

Distributionally robust, skeptical binary inferences in multi-label problems

12th International Symposium on Imprecise Probabilities:
Theories and Applications

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06 to 09 July 2021

Overview

- Multi-label classification problem
- Cautious inferences in multi-label problems
 - General case for the Hamming loss
 - Experimental results
- Conclusions and Perspectives

Multi-label classification problem

👉 **The goal of multi-label problem :**

Given a training data : $\mathcal{D} = \{\mathbf{x}^i, \mathbf{y}^i\}_{i=0}^N \subseteq \mathbb{R}^p \times \mathcal{Y}$

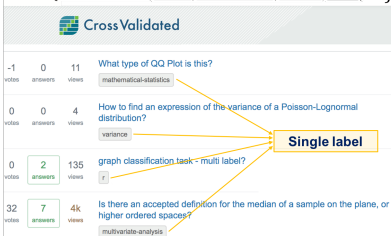
where : $\mathcal{Y} = \{0, 1\}^m, \quad |\mathcal{Y}| = 2^m$

Learning a multi-label classification rule : $\varphi : \mathbb{R}^p \rightarrow \mathcal{Y}$

👉 **Example :**

Classical classification

$\mathcal{H} = \{\text{mathematical-statistics, variance, poisson-distribution, lognormal, qq-plot, ...}\}$



CrossValidated

-1 0 11 votes answers views What type of QQ Plot is this?
mathematical-statistics

0 0 4 votes answers views How to find an expression of the variance of a Poisson-Lognormal distribution?
variance

0 2 135 votes answers views graph classification task - multi label?
r

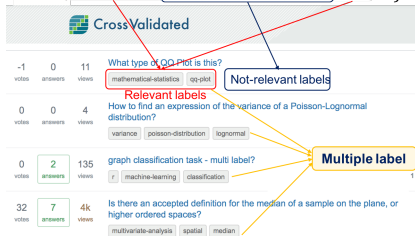
32 7 4k votes answers views Is there an accepted definition for the median of a sample on the plane, or higher ordered spaces?
multivariate-analysis

Single label



Multi-label classification

$\mathcal{H} = \{\text{mathematical-statistics, variance, poisson-distribution, lognormal, qq-plot, ...}\}$



CrossValidated

-1 0 11 votes answers views What type of QQ Plot is this?
mathematical-statistics qq-plot
Not-relevant labels

0 0 4 votes answers views How to find an expression of the variance of a Poisson-Lognormal distribution?
variance poisson-distribution lognormal

0 2 135 votes answers views graph classification task - multi label?
r machine-learning classification

32 7 4k votes answers views Is there an accepted definition for the median of a sample on the plane, or higher ordered spaces?
multivariate-analysis spatial median

Multiple label

Existing results for precise and cautious¹ inferences

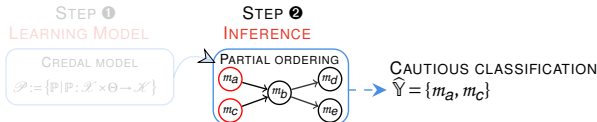
- ✌ Inference in precise case difficult, but there are
 - ✓ Efficient algorithms for specific losses [... ; [DEMBCZYŃSKI et al. 2012](#) ; [WAEGEMAN et al. 2014](#)]
 - ✓ Several simplified learning model : Binary relevance, Classifier chains [[READ et al. 2019](#)], ...
- ✂ This issue is poorly explored in IP [[DESTERCKE 2015](#) ; [ANTONUCCI et al. 2017](#)], and even less in other cautious settings [[NGUYEN et al. 2019](#) ; [PILLAI et al. 2013](#)].
- ✌ Our contribution consists in providing :
 - ✂ More efficient, dedicated algorithm for the Hamming Loss under the maximality criterion.
 - ✂ Polynomial-time inference on restricted credal sets \mathcal{P}_{PR} (imprecise Binary relevance).

1. Cautious and Skeptical are here used interchangeably.

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Cautious inferences in form of set-valued solutions



Problem setting and challenges :

✓ Step ① : The uncertainty model \mathcal{P} is known.

✗ Step ② : Under the maximality criterion and a generic loss matrix
 \Rightarrow the set-valued solutions require at worst $2^m(2^m-1) \propto 2^{2m}$ computations.

✍ **Example :** $|\mathcal{Y}| = 10$, it needs to $2^{10}(2^{10} - 1) = 1047552$ computations.

$$(0, 0, \dots, 0) \succ_{\ell}^{\mathcal{P}} (0, \dots, 1, 1) ?$$

$$(0, 0, \dots, 0) \succ_{\ell}^{\mathcal{P}} (0, \dots, 1, 0) ?$$

⋮
⋮
⋮
⋮



A set-valued solution

$$\hat{\mathcal{Y}}_{\ell, \mathcal{P}}^M = \begin{pmatrix} 1 & 1 & 0 & \dots & 0 \\ 0 & 1 & 1 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix}$$

👉 **Can we obtain cautious predictions efficiently ?**

General case for the Hamming case

Proposition 1 (Ceteris paribus comparison)

For a given set of indices $\mathcal{J} \subseteq \llbracket m \rrbracket$, let us consider an assignment $\mathbf{a}_{\mathcal{J}}$ and its complement $\bar{\mathbf{a}}_{\mathcal{J}}$. Then, for any two vectors $\mathbf{y}^1, \mathbf{y}^2$ such that $\mathbf{y}_{\mathcal{J}}^1 = \mathbf{a}_{\mathcal{J}}, \mathbf{y}_{\mathcal{J}}^2 = \bar{\mathbf{a}}_{\mathcal{J}}$ and $\mathbf{y}_{-\mathcal{J}}^1 = \mathbf{y}_{-\mathcal{J}}^2$, we have

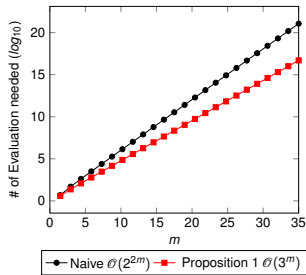
$$\mathbf{y}^1 >_{\ell}^{\mathcal{P}} \mathbf{y}^2 \iff \inf_{P \in \mathcal{P}} \sum_{i \in \mathcal{J}} P(Y_i = a_i) > \frac{|\mathcal{J}|}{2} \quad (1)$$

Prop. 1 amounts to focus on partial binary vector, e.g. $|\mathcal{Y}| = n + 3, \mathbf{a} = (0, 0, 0, *, \dots, *)$

$$(0, 0, 0, \underbrace{*, \dots, *}_{n \text{ labels}}) >_{\ell_H}^{\mathcal{P}} (1, 1, 1, \underbrace{*, \dots, *}_{n \text{ labels}})$$

1 comparison instead of 2^n .

✓ We can reduce : $\mathcal{O}(2^{2m}) \longrightarrow \mathcal{O}(3^m)$



Existing approximate results for Hamming loss

- The partial vector $\hat{\mathbf{y}}^* = (\hat{y}_1^*, \dots, \hat{y}_m^*) \in \mathfrak{Y} = \{0, 1, *\}$

$$\hat{y}_j^* = \begin{cases} 1 & \text{if } \underline{P}_{\mathbf{x}^*}(Y_j = 1) > 0.5 \\ 0 & \text{if } \overline{P}_{\mathbf{x}^*}(Y_j = 1) < 0.5 \\ * & \text{if } 0.5 \in [\underline{P}_{\mathbf{x}^*}(Y_j = 1), \overline{P}_{\mathbf{x}^*}(Y_j = 1)] \end{cases}$$

is an outer-approximation of $\hat{\mathcal{Y}}_{\ell_H, \mathcal{P}}^M$ [DESTERCKE 2015]

- Only requires to know imprecise marginal bounds \mathcal{P}_{Y_i} on each label.
- Note that not all cautious multi-label predictions can be exactly represented as a partial vector

$$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix} \Rightarrow \text{cannot be represented in } \mathfrak{Y} \quad \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = (*, *, 0) \in \mathfrak{Y}$$

Exact $\hat{Y}_{\ell_H, \mathcal{P}}^M$ vs. \hat{y}^* outer-approximation inferences

Imprecision — small — medium — high

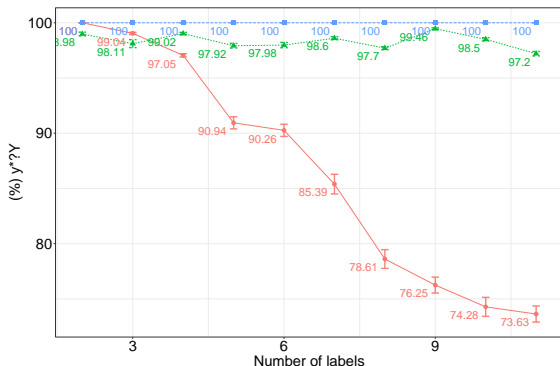


FIGURE – % of instances where $\hat{y}^* = \hat{Y}_{\ell_H, \mathcal{P}}^M$.

- ✓ The quality of \hat{y}^* decreases as the number of labels increases.
- ✓ The quality of \hat{y}^* seems to be the worst for moderate imprecision.

Exact $\hat{Y}_{\ell_H, \mathcal{P}}^M$ vs. \hat{y}^* outer-approximation inferences

Imprecision — small — medium — high

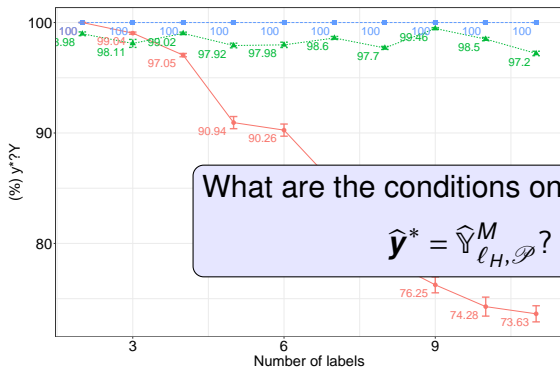


FIGURE — % of instances

What are the conditions on \mathcal{P} ensuring

$$\hat{y}^* = \hat{Y}_{\ell_H, \mathcal{P}}^M?$$

- ✓ The quality of \hat{y}^* decreases as the number of labels increases.
- ✓ The quality of \hat{y}^* seems to be the worst for moderate imprecision.

Binary relevance and partial vectors

Under the assumption of label independence :

$$\mathcal{P}_{BR} := \left\{ \prod_{\{i|y_i=1\}} p_i \prod_{\{i|y_i=0\}} (1-p_i) \mid p_i \in [\underline{p}_i, \bar{p}_i] \right\}.$$

Proposition 2 (Domain restriction on \mathcal{P})

Given a probability set \mathcal{P}_{BR} and the Hamming loss, $\hat{\mathcal{Y}}_{\ell_H, \mathcal{P}_{BR}}^M \in \mathfrak{Y}$.

- ✓ $\hat{\mathcal{Y}}_{\ell_H, \mathcal{P}_{BR}}^M$ can be represented as partial vector \mathfrak{Y} .
- ✓ $\hat{\mathcal{Y}}_{\ell_H, \mathcal{P}_{BR}}^M$ is equal to outer-approximation $\hat{\mathbf{y}}^*$ [DESTERCKE 2015].
- ✓ The time complexity becomes linear on m , i.e. $\mathcal{O}(m)$!

Dataset and experimental setting

Material/Imprecise Classifier/Metrics

- ☞ The data set issued from MULAN repository.

Data set	#Features	#Labels	#Instances	#Cardinality	#Density
emotions	72	6	593	1.90	0.31
yeast	103	14	2417	4.23	0.30
scene	294	6	2407	1.07	0.18

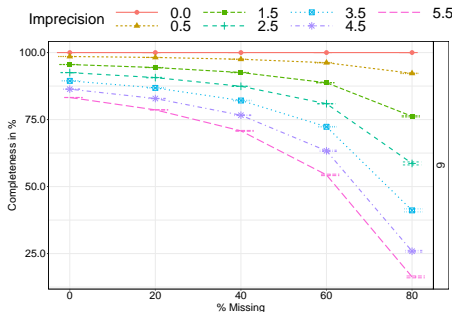
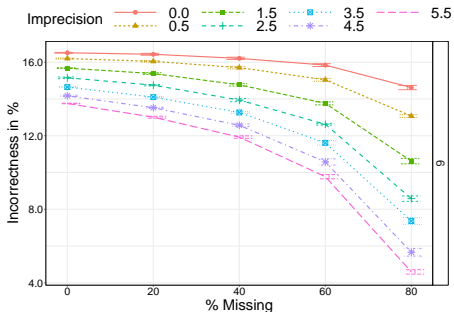
- ☞ Naive credal classifier (NCC) [ZAFFALON 2002] for each marginal credal \mathcal{P}_{Y_i} .
- ☞ Metric evaluations : (Q denotes the set of predicted label s.t. $\hat{y}_i = 1$ or $\hat{y}_i = 0$)

$$IC(\hat{Y}, \mathbf{y}) = \frac{1}{|Q|} \sum_{\hat{y}_i \in Q} 1_{(\hat{y}_i \neq y_i)} \quad \text{and} \quad CP(\hat{Y}, \mathbf{y}) = \frac{|Q|}{m}$$

Missing labels

We uniformly pick at random a percentage of missing labels $Y_{i,j}$ (the j th label of the i th instance) which are then removed from the training data, i.e. $Y_{i,j} = 1 \wedge 0 \rightarrow Y_{i,j} = *$

Features					Missing		
X_1	X_2	X_3	X_4	X_5	Y_1	Y_2	Y_3
107.1	25	Blue	60	1	1	*	0
-50	10	Red	40	0	1	0	*
200.6	30	Blue	58	1	*	0	0
...



Evolution of the incorrectness (left) and the completeness (right) in average (%) for each level of imprecision (a curve for each one), with respect to the % of missingness.

- ✗ The precise model ($s=0.0$) is not really affected by randomly missing labels.
- ☺ Our proposal, however, becomes more cautious as the number of missing labels increases.

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Conclusions and Perspective

- ① Works done in this paper :
 - ✌ Provide efficient algorithmic procedures to solve the maximality criterion under **Hamming loss** and **generic probability sets**.
 - ✌ When considering sets of distributions and cautious inferences, **it is not sufficient to consider marginal probabilities to get exact set-valued predictions**, as opposed to the case of precise distributions.
- ② What remains to do
 - ✗ Compare our proposal against those rejecting and abstaining approaches.
 - ✗ Solve the maximality criterion using other loss functions, e.g. ; ranking loss, Jaccard loss, F-measure, and so on.



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