# Machine Learning and Extremes for Anomaly Detection

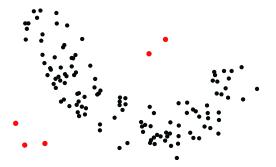
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## Anomaly Detection (AD)

'Finding patterns in the data that do not conform to expected behavior'



**Applications**: Network intrusions, credit card fraud detection, insurance, finance, military surveillance, predictive maintenance...

## Machine Learning context

## Different kinds of Anomaly Detection

- Supervised AD (not dealt with)
   Labels available for both normal data and anomalies (similar to rare class mining)
- Novelty Detection (our theoretical framework)
   Synonym: one-class classification. The algorithm learns on normal data only
- Outlier Detection (extended application framework)
   Training set (unlabeled) = normal + abnormal data (assumption: anomalies are very rare)



## Some literature in Anomaly Detection

#### Statistical AD techniques

[Hawkins 1980, Liu and Weng 1991, Eskin 2000, Agarwal 2006]

## K-nearest neighbors

[Breunig et al. 2000, Tang et al. 2002, Papadimitriou et al. 2002, Hautamaki et al. 2004]

## Support estimation

[Einmahl and Mason 92, Polonik 97, Schölkopf *et al.* 2000, Vert and Vert 2006, Scott and Nowak 2006]

## High-dimensional techniques

[Aggarwal and Yu 2001, Shyu et al. 2003, Shi and Horvath 2012, Liu et al. 2008]

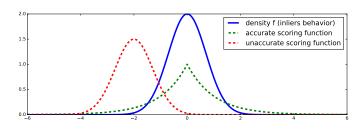
# Background: scoring functions

Notation: Normal behavior  $\rightarrow$  density f.

## AD algorithm returns a **scoring function** $s : \mathbb{R}^d \to \mathbb{R}$

- s defines a pre-order on  $\mathbb{R}^d$  = 'degree of normality'.
- s level sets are estimates of f level sets.
- ► s can be interpreted as a continuum of level sets estimates (at different levels).

**Remark.** Ideal scoring functions:  $s = T \circ f$  any increasing transform of f.



## Outline

Part I: Performance criterion for scoring functions

Part II: Learning accurate scoring functions on extreme regions

Part III: Heuristic contributions and perspectives

## Part I: Performance criterion for scoring functions

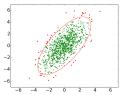
Part II: Learning accurate scoring functions on extreme regions

Part III: Heuristic contributions and perspectives

## Existing criterion: Mass-Volume curve

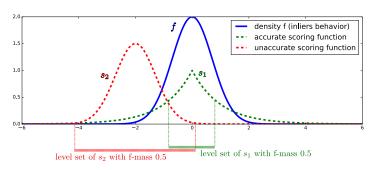
Minimum volume set [Einmahl and Mason 1992, Polonik 1997]

$$\Gamma_{\alpha}^{*} = \mathop{\arg\min}_{\Gamma \text{ borelian}} \quad \mathsf{Leb}(\Gamma) \quad \textit{s.t.} \quad \mathbb{P}(\mathbf{X} \in \Gamma) \geq \alpha$$

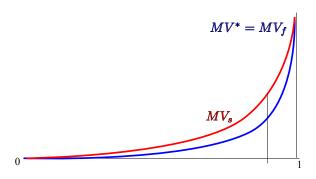


Mass Volume curve of a scoring function s [Clémençon and Jakubowicz, 2013]:

$$\begin{array}{ll} \mathit{MV}_s(\alpha) \ := \ \inf_{\Gamma \text{ level-set of } s} \big\{ \ \mathsf{Leb}(\Gamma) \quad \mathit{s.t.} \ \mathbb{P}(\mathbf{X} \in \Gamma) \geq \alpha \ \big\} \\ \mathit{MV}^*(\alpha) \ := \ \mathit{MV}_f(\alpha) \stackrel{\mathit{prop}}{=} \min_{\Gamma \text{ borelian}} \big\{ \ \mathsf{Leb}(\Gamma) \quad \mathit{s.t.} \ \mathbb{P}(\mathbf{X} \in \Gamma) \geq \alpha \ \big\} \end{array}$$



## Existing criterion: Mass-Volume curve



#### Main drawbacks of MV:

- When optimized w.r.t. different levels α over a finite class, produces not necessarily nested empirical level sets.
- ▶  $\rightarrow$  low convergence rates of order  $O(n^{-1/4})$ .
- MV diverges in 1 in case of unbounded support.

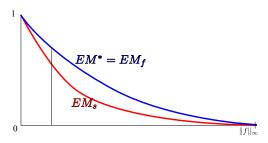
## Our contribution: Excess-Mass curve [Goix, Sabourin, Clémençon 2015]

# Excess-Mass [Polonik 1995] Excess-Mass curve

$$\begin{split} &\textit{EM}_{\textit{s}}(t) \ := \ \sup_{\Omega \text{ level-set of } \textit{s}} \ \left\{ \mathbb{P}(\mathbf{X} \in \Omega) \ - \ \textit{t} \mathsf{Leb}(\Omega) \right\} \\ &\textit{EM}^*(t) \ := \ \textit{EM}_{\textit{f}}(t) \stackrel{\textit{prop}}{=} \max_{\Omega \text{ borelian}} \ \left\{ \mathbb{P}(\mathbf{X} \in \Omega) - \textit{t} \mathsf{Leb}(\Omega) \right\} \end{split}$$

## Property: Previous drawbacks are fixed with EM.

- Produces nested empirical level sets.
- ▶  $\rightarrow$  convergence rates of order  $O(n^{-1/2})$ .
- ► EM curve **finite** even in case of unbounded support.



# Learning a scoring function with M-estimation

G: VC-class of sets.

Procedure: Fix 
$$t_0 > 0$$
For  $k = 1, \ldots, N$ ,
$$t_{k+1} = \frac{t_k}{(1 + \frac{1}{\sqrt{n}})}$$

$$\widehat{\Omega}_{t_{k+1}} = \underset{\Omega \in \mathcal{G}, \ \widehat{\Omega}_{t_k} \subset \Omega}{\arg \max} \quad \mathbb{P}_n(X \in \Omega) - t_{k+1} \mathsf{Leb}(\Omega)$$

$$s_N(x) := \sum_{j=1}^N (t_j - t_{j+1}) \mathbb{1}_{x \in \Omega_{t_j}}$$

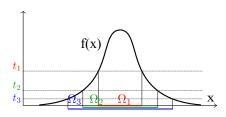
11

# Learning a scoring function with M-estimation

#### Theorem

Assume the density f bounded, with compact support and without flat parts and  $\mathcal{G}$  VC-class. Then if  $t_N = \mathcal{O}(n^{-1/2})$ , with probability at least  $1 - \delta$ ,

$$\sup_{t \in ]0,t_1]} |\mathit{EM}^*(t) - \mathit{EM}_{s_N}(t)| \ \leq \ \left[ A + \sqrt{2\log(1/\delta)} \right] \frac{1}{\sqrt{n}} + \mathit{bias}(\mathcal{G}).$$



Part I: Performance criterion for scoring functions

Part II: Learning accurate scoring functions on extreme regions

Part III: Heuristic contributions and perspectives

## Why dealing with extremes?

#### General ideas:

- Extreme observations play a special role when dealing with outlying data.
- But no anomaly detection algorithm has specific treatment for such multivariate extreme observations. Univariate EVT: [Roberts 99, Lee and Roberts 2008, Clifton et al. 2011]
- ▶ Our goal:
  - Define a notion of sparsity for extremes observations.
  - Provide a method which can improve performance of standard AD algorithms by combining them with a multivariate extreme analysis of the dependence structure, using this notion of sparsity.

## Purpose

$$\mathbf{X} = (X_1, \dots, X_5)$$

Goal: find the groups of features which can be large together

ex: 
$$\{X_1, X_2\}, \{X_1, X_3, X_4\}, \{X_5\}$$

Namely: characterize the extreme dependence structure

→ Anomalies = points which violate this structure

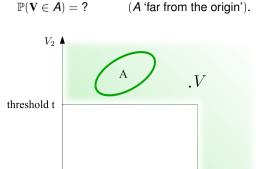
## Theoretical framework

#### Context

- Random vector  $\mathbf{X} = (X_1, \dots, X_d)$
- ► Margins:  $X_j \sim F_j$  ( $F_j$  continuous)
- Preliminary step: Standardization of each marginal
  - ▶ Standard Pareto:  $V_j = \frac{1}{1 F_j(X_j)}$   $\left( \mathbb{P}(V_j \ge x) = \frac{1}{x}, x \ge 1 \right)$

## Problematic of Extreme Value Theory

Describe V's distribution, when V exceeds some large threshold.



"Extremal region"

## Fundamental hypothesis and consequences

Standard assumption: let A extreme region,

$$\mathbb{P}[\mathbf{V} \in t \ A] \simeq t^{-1} \mathbb{P}[\mathbf{V} \in A]$$
 (radial homogeneity)

Formally:

regular variation (after standardization):

If 
$$0 \notin \overline{A}$$
,  $t\mathbb{P}[\mathbf{V} \in t \ A] \xrightarrow[t \to \infty]{} \mu(A)$ .  $\mu$ : exponent measure

Necessarily: 
$$\mu(tA) = t^{-1}\mu(A)$$

▶  $\Rightarrow$  angular measure on sphere  $S_{d-1}$ :  $\Phi(B) = \mu\{tB, t \ge 1\}$ 

## General model of multivariate EVT

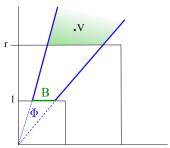
 $\mathbb{P}[V \in A] \simeq \mu(A)$ , if A extreme region.

#### Model for excesses

For a large r > 0 and a region B on the unit sphere:

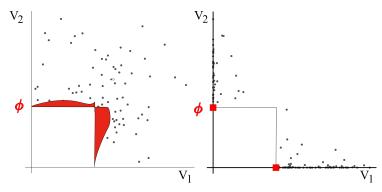
$$\mathbb{P}\left[\|\mathbf{V}\|>r,\ \frac{\mathbf{V}}{\|\mathbf{V}\|}\in B\right] \quad \mathop{\sim}_{r\to\infty}\quad \frac{1}{r}\,\Phi(B)=\mu(\{tB,t\geq r\})$$

 $\Rightarrow \Phi$  (or  $\mu$ ) rules the joint distribution of extremes (if margins are known).



## Angular distribution

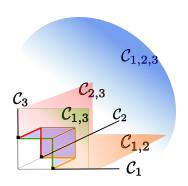
 $\Phi$  rules the joint distribution of extremes:



Asymptotic dependence:  $(V_1, V_2)$  may be large together.

Asymptotic independence: Only  $V_1$  or  $V_2$  may be large.

## General Case



- ▶ Sub-cones:  $C_{\alpha} = \{ \|v\| \ge 1, v_j > 0 \ (j \in \alpha), v_j = 0 \ (j \notin \alpha) \}$
- $\blacktriangleright \ \, \text{Corresponding sub-spheres:} \, \left\{\Omega_{\alpha}, \alpha \subset \{1, \ldots, \textit{d}\}\right\} \quad (\Omega_{\alpha} = \mathcal{C}_{\alpha} \cap \mathbf{S}_{\textit{d}-1})$

## Representation of extreme data

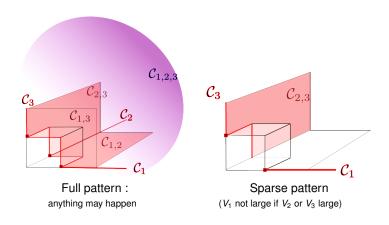
Natural decomposition of the angular measure :

$$\Phi = \sum_{\alpha \subset \{1, \dots, d\}} \Phi_\alpha \qquad \qquad \text{with } \Phi_\alpha = \Phi_{|\Omega_\alpha} \leftrightarrow \mu_{|\mathcal{C}_\alpha}$$

▶ ⇒ yields a representation

• Assumption:  $\frac{d\mu_{|C_{\alpha}}}{dv_{\alpha}} = O(1)$ .

# Sparse Representation?



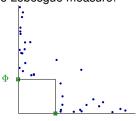
## **Estimation Problem**: $\mathcal{M}$ is an **asymptotic** representation

$$\mathcal{M} \ = \ \big\{ \ \Phi(\Omega_\alpha), \ \alpha \ \big\} \ = \ \big\{ \ \mu(\mathcal{C}_\alpha), \ \alpha \ \big\}$$

is the restriction of an asymptotic measure

$$\mu(\textit{A}) = \lim_{t \to \infty} t \mathbb{P}[\textit{\textbf{V}} \in \textit{t} \; \textit{A}]$$

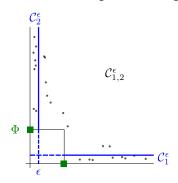
to a representative class of set  $\{\mathcal{C}_{\alpha}, \ \alpha\}$ , but only the central sub-cone has positive Lebesgue measure!



 $\Rightarrow$  Cannot just do, for large t:

$$\Phi(\Omega_{\alpha}) = \mu(\mathcal{C}_{\alpha}) \simeq t \widehat{\mathbb{P}}(t \mathcal{C}_{\alpha})$$

Fix  $\epsilon > 0$ . Affect data  $\epsilon$ -close to an edge, to that edge.



$$C_{\alpha} \to C_{\alpha}^{\epsilon} = \{ \|v\| \ge 1, \ v_j > \epsilon \ (j \in \alpha), \ v_j \le \epsilon \ (j \notin \alpha) \}.$$

New partition.

## Resulting estimation procedure

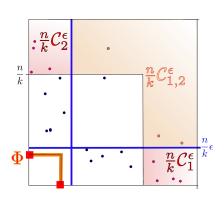
$$\hat{V}_i^j = \frac{1}{1 - \hat{F}_j(X_i^j)}$$
 with  $\hat{F}_j(X_i^j) = \frac{rank(X_i^j) - 1}{n}$ 

#### Recall that:

$$\mu(A) = \lim_{t \to \infty} t \mathbb{P}[\mathbf{V} \in t \ A]$$

 $\Rightarrow$  get an natural estimate of  $\Phi(\Omega_\alpha)$ 

$$\begin{split} \widehat{\Phi}(\Omega_{\alpha}) &:= \frac{n}{k} \mathbb{P}_n(\hat{V} \in \frac{n}{k} \mathcal{C}_{\alpha}^{\epsilon}) \\ &(\frac{n}{k} \text{ large, } \epsilon \text{ small}) \end{split}$$



 $\Rightarrow$  we obtain

$$\widehat{\mathcal{M}} := \big\{ \ \widehat{\Phi}(\Omega_\alpha), \ \alpha \ \big\}$$

## Statistical guaranties

#### Theorem [Goix, Sabourin, Clémençon 2016]

There is an absolute constant C>0 such that for any  $n>0,\ k>0,\ 0<\epsilon<1,\ \delta>0$  such that  $0<\delta< e^{-k}$ , with probability at least  $1-\delta$ ,

$$\|\widehat{\mathcal{M}} - \mathcal{M}\|_{\infty} \le Cd\left(\sqrt{\frac{1}{\epsilon k}\log\frac{d}{\delta}} + Md\epsilon\right) + \operatorname{bias}(\epsilon, k, n)$$

#### Comments:

- $M \simeq \sum_{\alpha} \sup(\text{density on cones } \alpha)$
- Existing literature (for spectral measure) [Einmahl and Segers 09, Einmahl et al. 01]

$$d = 2$$
, asymptotic behavior, rates in  $1/\sqrt{k}$ .

▶ Here:  $1/\sqrt{k} \rightarrow 1/\sqrt{\varepsilon k} + \varepsilon$ . Price to pay for biasing our estimator with  $\varepsilon$ .

# Theorem's proof: key ingredient

Would like to use concentration inequality...

In our case: 
$$\sup_{A \in \mathcal{A}} \frac{\frac{n}{k}}{k} \left| (\mathcal{P} - \mathcal{P}_n) \left( \frac{n}{k} A \right) \right|$$
But usually: 
$$\sup_{A \in \mathcal{A}} \left| (\mathcal{P} - \mathcal{P}_n) (A) \right|$$

- ightharpoonup scaling  $\frac{n}{k}$
- ► classical VC-inequality:  $\frac{n}{k}$  nice but not used ! → high proba bound in

$$\frac{n}{k} \times \sqrt{\frac{1}{n} \log \frac{1}{\delta}} \longrightarrow \infty !!$$

 $\Rightarrow$  Needs to take into account that the proba of  $\frac{n}{k}A$  is small.

28

# Theorem's proof: key ingredient

**Key:** VC-inequality adapted to rare regions  $\rightarrow$  bound in

$$\sqrt{\mathbf{p}} \, \frac{n}{k} \sqrt{\frac{d}{n} \log \frac{1}{\delta}}$$

with p the probability to be in the union class  $\bigcup_{A \in \mathcal{A}} A$ .

$$\mathbf{p} \leq d \frac{k}{n}$$

 $\Rightarrow$  bound in

$$d\sqrt{\frac{1}{k}\log\frac{1}{\delta}}$$

 $k \propto$  number of data considered as extreme (data used for estimation)

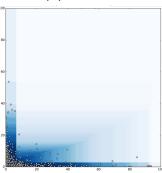
# Application to Anomaly Detection

Recall that after standardization of marginals:  $\mathbb{P}[R > r, \mathbf{W} \in B] \simeq \frac{1}{r} \Phi(B)$ 

 $\rightarrow$  scoring function =  $\Phi_n^{\epsilon} \times 1/r$ :

$$\textbf{\textit{S}}_{\textit{n}}(\textbf{\textit{x}}) := (1/\|\boldsymbol{\hat{\mathcal{T}}}(\textbf{\textit{x}})\|_{\infty}) \sum_{\alpha} \Phi^{\alpha,\varepsilon}_{\textit{n}} \mathbb{1}_{\boldsymbol{\hat{\mathcal{T}}}(\textbf{\textit{x}}) \in \mathcal{C}^{\varepsilon}_{\alpha}}.$$

where 
$$\hat{T}: \mathbf{X} \mapsto \mathbf{V}$$
  $(\hat{V}_j = \frac{1}{1 - \hat{F}_j(X_j)})$ 



Part I: Performance criterion for scoring functions

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Part III: Heuristic contributions and perspectives

#### EM and MV curves for model selection?

#### Practical motivations:

Most of the time, data come without any label.

 $\rightarrow$  no ROC or PR curves!

#### **Estimation:**

$$\begin{split} \widehat{\mathit{MV}}_{\mathcal{S}}(\alpha) &= \inf_{u \geq 0} \quad \mathsf{Leb}(s \geq u) \quad \textit{s.t.} \quad \mathbb{P}_{n}(s \geq u) \geq \alpha \\ \widehat{\mathit{EM}}_{\mathcal{S}}(t) &= \sup_{u \geq 0} \quad \mathbb{P}_{n}(s \geq u) \ - \ t\mathsf{Leb}(s \geq u) \end{split}$$

[Thomas et al. 2015]

#### Issue in large dimensions:

The volume Leb(s > u) has to be estimated!

#### Heuristic extension for large dimension:

## Random projection and averaging [Goix 2016]

**Inputs**: AD algorithm  $\mathcal{A}$ , data set X size  $n \times d$ , feature sub-sampling size d', number of draws m.

for 
$$k = 1, \ldots, m$$
 do

- -randomly select a sub-group  $F_k$  of d' features
- -compute the associated scoring function  $s_k = \mathcal{A}((x_i^j)_{1 \le i \le n, i \in F_k})$
- -compute  $\widehat{\mathcal{C}}_k^{EM} = \|\widehat{EM}_{s_k}\|_{L^1(I)}$  or  $\widehat{\mathcal{C}}_k^{MV} = \|\widehat{MV}_{s_k}\|_{L^1(J)}$

#### end for

Return performance criteria:

$$\widehat{\mathcal{C}}_{\mathit{high\_dim}}^{\mathit{EM}}(\mathcal{A}) = \frac{1}{m} \sum_{k=1}^{m} \widehat{\mathcal{C}}_{k}^{\mathit{EM}} \quad \text{or} \quad \widehat{\mathcal{C}}_{\mathit{high\_dim}}^{\mathit{MV}}(\mathcal{A}) = \frac{1}{m} \sum_{k=1}^{m} \widehat{\mathcal{C}}_{k}^{\mathit{MV}} \; .$$

Seems to work in practice but no statistical guaranties.

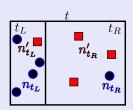
## Random Forests for one-class classification

## Two-class Random Forests [Breiman, 2001]

#### Two-Class impurity decrease

$$I_G(t_L, t_R) = \frac{n_{t_L} n'_{t_L}}{n_{t_L} + n'_{t_L}} + \frac{n_{t_R} n'_{t_R}}{n_{t_R} + n'_{t_R}}.$$

 $n_t$ : nb of observations with label 0 in node t.  $n_t'$ : nb of observations with label 1 in node t.



#### Random Forests for one-class classification

Two-Class: 
$$I_G(t_L, t_R) = \frac{n_{t_L} n'_{t_L}}{n_{t_L} + n'_{t_I}} + \frac{n_{t_R} n'_{t_R}}{n_{t_R} + n'_{t_R}}$$
.

One-Class:  $n'_{t_l}$ ,  $n'_{t_p} = ?$ 

Existing literature: [Désir et al., 2013, Liu et al., 2008, Shi and Horvath, 2012]. Based on **second-class sampling**.

## Random Forests for one-class classification

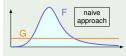
Two-Class: 
$$I_G(t_L, t_R) = \frac{n_{t_L} n'_{t_L}}{n_{t_L} + n'_{t_L}} + \frac{n_{t_R} n'_{t_R}}{n_{t_R} + n'_{t_R}}$$
.

One-Class:  $n'_{t_L}$ ,  $n'_{t_R} = ?$ 

One-Class splitting criterion [Goix, Brault, Drougard, Chiapino 2016]:

$$\begin{array}{llll} \text{Naive approach:} & \textit{n}'_{\textit{l}_L} \rightarrow \mathbf{n}_{\frac{\mathsf{Leb}(\textit{l}_L)}{\mathsf{Leb}(\textit{l}_0)}}^{\mathsf{Leb}(\textit{l}_L)} & \text{and} & \textit{n}'_{\textit{l}_R} \rightarrow \mathbf{n}_{\frac{\mathsf{Leb}(\textit{l}_R)}{\mathsf{Leb}(\textit{l}_0)}}^{\mathsf{Leb}(\textit{l}_R)} & (\textbf{t}_0 \text{ root node}) \\ \text{Adaptive approach:} & \textit{n}'_{\textit{l}_\ell} \rightarrow \mathbf{n}_t \frac{\mathsf{Leb}(\textit{l}_R)}{\mathsf{Leb}(\mathsf{l}_1)} & \text{and} & \textit{n}'_{\textit{l}_R} \rightarrow \mathbf{n}_t \frac{\mathsf{Leb}(\textit{l}_R)}{\mathsf{Leb}(\mathsf{l}_1)} \\ \end{array}$$

$$n_{t_L}' o n_t rac{\mathsf{Leb}(t_0)}{\mathsf{Leb}(t)}$$



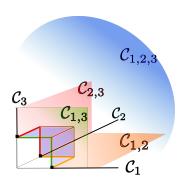




*F* is the inliers distribution, *G* is the resulting outliers distribution.

Theoretical guaranties ? [Biau et al. 2008, Biau and Scornet, 2016]

# Perspectives on AD with Extremes



- ▶ How to choose  $\epsilon$  in practice?
- Refine our representation?
- An alternative notion of sparsity?

#### Some references:

- Agarwal 2006, Detecting anomalies in cross-classified streams: a bayesian approach.
- Aggarwal and Yu 2001, Outlier detection for high dimensional data.
- Chandola, Banerjee, and Kumar 2009, Anomaly detection: A survey.
- Clifton, Hugueny and Tarassenko 2011, Novelty detection with multivariate extreme value statistics.
- Désir, Bernard, Petitjean and Heutte 2012, A New Random Forest Method for One-Class Classification.
- Einmahl and Mason 1992, Generalized quantile processes.
- Einmahl, Krajina and Segers 2012, An m-estimator for tail dependence in arbitrary dimensions.
- Eskin 2000, Anomaly detection over noisy data using learned probability distributions.
- Goix, Sabourin and Clémençon 2015, Learning the dependence structure of rare events: a non-asymptotic study.
- Goix, Sabourin and Clémençon 2016, Sparse Representation of Multivariate Extremes with Applications to Anomaly Ranking.
- Goix, Sabourin and Clémençon 2015, On Anomaly Ranking and Excess-Mass Curves.
- Goix 2016, How to Evaluate the Quality of Unsupervised Anomaly Detection Algorithms?
- Goix, Brault, Drougard and Chiapino 2016, One Class Splitting Criteria for Random Forests with Application to Anomaly Detection.
- Hautamaki, Karkkainen and Franti 2004. Outlier detection using k-nearest neighbour graph.
- de Haan and Ferreira, Extreme value theory, 2006.
- Hawkins 1980. Identification of outliers.
- Lee and Roberts 2008, On-line novelty detection using the Kalman filter and extreme value theory.

#### Some references:

- Liu, Ting, Zhou 2008, Isolation forest.
- Liu and Weng 1991, Detection of outlying data in bioavailability/bioequivalence studies.
- Papadimitriou, Kitagawa, Gibbons and Faloutsos 2002, Loci: Fast outlier detection using the local correlation integral.
- Polonik 1995, Measuring mass concentrations and estimating density contour cluster-an excess mass approach.
- Polonik 1997, Minimum volume sets and generalized quantile processes.
- Qi 1997, Almost sure convergence of the stable tail empirical dependence function in multivariate extreme statistics.
- Resnick 1987, Extreme Values, Regular Variation, Point Processes.
- Roberts 1999, Novelty detection using extreme value statistics.
- Schölkopf, Platt, Shawe-Taylor, Smola, and Williamson 2001, Estimating the support of a high-dimensional distribution.
- Scott and Nowak 2006, Learning minimum volume sets.
- J. Segers 2012, Max-stable models for multivariate extremes.
- ▶ Shi and Horvath 2012, Unsupervised learning with random forest predictors.
- Shyu, Chen, Sarinnapakorn and Chang 2003, A novel anomaly detection scheme based on principal component classifier
- Tang, Chen, Fu, and W.Cheung 2002. Enhancing effectiveness of outlier detections for low density patterns.
- ▶ Thomas, Feuillard and Gramford 2015, Calibration of One-Class SVM for MV set estimation.
- Thomas, Clémençon, Feuillard and Gramford 2016, Learning Hyperparameters for Unsupervised Anomaly Detection.
- Vert and Vert 2006, Consistency and Convergence Rates of One-Class SVMs and Related Algorithms

# Damex algorithm

## DAMEX in $O(dn \log n)$

```
Input: parameters \epsilon > 0, k = k(n)
for i = 1, \ldots, n do
   # Standardize via marginal rank-transformation:
   \hat{V}_i := (1/(1-\hat{F}_j(X_i^j)))_{i=1}
   if \hat{V}_i > \frac{n}{k} then
       # Assign to each \hat{V}_i the cone \frac{n}{\nu}C_{\alpha}^{\epsilon} it belongs to:
       \alpha = \alpha(V_i)
       C_{\alpha} ++
   end if
end for
\Phi_n^{\alpha,\epsilon} := \frac{n}{k} c_{\alpha}
```

**Output:** (sparse) representation of the dependence structure:  $\Phi_n^{\alpha,\epsilon} = \widehat{\Phi}(\Omega_\alpha) = \frac{n}{k} \mathbb{P}_n(\widehat{V} \in \frac{n}{k} \mathcal{C}_\alpha^\epsilon)$ , estimate of the  $\alpha$ -mass of  $\Phi$  for every  $\alpha$ .

$$\widehat{\mathcal{M}} := (\Phi_n^{\alpha,\varepsilon})_{\alpha \subset \{1,\dots,d\},\Phi_n^{\alpha,\,\varepsilon} > \Phi_{\text{min}}}$$

# Does performance in term of EM/MV correspond to performance in term of ROC/PR?

Experiments: 12 datasets, 3 AD algorithms (LOF, OCSVM, iForest) → 36 possible pairwise comparisons:

$$\left\{ \begin{array}{l} \left( A_1 \text{ on } \mathcal{D}, \ A_2 \text{ on } \mathcal{D} \right), \ A_1, A_2 \in \{\text{iForest, LOF, OCSVM}\}, \\ \\ \mathcal{D} \in \{\text{adult, http,} \dots, \text{spambase}\} \end{array} \right\}.$$

Results: If we only consider the pairs s.t. ROC and PR agree on which algorithm is the best, we are able (with EM and MV scores) to recover it in 80% of the cases.

## EM/MV random projection benchmark

Table: Results for the novelty detection setting. One can see that ROC, PR, EM, MV often do agree on which algorithm is the best (in bold), which algorithm is the worse (underlined) on some fixed datasets. When they do not agree, it is often because ROC and PR themselves do not, meaning that the ranking is not clear.

Dataset	Dataset iForest				OCSVM				LOF			
	ROC	PR	EM	MV	ROC	PR	EM	MV	ROC	PR	EM	MV
adult	0.661	0.277	1.0e-04	7.5e01	0.642	0.206	2.9e-05	4.3e02	0.618	0.187	1.7e-05	9.0e02
http	0.994	0.192	1.3e-03	9.0	0.999	0.970	6.0e-03	2.6	0.946	0.035	8.0e-05	3.9e02
pima	0.727	0.182	5.0e-07	1.2e04	0.760	0.229	5.2e-07	1.3e04	0.705	0.155	3.2e-07	2.1e04
smtp	0.907	0.005	1.8e-04	9.4e01	0.852	0.522	1.2e-03	8.2	0.922	0.189	1.1e-03	5.8
wilt	0.491	0.045	4.7e-05	2.1e03	0.325	0.037	5.9e-05	4.5e02	0.698	0.088	2.1e-05	1.6e03
annthyroid	0.913	0.456	2.0e-04	2.6e02	0.699	0.237	6.3e-05	2.2e02	0.823	0.432	6.3e-05	1.5e03
arrhythmia	0.763	0.487	1.6e-04	9.4e01	0.736	0.449	1.1e-04	1.0e02	0.730	0.413	8.3e-05	1.6e02
forestcov.	0.863	0.046	3.9e-05	2.0e02	0.958	0.110	5.2e-05	1.2e02	0.990	0.792	3.5e-04	3.9e01
ionosphere	0.902	0.529	9.6e-05	7.5e01	0.977	0.898	1.3e-04	5.4e01	0.971	0.895	1.0e-04	7.0e01
pendigits	0.811	0.197	2.8e-04	2.6e01	0.606	0.112	2.7e-04	2.7e01	0.983	0.829	4.6e-04	1.7e01
shuttle	0.996	0.973	1.8e-05	5.7e03	0.992	0.924	3.2e-05	2.0e01	0.999	0.994	7.9e-06	2.0e06
spambase	0.824	0.371	9.5e-04	4.5e01	0.729	0.230	4.9e-04	1.1e03	0.754	0.173	2.2e-04	4.1e04

## **OCRF Benchmark**

Table: Results for the novelty detection setting (novelty detection framework).

Datasets	OneClassRF	iForest	OCRFsampl.	OCSVM	LOF	Orca	LSAD	RFC
	ROC PR	ROC PR	ROC PR	ROC PR	ROC PR	ROC PR	ROC PR	ROC PR
adult	0.665 0.278	0.661 0.227	NA NA	0.638 0.201	0.615 0.188	0.606 0.218	0.647 0.258	NA NA
annthyroid	<b>0.936</b> 0.468	0.913 0.456	0.918 0.532	0.706 0.242	0.832 0.446	0.587 0.181	0.810 0.327	NA NA
arrhythmia	0.684 0.510	0.763 0.492	0.639 0.249	0.922 0.639	0.761 0.473	0.720 0.466	0.778 0.514	0.716 0.299
forestcover	0.968 0.457	0.863 0.046	NA NA	NA NA	0.990 0.795	0.946 0.558	0.952 0.166	NA NA
http	0.999 0.838	0.994 0.197	NA NA	NA NA	NA NA	0.999 0.812	0.981 0.537	NA NA
ionosphere	0.909 0.643	0.902 0.535	0.859 0.609	0.973 0.849	0.959 0.807	0.928 0.910	<b>0.978</b> 0.893	0.950 0.754
pendigits	0.960 0.559	0.810 0.197	0.968 0.694	0.603 0.110	0.983 0.827	0.993 0.925	0.983 0.752	NA NA
pima	0.719 0.247	0.726 0.183	0.759 0.266	0.716 0.237	0.700 0.152	0.588 0.175	0.713 0.216	0.506 0.090
shuttle	0.999 0.998	0.996 0.973	NA NA	0.992 0.924	<b>0.999</b> 0.995	0.890 0.782	0.996 0.956	NA NA
smtp	0.922 0.499	0.907 0.005	NA NA	0.881 0.656	<b>0.924</b> 0.149	0.782 0.142	0.877 0.381	NA NA
spambase	<b>0.850</b> 0.373	0.824 0.372	0.797 0.485	0.737 0.208	0.746 0.160	0.631 0.252	0.806 0.330	0.723 0.151
wilt	0.593 0.070	0.491 0.045	0.442 0.038	0.323 0.036	0.697 0.092	0.441 0.030	0.677 0.074	0.896 0.631
average:	0.850 0.495	0.821 0.311	0.769 0.410	0.749 0.410	0.837 0.462	0.759 0.454	<b>0.850</b> 0.450	0.758 0.385
cum. train time:	61s	68s	NA	NA	NA	2232s	73s	NA

# **Datasets**

Datasets	nb of samples	nb of features	anomaly class			
adult	48842	6	class '> 50K'	(23.9%)		
annthyroid	7200	6	classes ≠ 3	(7.42%)		
arrhythmia	452	164	classes ≠ 1 (features 10-14 removed)	(45.8%)		
forestcover	286048	10	class 4 (vs. class 2)	(0.96%)		
http	567498	3	attack	(0.39%)		
ionosphere	351	32	bad	(35.9%)		
pendigits	10992	16	class 4	(10.4%)		
pima	768	8	pos (class 1)	(34.9%)		
shuttle	85849	9	classes ≠ 1 (class 4 removed)	(7.17%)		
smtp	95156	3	attack	(0.03%)		
spambase	4601	57	spam	(39.4%)		
wilt	4839	5	class 'w' (diseased trees)	(5.39%)		