

## Outlier mining in high-dimensional datasets based on Jensen-Shannon distance and graph structure analysis

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*Complex Networks*  
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# An outlier or an anomaly?

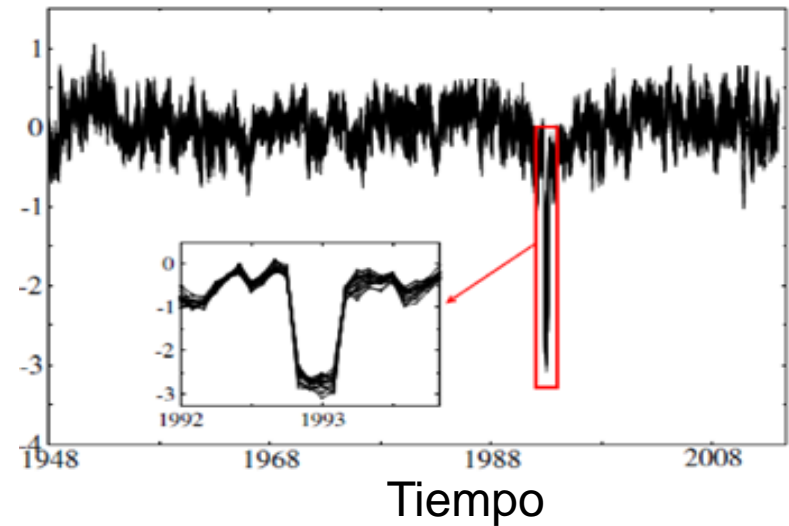
- *Outlier*: a legitimate data point that is far from the center of the distribution that characterizes the process
- *Anomaly*: a data point that cannot be explained given current knowledge of the process generating the data.
- Types:
  - *Point anomalies*: a data point that is anomalous with respect to the rest of the data.
  - *Contextual anomalies*: a data point that is anomalous in a specific context.
  - *Collective anomalies*: a set of data points that are not anomalies by themselves, but their collective occurrence is anomalous.

V. Chandola et al., *ACM Comput. Surveys* 41, 15 (2009)

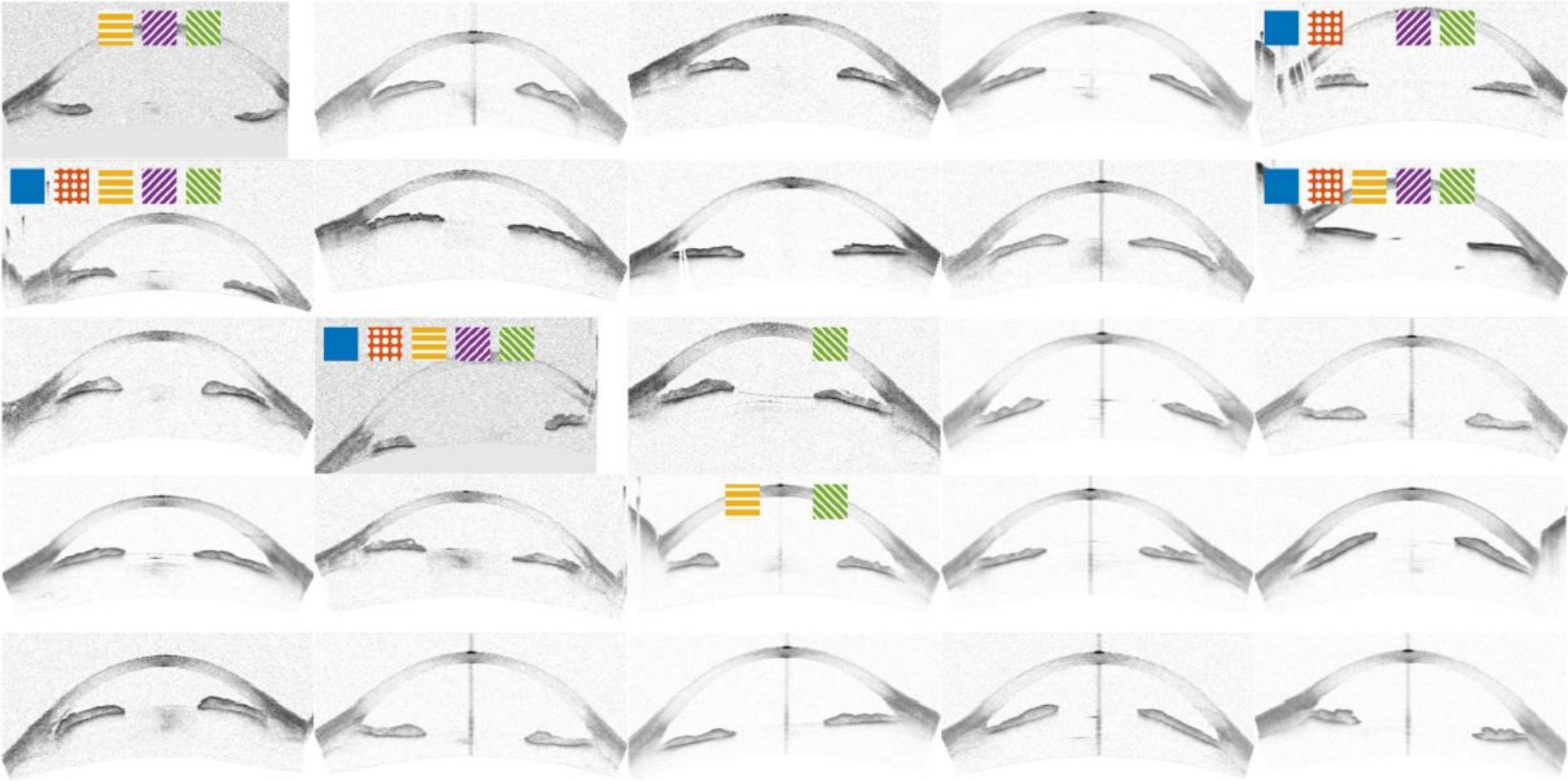
# Outlier/anomaly detection algorithms: many applications








- Intrusion detection
- Failure detection
- Machine learning: filtering outliers from the training data improves algorithm performance.



# Our motivation: analysis of OCT anterior chamber images



*P. Amil, N. Almeida and C. Masoller: Outlier Mining Methods Based on Graph Structure Analysis, Front. Phys. 7, 194 (2019).*

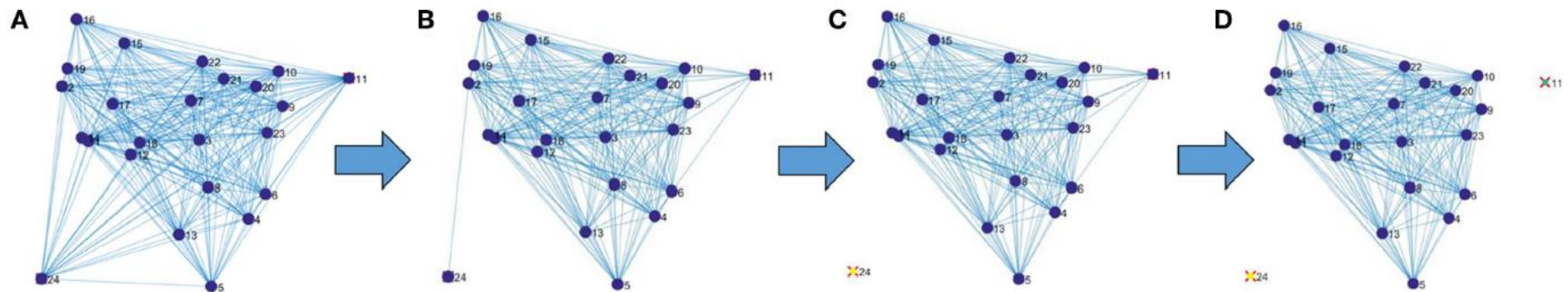
|   |             |
|---|-------------|
|  | OCSVM       |
|  | d2CM        |
|  | IsoMap      |
|  | Percolation |
|  | Ramaswamy   |

**We consider high-dimensional datasets where a distance can be defined between items of the dataset**

Feature vectors of items  $i$  and  $j$ :  $\{f_{i1} \dots f_{iM}\}$   $\{f_{j1} \dots f_{jM}\}$

Distance between them: 
$$d_{ij} = \sqrt{\sum_{k=1}^M (f_{ik} - f_{jk})^2}$$

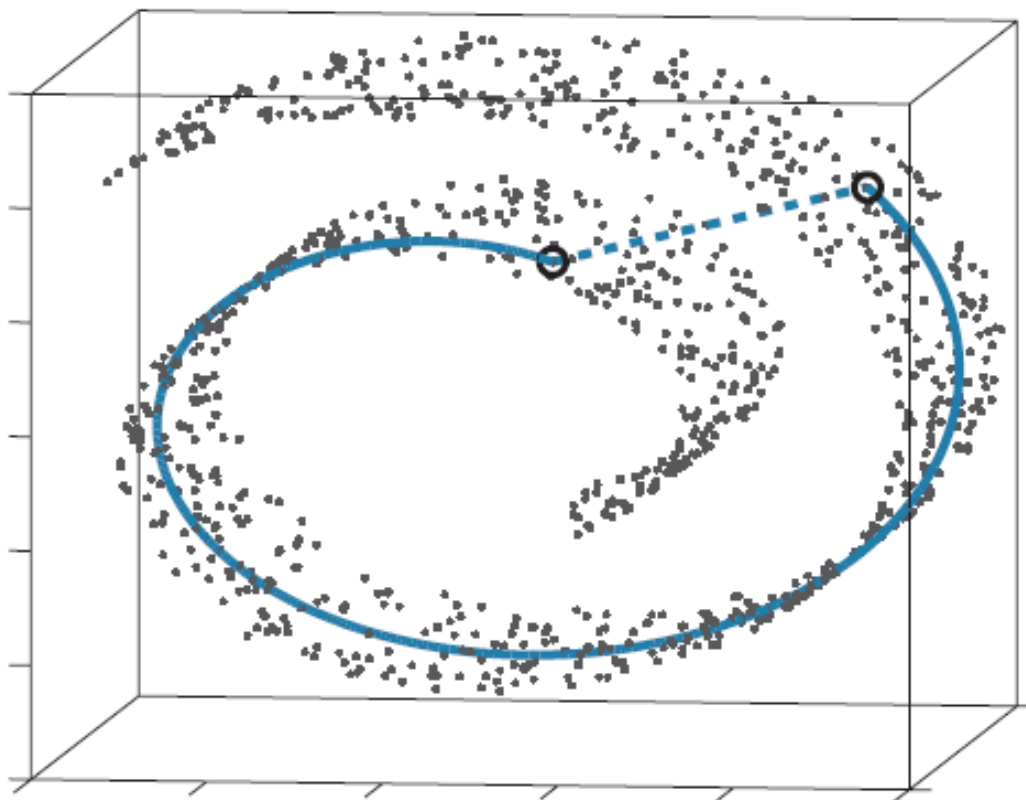
**First method: Outlier detection using percolation (OP)**



Outlier score OP = order in which elements disconnect from the giant component. **Parameter free.**

## Second method: nonlinear dimensionality reduction

- *Main idea: how well or how poorly an element fits in the learned manifold.*



Distance in the high dimensional space (dash) and distance in the learned (lower dimensional) manifold (solid).

*ISOMAP, Tenenbaum et al., Science 290, 2319 (2000).*

*P. Amil, N. Almeida and C. Masoller, Front. Phys. 7, 194 (2019).*

# Steps

- Apply *IsoMap* to the distance matrix  $\mathbf{D}_{ij}$  to obtain
  - a new set of features
  - a new distance matrix in the geodesic space,  $\mathbf{D}^G_{ij}$
- With the new features, recalculate the distance matrix  $\mathbf{D}'_{ij}$
- For each element, calculate correlation between  $\mathbf{D}^G_{ij}$  and  $\mathbf{D}'_{ij}$
- $AL_i = 1 - \rho_i^2$
- Two parameters (integers):
  - Dimension of reduced space
  - # of geodesic neighbors

*Note: we don't use the features returned by Isomap to assign outlier scores*

# Comparison with other outlier detection methods

- Distance to center of mass (d2CM): an outlier score is assigned according to the distance of an element to the center of mass.
- Ramaswamy: an outlier score is assigned according to the distance of an element to its  $k$ th nearest neighbor.
- One Class Support Vector Machine (OCSVM): uses the scalar product to define a function that returns +1 in the region where normal elements are located and -1 elsewhere.

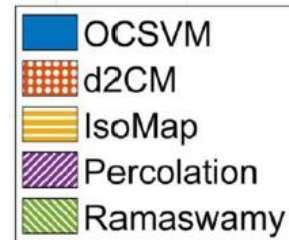
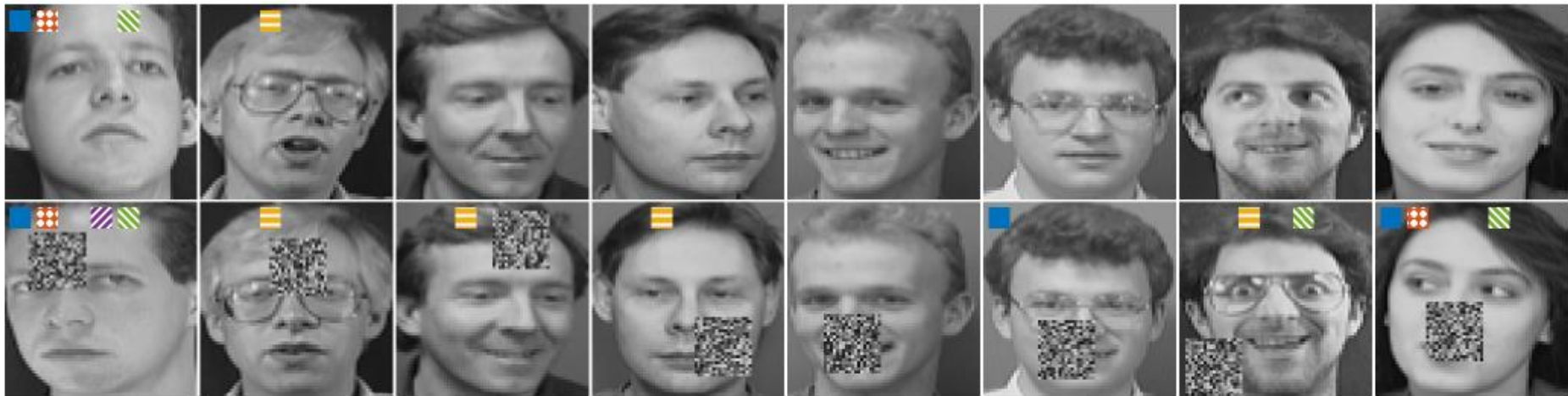
*Ramaswamy et al., Efficient algorithms for mining outliers from large data sets. ACM Sigmod Record (Vol. 29, No. 2, pp. 427-438, 2000).*  
*Schölkopf et al., Estimating the support of a high-dimensional distribution. Neural computation 13, 1443-1471, 2001.*



# Dataset and performance measures

<http://www.cl.cam.ac.uk/research/dtg/attarchive/facedatabase.html>

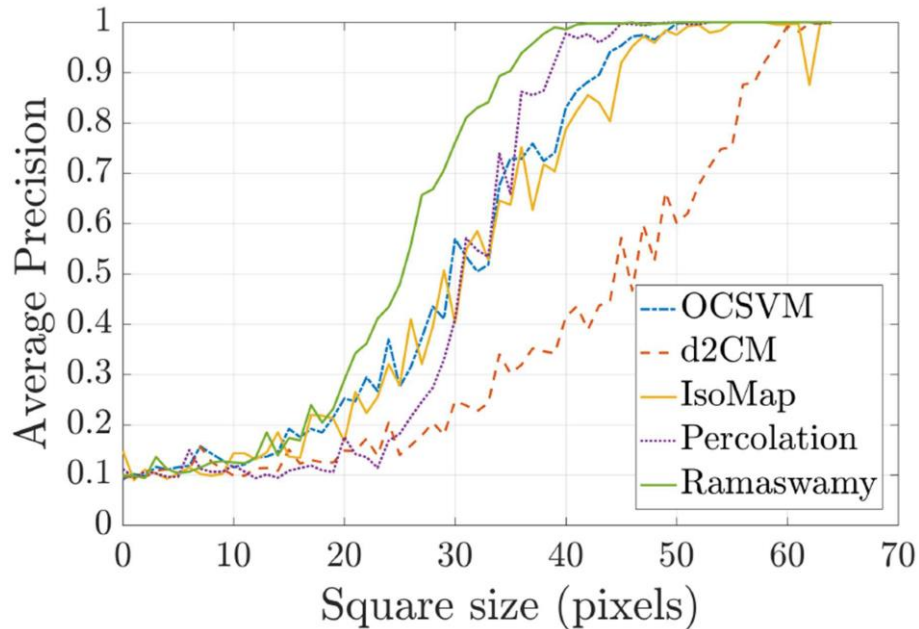
We added to some random images a square with gray-scale pixels whose color distribution is the same as that of the image.



Performance quantification: average precision  
(area under the Precision-Recall curve,  $TP/(TP+FP)$  vs  $TP$ )

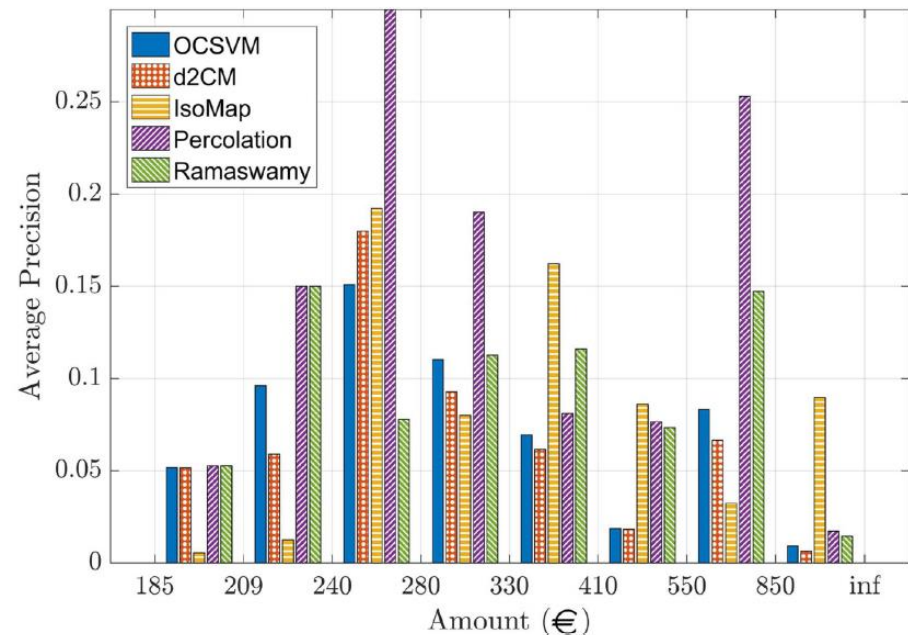
# Results

## Face database



How about other types of elements?

Credit card transactions (some identified as frauds); each transaction has 28 features from PCA  
<https://www.kaggle.com/mlg-ulb/creditcardfraud>



*P. Amil, N. Almeida and C. Masoller, Front. Phys. 7, 194 (2019).*

## The methods' performance depends on the data. How do they compare in terms of execution time?

For a database of 1,000 elements with 30 dimensions,  
run on *Matlab* on an Intel i7-7700HQ laptop:

|                                  |        |
|----------------------------------|--------|
| Distance to center of mass       | 0.01 s |
| Ramaswamy                        | 0.04 s |
| One Class Support Vector Machine | 0.2 s  |
| Percolation                      | 6 s    |
| IsoMap                           | 18 s   |

Can we do better?

## Two new outlier mining methods

Feature vectors of items  $i$  and  $j$

$$\{f_{i1} \dots f_{iM}\} \quad \{f_{j1} \dots f_{jM}\}$$

Euclidean distance between them:

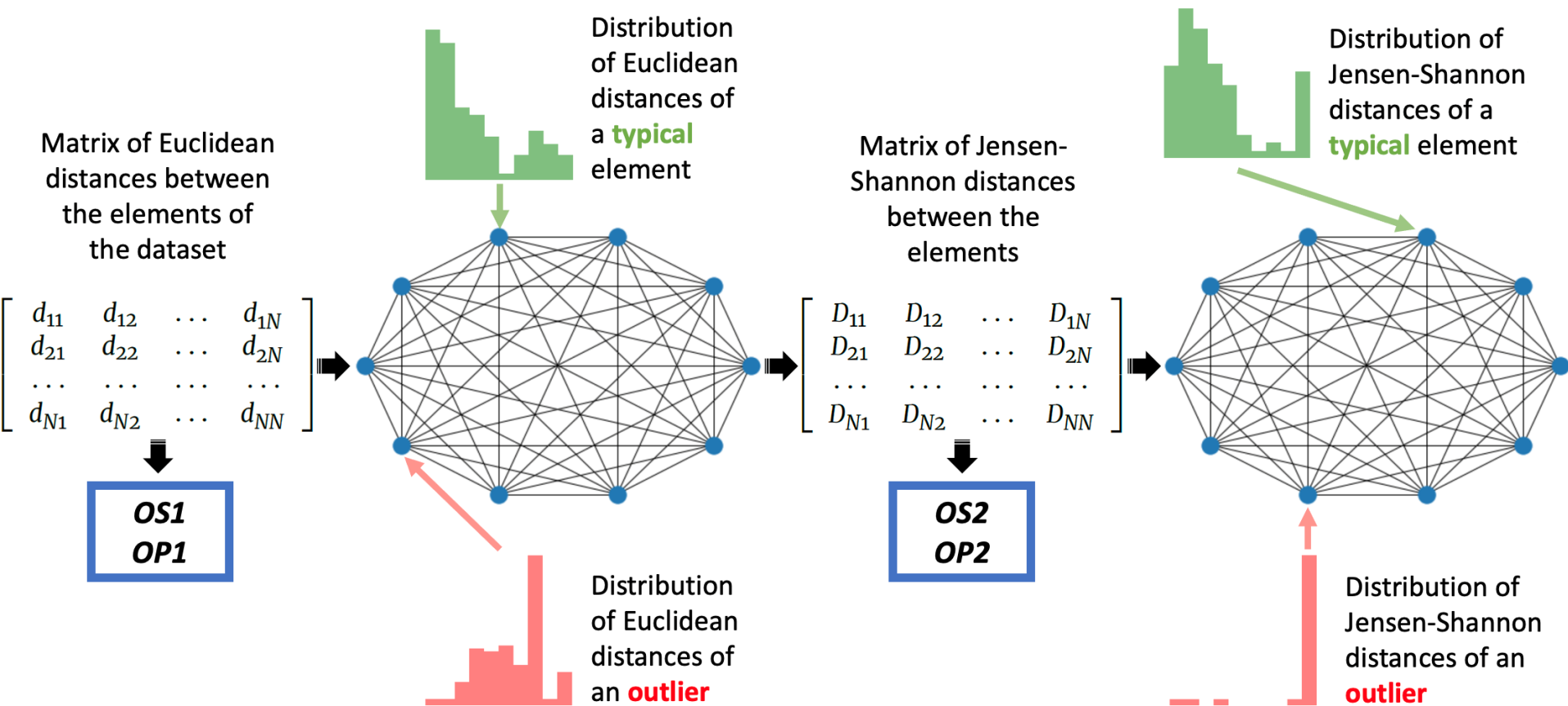
$$d_{ij} = \sqrt{\sum_{k=1}^M (f_{ik} - f_{jk})^2}$$

$$OS1_i = \frac{1}{N} \sum_{l=1}^N d_{il}$$

Instead of the Euclidean distance, we can use the distance between the distributions of distances  $\{d_{il}\}$  and  $\{d_{jl}\}$ : the Jensen-Shannon distance

$$D_{ij} = JS[P_i, P_j] = H[(P_i + P_j)/2] - H[P_i]/2 - H[P_j]/2,$$

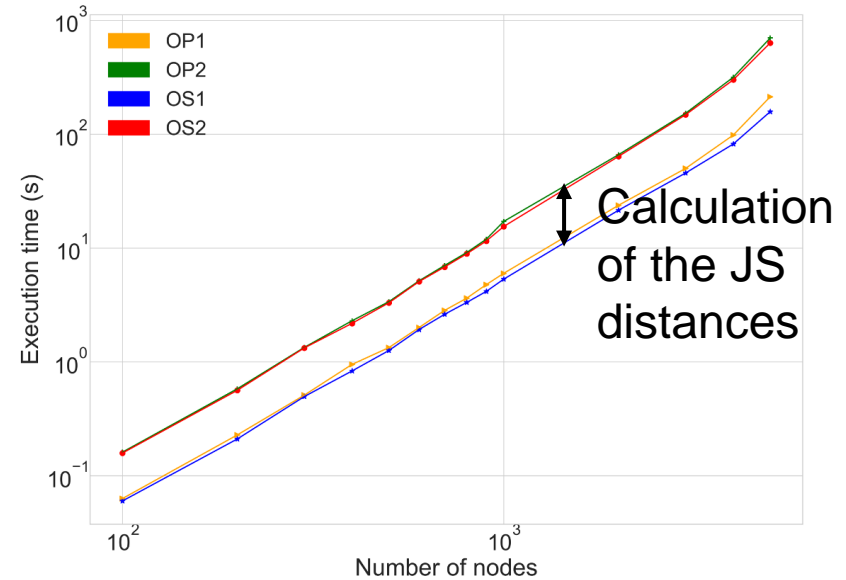
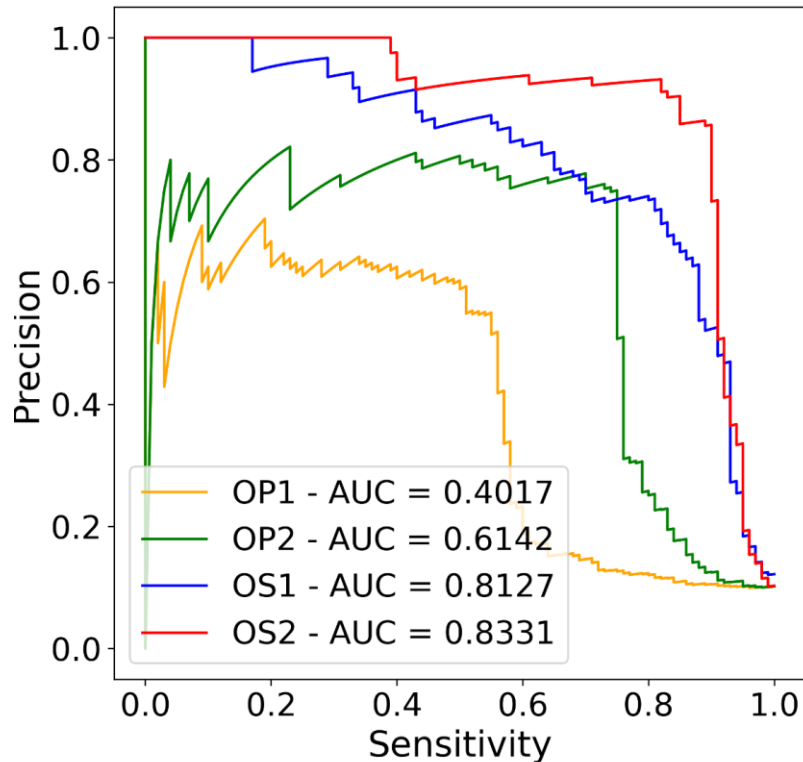
$$OS2_i = \frac{1}{N} \sum_{l=1}^N D_{il}$$



OS1, OS2: Outlier score defined by the sum of distances  
 OP1, OP2: Outlier score defined by the percolation order

# Results for the credit card database, 1000 transactions

10% fraud  
(similar with 5% fraud)



Python, iMac core i7  
with 32 GB RAM:

|     | t(s)  |
|-----|-------|
| OP1 | 5.99  |
| OP2 | 17.12 |
| OS1 | 5.33  |
| OS2 | 16.45 |

**Conclusion:** The methods are suitable for high dimensional, not too large databases because the execution time grows with the number of features and at least as  $N \times N$  with the size of the dataset.

P. Amil, N. Almeida and C. Masoller, *Outlier Mining Methods Based on Graph Structure Analysis*, *Frontiers in Physics* 7, 194 (2019).

A. S. O. Toledo et al., *Outlier mining in high-dimensional data using the Jensen-Shannon divergence and graph structure analysis*, under review (2022).

**Thank you for your attention !**

