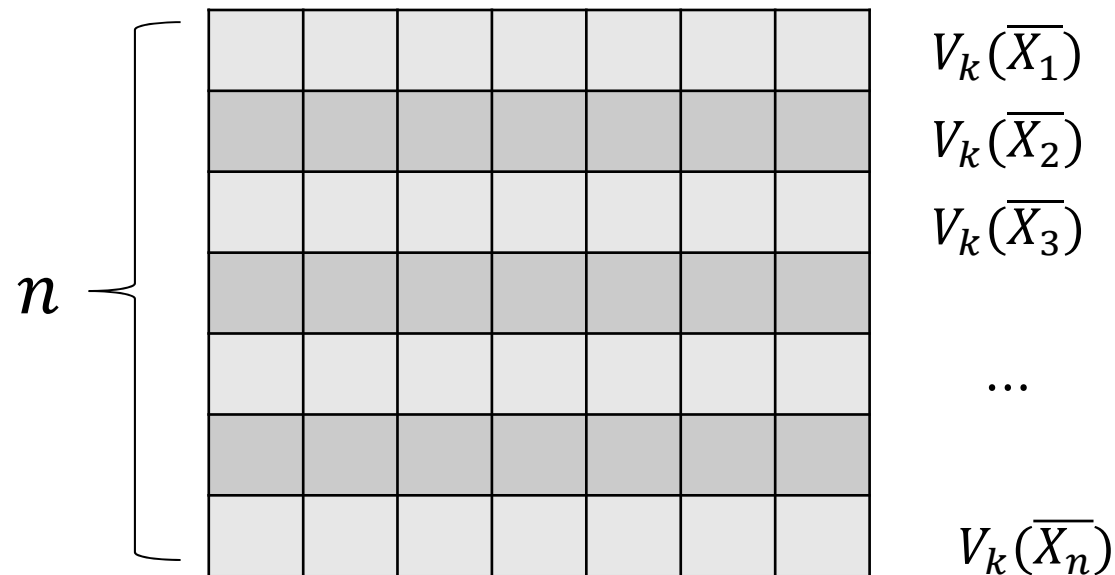


2. Find the k -th **smallest** value in each row

The Naïve Approach for Finding Top r -Outliers



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



2. Find the k -th **smallest** value in each row
3. Choose r data points with **largest** $V_k(\cdot)$

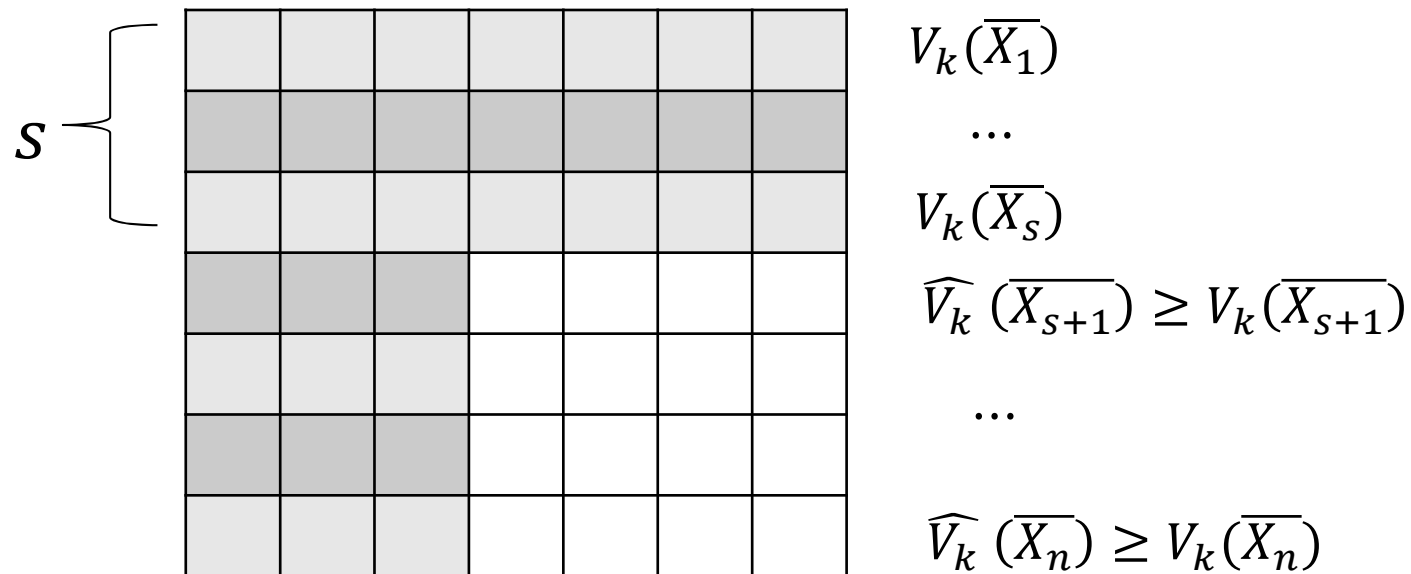


Diagram illustrating a sparse matrix structure. The matrix is represented as a grid of cells. The first row is shaded gray. The first three columns are shaded gray. The intersection of the first three rows and first three columns is shaded dark gray. A bracket on the left indicates the first row is part of a set of size s . The text $s \ll n$ is on the right.



Pruning Methods—Sampling

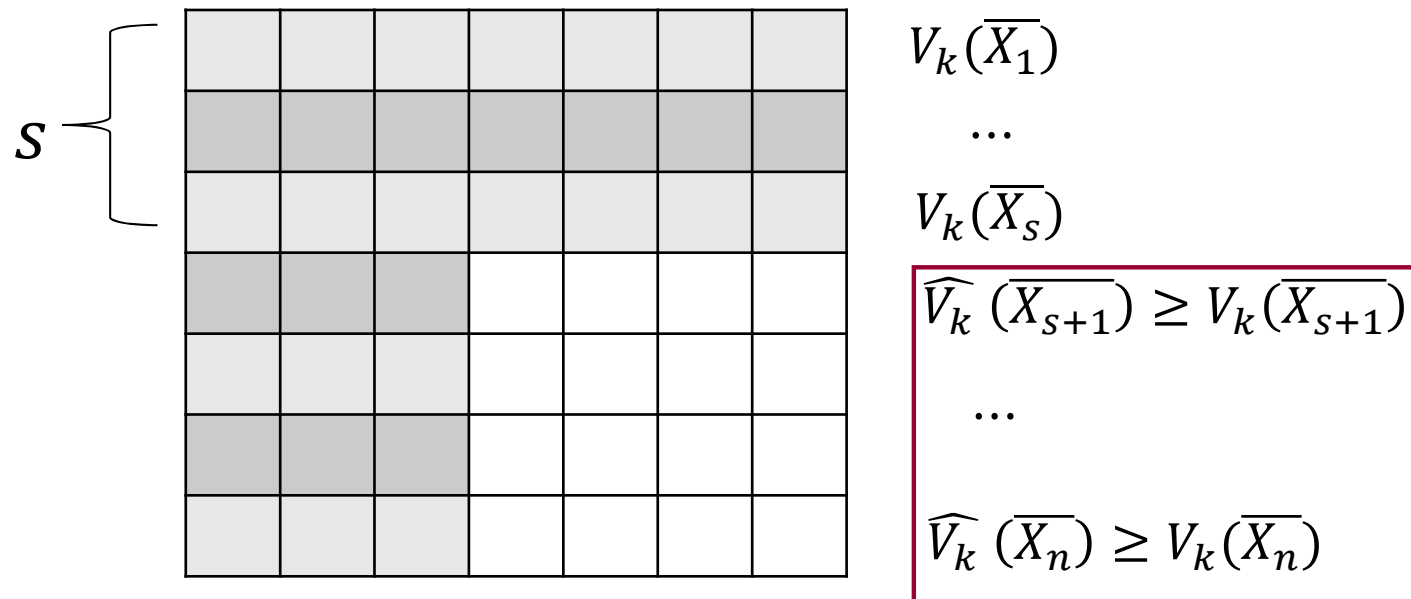
1. Evaluate a $s \times n$ distance matrix



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

Pruning Methods—Sampling

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



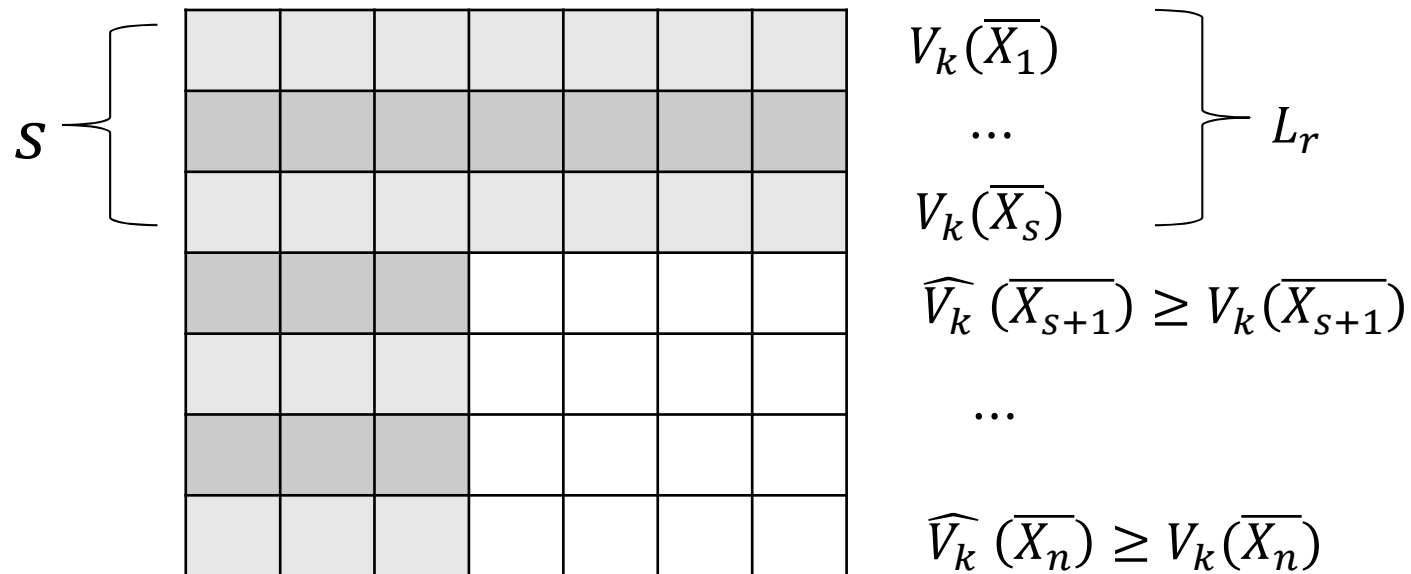
2. Find the k -th smallest value in each row

Il valore stimato della distanza dal k -esimo vicino è certamente un limite superiore del valore vero



Pruning Methods—Sampling

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



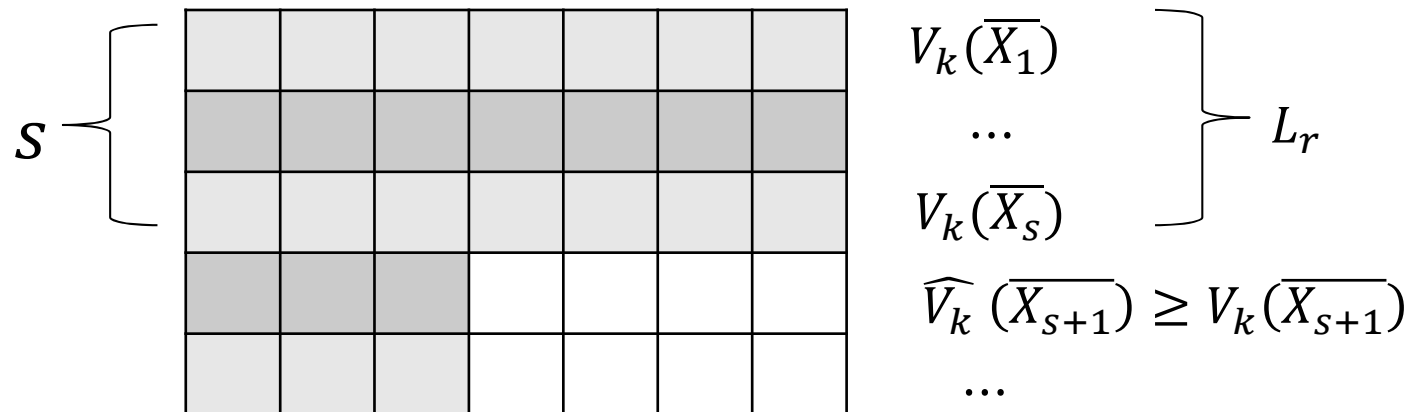
2. Find the k -th smallest value in each row

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



Pruning Methods—Sampling

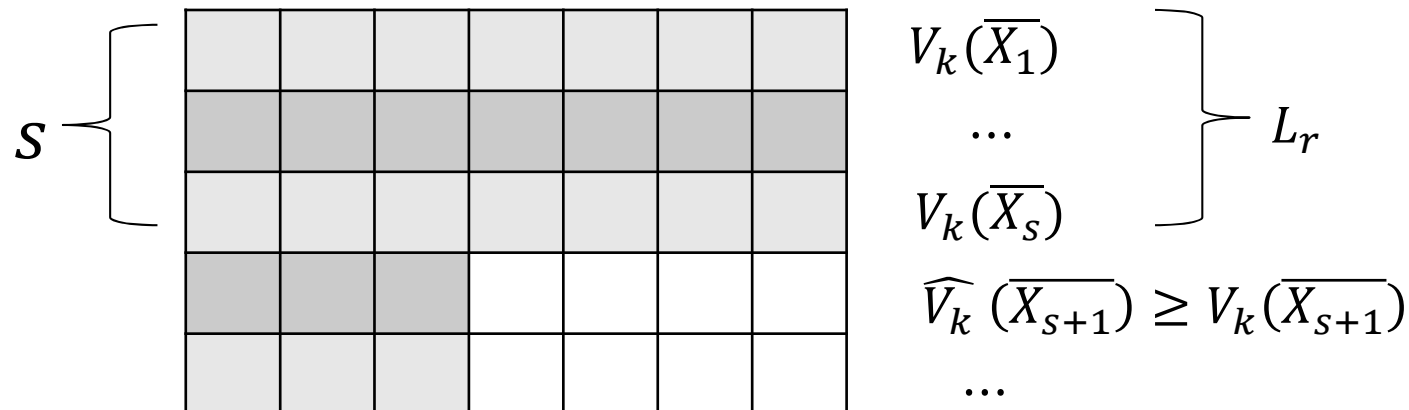
1. Evaluate a $s \times n$ distance matrix



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—Sampling

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



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

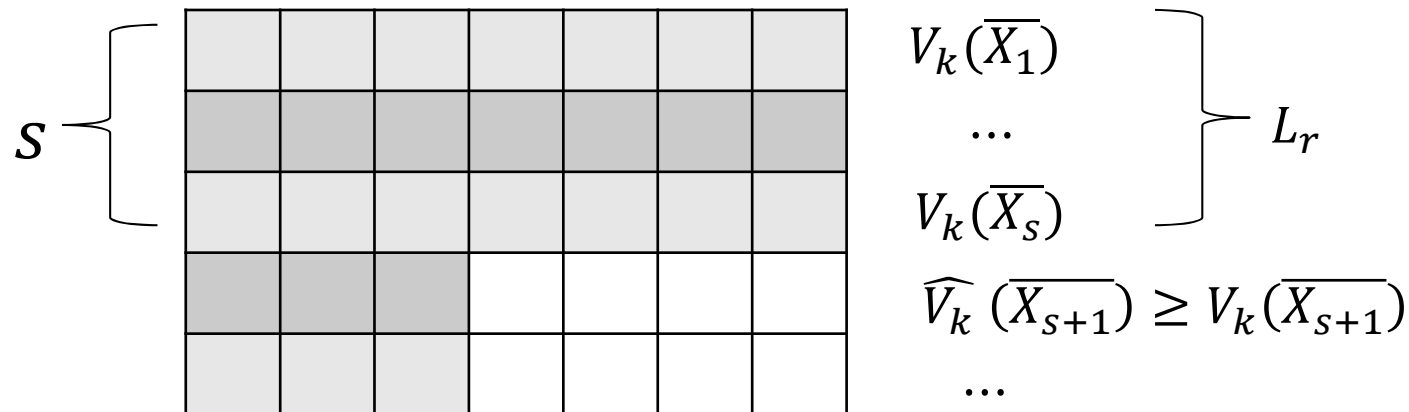
3. Identify the r -th score in top s -rows

4. Remove points with $\widehat{V}_k(\cdot) \leq L_r$

Il "limite superiore" alla loro distanza dal k -esimo vicino è certamente più piccolo del minimo degli r top outliers

Pruning Methods—Sampling

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



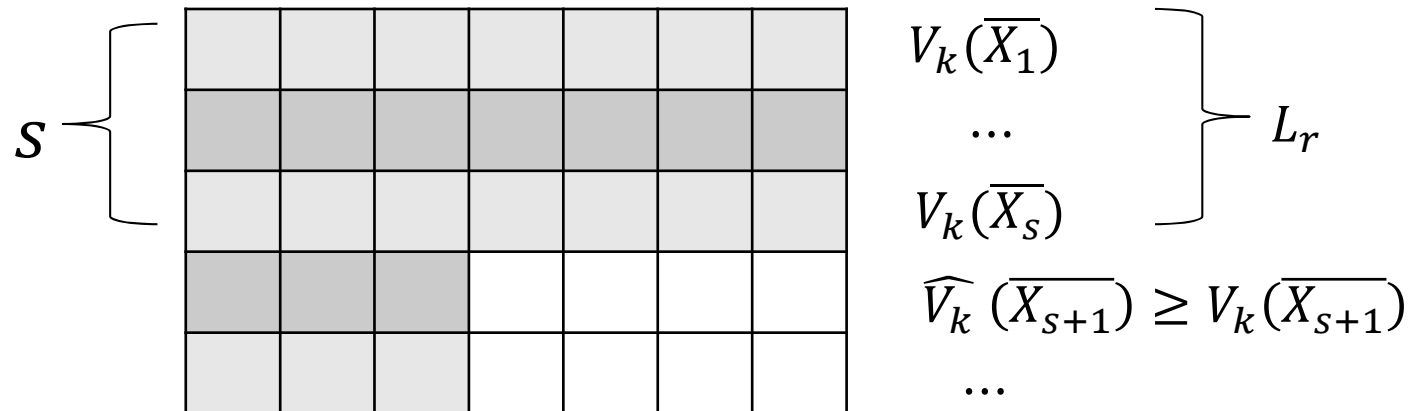
A questo punto è necessario calcolare le distanze rimanenti per individuare i veri r top outliers

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



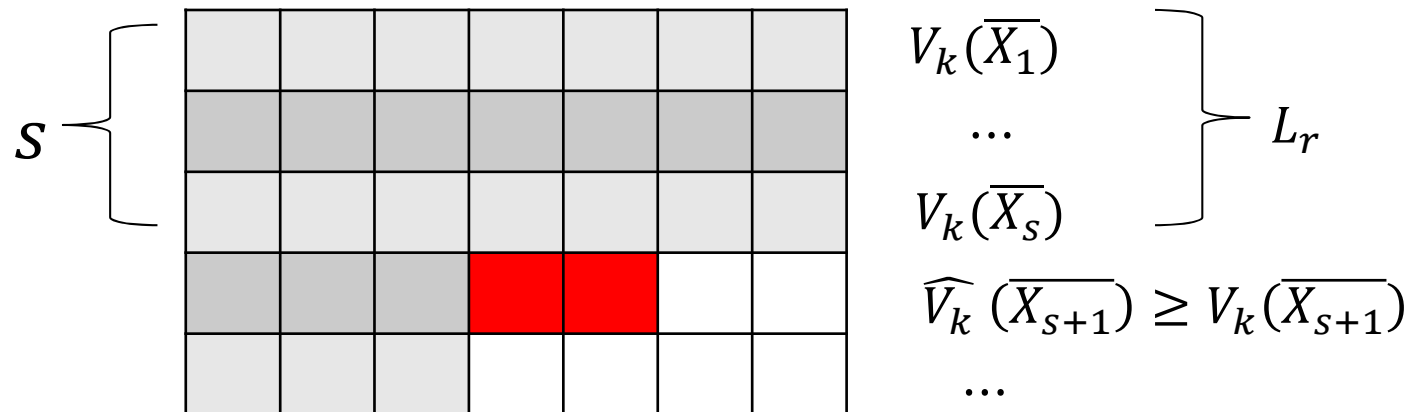
□ When completing the empty area



Pruning Methods—Early Termination



- When completing the empty area

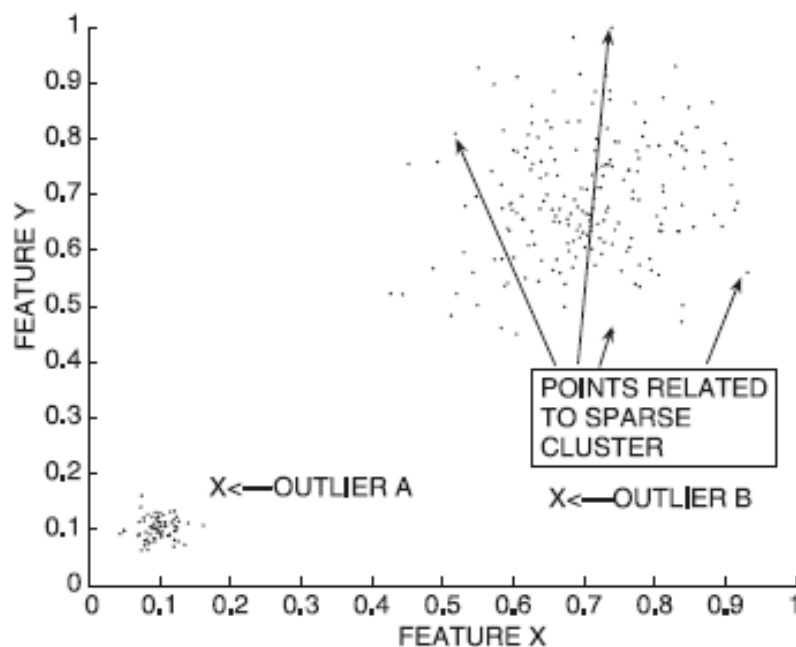


- Update $\widehat{V}_k(\cdot)$ when more distances are known
- Stop if $\widehat{V}_k(\cdot) \leq L_r$
- Update L_r if necessary

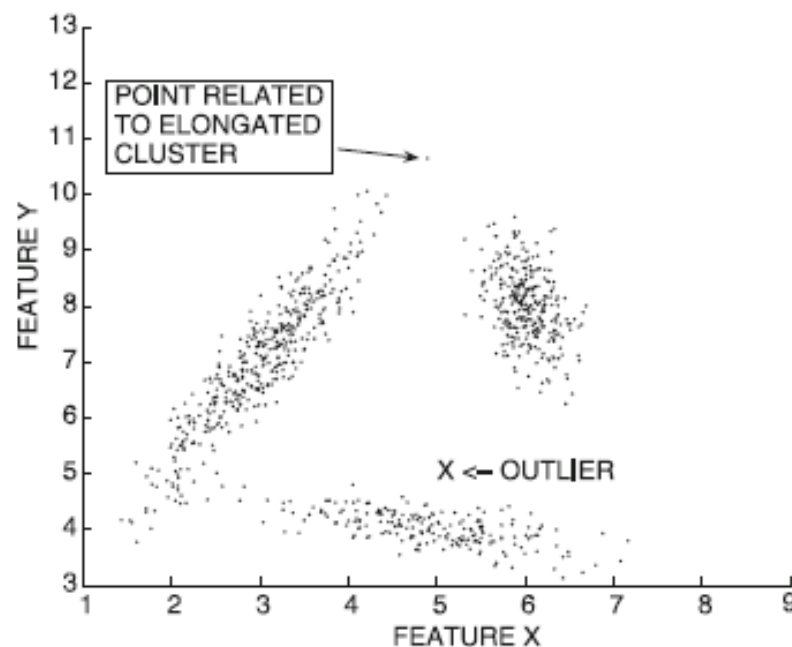
Local Distance Correction Methods



□ Impact of Local Variations



(a) Varying cluster density



(b) Varying cluster shape

La distanza euclidea non è un rank corretto per gli outlier.

E' necessario calcolare delle distanze "normalizzate" rispetto alla struttura locale dei cluster.



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

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

- 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

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

□ Local Outlier Factor

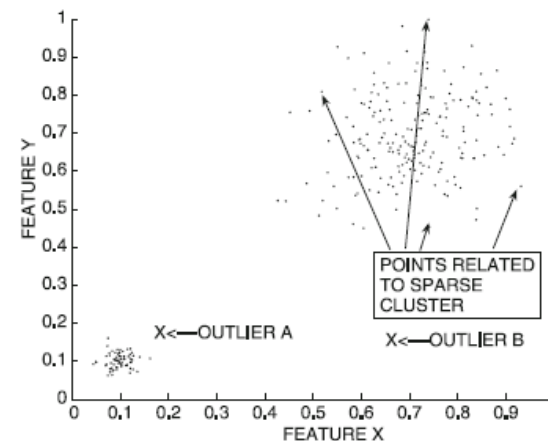
$$LOF_k(\bar{X}) = \text{MEAN}_{\bar{Y} \in L_k(\bar{X})} \frac{AR_k(\bar{X})}{AR_k(\bar{Y})}$$

I valori di $AR_k(X)$ e $LOF_k(X)$ sono calcolati rispetto alla Reachability dei punti in un intorno di X introducendo così il concetto di “normalizzazione” della distanza

- 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 $L^k(\bar{X})$

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

□ Instance-specific Mahalanobis score

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

□ Outlier score

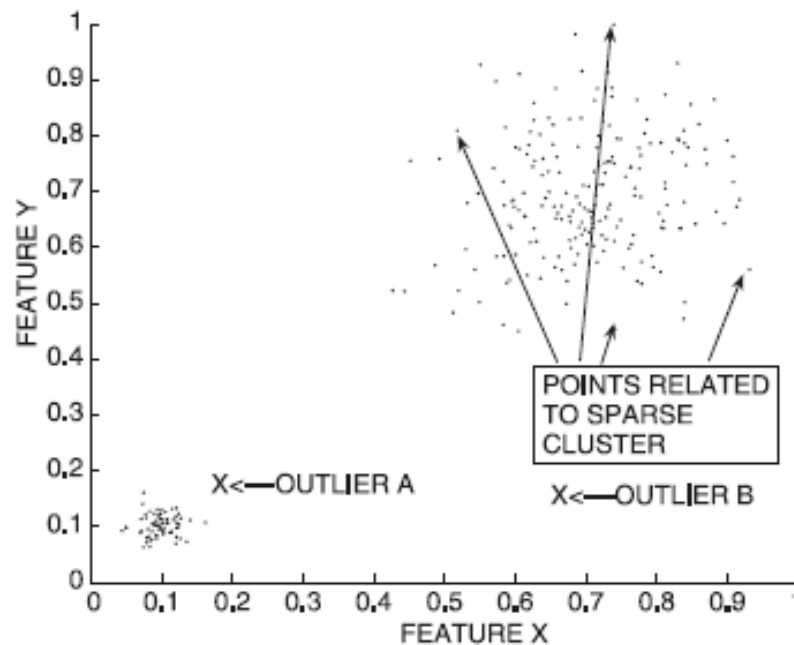
$$\max_k LMaha_k(\bar{X})$$

Il calcolo della matrice di covarianza locale introduce il concetto di “normalizzazione” della distanza

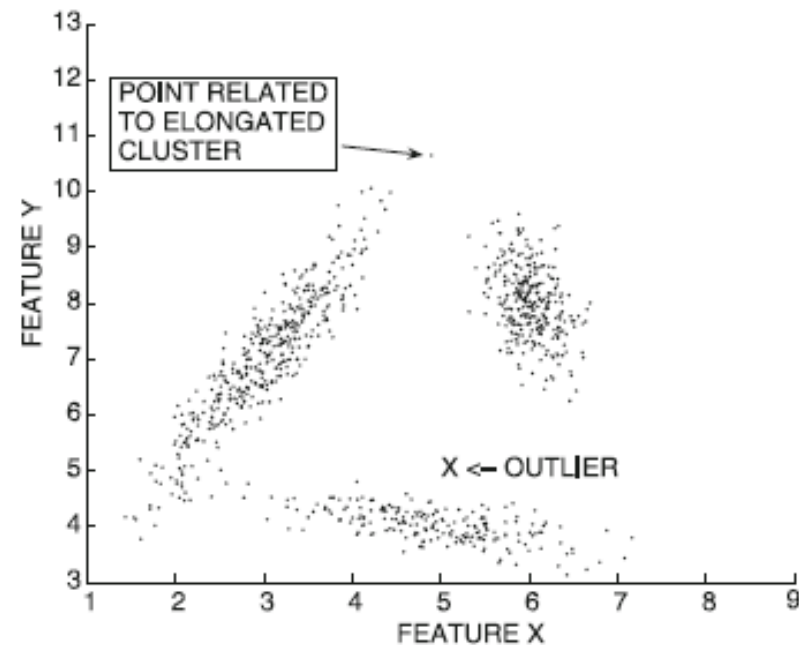
Instance-Specific Mahalanobis Distance (3)



□ Can be applied to both cases



(a) Varying cluster density



(b) Varying cluster shape

□ Relation to clustering-based approaches



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- ☐ Information-Theoretic Models
- ☐ Outlier Validity
- ☐ Summary

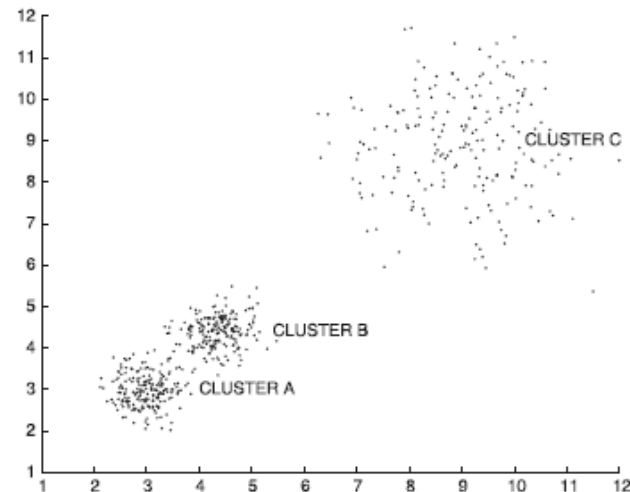
Density-Based Methods

□ The Key Idea

- Determine sparse regions in the underlying data

□ Limitations

- Cannot handle variations of density



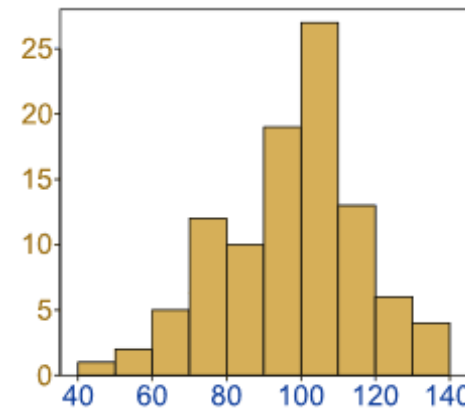
Histogram- and Grid-Based Techniques



□ Histogram for 1-dimensional data

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

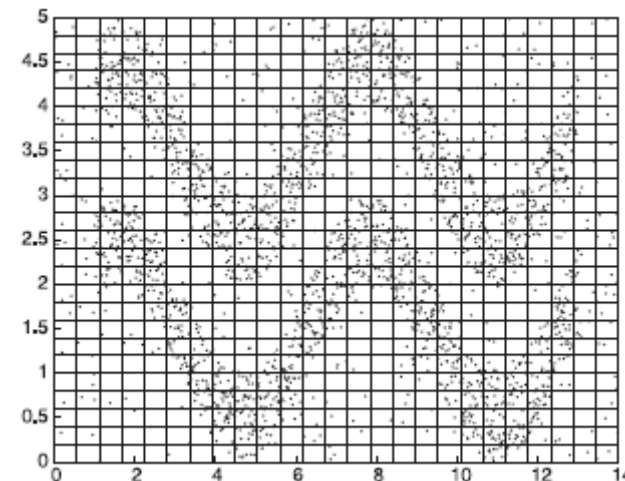
<https://www.mathsisfun.com/data/histograms.html>



□ Grid for high-dimensional data

□ Challenges

- Size of grid
- Too local
- Sparsity



Kernel Density Estimation

- Nella Kernel Density Estimation (KDE) la densità in un punto dello spazio \mathbb{R}^d viene stimata attraverso una *composizione di funzioni kernel* $K(\cdot)$ centrate nei vari punti del dataset \mathcal{D} :

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

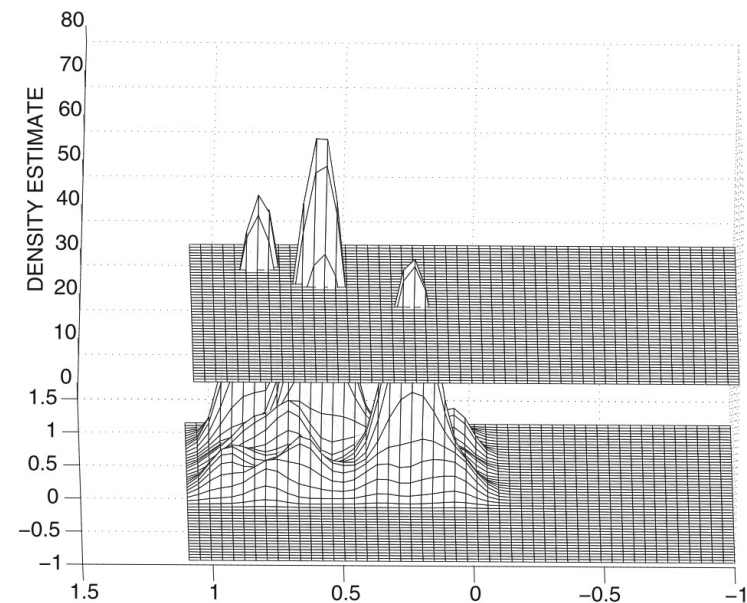
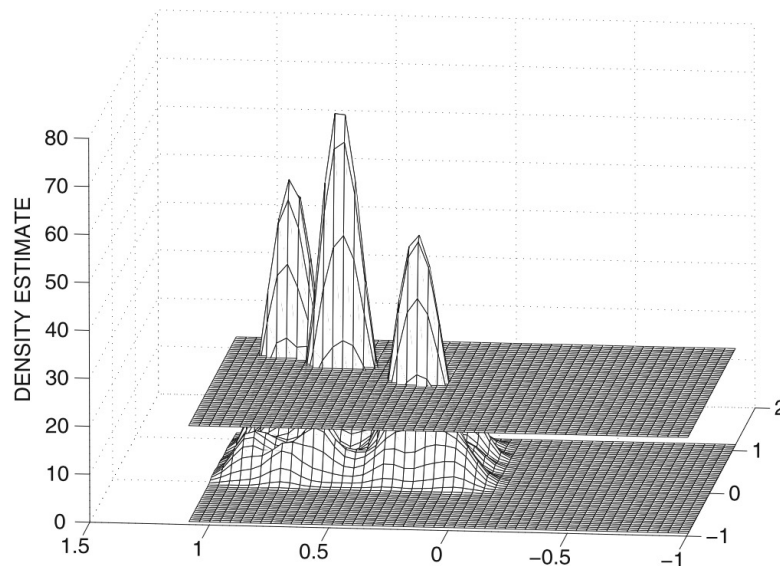
- Un a scelta tipica è quella del kernel gaussiano:

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

- Il parametro h definisce una misura di *smoothness* della stima e viene scelto euristicamente dai dati

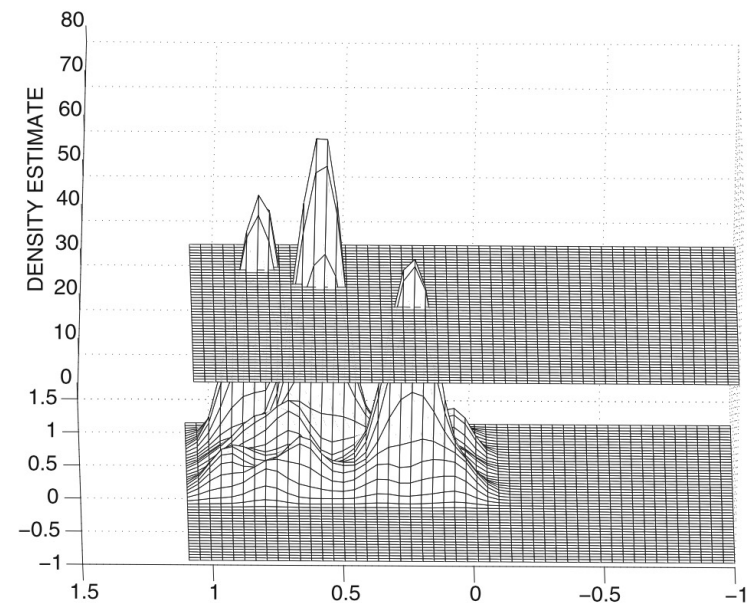
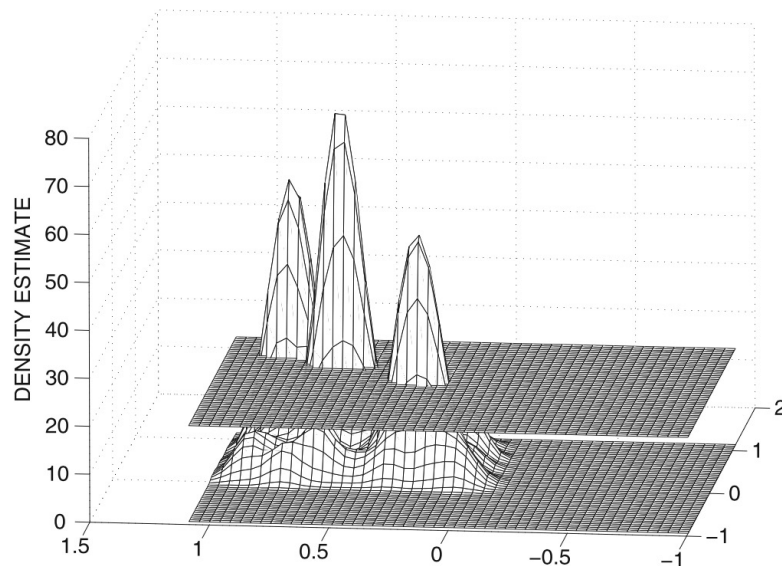
DENCLUE clustering tramite KDE

- DENCLUE cerca i cluster come i profili di intersezione della KDE con una soglia τ di densità
- Tutti i punti per cui $f(\cdot) < \tau$ sono considerati *outlier*
- La ricerca di τ è empirica: dipende dai dati ed è difficile determinarla



DENCLUE clustering tramite KDE

- DENCLUE usa il concetto di *attrattore di densità*:
 - Ogni picco di $f(\cdot)$ sarà un attrattore verso cui tendono i punti appartenenti a quel picco



DENCLUE clustering tramite KDE

- DENCLUE utilizza un approccio di tipo gradient ascent iterativo applicato ai punti di \mathcal{D} fino alla convergenza verso un massimo locale che sarà l'attrattore del cluster i -esimo

$$\overline{X^{(t+1)}} = \overline{X^{(t)}} + \alpha \nabla f(\overline{X^{(t)}})$$

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

DENCLUE clustering tramite KDE

- La forma del gradiente $\nabla f(\cdot)$ dipende dalla forma di $K(\cdot)$
- Il kernel gaussiano è una buona scelta perché si può mostrare che:

$$\nabla K(\bar{X} - \bar{X}_i) \propto (\bar{X}_i - \bar{X}) K(\bar{X} - \bar{X}_i)$$

DENCLUE clustering tramite KDE

- Alternativamente, se ottimizziamo ponendo $\nabla f(\cdot)=0$:

$$\sum_{i=1}^n \bar{X} K(\bar{X} - \bar{X}_i) = \sum_{i=1}^n \bar{X}_i K(\bar{X} - \bar{X}_i)$$

- Da cui viene una semplice regola di aggiornamento dei punti che converge più velocemente dell'altra

$$\bar{X}^{(t+1)} = \frac{\sum_{i=1}^n \bar{X}_i K(\bar{X}^{(t)} - \bar{X}_i)}{\sum_{i=1}^n K(\bar{X}^{(t)} - \bar{X}_i)}$$

DENCLUE clustering tramite KDE

- Complessità computazionale $O(n^2)$ come DBSCAN
 - n computazioni di $f(\cdot)$ ad ogni iterazione
- Si possono trascurare i contributi delle gaussiane centrate in punti lontani oltre $3h$
 - Si usano delle griglie per questa pre-computazione
- DBSCAN caso particolare di DENCLUE in cui:

$$K(\bar{X} - \bar{X}_i) = \begin{cases} 1, & \| \bar{X} - \bar{X}_i \|^2 < Eps \\ 0, & \text{altrimenti} \end{cases}$$



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Information-Theoretic Models

□ An Example

ABABABABABABABABABABABABABABABABABAB

ABABACABABABABABABABABABABABABABABAB

- 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



Information-Theoretic Models

□ An Example

ABABABABABABABABABABABABABABABABABAB

AB17

ABABACABABABABABABABABABABABABABABAB

- 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



Information-Theoretic Models

□ An Example

ABABABABABABABABABABABABABABABABABAB

AB17

ABABACABABABABABABABABABABABABABABAB

AB2A1C1AB14

- 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

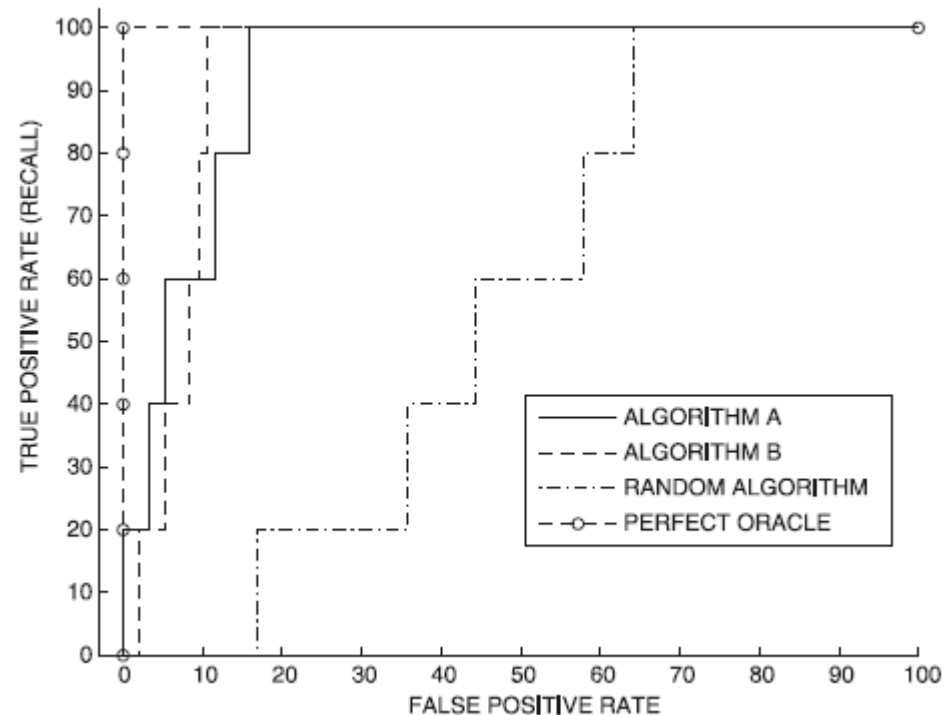
$$FPR(t) = 100 * \frac{|\mathcal{S}(t) - \mathcal{G}|}{|\mathcal{D} - \mathcal{G}|}$$

- 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