Machine Learning and Extremes for Anomaly Detection

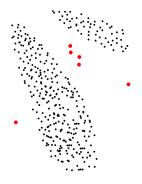
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PhD Defense, Telecom Paristech, November 28th 2016

Anomaly Detection (AD)

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



Huge number of applications: Network intrusions, credit card fraud detection, insurance, finance, military surveillance,...

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)
 The algorithm learns on normal data only
- Outlier Detection (extended application framework)
 Training set (unlabeled) = normal + abnormal data (assumption: anomalies are very rare)

Some litterature 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

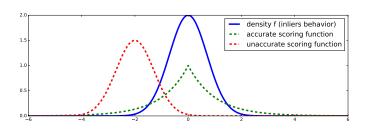
[Aggarwal and Yu 2001, Shyu et al. 2003, Shi and Horvath 2012, Liu et al. 2008]

Background: scoring functions

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

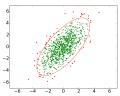
Part II: Learning accurate scoring functions on extreme regions

Part III: Heuristic contributions and perspectives

Existing criterion: Mass-Volume curve

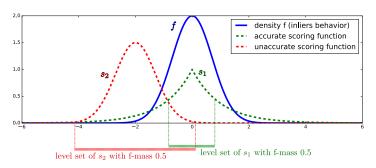
Minimum volume set [Einmahl and Mason 1992, Polonik 1997]

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

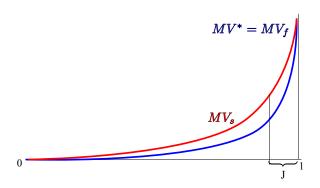


Mass Volume curve of a scoring function s [Clémençon and Jakubowicz, 2013]:

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



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.

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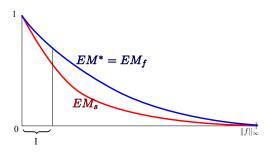
Our solution: Excess-Mass curve

Excess-Mass curve [G., Sabourin, Clémençon 2015]

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

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

We are looking for nearly optimal scoring functions of the form $s(x) = \sum_{j=1}^N a_j \mathbb{1}_{x \in \Omega_j}$, with $a_j \ge 0$, $\Omega_j \in \mathcal{G}$ a VC-class.

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

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

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

$$f(x)$$

$$p(X \in \Omega_1)$$

$$p(X \in \Omega_2)$$

$$p(X \in \Omega_1)$$

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$$p(X \in \Omega_2)$$

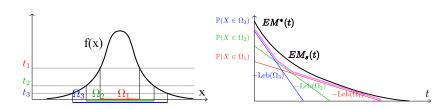
$$p(X \in \Omega_1)$$

Learning a scoring function with M-estimation

Theorem [G., Sabourin, Clémençon 2015]

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

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

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

 \rightarrow Anomalies = points which violate this structure

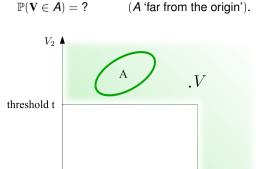
Theoretical framework

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

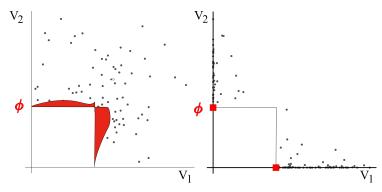
For a large r > 0 and a region B on the unit sphere:

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

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

Angular distribution

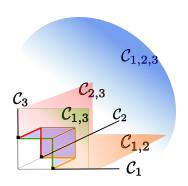
 Φ rules the joint distribution of extremes:



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

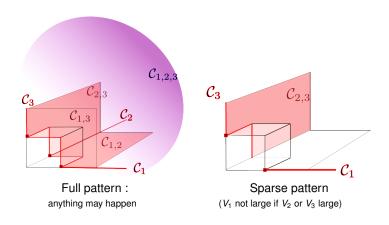
Natural decomposition of the angular measure :

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

▶ ⇒ yields a representation

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

Sparse Representation?



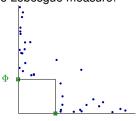
Estimation Problem: \mathcal{M} is an **asymptotic** representation

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

is the restriction of an asymptotic measure

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

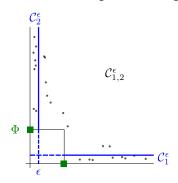
to a representative class of set $\{\mathcal{C}_{\alpha}, \ \alpha\}$, but only the central sub-cone has positive Lebesgue measure!



 \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 ϵ -close to an edge, to that edge.



$$\mathcal{C}_{\alpha} \to \mathcal{C}_{\alpha}^{\varepsilon} = \{\|v\| \geq 1, \ v_j > \varepsilon \ (j \in \alpha), \ v_j \leq \varepsilon \ (j \notin \alpha)\}.$$

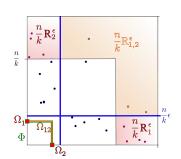
New partition of S_{d-1} .

Resulting estimation procedure

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

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

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



 \Rightarrow we obtain

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

Statistical guaranties

Theorem [G., 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* = sup(density on sub-cones)
- Existing litterature (for spectral measure) [Einmahl and Segers 09, Einmahl et al. 01]

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

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

Theorem's proof: key ingredient

Would like to use concentration inequality...

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

- ▶ scaling $\frac{n}{k}$
- ► classical VC-inequality: $\frac{k}{n}$ 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 $\frac{k}{n}A$ is small.

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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)

Corresponding 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}{k}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 α -mass of Φ for every α .

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

Application to Anomaly Detection

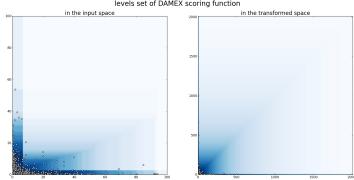
Recall that after standardization of marginals: $\mathbb{P}[R > r, \mathbf{W} \in B] \simeq \frac{1}{r} \Phi(B)$

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

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

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

levels set of DAMEX scoring function



Experiments

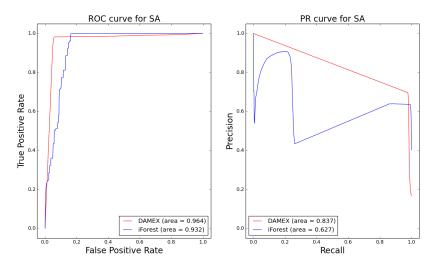


Figure: ROC and PR curve on SA dataset

Part I: Performance criterion for scoring functions

Part II: Learning accurate scoring functions on extreme regions

Part III: Heuristic contributions and perspectives

In moderate dimension: [Thomas et al. 2015, 2016]

Practical motivations:

Most of the time, data come without any label.

 \rightarrow no ROC or PR curves!

Implicit (natural) simplification of the problem:

How good is an anomaly detection algorithm?

 \rightarrow How good is it estimating the level sets of the inliers distribution?

Estimation:

$$\begin{split} \widehat{\mathit{MV}}_s(\alpha) &= \inf_{u \geq 0} \quad \mathsf{Leb}(s \geq u) \quad \textit{s.t.} \quad \mathbb{P}_n(s \geq u) \geq \alpha \qquad \to \widehat{\mathcal{C}}^{\mathit{EM}}(s) = \|\mathit{MV}_s\|_{1,J} \\ \widehat{\mathit{EM}}_s(t) &= \sup_{u > 0} \quad \mathbb{P}_n(s \geq u) \quad - t \mathsf{Leb}(s \geq u) \qquad \to \widehat{\mathcal{C}}^{\mathit{MV}}(s) = \|\mathit{EM}_s\|_{1,J} \end{split}$$

Issue in large dimension: The volume Leb($s \ge u$) has to be estimated!

Heuristic extension for large dimension:

Random projection and averaging

Inputs: AD algorithm 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 $s_k=\mathcal{A}\big((x_i^j)_{1\leq i\leq n,\ j\in F_k}\big)$ -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

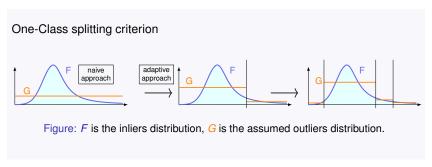
Return performance criteria:

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

Seems to work in pratice but no statistical guaranties.

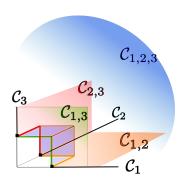
One Class Random Forests

Existing litterature: [Désir et al., 2013, Liu et al., 2008, Shi and Horvath, 2012].



Does theorical guaranties on RFs apply ? [Biau et al. 2008, Biau and Scornet, 2016]

AD and Extremes perspectives



A more accurate sparse representation?

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- ▶ 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.
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	number of samples	number of features
shuttle	85849	9
forestcover	286048	54
SA	976158	41
SF	699691	4
http	619052	3

Table: Datasets characteristics

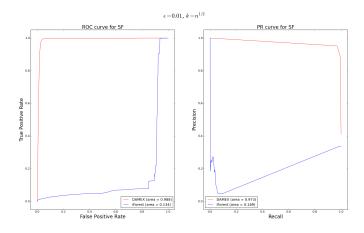


Figure: ROC and PR curve on SF dataset

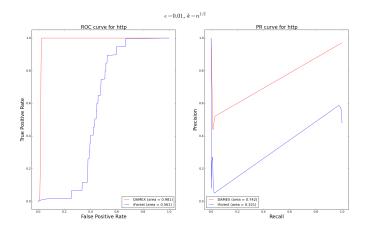


Figure: ROC and PR curve on http dataset

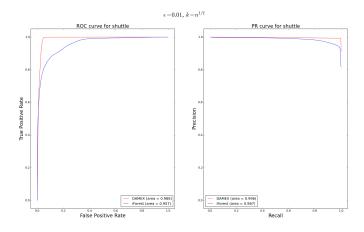


Figure: ROC and PR curve on shuttle dataset

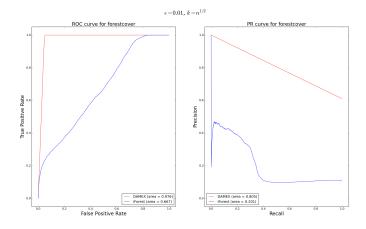


Figure: ROC and PR curve on forestcover dataset

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:

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

▶ **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.

Table: Original Datasets characteristics

	nb of samples	nb of features	anomaly class				
adult	48842	6	class '> 50 <i>K</i> '	(23.9%)			
http	567498	3	attack	(0.39%)			
pima	768	8	pos (class 1)	(34.9%)			
smtp	95156	3	attack	(0.03%)			
wilt	4839	5	class 'w' (diseased trees)	(5.39%)			
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%)			
ionosphere	351	32	bad	(35.9%)			
pendigits	10992	16	class 4	(10.4%)			
shuttle	85849	9	classes \neq 1 (class 4 removed)	(7.17%)			
spambase	4601	57	spam	(39.4%)			

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	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