Methods and Evaluation

Imbalanced Domains and Rare Event Detection

Performance Evaluation

Why is performance evaluation a challenge?

- Standard metrics (e.g. error rate or mean squared error) describe the average predictive performance of the models
- When the user is focused on a small subset of rare values, the average is not a good idea
- These metrics will be mostly influenced by the performance of the models on cases that are irrelevant for the user

An Example from Classification

Fraud Detection

- Two classes: Fraud and Normal
- Fraudulent cases are roughly 1% of the training sample
- A classifier that always predicts Normal would achieve on average 99% accuracy!
- This classifier is completely useless!
- Because frauds are very rare, failing them or correctly predicting them will have a minor impact on the accuracy (or error rate) metric.

An Example from Regression

Forecasting Stock Market Returns

- Very high or low returns (% variations of prices) are interesting
- Near-zero returns are very common but uninteresting for traders - unable to cover transaction costs
- Examples:
  - Forecasting a future return of 3% and then it happens -5% is a very bad error!
  - Forecasting a return of 3% and then it happens 11% has the same error amplitude but it is not a serious error
  - Forecasting 0.2% for a true value of 0.4% is reasonably accurate but irrelevant!
  - Forecasting -7.5% for a true value of -8% is a good an useful prediction
- Because near 0 returns are very common a model that always forecasts 0 is hard to beat in terms of Mean Squared Error. But this model is useless!

Metrics and the Available Information

- Different applications may involve different type of information on the user preferences
- This may have an impact on the metrics you can and/or should calculate
- Independently, there are two classes of metrics: scalar and graphical

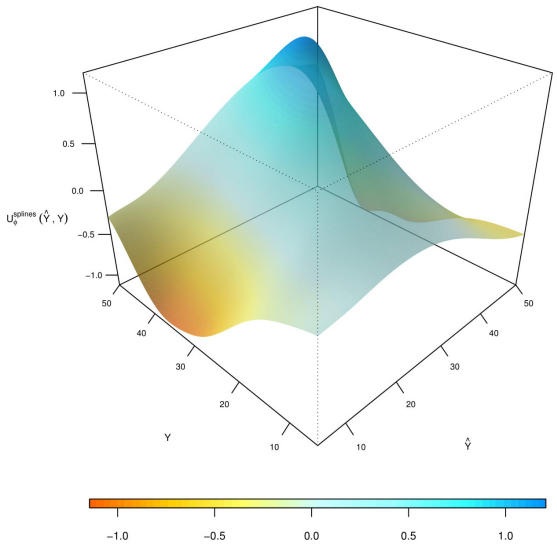
Evaluation with Full Utility Information

Utility Matrices

Table where each entry specifies the cost (negative benefit) or benefit of each type of prediction

		Pred.		
		c_1	c_2	c_3
Obs.	c_1	$B_{1,1}$	$C_{1,2}$	$C_{1,3}$
	c_2	$C_{2,1}$	$B_{2,2}$	$C_{2,3}$
	c_3	$C_{3,1}$	$C_{3,2}$	$B_{3,3}$

- Models are then evaluated by the total utility of their predictions, i.e. the sum of the benefits minus the costs.
- Similar setting for regression using Utility Surfaces (Ribeiro, 2011)



R. Ribeiro (2011). "Utility-based Regression". PhD on Computer Science, Univ. Porto.

The Precision/Recall Framework

Classification

- Problems with two classes
- One of the classes is much less frequent and it is also the most relevant

		Preds.	
		Pos	Neg
Obs.	Pos	True Positives (TP)	False Negatives (FN))
	Neg	False Positives (FP)	True Negatives (TN)

The Precision/Recall Framework

Classification - 2

		Preds.	
		P	N
Obs.	P	TP	FN
	N	FP	TN

- *Precision* - proportion of the signals (events) of the model that are correct

$$Prec = \frac{TP}{TP + FP}$$

- *Recall* - proportion of the real events that are captured by the model

$$Rec = \frac{TP}{TP + FN}$$

The F-Measure

Combining Precision and Recall into a single measure

- Useful to have a single measure - e.g. optimization within a search procedure
- Maximizing one of them is easy at the cost of the other (it is easy to have 100% recall - always predict "P").
- What is difficult is to have both of them with high values

The F-Measure

Combining Precision and Recall into a single measure

- Useful to have a single measure - e.g. optimization within a search procedure
- Maximizing one of them is easy at the cost of the other (it is easy to have 100% recall - always predict "P").
- What is difficult is to have both of them with high values
- The F-measure is a statistic that is based on the values of precision and recall and allows establishing a trade-off between the two using a user-defined parameter (β),

$$F_\beta = \frac{(\beta^2 + 1) \cdot Prec \cdot Rec}{\beta^2 \cdot Prec + Rec}$$

where β controls the relative importance of *Prec* and *Rec*. If $\beta = 1$ then F is the harmonic mean between *Prec* and *Rec*; When $\beta \to 0$ the weight of *Rec* decreases. When $\beta \to \infty$ the weight of *Prec* decreases.

The G-Mean and Adjusted G-Mean

$$Gm = \sqrt{\frac{TP}{TP+FN} \times \frac{TN}{TN+FP}} = \sqrt{sensitivity \times specificity}$$

$$AGm = \begin{cases} \frac{Gm + Specificity \times N_n}{1+N_n} & sensitivity \geq 0 \\ 0 & sensitivity = 0 \end{cases}$$

where N_n is the proportion of majority class examples in the data set.

M. Kubat and S. Matwin. "Addressing the curse of imbalanced training sets: one-sided selection." In Proc. of 14th Int. Conf. on Machine Learning, 1997, Nashville, USA, pp.179-186

R. Batuwita and V. Palade. "A new performance measure for class imbalance learning. Application to bioinformatics problems." In ICMLA'09, pp.545–550. IEEE, 2009.

Metrics for Multiclass Imbalance Problems

- $\phi(i)$ is the relevance of class i.
- Different ways to obtain $\phi()$ depending on the available domain information (Branco, 2017).

$$Rec^{\phi} = \frac{1}{\sum_{i=1}^{C} \phi(i)} \sum_{i=1}^{C} \phi(i) \cdot recall_i \qquad Prec^{\phi} = \frac{1}{\sum_{i=1}^{C} \phi(i)} \sum_{i=1}^{C} \phi(i) \cdot precision_i$$

$$F_{\beta}^{\phi} = \frac{(1+\beta^2) \cdot Prec^{\phi} \cdot Rec^{\phi}}{(\beta^2 \cdot Prec^{\phi}) + Rec^{\phi}} \qquad AvF_{\beta}^{\phi} = \frac{1}{\sum_{i=1}^{C} \phi(i)} \sum_{i=1}^{C} \frac{\phi(i) \cdot (1+\beta^2) \cdot precision_i \cdot recall_i}{(\beta^2 \cdot precision_i) + recall_i}$$

$$CBA^{\phi} = \sum_{i=1}^{C} \phi(i) \cdot \frac{mat_{i,i}}{max\left(\sum_{j=1}^{C} mat_{i,j}, \sum_{j=1}^{C} mat_{j,i}\right)}$$

P. Branco, L. Torgo, and R. Ribeiro. "Relevance-based evaluation metrics for multi-class imbalanced domains." PAKDD. Springer, Cham, pp.698-710 (2017).

The Precision/Recall Framework

Regression

For forecasting rare extreme values, the concepts of Precision and Recall were also adapted to regression (Torgo and Ribeiro, 2009; Branco, 2014),

$$prec^{\phi} = \frac{\sum_{\phi(\hat{y}_i)>t_R}(1 + U(\hat{y}_i, y_i))}{\sum_{\phi(\hat{y}_i)>t_R}(1 + \phi(\hat{y}_i))}$$

$$rec^{\phi} = \frac{\sum_{\phi(y_i)>t_R}(1 + U(\hat{y}_i, y_i))}{\sum_{\phi(y_i)>t_R}(1 + \phi(y_i))}$$

L. Torgo and R. P. Ribeiro (2009). "Precision and Recall for Regression". In: Discovery Science'2009. Springer.

P. Branco (2014). "Re-sampling Approaches for Regression Tasks under Imbalanced Domains". MSc on Computer Science, Univ. Porto.

Summary of Scalar Metrics for Imbalanced Domains

Metric type	Task type		Metric	Main References
Scalar	Classification	binary	$TP_{rate}(recall\ or\ sensitivity)$, $TN_{rate}(specificity)$, FP_{rate}, FN_{rate}, $PP_{value}(precision)$, NP_{value}, F_β, $G-Mean$, $dominance$, $IBA_\alpha(M)$, CWA, $balanced\ accuracy$, $optimized\ precision$, $adjusted\ G-Mean$, B_{42}	Rijsbergen [1979], Kubat et al. [1998], Estabrooks and Japkowicz [2001], Cohen et al. [2006], Ranawana and Palade [2006], García et al. [2008, 2009], Batuwita and Palade [2009], Brodersen et al. [2010], García et al. [2010], Thai-Nghe et al. [2011], Batuwita and Palade [2012]
		multiclass	$recall(c)$, $precision(c)$, $F_\beta(c)$, Rec_μ, $Prec_\mu$, Rec_M, $Prec_M$, MF_β, $MF_{\beta\mu}$, $MF_{\beta M}$, $MAvA$, $MAvG$, CWA, $Prec^{Prev}$, Rec^{Prev}, F_β^{Prev}, CBA^{Prev}, $Prec^{TO}$, Rec^{TO}, F_β^{TO}, CBA^{TO}, $Prec^{PO}$, Rec^{PO}, F_β^{PO}, CBA^{PO}, $Prec^{\phi}$, Rec^{ϕ}, F_β^{ϕ}, CBA^{ϕ}	Sun et al. [2006], Ferri et al. [2009], Sokolova and Lapalme [2009], Branco et al. [2017b]
	Regression		NMU, $precision^u$, $recall^u$, $precision^\phi$, $recall^\phi$	Torgo and Ribeiro [2007, 2009], Ribeiro [2011], Branco [2014]

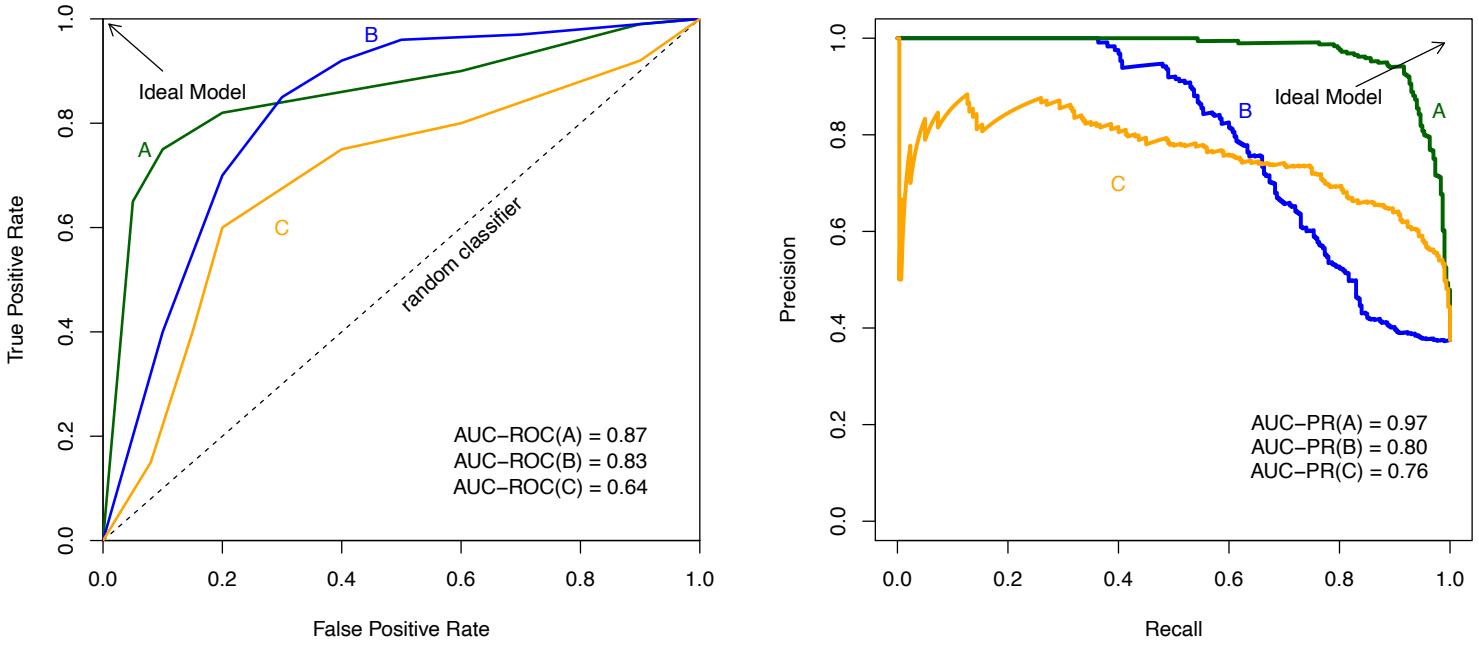
Adapted from:

P. Branco, L. Torgo and R. Ribeiro. "A Survey of Predictive Modeling on Imbalanced Domains". In: ACM Comput. Surv. 49-2, 1–31 (2016).

P. Branco (2018). "Utility-based Predictive Analytics". PhD on Computer Science, Univ. Porto.

ROC curve and Precision-Recall Curve

Classification

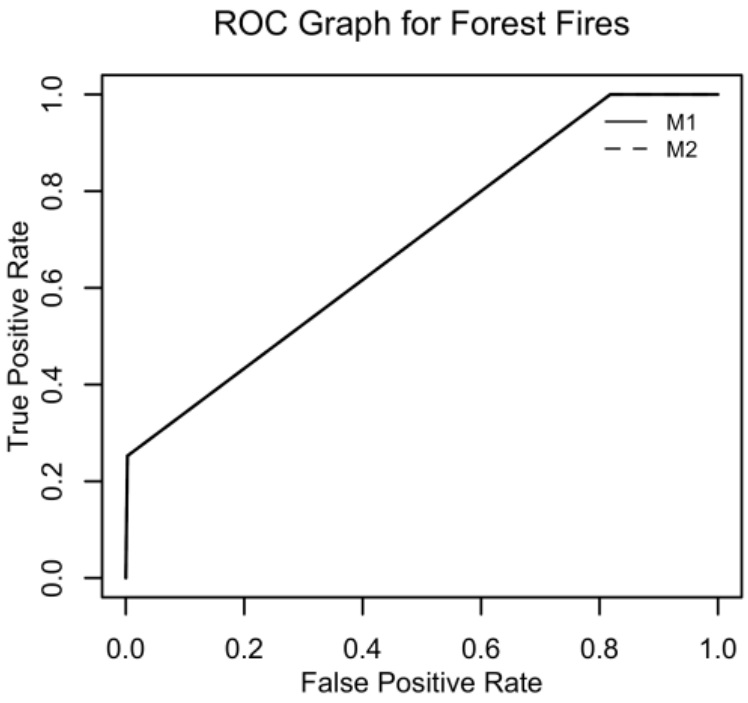


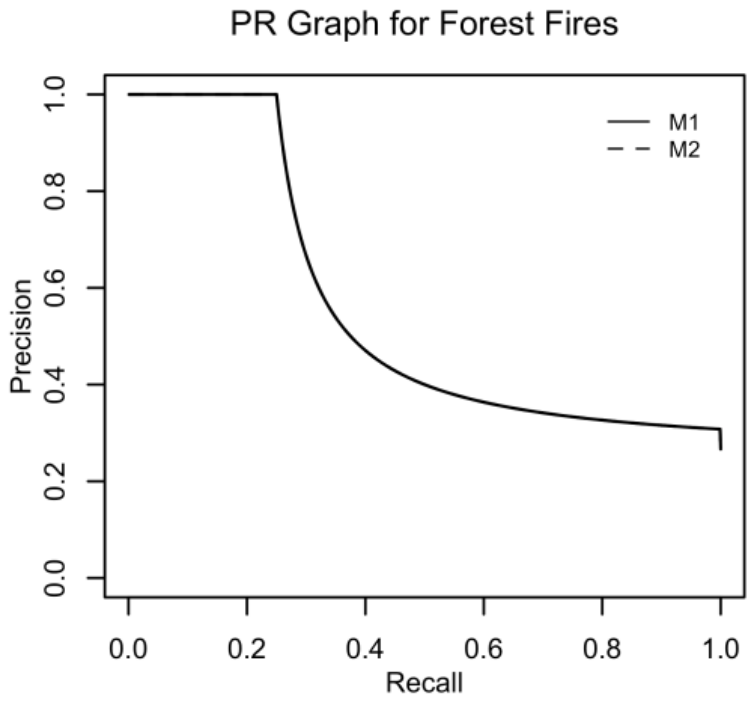
Taken from:

P. Branco (2018). "Utility-based Predictive Analytics". PhD on Computer Science, Univ. Porto.

ROC curve and Precision-Recall Curve

Regression





Taken from:

R. Ribeiro (2011). "Utility-based Regression". PhD on Computer Science, Univ. Porto.

Summary of Graphical Metrics for Imbalanced Domains

Metric type	Task type		Metric	Main References
Graphical	Classification	binary	*ROC curve*, *AUC*, *ProbAUC*, *ScoredAUC*, *WAUC*, *PR curve*, *Cost curve*, *Brier curve*,	Egan [1975], Metz [1978], Bradley [1997], Provost and Fawcett [1997], Provost et al. [1998], Drummond and Holte [2000a], Ferri et al. [2005], Davis and Goadrich [2006], Fawcett [2006b], Wu et al. [2007], Weng and Poon [2008], Hand [2009], Ferri et al. [2011b,a]
		multiclass	*ROC surface*, *AUNU*, *AUNP*, *AU1U*, *AU1P*, *SAUC*, *PAUC*	Mossman [1999], Ferri et al. [2009], Alejo et al. [2013], Sánchez-Crisostomo et al. [2014]
	Regression		$AUC-ROC^{\phi}$, $AUC-PR^{\phi}$, $AUC-ROCIV^{\phi}$, $AUC-PRIV^{\phi}$, *REC surface*	Torgo [2005], Ribeiro [2011]

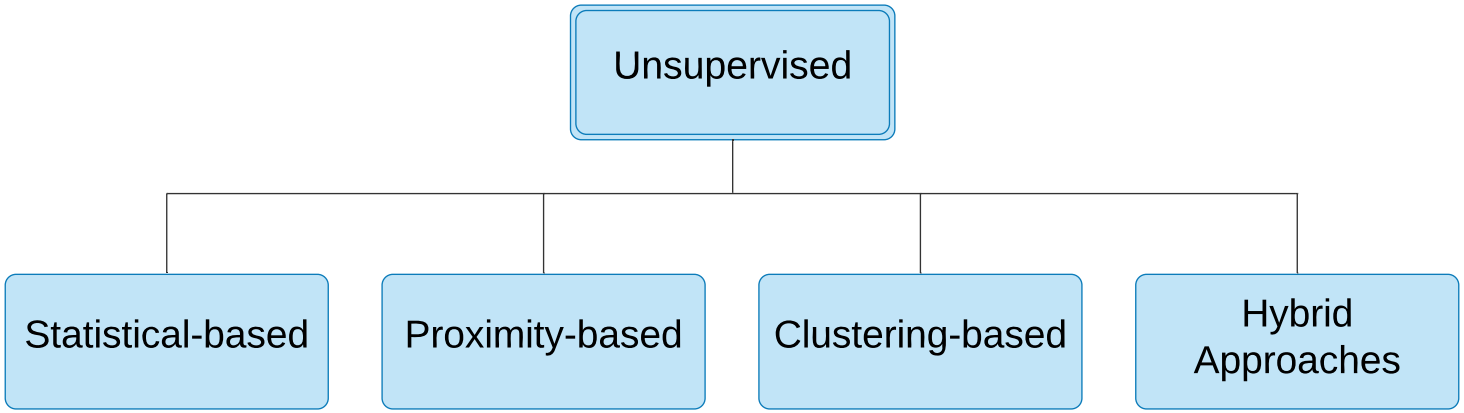
Adapted from:
P. Branco, L. Torgo and R. Ribeiro. "A Survey of Predictive Modeling on Imbalanced Domains". In: ACM Comput. Surv. 49-2, 1–31 (2016).

P. Branco (2018). "Utility-based Predictive Analytics". PhD on Computer Science, Univ. Porto.

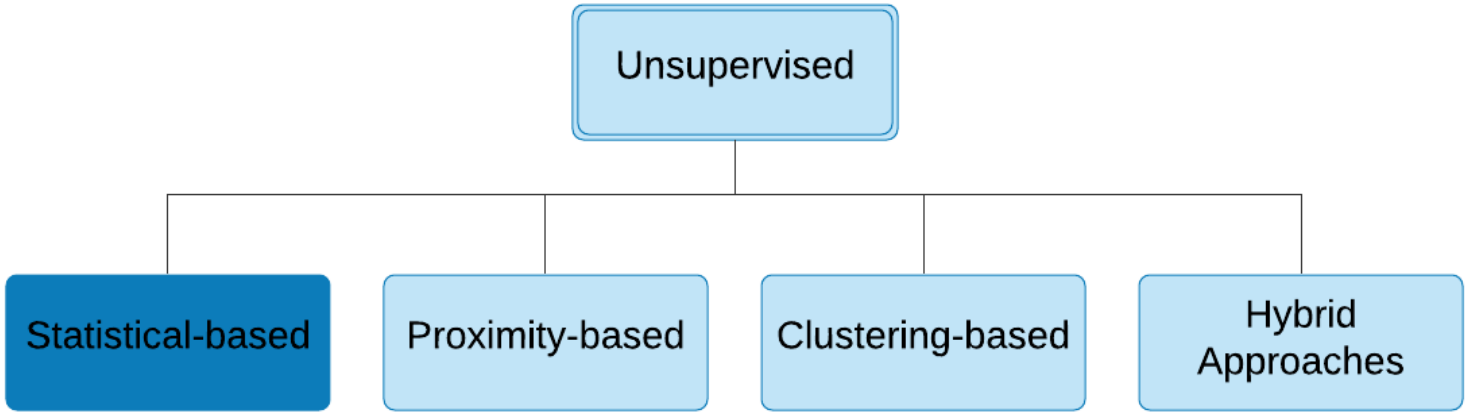
Imbalanced Domains and Rare Event Detection

Unsupervised Methods

Unsupervised Methods



Unsupervised Methods



Statistical-based Methods

Parametric

Assumption

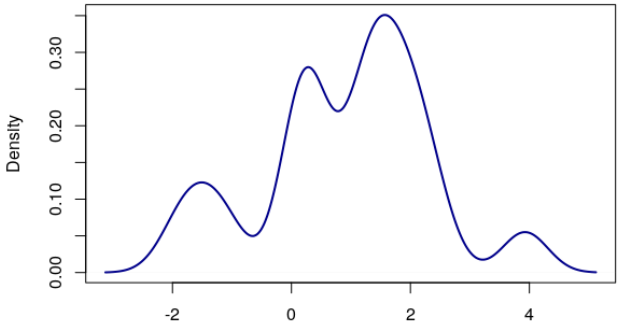
Normal instances occur in high probability regions of a stochastic model.
Anomalies occur in the low probability regions of the stochastic model.

- Gaussian Model Based
- Regression Model Based
- Mixture of Parametric Distributions Based

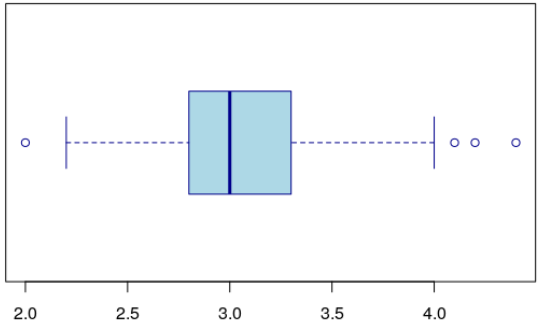
Statistical-based Methods

Parametric

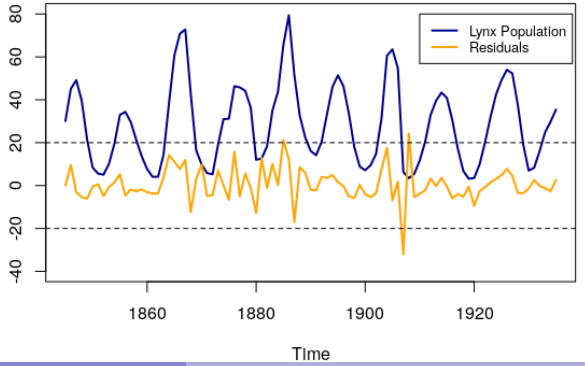
- Grubb's test
  $z = \frac{|x-\mu|}{\sigma}$



- Box Plot Rule



- Regression model based
  - fit a regression model
  - use the residuals to determine the anomaly score



Statistical-based Methods

Non-parametric

Assumption

The model structure is not determined a priori but is determined from the given data. Few assumptions regarding the data when compared to parametric techniques.

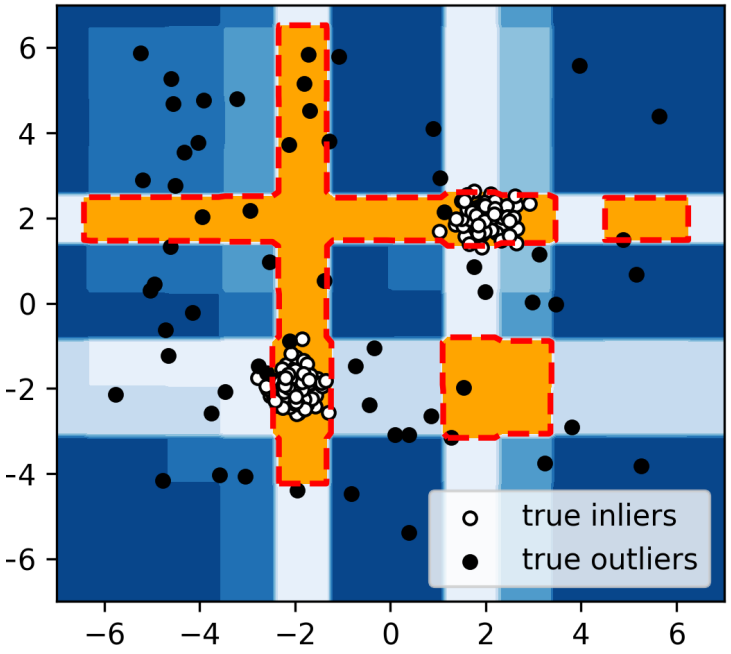
- Histogram Based
- Kernel Function Based

Statistical-based Methods

Non-parametric

Histogram Based

- build histogram
- for a new test instance, check if it falls in a bin of the histogram. If it does: normal, otherwise: anomaly.
- Variant: assign an anomaly score based on the bin frequency



Statistical-based Methods

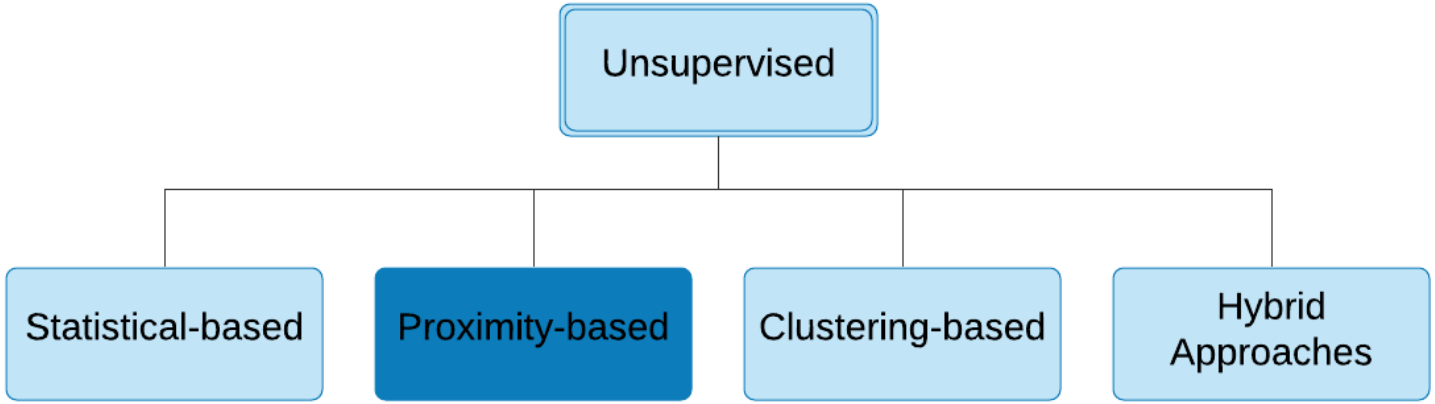
Non-parametric

Kernel Function Based

- Non-parametric techniques for probability density estimation
- Example: parzen windows estimation (Parzen, 1962)
- Use kernel functions to approximate the actual density.
- Similar to parametric methods. Difference: the density estimation technique used

Parzen, E. (1962) On the estimation of a probability density function and mode. Annals of Mathematical Statistics 33, 1065–1076.

Unsupervised Methods



Proximity-based Methods

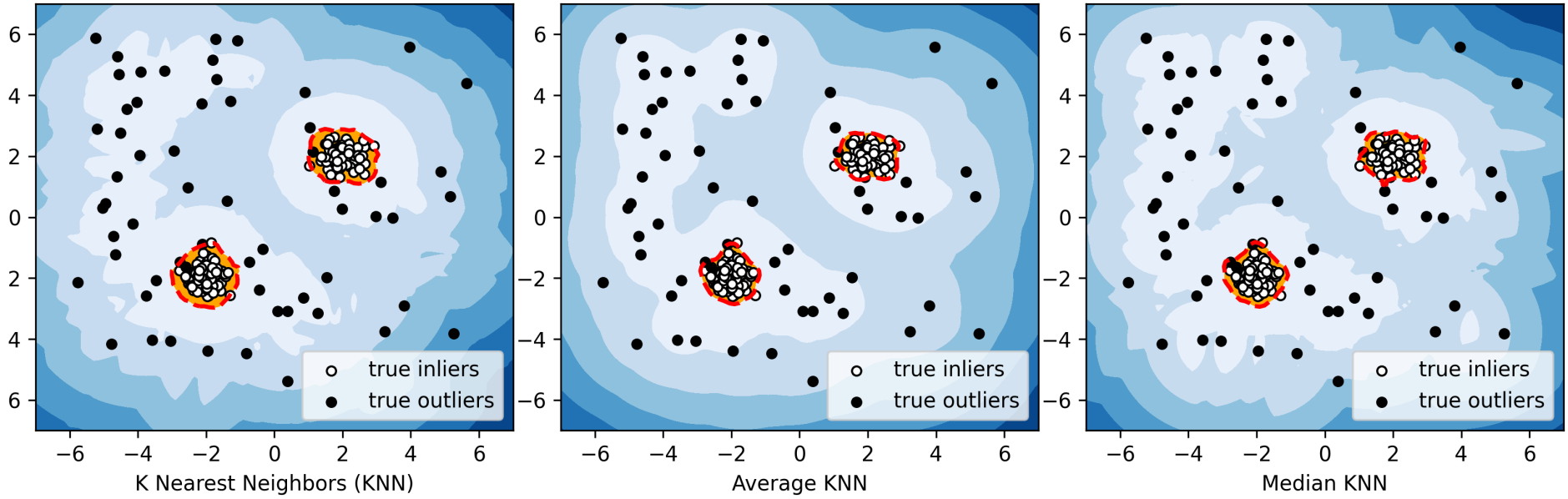
Distance-based: Nearest Neighbors (NN) Approach

- The anomaly score of a case is its distance to the kth nearest neighbor
- Apply a threshold on the anomaly score to determine is a case is anomalous or not.
- Examples of applications: land mines detection from satellite ground images, detect anomalies in large synchronous turbine-generators

Ramaswamy, S.,Rastogi, R. and Shim., K. "Efficient algorithms for mining outliers from large data sets." Proceedings of the 2000 ACM SIGMOD international conference on Management of data. 2000.

Proximity-based Methods

Distance-based: Nearest Neighbors (NN) Approach



Proximity-based Methods

Distance-based: Nearest Neighbors (NN) Approach

- Alternative way for computing the anomaly score: count the number of nearest neighbors that are not more than d distance apart from the case.
- Can be viewed as a way to obtain an estimate of the global density for each case.

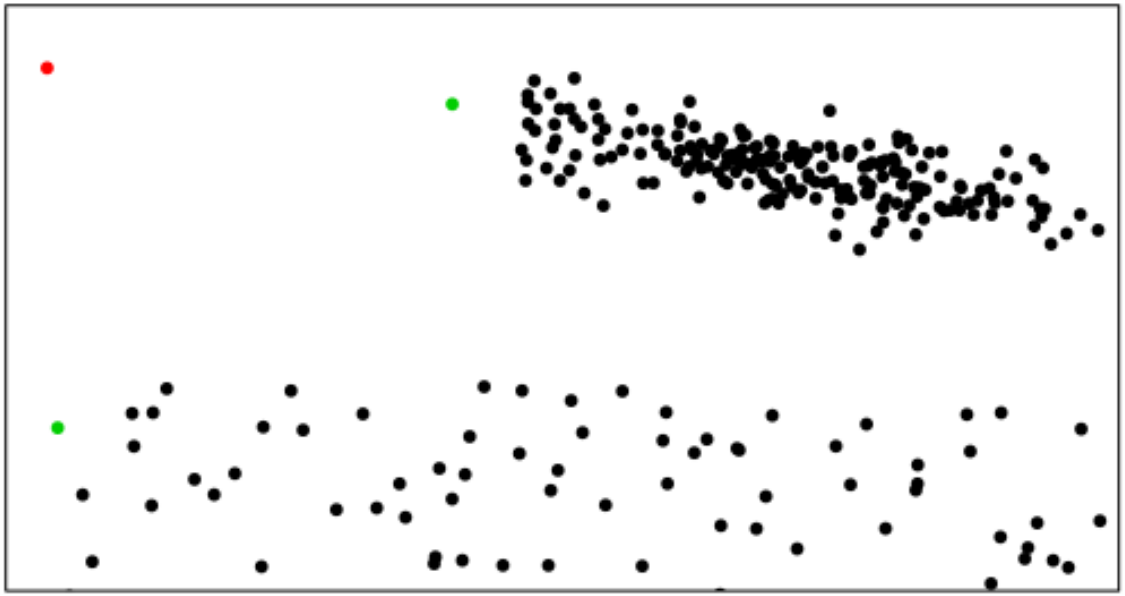
Knorr, E. M., and Ng, R. T. "Algorithms for mining distance based outliers in large datasets." Proceedings of the international conference on very large data bases. 1998.

Proximity-based Methods

LOF-based

Local Outlier Factor (LOF) (Breunig et al., 2000)

Each point has a score that captures the relative degree of isolation of the point from its surrounding neighbourhood.



Breunig, M. M., Kriegel, H. P., Ng, R., and Sander, J. (2000). "LOF: Identifying density-based local outliers." In Chen, W., Naughton, J. F., and Bernstein, P. A., editors, Proceedings of ACM SIGMOD 2000 International Conference on Management of Data. ACM Press.

Proximity-based Methods

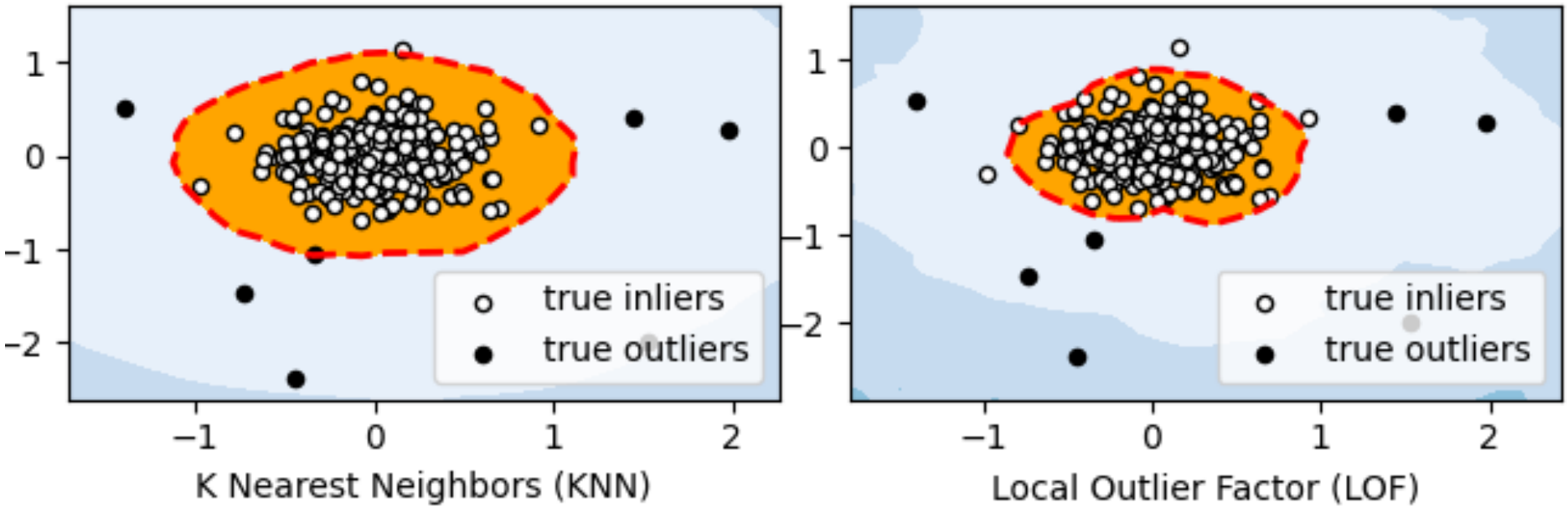
LOF-based

LOF Approach

- MinPts: number of nearest neighbors used in defining the local neighborhood
- For each point x compute distance to the kth nearest neighbor $(k - dist)$
- Compute reachability distance: $reach - dist_k(x, p) = max\{k - dist(p), d(x, p)\}$
- Compute local reachability density: $lrd_{MinPts}(x) = \frac{MinPts}{\sum_p reach - dist_{MinPts}(x,p)}$
- Compute LOF score: $LOF_{MinPts}(x) = \frac{1}{MinPts} \cdot \sum_p \frac{lrd_{MinPts}(p)}{lrd_{MinPts}(x)}$

Proximity-based Methods

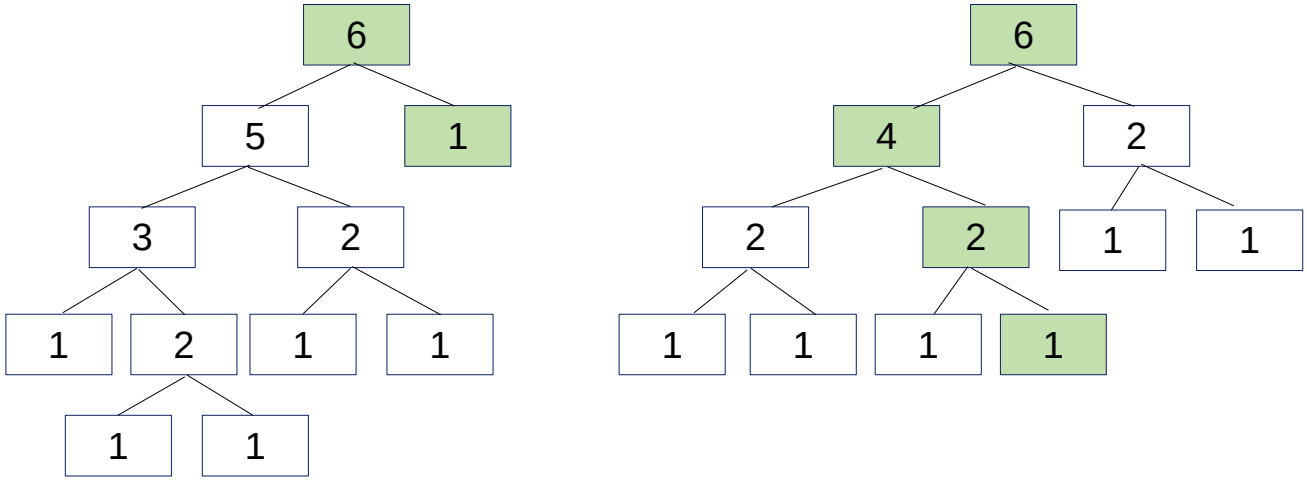
KNN-based vs LOF-based



Proximity-based Methods

Isolation Forest

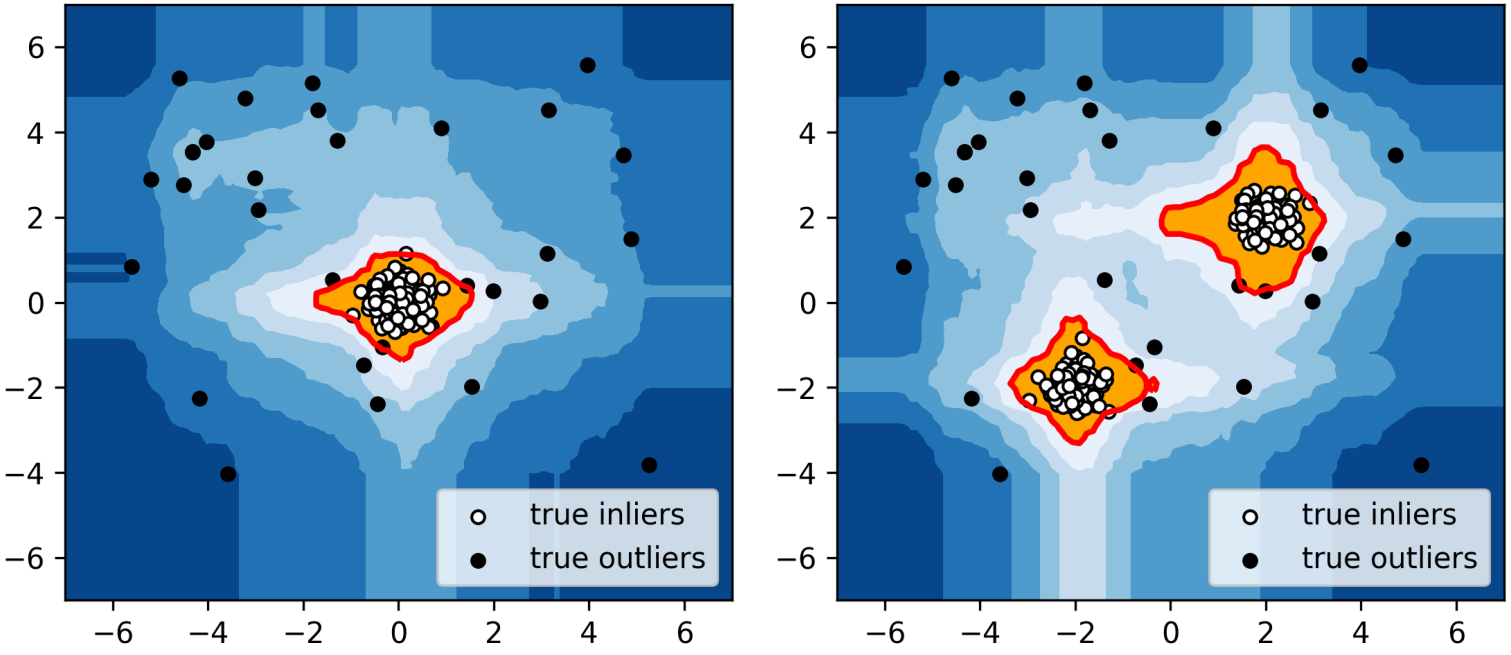
- Anomalies are **few and different**.
  - Collection of isolation trees (iTrees)
  - Each iTree isolates every case from the remaining cases for a given sample
  - Anomalies should be more susceptible to isolation, i.e., they exhibit a shorter average path
  - $Score(x) = \frac{1}{t}\sum_{i=1}^{t} l_i(x)$, where $l_i(x)$ is the path length of observation x in tree i



[1] Liu, Fei Tony; Ting, Kai Ming; Zhou, Zhi-Hua (2008). "Isolation Forest". 2008 Eighth IEEE International Conference on Data Mining: 413–422.

Proximity-based Methods

Isolation Forest



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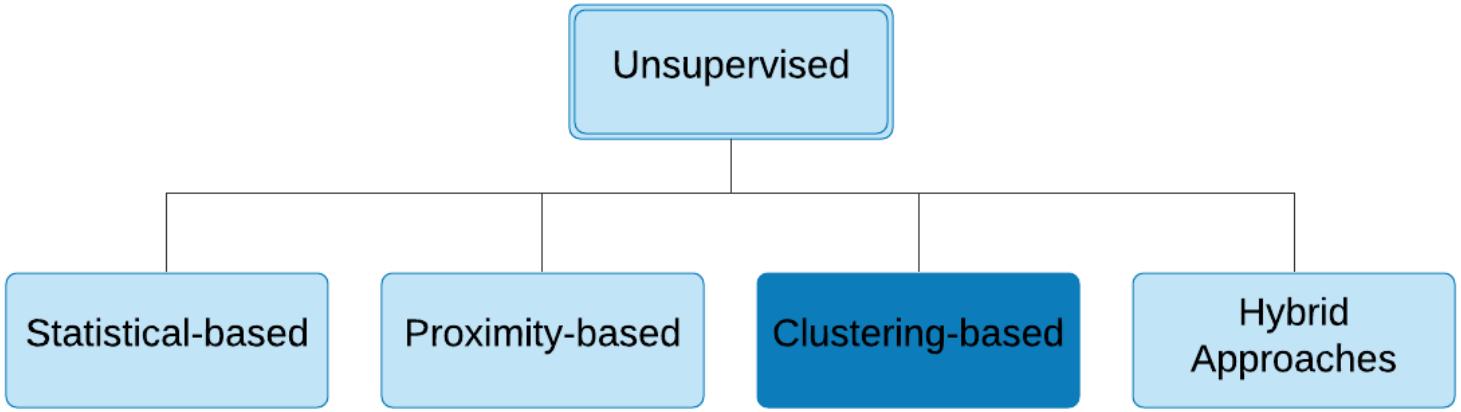
Unsupervised Methods



Clustering-based Methods

DBSCAN

- Idea: find the areas that satisfy a simple minimum density level, and which are separated by areas with lower density.
- Parameters: *MinPts*: threshold for the number of neighbors, ϵ: radius
- Objects with more than *MinPts* neighbors within a radius of ϵ (including the query point) are considered to be core points.

Ester, Martin, et al. "A density-based algorithm for discovering clusters in large spatial databases with noise." KDD. Vol. 96. No. 34. 1996.

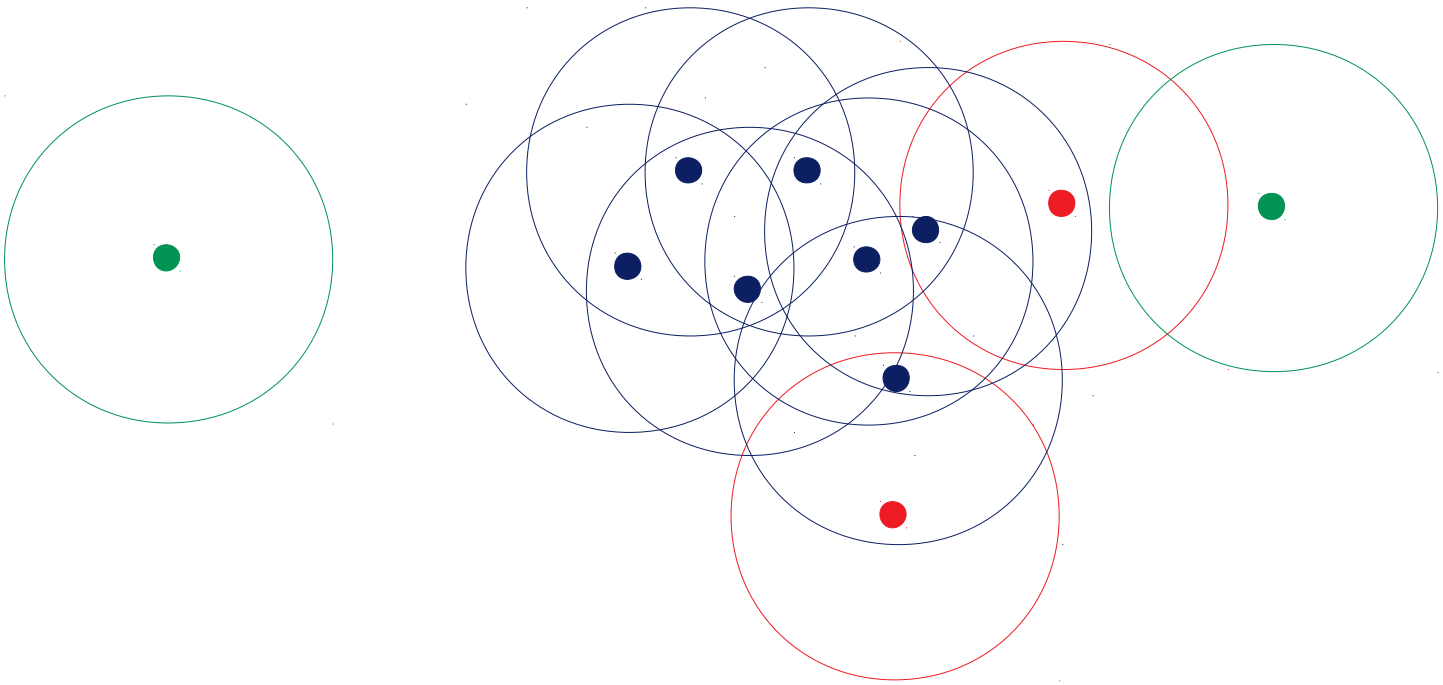
Schubert, Erich, et al. "DBSCAN revisited, revisited: why and how you should (still) use DBSCAN." ACM TODS 42.3 (2017): 1-21.

Clustering-based Methods

DBSCAN

Steps

- Compute neighbors of each point and identify core points
- Join neighboring core points into clusters
- for each non-core point
  - Add to a neighboring core point if possible
  - Otherwise, add to noise

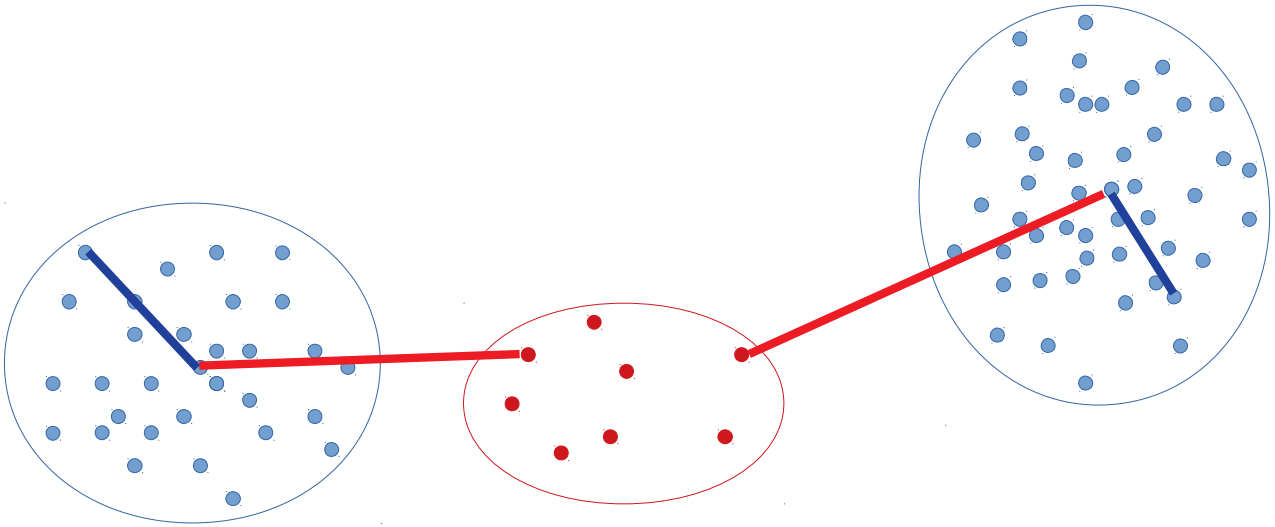


Clustering-based Methods

CBLOF

Cluster-based Local Outlier Factor (He, 2003)

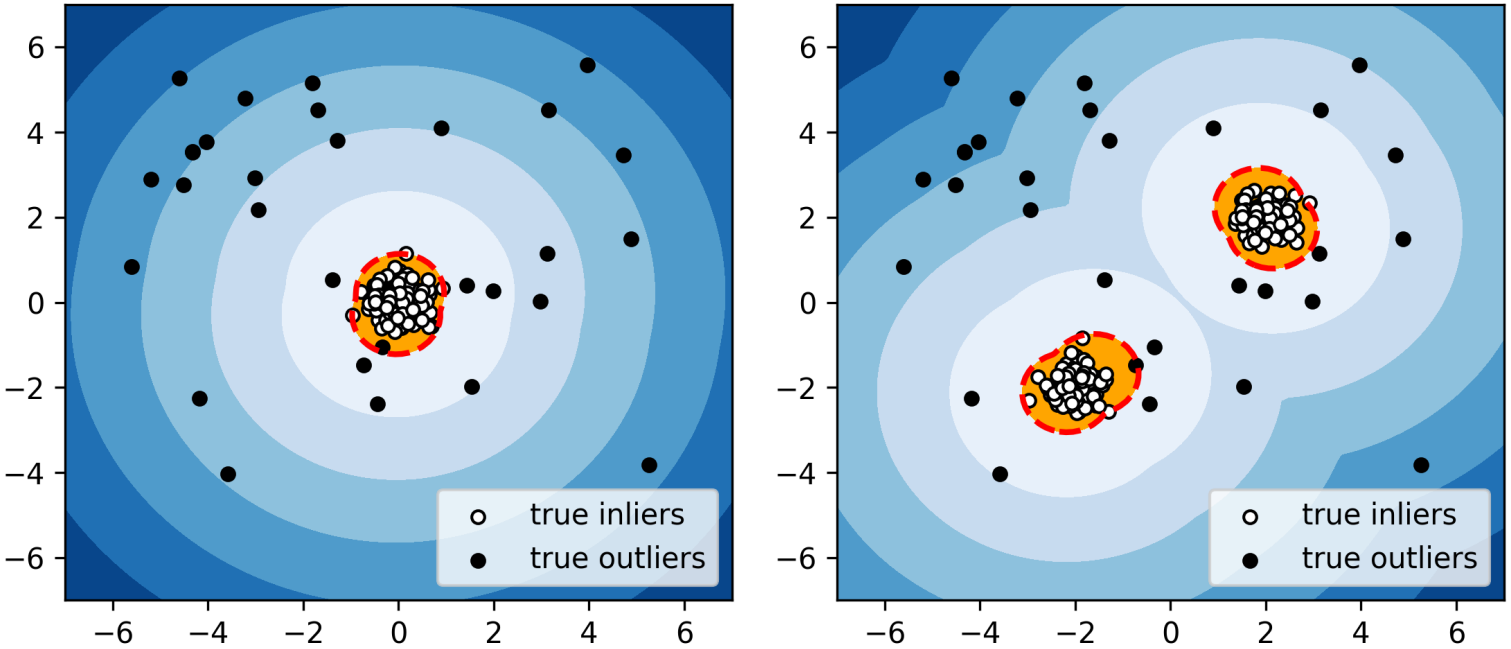
- Two parameters:
  - α: ratio of the data set that is expected to be normal
  - β: minimum ratio of the size of the large cluster to the small clusters
- Idea: Anomaly score of a case is equal to the distance to the nearest large cluster multiplied by the size of the cluster the case belong to.



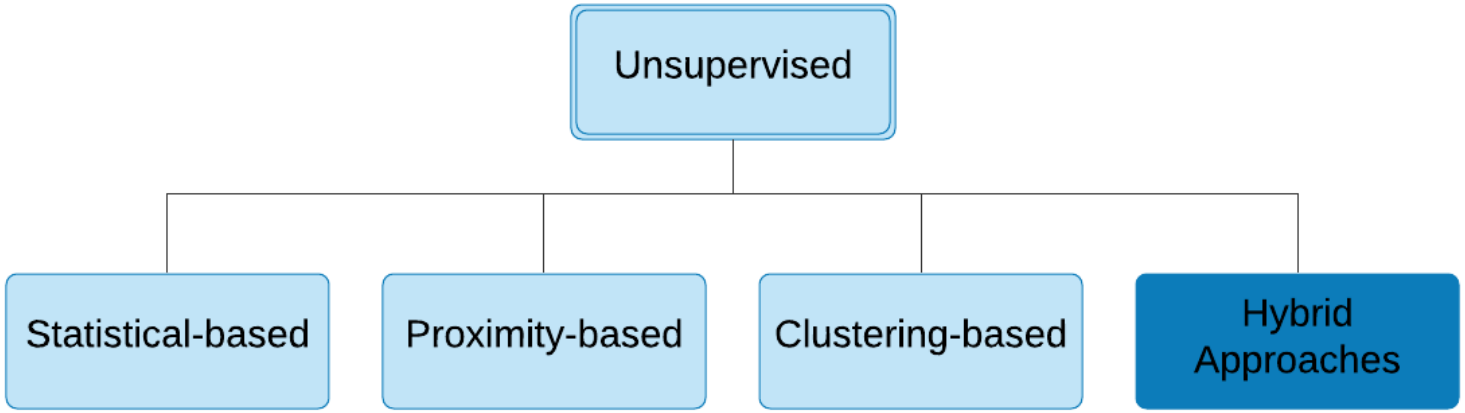
He, Zengyou, Xiaofei Xu, and Shengchun Deng. "Discovering cluster-based local outliers."

Clustering-based Methods

CBLOF



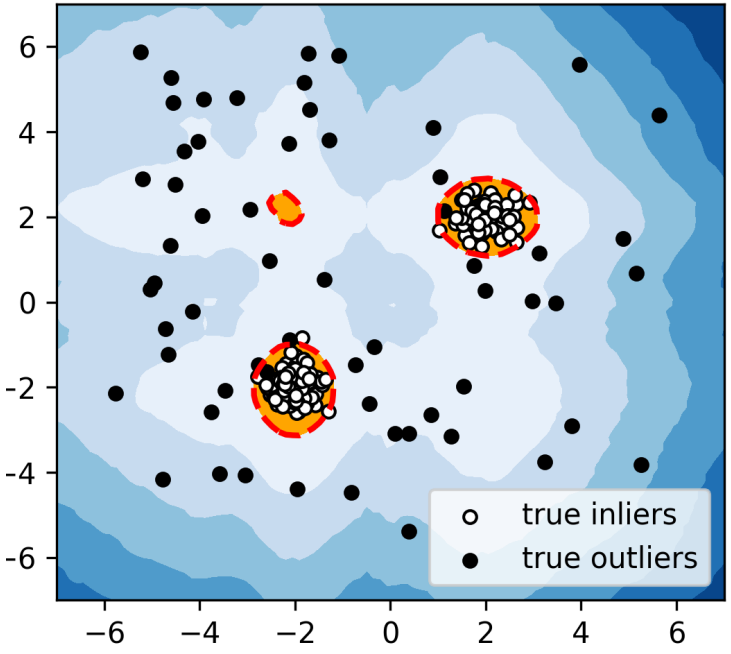
Unsupervised Methods



Hybrid Approaches

Feature Bagging for Outlier Detection

- Feature Bagging for Outlier Detection runs LOF method on multiple projections of the data and combines the results for improved detection qualities in high dimensions.
- First ensemble learning approach to outlier detection.



Lazarevic, A. and Kumar, V., 2005, Feature bagging for outlier detection. In KDD '05. 2005.

Up next ...

- Semi-supervised Methods
- Class-based Anomaly Detection
- Explanation of Rare Events

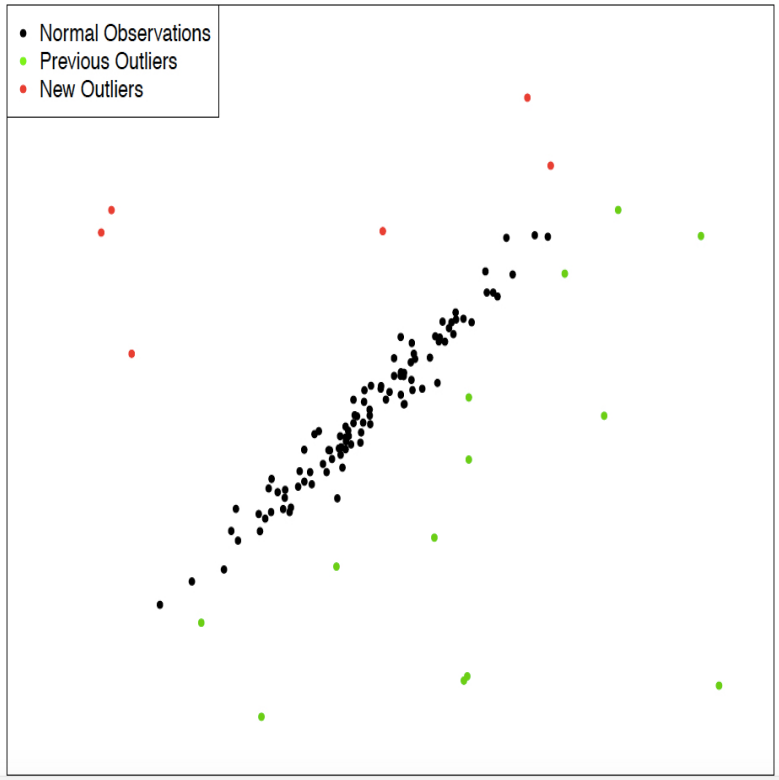
Semi-supervised outlier detection

training data has labeled instances only for one class

the most common - only normal data available, labeled outliers are missing

more robust than unsupervised methods

can outperform supervised ones if we are not sure about representativness of labeled outliers



Jason Sopheap Tun, Semi-Supervised Outlier Detection Algorithms, U. California 2018

Methods

One-class learning: disadvantage: can be sensitive (as One-class SVM) to outliers and thus does not perform very well (see also Aggarwal for details)

any unsupervised anomaly detection algorithm can be used

- learning set contains only normal instances, test set both
- = (a sort of) novelty detection
- Evaluation: outliers lie outside the area

Novelty detection is more general: can result even in a dense cluster that is far from normal points.

Example: sckit-learn