# A first glance at multi-label chaining using imprecise probabilities

ECML/PKDD 2020 Tutorial and Workshop on Uncertainty in Machine Learning

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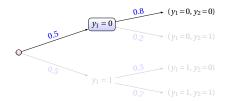




# Our approach in a nutshell

### What?

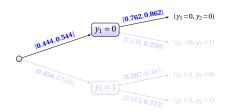
Multi-label chaining using a set of probability models [5] instead of a single probability model.



Chaining with precise probabilistic models

$$\mathbb{P}$$

$${}_{P(Y_{j}|Y_{1},...,Y_{j-1},X)}$$
 widely studied!



Chaining with imprecise probabilistic models

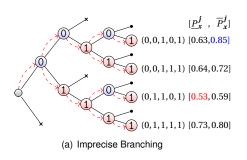
$$\mathscr{P}$$

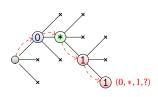
$$[\underline{P}(Y_j|Y_1,...,Y_{j-1},X),\overline{P}(Y_j|Y_1,...,Y_{j-1},X)]$$
how can we do it?

# Our approach in a nutshell

# How can doing it?

- We propose two strategies to get probability bounds  $[\underline{P}, \overline{P}]$ Imprecise Branching
  - Marginalization





(b) Marginalization (\* =  $\{0, 1\}$ )

# Our approach in a nutshell

## Why?

- Recognizing hard instances to predict in order to avoid making mistakes → Making a cautious decision.
- Trying to avoid to propagate unsure predictions in the chaining.

#### Results?

- Our proposal overcomes precise ones in noisy setting.
- Good balance between abstained labels and performance.



### **Overview**

- Introduction to multi-label classification
- Multi-label chaining with imprecise probabilities
- Evaluation
  - Settings and Datasets
  - Experimental results
- Conclusions and Perspectives

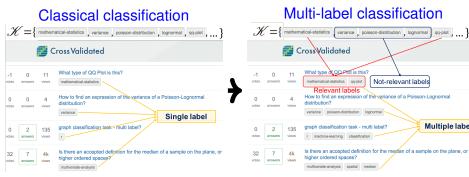


# Multi-label classification problem

#### □ Problem statement:

Let  $\mathcal{H} = \{m_1, \dots, m_K\}$  be a set of labels and let  $\mathbf{x} \in \mathbb{R}^p$  be an unlabelled instance, attribute it a set of relevant labels  $\mathcal{S}(x) \subseteq \mathcal{K}$ .

#### Example:





Multiple label



# Multi-label classification problem

#### The goal of multi-label problem:

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

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

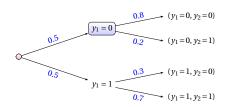
## Learning a multi-label classification rule : $\varphi : \mathbb{R}^p \to \mathscr{Y}$

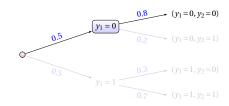
Example of training data:

$X_1$	$X_1$ $X_2$		$X_4$	<i>y</i> 1	$y_2$	<i>y</i> 3				
107.1	25	Blue Red Blue	60	1	0	0				
-50	10	Red	40	1	0	1				
200.6	30	Blue	58	0	1	0				

## Multi-label classification problem

- Why we want to use the multi-label chaining.
- Decomposition techniques ignore the label dependencies.
- Probabilistic tree chains require to scan all possible predictions.





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#### **Basic notations**

Let us denote the probability of the label  $Y_i$  conditioned on previous labels by

$$P_{\mathbf{x}}^{j}(Y_{j}=1) := P_{\mathbf{x}}(Y_{j}=1|Y_{\mathcal{J}_{\mathcal{R}}^{j-1}}=1,Y_{\mathcal{J}_{\mathcal{J}}^{j-1}}=0)$$
 (1)

where  $\mathscr{I}_{*}^{j}$  is the set of indices of the labels among the j first predicted as

- 1. (relevant labels)  $\mathscr{I}_{\mathscr{Q}}^{j} \subseteq [j]^{1}$ ,  $\forall i \in \mathscr{I}_{\mathscr{Q}}^{j}$ ,  $y_{i} = 1$ ,
- 2. (irrelevant labels)  $\mathscr{I}_{\alpha}^{j} \subseteq [j], \mathscr{I}_{\alpha}^{j} \cap \mathscr{I}_{\alpha}^{j} = \emptyset, \forall i \in \mathscr{I}_{\alpha}^{j}, y_{i} = 0,$
- 3. (abstained labels)  $\mathscr{I}_{\mathcal{A}}^{j} = [\![j]\!] \setminus (\mathscr{I}_{\mathcal{A}}^{j} \cup \mathscr{I}_{\mathcal{A}}^{j}), \forall i \in \mathscr{I}_{\mathcal{A}}^{j}, \gamma_{i} = \{0,1\} := *.$

<sup>1.</sup>  $[i] = \{1, ..., i\}$  set of the first i integers

# (Precise) Multi-label chaining

#### Learning a multi-label chaining

• Learning a binary classifier at each step of the chaining [3]:

$$\varphi_i: \mathbb{R}^p \times \{0,1\}^{i \le m} \to \{0,1\}$$

Decision step under a binary classifier  $\ell(y_i, \hat{y}_i) \rightarrow$ 

"Optimal" decision [4] : 
$$\varphi_i := \hat{y}_j = \begin{cases} 1 & P_x^j(Y_j = 1) \ge 0.5 \\ 0 & otherwise \end{cases}$$

#### An example of multi-label chaining

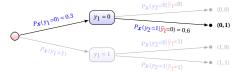


FIGURE - Precise multi-label chaining with two labels.





# (Imprecise) Multi-label chaining

#### Learning a multi-label chaining using imprecise probabilities

 Learning an imprecise classifier model at each step of the chaining :

$$[P_x^j]: \mathbb{R}^p \times \{0,1\}^{j \le m} \to [\underline{P}_x^j, \overline{P}_x^j]$$

Making a cautious decision

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

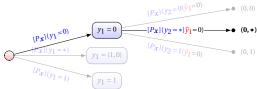


FIGURE - An example of multi-label chaining using imprecise



# Strategy **0**: Imprecise branching

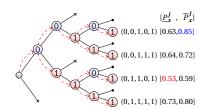
Considering all possible branching in the chaining as soon as there is an abstained label.

$$\begin{split} & \underline{P}_{\boldsymbol{x}}^{\boldsymbol{j}}(Y_{j}=1) = \min_{\boldsymbol{y} \in \{0,1\}^{|\mathcal{I}_{\mathcal{A}}|}} \underline{P}_{\boldsymbol{x}}(Y_{j}=1 | Y_{\mathcal{I}_{\mathcal{R}}^{j-1}} = 1, Y_{\mathcal{I}_{\mathcal{I}}^{j-1}} = 0, Y_{\mathcal{I}_{\mathcal{A}}^{j-1}} = \boldsymbol{y}), \\ & \overline{P}_{\boldsymbol{x}}^{\boldsymbol{j}}(Y_{j}=1) = \max_{\boldsymbol{y} \in \{0,1\}^{|\mathcal{I}_{\mathcal{A}}|}} \overline{P}_{\boldsymbol{x}}(Y_{j}=1 | Y_{\mathcal{I}_{\mathcal{R}}^{j-1}} = 1, Y_{\mathcal{I}_{\mathcal{I}}^{j-1}} = 0, Y_{\mathcal{I}_{\mathcal{A}}^{j-1}} = \boldsymbol{y}). \end{split}$$

#### Example:

Computing the probability of the label  $Y_5 = 1$  conditioned on previous labels

$$\{\hat{Y}_1 = 0, \hat{Y}_2 = *, \hat{Y}_3 = 1, \hat{Y}_4 = *\}$$





# Strategy 2: Marginalization

Ignore unsure predictions chaining in the interests of not propagating imprecision in the tree.

$$\begin{split} \underline{P_{x}^{j}}(Y_{j} = 1) &= \underline{P_{x}}(Y_{j} = 1 | Y_{\mathcal{J}_{\mathcal{R}}^{j-1}} = 1, Y_{\mathcal{J}_{\mathcal{J}}^{j-1}} = 0, Y_{\mathcal{J}_{\mathcal{J}}^{j-1}} = \{0, 1\}^{|\mathcal{J}_{\mathcal{J}}^{j-1}|}), \\ &= \min_{P \in \mathcal{P}^{*}} P_{x}(Y_{j} = 1 | Y_{\mathcal{J}_{\mathcal{R}}^{j-1}} = 1, Y_{\mathcal{J}_{\mathcal{J}}^{j-1}} = 0), \\ \overline{P_{x}^{j}}(Y_{j} = 1) &= \overline{P_{x}}(Y_{j} = 1 | Y_{\mathcal{J}_{\mathcal{R}}^{j-1}} = 1, Y_{\mathcal{J}_{\mathcal{J}}^{j-1}} = 0, Y_{\mathcal{J}_{\mathcal{J}}^{j-1}} = \{0, 1\}^{|\mathcal{J}_{\mathcal{J}}^{j-1}|}), \\ &= \max_{P \in \mathcal{P}^{*}} P_{x}(Y_{j} = 1 | Y_{\mathcal{J}_{\mathcal{R}}^{j-1}} = 1, Y_{\mathcal{J}_{\mathcal{J}}^{j-1}} = 0). \end{split}$$
 (MAR)

where  $\mathscr{P}^*$  is the set of joint probability distributions described by the imprecise probabilistic tree [2].

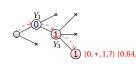
# Strategy 2: Marginalization

An example with four labels.

$$\begin{split} \underline{P_{x}^{4}(Y_{4}=1)} &= \min_{P_{x}^{4} \in \mathscr{P}^{*}} P_{x}(Y_{4}=1|Y_{1}=0, (Y_{2}=0 \cup Y_{2}=1), Y_{3}=1) \\ &= \min_{P_{x}^{4} \in \mathscr{P}^{*}} \frac{\sum_{y_{2} \in \{0,1\}} P_{x}(Y_{4}=1, Y_{1}=0, Y_{2}=y_{2}, Y_{3}=1)}{\sum_{y_{2} \in \{0,1\}} P_{x}(Y_{1}=0, Y_{2}=y_{2}, Y_{3}=1)} \\ &= \min_{P_{x}^{4} \in \mathscr{P}^{*}} P_{x}(Y_{4}=1|Y_{1}=0, Y_{3}=1). \end{split}$$

- The optimization problem can be tricky.
- But, we propose to use NCC classifier to compute  $P_r$







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## **Datasets and experimental setting**

#### Material and method

3 data sets issued from MULAN repository.

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

■ 10×10-fold cross-validation procedure.

Naive imprecise classifier (NCC) [1]

Applying minimax strategy to compare precise approaches.

e.g. 
$$(0, *, 1) \xrightarrow{minimax} (0, 1, 1)$$

### Missing and Noise labels

- **1. Missing (miss)**  $Y_{j,i} = 0 \land 1 \longrightarrow Y_{j,i} = *$ .
- 2. Noise
  - 2.1 Reversing (rev)  $Y_{i,i} = 1 \longrightarrow Y_{i,i} = 0$  or  $Y_{i,i} = 0 \longrightarrow Y_{i,i} = 1$ ).
  - 2.2 **Flipping (flip)**  $Y_{i,i} \sim \mathcal{B}er(\beta), \beta := P(Y_{i,i} = 1), \beta \in \{0.2, 0.8\}.$





# **Experimental results**

TABLE – Average (%) of the IC on missing and noise settings for s=2 and  $\beta=0.8$ 

(a) Imprecise Branching							(b) Marginalization								
Data set	%	<sub>ov</sub> Mis	SING	ING REVERSING		FLIPPING		Data set	%	Missing		REVERSING		FLIPPING	
Dala Sel	%	CC	ICC	CC	ICC	CC	ICC	Dala Sel	70	CC	ICC	CC	ICC	CC	ICC
	0.0	21.87	22.70	_	_	_	_		0.0	21.76	22.83	_	_	_	_
Emotion	0.4	21.82	23.02	32.02	32.75	27.71	27.74	Emotion	0.4	21.84	23.24	31.71	32.59	27.75	27.79
	8.0	21.61	23.17	74.64	73.58	39.51	34.80		0.8	21.64	24.35	74.74	73.72	40.04	35.29
	0.0	16.03	16.94	_	_	_	_	Scene	0.0	16.03	16.98	_	_	_	_
Scene	0.4	15.74	17.21	30.38	31.54	28.22	28.70		0.4	15.73	17.31	30.62	31.73	28.20	28.74
	8.0	14.07	18.38	74.92	73.68	38.33	34.91		8.0	14.14	18.77	74.92	73.67	38.37	34.85
	0.0	29.59	33.00	_	_	_	_		0.0	29.67	33.69	_	_	_	
Yeast	0.4	28.96	34.54	40.50	41.85	36.45	38.34	Yeast	0.4	28.86	34.80	40.50	41.84	36.45	38.19
	8.0	26.17	40.10	67.49	64.58	53.15	50.55		0.8	26.17	42.29	67.54	64.73	53.17	50.59



# **Experimental results**

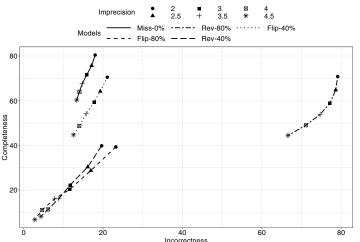


FIGURE – Evolution of the incorrectness and completeness for the imprecise branching strategy and Emotion dataset.



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# **Conclusions and Perspectives**

- We propose two new innovative strategies to treat the multi-label chaining under uncertainty.
- Our proposal overcomes those precise ones in the noise setting.
- How to come up with general but efficient optimisation methods to solve Equations (IB) and (MAR).
- Investigating the performance of our proposed strategies on other imprecise classifier (eg. continuous classifier).





#### References



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