Multi-Label Classification based on Sum-Product Networks

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Resumo

Villanueva, J. G. **Classificação Multi-Rótulo baseada em Redes Soma-Produto**. 2017. 43 f. Dissertação Mestrado - Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, 2017.

A classificação Multi-Rótulo consiste em aprender uma função que seja capaz de mapear um objeto para um conjunto de rótulos relevantes. Ela possui aplicações como associação de genes com funções biológicas, classificação semântica de cenas e categorização de texto. A classificação tradicional, de rótulo único é, portanto, um caso particular da Classificação Multi-Rótulo, onde cada objeto está associado com exatamente um rótulo.

Uma abordagem bem sucedida para classificação é obter um modelo probabilístico da relação entre atributos do objeto e rótulos. Esse modelo pode então ser usado para classificar objetos, encontrando a predição mais provável por meio da probabilidade marginal ou a explicação mais provável dos rótulos dados os atributos. Dependendo da família de modelos probabilísticos escolhidos, tais inferências podem ser intratáveis quando o número de rótulos é grande.

As redes Soma-Produto (SPN, do inglês Sum Product Network) são modelos probabilísticos profundos, que permitem inferência marginal tratável. No entanto, como em muitos outros modelos probabilísticos, a inferência da explicação mais provável é NP-difícil. Embora SPNs já tenham sido usadas com sucesso para tarefas de classificação tradicionais, não existe investigação aprofundada no uso de SPNs para classificação Multi-Rótulo.

Neste trabalho, investigamos o uso de SPNs para classificação Multi-Rótulo. Comparamos vários algoritmos de aprendizado de SPNs combinados com diferentes abordagens propostos para classificação. Mostramos que os classificadores Multi-Rótulos baseados em SPN são competitivos contra classificadores estado-da-arte, como Random k-Labelsets usando Máquinas de Suporte Vetorial e inferência exata da explicação mais provável em CutNets, em uma coleção de conjuntos de dados de referência.

Palavras-chave: Classificação Multi-Rótulo, modelos probabilísticos, redes soma-produto.

Abstract

Villanueva , J. G. **Multi-Label Classification based on Sum-Product Networks**. 2017. 43 f. Dissertação Mestrado - Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, 2017.

Multi-label classification consists of learning a function that is capable of mapping an object to a set of relevant labels. It has applications such as the association of genes with biological functions, semantic classification of scenes and text categorization. Traditional classification (i.e., single-label) is therefore a particular case of multi-label classification in which each object is associated with exactly one label.

A successful approach to constructing classifiers is to obtain a probabilistic model of the relation between object attributes and labels. This model can then be used to classify objects, finding the most likely prediction by computing the marginal probability or the most probable explanation (MPE) of the labels given the attributes. Depending on the probabilistic models family chosen, such inferences may be intractable when the number of labels is large.

Sum-Product Networks (SPN) are deep probabilistic models, that allow tractable marginal inference. Nevertheless, as with many other probabilistic models, performing MPE inference is NP-hard. Although, SPNs have already been used successfully for traditional classification tasks (i.e. single-label), there is no in-depth investigation on the use of SPNs for Multi-Label classification.

In this work we investigate the use of SPNs for Multi-Label classification. We compare several algorithms for learning SPNs combined with different proposed approaches for classification. We show that SPN-based multi-label classifiers are competitive against state-of-the-art classifiers, such as Random k-Labelsets with Support Vector Machine and MPE inference on CutNets, in a collection of benchmark datasets.

Keywords: Multi-label classification, probabilistic graphical models, sum-product networks.

Contents

List of Abbreviations	ix
List of Symbols	xi
List of Figures	xiii
List of Tables	xv
1 Introduction	1
1.1 Objectives	1
1.2 Contributions	2
1.3 Organization	2
2 Sum-Product Networks	3
2.1 Preliminary Considerations	3
2.2 Sum-Product Networks	3
2.2.1 Sum-Product Networks Properties	4
2.3 Probability of Evidence	4
2.4 Most Probable Explanation	5
2.5 Sum-Product Networks Structure Learning	6
2.5.1 LearnSPN	6
2.5.2 Deepening by limiting node splits (LL)	8
2.5.3 Regularization by tractable multivariate distribution hybridization (LC)	9
2.5.4 Learning with Direct and Indirect Variable Interactions (ID)	10
3 Multi-Label Classification	15
3.1 Methods for Multi-Label Classification	16
3.1.1 Binary Relevance	16
3.1.2 Chain Classifier	16
3.1.3 Label Power-Set	17
3.1.4 Probabilistic Graphical Models	17
4 Multi-Label Classification based on Sum-Product Networks	19
4.1 Max-Prod Classification (MC)	21
4.2 Exhaustive Classification (EC)	21
4.3 Sequential Classification (SC)	23

4.4	Pool of Classifications (PC)	25
4.5	Complexity Analysis	27
5	Experiments	29
5.1	Datasets	29
5.2	Metrics	30
5.2.1	Hamming Score (HS)	30
5.2.2	Exact Match (EM)	30
5.2.3	Accuracy (Acc)	30
5.3	Algorithms	31
5.3.1	Multi-label Classifiers based on SPN	31
5.3.2	State-Of-Art Multi-Label Classifiers	32
5.4	Results and Discussion for Multi-Label Classifiers based on SPN and State-of-art	32
5.4.1	Comparing classifiers with Wilcoxon signed-rank test	34
5.4.2	Comparing classifiers with Bayesian signed-rank test	34
6	Conclusions	39
6.1	Suggestions for Future Research	39
	Bibliography	41

List of Abbreviations

MLC	Multi-Label Classification
MPE	Most Probable Explanation
SPN	Sum-Product Network
SVM	Support Vector Machine
RCNET	Multi-label classification on CutNets with MPE exact computation
RSVM	Multi-label classification Random k-labelset using SVM
RV	Random Variable
MCC	Multi-Class Classification
BC	Binary Classification
LL	Learning SPN algorithm limiting node splits
LC	Learning SPN algorithm with Chow-Liu Trees as leaves
ID	Learning SPN algorithm with direct and indirect variable interactions
BR	Binary Relevance approach for MLC
CC	Classifier Chain approach for MLC
LP	Label Power-set approach for MLC
PGM	Probabilistic Graphical Models
EC	Exhaustive Classification approximate MPE algorithm
MC	Max-Prod Classification approximate MPE algorithm
SC	Sequential Classification approximate MPE algorithm
PSC	Pool of Sequential Classification approximate MPE algorithm
PEC	Pool of Exhaustive Classification approximate MPE algorithm
Acc	Accuracy metric for Multi-Label Classification
HS	Hamming Score metric for Multi-Label Classification
EM	Exact Match metric for Multi-Label Classification
EC+LL	Multi-Label Classifier based on SPNs using EC and LL algorithms
EC+LC	Multi-Label Classifier based on SPNs using EC and LC algorithms
EC+ID	Multi-Label Classifier based on SPNs using EC and ID algorithms
MC+LL	Multi-Label Classifier based on SPNs using MC and LL algorithms
MC+LC	Multi-Label Classifier based on SPNs using MC and LC algorithms
MC+ID	Multi-Label Classifier based on SPNs using MC and ID algorithms

SC+LL	Multi-Label Classifier based on SPNs using SC and LL algorithms
SC+LC	Multi-Label Classifier based on SPNs using SC and LC algorithms
SC+ID	Multi-Label Classifier based on SPNs using SC and ID algorithms
PSC+LL	Multi-Label Classifier based on SPNs using PSC and LL algorithms
PSC+LC	Multi-Label Classifier based on SPNs using PSC and LC algorithms
PSC+ID	Multi-Label Classifier based on SPNs using PSC and ID algorithms
PEC+LL	Multi-Label Classifier based on SPNs using PEC and LL algorithms
PEC+LC	Multi-Label Classifier based on SPNs using PEC and LC algorithms
PEC+ID	Multi-Label Classifier based on SPNs using PEC and ID algorithms

List of Symbols

$\mathcal{S}$	Sum-Product Network
$\mathcal{P}_{\mathcal{S}}$	SPN distribution
$\mathcal{S}_i$	Sub-SPN rooted at node i
$\mathcal{S}^m$	Max-Product Network
V	Random Variable
$\mathbf{V}$	Set of Random variables
$val(V)$	Set of values of V
v	A value of V , where $v \in val(V)$
$\mathcal{Z}$	Partition function
α	Parameter for Laplace smooth
$\mathcal{M}$	A Markov Network
$\mathcal{P}_{\mathcal{M}}$	Markov Network distribution
$\emptyset$	Empty set
Δ_{ll}	Increase of log-likelihood
Δ_e	Increase of edges
γ	User defined weight
$\mathcal{C}$	Classifier
$\mathcal{D}$	Training set
$\mathcal{D}_j$	Training subset
θ	Labels ordering
$\mathcal{CS}$	Set of classifications

List of Figures

2.1	Sum-Product Networks examples	3
2.2	Sum-Product Networks properties	4
2.3	Example of computation evidence probability on SPN	5
2.4	Example of Max-Product algorithm on SPNs	6
2.5	Algorithm LearnSPN	7
2.6	Algorithm LearnSPN limiting on node splits	8
2.7	Algorithm LearnSPN with multivariate distribution hybridization	10
2.8	Arithmetic Circuit	11
2.9	Example of SPN learned with ID algorithm	12
2.10	ID learning SPN	14
3.1	Multi-Label Dataset representation	15
3.2	Examples of Traditional, Multi-Class and Multi-Label classifications	15
3.3	Example of Binary Relevance training dataset transformation	16
3.4	Example of Chain Classifier training dataset transformation	16
3.5	Label Power-Set training dataset Transformation	17
3.6	An example of a probabilistic model	18
4.1	Multi-label classifier based on SPN adopting BR approach	19
4.2	Multi-label classifier based on SPN adopting CC approach	20
4.3	Probability distributions of variable A and B	20
4.4	Multi-label classifier based on SPN using Max-Prod classification	21
4.5	An example of EC optimization	22
4.6	An example of Exhaustive classification	23
4.7	An example of sequential classification	24
4.8	An example of pool classification	25
4.9	An example of Pool Sequential Classification	26
4.10	An example of Pool Exhaustive Classification	27
5.1	Pairwise Bayesian signed-rank test for Accuracy metric	35
5.2	Pairwise Bayesian signed-rank test for Exact Match metric	36
5.3	Pairwise Bayesian signed-rank test for Hamming Score metric	37
5.4	Posterior graphic from the Bayesian signed-rank test for Accuracy, Exact Match and Hamming Score	38

List of Tables

5.1	Multi-Label Datasets	29
5.2	Multi-Label Classifiers based on Sum-Product Networks	31
5.3	Comparison Hamming Score	32
5.4	Comparison Exact Match	33
5.5	Comparison Accuracy	33
5.6	P-value obtained from the Wilcoxon signed-rank test on the Compared classifiers for each Metric	34

Chapter 1

Introduction

Multi-Label Classification (MLC) consists in learning a function that associates each example, represented by a feature vector, to a set of (relevant) labels. It therefore generalizes traditional (single-label) classification problem, where each example is associated with a single label. Categorizing music into emotions [TTKV08], associating genes to biological functions [CK01] and performing semantic classification of scenes [BLSB04] are some examples of MLC applications.

A popular and often effective approach to MLC is to transform the problem into one or many single-label classification problems. For example, the Binary Relevance approach consists in independently learning a binary classifier for each distinct label using only the feature vectors [TK06]. Even though it ignores label correlations, this approach often performs reasonably.

A different approach that tries to capture label correlation is the Classifier Chain [DWCH12]. This approach takes an ordering of the labels and sequentially learns a single-label classifier using (in addition to the original attributes) the smaller labels as attributes [RPHF11]. Selecting an ordering of the labels is not trivial and might greatly affect the classification performance.

A caveat of both these approaches is that they require learning a number of classifiers that is equal to the number of labels; since learning a classifier is usually expensive, this might scale poorly to problems with hundreds or even thousands of labels, as is the case in many real domains.

A more principled approach to capture label correlations while dispensing with the need of learning a large number of models is to learn a single joint probabilistic model, such as a Bayesian Network or a Markov Network, over the features and label variables [CAMG14, ACMG13, FGG97, LMP01]. The probabilistic model can then be used to classify the labels either by maximizing the marginal probability of each label given the features, which can result in inconsistent predictions; or by computing the Most Probable Explanation (MPE) of the labels given the features, that maximizes the join probability of the classification given the features.

Sum-product networks (SPNs) are a relatively new class of deep probabilistic models that have obtained impressive results in many tasks such as image completion [PD11] and image (single-label) classification [GD12, SC16, ABG15]. An SPN represents a probability distribution over a set of random variables by a rooted directed-acyclic graph with tractable distributions as leaves, sums and products as inner nodes and weighted edges. Although SPNs have already been shown to perform well in specific MLC tasks (e.g., image completion), there has been no in-depth investigation of the use of SPNs to tackle general MLC problems.

1.1 Objectives

This work aims to investigate the adequacy of SPNs for MLC. Our approach learns a single SPN from data and then uses it to obtain the classification given features as evidence. We experiment with several different state-of-the-art structure learning algorithms for learning SPNs.

An approach for classification using a SPN is to maximize the marginal probability for each label given the features as evidence, this approach is often effective since SPNs compute marginal inference in linear time in its size. However it can result in low probability label sets.

Another approach consists in compute the MPE for the labels, finding the most probable configuration of relevant labels given the features, as a consequence obtains predictions with high joint probability. Unfortunately compute exact MPE on SPNs is NP-hard [PGPD16].

Aiming to construct efficient classifiers based on SPNs, which map objects to consistent predictions in a reasonable time, we propose several new classification algorithms, and compare them against each other, the widely-used max-product algorithm [PD11], which approximates the MPE by replacing sum by maximizations in the evaluation of the SPN, the state-of-the-art Multi-Label classifiers RSVM and RCNET.

1.2 Contributions

The main contributions of this work are the proposed algorithms for Multi-Label classification using a single Sum-Product Network, which are described below:

- **Exhaustive Classification**

Search exhaustively for the most likely prediction in a set of candidates, these candidates are obtained by choosing all distinct classifications on the training set, and then selects the relevant labels that maximize the probability of each candidate given the features.

- **Sequential Classification**

In the spirit of the Classifier Chain, takes a linear ordering over the labels and sequentially selects the maximum probability value for the current label given the smaller labels and features. We apply two criteria for choosing that label ordering: Static Best-First, orders label by the marginal probability of relevance given features only. Dynamic Best-First selects at each iteration the label with the current highest probability of relevance given features and previously selected labels.

- **Pooling classifications**

Based on ensemble of classifications, obtains a set of classification from Sequential Classification using random orderings or from the set of most probable predictions by Exhaustive Classification. Combines these classifications by computing the weighted average of each marginal probability (given features and previous labels), computing the majority voting for each label, and simply selecting the classification with higher probability.

Our results show that our proposed SPN-based Multi-label classifiers, obtained by different combinations of learning and classification algorithms, in average for Accuracy, Hamming Score and Exact Match metrics, outperforms the state-of-the-art Multi-Label classifiers RSVM, that adopts the Random k-labelset approach with Support Vector Machines as basis multi-class classifier and RCNET, that compute exact MPE on CutsetNets in a collection of benchmark datasets.

Part of the contributions of this work was published in the 6th Brazilian Conference on Intelligent Systems (BRACIS) [LM17].

1.3 Organization

The remainder of the paper is organized as follows. In Chapter 2, we introduce some basic knowledge about SPNs and discuss state-of-the-art methods for structure learning. In Chapter 3, we introduce basic concepts about Multi-Label Classification. In Chapter 4 we present our approach for MLC based on SPNs. In Chapter 5 we describe the experiments and show the experimental results of the proposed classifiers. Finally, we conclude the work and discuss possible improvements in Chapter 6.

Chapter 2

Sum-Product Networks

2.1 Preliminary Considerations

We begin by establishing some notation. Random variables (RV) are denoted by upper-case letters (V). The set of values of an RV V is denoted by $\text{val}(V)$, where $v \in \text{val}(V)$. Sets of RVs are written in bold ($\mathbf{V}$). For RVs set $\mathbf{V} = \{V_1, V_2, \dots, V_N\}$, we define $\text{val}(\mathbf{V}) = \times_{n=1}^N \text{val}(V_n)$, where $\mathbf{v} \in \text{val}(\mathbf{V})$.

2.2 Sum-Product Networks

An SPN is a rooted directed acyclic graph with tractable distributions as leaves, sums and products as internal nodes, and non-negative weights associated to the edges connecting sum nodes to their children [PD11]. An SPN $\mathcal{S}$ represents a tractable non-normalized probability distribution $\mathcal{P}_{\mathcal{S}}$ over a set of RVs $\mathbf{V}$. A distribution is called *tractable* if any marginal probability induced by it can be computed in linear time.

Figure 2.1 contains examples of valid SPNs, that is SPNs representing valid distributions, Figure 2.1a shows an SPN with univariate distributions as leaves, while Figure 2.1b shows a SPN with multivariate distributions (Chow-Liu Trees¹ [CL68]) as leaves.

Figure 2.1: SPNs with univariate distributions (2.1a) and Chow-Liu trees (2.1b) as leaves. The numbers below the leaves in (2.1a) denote the probability that the corresponding variables takes on value 1.

¹Chow-Liu Trees are Bayesian Networks where each node have at most one parent

2.2.1 Sum-Product Networks Properties

The *scope* of an SPN, is the set of RVs appearing in their leaves distribution. The scope of a node is the scope of the corresponding Sub-SPN rooted at that node. The set of all nodes of an SPN satisfies the following properties to ensure that it represents a valid distribution:

- The children of a sum node have identical scope (*Completeness*).
- The children of a product node have pairwise disjoint scopes (*Decomposability*).

The Figure 2.2 shows that the Sum-Product Network at the Figure 2.1a represent a valid distribution and satisfies completeness and decomposability properties.

Figure 2.2: *Completeness and Decomposability properties in the SPN of the Figure 2.1a*

2.3 Probability of Evidence

For the SPN $\mathcal{S}$ with scope $\mathbf{V}$, we write $\mathcal{S}(\mathbf{e})$ to denote the network evaluation at $\mathbf{e}$, where $\mathbf{E} \subseteq \mathbf{V}$. An SPN defines a (normalized) probability distribution by:

$$\mathcal{P}_{\mathcal{S}}(\mathbf{E} = \mathbf{e}) = \frac{\mathcal{S}(\mathbf{e})}{\mathcal{Z}}, \quad (2.1)$$

where $\mathcal{Z} = \sum_{\mathbf{v}} \mathcal{S}(\mathbf{v})$ is the *partition function* of the network. If the weights at each sum node in $\mathcal{S}$ add to one and the distributions at the leaves are normalized, then $\mathcal{Z} = 1$ and $\mathcal{S}$ defines a probability distribution by:

$$\mathcal{P}_{\mathcal{S}}(\mathbf{E} = \mathbf{e}) = \mathcal{S}(\mathbf{e}) \quad (2.2)$$

The upward evaluation of the network $\mathcal{S}$ at $\mathbf{e}$ is computed as follows:

- First evaluates the leaves values. Let $\mathbf{A}$ be the set of variables in the leaf i :
 - If $\mathbf{A} \subseteq \mathbf{E}$, the value of i in $\mathcal{S}$ is simply the value $\mathcal{S}_i(\mathbf{e}) = \mathcal{P}_i(\mathbf{A} = \mathbf{a})$ of the corresponding probability distribution $\mathcal{P}_i$.
 - Otherwise the value of i in $\mathcal{S}$ is one, $\mathcal{S}_i(\mathbf{e}) = 1$, summing over the variables in $\mathbf{A}$.
- The value of a sum node i is $\mathcal{S}_i(\mathbf{e}) = \sum_{j \in \mathcal{S}} w_{ij} \mathcal{S}_j(\mathbf{e})$, where the sum ranges over the children of i and w_{ij} is the weight associated with the edge $i \rightarrow j$.
- The value of a product node i is $\mathcal{S}_i(\mathbf{e}) = \prod_{j \in \mathcal{S}} \mathcal{S}_j(\mathbf{e})$, where j and $i \rightarrow j$ are as before.

- Finally, the SPN value at $\mathbf{e}$, $\mathcal{S}(\mathbf{e})$, is the value of its root.

For example, in the SPN in Figure 2.1a:

- For $\mathbf{e} = \{V_1=1, V_2=0\}$, $\mathcal{S}(\mathbf{e}) = 0.4(0.8 \times 0.3) + 0.6(0.4 \times 0.4) = 0.192$.
- For $\mathbf{e} = \{V_1 = 0\}$, $\mathcal{S}(\mathbf{e}) = 0.4(0.2 \times 1) + 0.6(0.6 \times 1) = 0.44$. Figure 2.3 shows the computation of probability on the network.

Figure 2.3: Computation of the probability of evidence on the SPN in the Figure 2.1a and $\mathbf{e} = \{V_1 = 0\}$, where the node value is in purple above of the corresponding node. The resulting probability is $\mathcal{P}_{\mathcal{S}}(\mathbf{e}) = 0.44$

2.4 Most Probable Explanation

The problem of finding a most probable configuration given evidence has many applications such as Multi-Label Classification, that aims to find the most probable configuration of relevant labels given the object features.

Since an SPN defines a distribution, we can obtain the *Most Probable Explanation* (MPE) of a network $\mathcal{S}$ by:

$$\operatorname{argmax}_{\mathbf{q}} \mathcal{P}_{\mathcal{S}}(\mathbf{q}|\mathbf{e}) = \operatorname{argmax}_{\mathbf{q}} \mathcal{P}_{\mathcal{S}}(\mathbf{q}, \mathbf{e}), \quad (2.3)$$

where $\mathbf{e}$ is a configuration of the observed variables $\mathbf{E}$, $\mathbf{Q}$ is a set of query variables and $\mathbf{E}, \mathbf{Q} \subset \mathbf{V}$. Unfortunately, to find a MPE on Sum-Product Networks is NP-hard [PGPD16], even when restricted to binary RVs.

A popular approximate algorithm proposed by Poon and Domingos consists in obtaining a Max-Product Network (MPN) $\mathcal{S}^m$ by replacing the sums nodes in an SPN $\mathcal{S}$ with maximization nodes [PD11], and traverse the network $\mathcal{S}^m$ twice:

- The first pass computes a lower bound on the probability of the MPE by evaluating the network bottom-up as usual, but labeling maximizers at each max node.
- The second pass finds the corresponding configuration by starting at the root and then recursively selecting a highest-valued child of a max node, all children of a product node and an MPE of each leaf.

For example, for the SPN in Figure 2.1a to find the approximate MPE of V_1 given $V_2 = 1$, $\operatorname{argmax}_{v_1} \mathcal{P}_{\mathcal{S}}(v_1|V_2 = 1)$, first obtains the MPN from the SPN and execute the first pass:

$\max(0.4(0.8 \times 0.3), 0.6(0.6 \times 0.4)) = 0.144$ and finally recovers the correspondent value $V_1 = 0$ in the MPN path on the second pass. The Figure 2.4 shows in more detail this procedure for the given example.

Figure 2.4: MPE approximation by Max-Prod algorithm on the SPN in Figure 2.1a. For $\mathbf{Q} = \{V_1\}$ and $\mathbf{e} = \{V_2=1\}$. The Figure 2.4a shows the first pass, obtaining the value of each node (number in purple above of the correspondent node), and the Figure 2.4b shows the second pass on the network recovering the MPE for $\mathbf{Q}$ (the selected path on the MPN is in blue).

Unfortunately, computing MPE by the approximate MPN algorithm does not always generate correct results. For the previous example, the MPE calculate by MPN is $V_1 = 0$ given $V_2 = 0$ as evidence, while the exact MPE obtained by computing $\mathcal{P}_{\mathcal{S}}(V_1 = 0, V_2 = 0) = 0.168$ and $\mathcal{P}_{\mathcal{S}}(V_1 = 1, V_2 = 0) = 0.192$ is $V_1 = 1$.

2.5 Sum-Product Networks Structure Learning

There are several methods for learning the structure and parameters of an SPN from data [PD11, GD13, DV12, PGP13]. In this work we consider several variants of LearnSPN, that is a simple and popular method to learn both structure and parameters of an SPN [GD13].

2.5.1 LearnSPN

LearnSPN is an algorithm schema, that can incorporate a variety of methods for splitting variables and examples into subsets [GD13].

Given a dataset of i.i.d. ² examples (configurations) $\mathbf{t}$ of categorical RVs $\mathbf{V}$ (for each $t \in \mathbf{t}, t \in \text{val}(\mathbf{V})$), LearnSPN operates recursively as follows:

- If $\mathbf{V}$ contains only one variable, return the corresponding univariate distribution (obtained e.g. by maximum likelihood estimation).
- If $\mathbf{V}$ contains more than one variable execute recursive calls for subsets with fewer variables or examples obtained as follows:
 - If it is able to split $\mathbf{V}$ into mutually independent subsets (according to the result of some statistical test, such as G-test of pairwise independence), returns a product node whose children are the resulting SPNs obtained from the execution of the recursive calls on each of the mutually independent subsets.

²Independent and identically distributed RVs

- Otherwise, it performs clustering on the examples $\mathbf{t}$ (according to some clustering algorithm such as Expectation Maximization), creates a sum node whose children are the SPNs retrieved from recurring the procedure in each of the obtained subsets, and whose weights are the proportions of examples in the corresponding subsets.

This method for learning structure and parameters of an SPN is summarized in the Algorithm 1 and illustrated in the Figure 2.5.

Algorithm 1: $LearnSPN(\mathbf{t}, \mathbf{V})$

input : Set of examples $\mathbf{t}$ and set of variables $\mathbf{V}$
output: An SPN representing the probability distribution of $\mathbf{V}$ learned from $\mathbf{t}$

```

1 if  $|\mathbf{V}| = 1$  then
2    $\mathcal{S} \leftarrow UnivariateDistribution(\mathbf{t}, \mathbf{V})$ 
3 else
4   partition  $\mathbf{V}$  into approximately independent subsets  $\mathbf{V}_j$ 
5   if success then
6      $\mathcal{S} \leftarrow \prod_j LearnSPN(\mathbf{t}, \mathbf{V}_j)$ 
7   else
8     partition  $\mathbf{t}$  into subsets of similar examples  $\mathbf{t}_i$ 
9      $\mathcal{S} \leftarrow \sum_i \frac{|\mathbf{t}_i|}{|\mathbf{t}|} LearnSPN(\mathbf{t}_i, \mathbf{V})$ 
10  end
11 end
12 return  $\mathcal{S}$ 

```

Figure 2.5: Algorithm $LearnSPN$, that learns the structure and parameters of an SPN from data. The numbers in blue rectangles represent the associate lines number in the Algorithm 1.

2.5.2 Deepening by limiting node splits (LL)

This method improves over LearnSPN by limiting the number of node's children while learning, resulting in deeper networks, and potentially less edges and parameters [VDME15]. The number of subsets in which the current set can be split is usually set to two.

The Algorithm 2 shows the previously described improves over LearnSPN, establishing thresholds for the number of variables partitions (I) and for the examples partitions (C). Additionally limits the minimum number of examples to be evaluated, if an example partition is performed with a number of examples under m creates and returns a product node with univariate distributions as leaves (Naive Factorization). The Figure 2.6 illustrates the LL learning method.

Figure 2.6: Algorithm LearnSPN limiting node splits to two ($I = 2$ and $C = 2$). The numbers in blue rectangles represent the associate line number in the Algorithm 2.

Algorithm 2: *LearnSPNL*($\mathbf{t}, \mathbf{V}, \alpha, m$)

input : Set of examples $\mathbf{t}$, set of variables $\mathbf{V}$, minimum number of examples for partition m and the parameter for Laplace smooth α
output: An SPN representing the probability distribution of $\mathbf{V}$ learned from $\mathbf{t}$

```

1 if  $|\mathbf{V}| = 1$  then
2    $\mathcal{S} \leftarrow \text{UnivariateDistribution}(\mathbf{t}, \mathbf{V}, \alpha)$ 
3 else if  $|\mathbf{t}| < m$  then
4    $\mathcal{S} \leftarrow \text{NaiveFactorization}(\mathbf{t}, \mathbf{V}, \alpha)$ 
5 else
6   partition  $\mathbf{V}$  into  $I$  approximately independent subsets  $\mathbf{V}_j$ 
7   if success then
8      $\mathcal{S} \leftarrow \prod_{j=1}^I \text{LearnSPNL}(\mathbf{t}, \mathbf{V}_j, \alpha, m)$ 
9   else
10    partition  $\mathbf{t}$  into  $C$  subsets of similar examples  $\mathbf{t}_i$ 
11     $\mathcal{S} \leftarrow \sum_{i=1}^C \frac{|\mathbf{t}_i|}{|\mathbf{t}|} \text{LearnSPNL}(\mathbf{t}_i, \mathbf{V}, \alpha, m)$ 
12  end
13 end
14 return  $\mathcal{S}$ 

```

Algorithm 3: Naive Factorization ($\mathbf{t}, \mathbf{V}, \alpha$)

input : Set of examples $\mathbf{t}$, set of variables $\mathbf{V}$ and Laplace smoothing parameter α
output: An SPN $\mathcal{S}$ encoding a product of factors $\mathbf{V}$ estimated from $\mathbf{t}$

```

1 return  $\mathcal{S} \leftarrow \prod_{j=1}^{|\mathbf{V}|} \text{Univariate Distribution}(\mathbf{t}, \mathbf{V}_j, \alpha)$ 

```

2.5.3 Regularization by tractable multivariate distribution hybridization (LC)

Builds on LL, by replacing the naive factorizations by *directed tree distributions* (Chow-Liu distribution) as the leaves [VDME15]. This increases network data likelihood by enabling the capture of finer local dependencies, while maintaining the overall computational complexity and tractability of distributions (since both marginal inference and MPE can be computed efficiently in directed trees).

For the implementation of the described improvement it is necessary a modification of the Algorithm 2 replacing the line 4. $\mathcal{S} \leftarrow \text{NaiveFactorization}(\mathbf{t}, \mathbf{V}, \alpha)$ (creation of naive factorizations) by 4. $\mathcal{S} \leftarrow \text{CLTree}(\mathbf{t}, \mathbf{V}, \alpha)$ (directed tree distributions learning). *CLTree* procedure builds the maximum spanning tree on the graph obtained by calculating the mutual information for each pair of variables in $\mathbf{V}$, then transforms the resulting non-directed tree into a directed tree by randomly selecting a root and visiting each node exactly once. Therefore, the leaves of the network are Chow-Liu (multivariate) distributions instead of univariate distributions. The *CLTree* procedure is summarized in Algorithm 4 and the learning algorithm is illustrated in Figure 2.7.

Algorithm 4: *CLTree*($\mathbf{t}, \mathbf{V}, \alpha$)

input : Set of examples $\mathbf{t}$, set of variables $\mathbf{V}$ and the parameter for Laplace smooth α
output: A Chow-Liu Tree $\mathcal{T}$ over $\mathbf{V}$ learned from $\mathbf{t}$

```

1  $M \leftarrow O_{|\mathbf{V}| \times |\mathbf{V}|}$ 
2 foreach  $X_u, X_v \in \mathbf{V}$  do
3    $M_{u,v} \leftarrow \text{estimateMutualInformation}(X_u, X_v, \alpha)$ 
4 end
5  $\mathcal{T} \leftarrow \text{maximumSpanningTree}(M)$ 
6 return Transforms  $\mathcal{T}$  into a directed tree

```

Figure 2.7: Algorithm LearnSPN limiting node splits and Chow-Liu distributions, instead of Naive Factorizations, as leaves. The numbers in blue rectangles represent the associate line number in the Algorithm 2.

2.5.4 Learning with Direct and Indirect Variable Interactions (ID)

LearnSPN (or LL or LC) captures variable interactions indirectly using bottom-up clustering to find mixtures. In contrast, most work on learning graphical models (e.g., Bayesian networks or Markov Networks), has focused on finding direct interactions among variables.

Learning Markov Networks with Arithmetic Circuits (ACMN)

A *Markov Network* (MN) represents a probability distribution over $\mathbf{V}$ as a normalized product of factors (potentials).

$$\mathcal{P}_{\mathcal{M}}(\mathbf{V}) = \frac{1}{Z} \prod_c \phi_c(\mathbf{D}_c). \quad (2.4)$$

where each ϕ_c is a non-negative real-value function, $\mathbf{D}_c \subset \mathbf{V}$ represents the factor domain c , and Z is the partition function. The distribution also can be represented by equivalent log-linear model:

$$\log \mathcal{P}_{\mathcal{M}}(\mathbf{V}) = \sum_i w_i f_i(\mathbf{D}_i) - \log Z. \quad (2.5)$$

where f_i is a real-value feature function with domain $\mathbf{D}_i$ and, w_i is a real-value weight. f_i can be given by a logical conjunction of variables evaluated as 1 if the expression is satisfied and 0 otherwise, for example $f_1(V_1, V_3, V_8) = v_1 \wedge \bar{v}_3 \wedge v_8$.

An *Arithmetic Circuit* (AC) is a rooted, directed acyclic graph, whose interior nodes are sums and products, and its leaves contain parameters (numerical values) or indicator variables. The evaluating or differentiating of an AC with or without evidence can be done in linear time in the

size of the circuit [LR13]. The Figure 2.8 shows an example of AC that encodes a two variables Markov Network.

Figure 2.8: Arithmetic Circuit example that encodes a Markov Network with two variables, where θ_1 and θ_2 are parameters and $v_1, \bar{v}_1, v_2$ and $\bar{v}_2$ are indicator functions of variables V_1 and V_2

The algorithm ACMN executes a greedy search through the structure space, generating an arithmetic circuit representing a tractable Markov Network [LR13]. The initial structure is the set of all single-variable feature functions. The *split* operation consists of selecting a feature in the MN, f , and combine it with another variable, V , creating two new features: $f \wedge v$ and $f \wedge \bar{v}$. Splits are scored according to their effect on the log-likelihood of the MN and the size of the corresponding Arithmetic Circuit (AC):

$$score(s) = \Delta_{ll}(s) - \gamma \Delta_e(s). \quad (2.6)$$

where $\Delta_{ll}(s)$ is a measure of how much the split s will increase the log-likelihood, $\Delta_e(s)$ denotes the number of edges that would be added to the AC if this split were included. γ determines the relative weightings of the two terms.

Algorithm 5: ACMN($\mathbf{t}, \mathbf{V}$)

input : Set of examples $\mathbf{t}$ and set of variables $\mathbf{V}$
output: A model $\mathcal{M}$ and an arithmetic circuit C

- 1 initialize model $\mathcal{M}$ and circuit C as product of marginals
- 2 initialize priority queue Q with initial candidate splits
- 3 **Loop**
- 4 Update edge and likelihood gain for each split in Q .
- 5 $s \leftarrow Q.pop()$ // Select best split
- 6 $(\mathcal{M}, C, f, \theta, f', \theta') \leftarrow \text{split}(s, \mathcal{M}, C)$
- 7 **for** $V \in \mathbf{V}$ **do**
- 8 Add the new split (f, θ, V) and (f', θ', V) to Q .
- 9 **end**
- 10 **EndLoop**
- 11 **return** $(\mathcal{M}, C)$

SPN Learning Direct and Indirect Variable Interactions

SPN Learning Direct and Indirect Variable Interactions (ID) [RL14] unifies these two approaches by learning an SPN and an MN from the same dataset and then selecting the one that best represents the data (maximizes the likelihood). The Figure 2.9 shows an Sum-Product network with arithmetic circuits as leaves learned with the ID algorithm).

Figure 2.9: Sum-Product network with Markov networks, represented by arithmetic circuits, as leaves

The ID algorithm learns simultaneously at each execution of *extend* operation an MN, represented by an AC and an SPN with ACs as leaves using the same dataset, and then selects the structure with highest likelihood (the number of times that it executes the extend operation is defined by the user). If the algorithm never selects an AC, the final model is SPN with univariate distribution as leaves. In the other hand if the algorithm selects the AC in the first extend operation and can not find a structure with better likelihood, the final model is a Markov network. The Algorithms 6, 7 summarize the ID algorithm and the extend operation, and the Figure 2.10 illustrates the Algorithm 7.

Algorithm 6: ID($\mathbf{t}, \mathbf{V}$)

input : Set of examples $\mathbf{t}$ and set of variables $\mathbf{V}$.
output: SPN model.

- 1 $n \leftarrow \text{ACMN}(\mathbf{t})$
- 2 $S \leftarrow n$
- 3 $N \leftarrow n$
- 4 **while** $N \neq \emptyset$ **do**
 - 5 $n \leftarrow$ remove the node with more examples from N
 - 6 $(\mathbf{t}_{i,j}, \mathbf{V}_j) \leftarrow$ set of samples and variables used for learning n
 - 7 $\text{subS} \leftarrow \text{extend}(n, \mathbf{t}_{i,j}, \mathbf{V}_j)$
 - 8 $S' \leftarrow S$ with n replaced by subS
 - 9 **if** $\log\text{-likelihood of } S' > \log\text{-likelihood } S$ **then**
 - 10 $S \leftarrow S'$
 - 11 $N \leftarrow N \cup \text{subS.leaves}()$
 - 12 **end**
- 13 **end**
- 14 **return** S

Algorithm 7: *extend*($n, \mathbf{t}, \mathbf{V}$)

input : Set of examples $\mathbf{t}$ and set of variables $\mathbf{V}$ used for learning the node n in an AC.
output: A sub-SPN subS representing the distribution of $\mathbf{V}$ learned from $\mathbf{t}$

```

1 p-success  $\leftarrow$  partition  $\mathbf{V}$  into approximately independent subsets  $\mathbf{V}_j$  using  $\mathbf{t}$ 
2 if p-success then
3   // Learn a product node
4   foreach  $\mathbf{V}_j$  do
5     let  $\mathbf{t}_j$  be the data samples projected into  $\mathbf{V}_j$ 
6     s-success  $\leftarrow$  partition  $\mathbf{t}_j$  into subsets of similar examples  $\mathbf{t}_{i,j}$ 
7     if s-success then
8       // Learn a sum node
9       foreach  $\mathbf{t}_{i,j}$  do
10        |  $n_{i,j} \leftarrow \text{ACMN}(\mathbf{t}_{i,j}, \mathbf{V}_j)$ 
11      end
12       $n_i \leftarrow \sum_i \frac{|\mathbf{t}_{i,j}|}{|\mathbf{t}_j|} n_{i,j}$ 
13    else
14      |  $n_i \leftarrow \text{ACMN}(\mathbf{t}_j, \mathbf{V}_j)$ 
15    end
16  end
17  subS  $\leftarrow \prod_i n_i$ 
18 else
19   s-success  $\leftarrow$  partition  $\mathbf{t}$  into subsets of similar examples  $\mathbf{t}_i$ 
20   if s-success then
21     // Learn a sum node
22     foreach  $\mathbf{t}_i$  do
23       |  $n_i \leftarrow \text{ACMN}(\mathbf{t}_i, \mathbf{V})$ 
24     end
25     subS  $\leftarrow \sum_i \frac{|\mathbf{t}_i|}{|\mathbf{t}|} n_i$ 
26   else
27     // If extend fails
28     subS  $\leftarrow n$ 
29   end
30 end
31 return subS

```

Figure 2.10: Sum-Product network with Markov networks, represented by arithmetic circuits, as leaves. The numbers in blue rectangles represent the associate lines number in the Algorithm 7.

Chapter 3

Multi-Label Classification

Let $\mathcal{D}$ be a *training set* with N examples $(\mathbf{x}^i, \mathbf{y}^i)$, where each $\mathbf{x}^i = (x_1^i, x_2^i, \dots, x_M^i)$ represents a vector of real numbers called *feature vector* and $\mathbf{y}^i = (y_1^i, y_2^i, \dots, y_R^i)$ is a Boolean vector representing the *relevance labels vector*. A coordinate $y_j^i = 1$ indicates that the j th label is present/relevant, while a coordinate $y_j^i = 0$ indicates that the j th label is absent/irrelevant. The Figure 3.1 illustrates the representation described for Multi-Label datasets.

$\mathbf{x}$				$\mathbf{y}$			
x_1^1	x_2^1	$\dots$	x_M^1	y_1^1	y_2^1	$\dots$	y_R^1
x_1^2	x_2^2	$\dots$	x_M^2	y_1^2	y_2^2	$\dots$	y_R^2
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
x_1^N	x_2^N	$\dots$	x_M^N	y_1^N	y_2^N	$\dots$	y_R^N

Figure 3.1: Multi-Label Dataset representation, $\mathbf{x}$ denotes the feature vector and $\mathbf{y}$ the relevance labels vector

The goal of Multi-Label Classification (MLC) is to obtain a classifier $\mathcal{C}$ using $\mathcal{D}$ that, given a feature vector $\mathbf{x}$, returns a relevance labels vector $\mathbf{y} = (y_1, \dots, y_R)$.

MLC generalizes traditional classification as follows. If for each example only one coordinate is present (i.e., $y_j^i = 1$ for $1 \leq j \leq R$), the problem is called a *single-label (multi-class) classification* (MCC). If $R = 1$, the problem is called *binary (single-label) classification* (BC). The Figure 3.2 shows examples for MLC, MCC and BC.

Figure 3.2: Examples of Traditional (binary), Multi-Class and Multi-Label Classifications represented in the tables on the right side BC, MCC and MLC

3.1 Methods for Multi-Label Classification

3.1.1 Binary Relevance

The Binary Relevance method (BR) or One-vs-All, consist of decomposing a MLC problem into several binary classification problems [CMM11]. Initially, BR transforms the original Multi-Label training dataset $\mathcal{D}$ in R subsets $\mathcal{D}_j$, where each $\mathcal{D}_j$ contains all the examples $(\mathbf{x}^i, y_j^i)$ from the original dataset. The Figure 3.3 shows a training set transformation for three labels.

$\mathbf{x}$				$\mathbf{y}$		
x_1^1	x_2^1	$\cdots$	x_M^1	y_1^1	y_2^1	y_3^1
x_1^2	x_2^2	$\cdots$	x_M^2	y_1^2	y_2^2	y_3^2
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
x_1^N	x_2^N	$\cdots$	x_M^N	y_1^N	y_2^N	y_3^N

(a)

$\mathbf{x}$	y_1
$\mathbf{x}^1$	y_1^1
$\mathbf{x}^2$	y_1^2
$\vdots$	$\vdots$
$\mathbf{x}^N$	y_1^N

(b)

$\mathbf{x}$	y_2
$\mathbf{x}^1$	y_2^1
$\mathbf{x}^2$	y_2^2
$\vdots$	$\vdots$
$\mathbf{x}^N$	y_2^N

(c)

$\mathbf{x}$	y_3
$\mathbf{x}^1$	y_3^1
$\mathbf{x}^2$	y_3^2
$\vdots$	$\vdots$
$\mathbf{x}^N$	y_3^N

(d)

Figure 3.3: Binary Relevance transformation on the training dataset with three labels at left 3.3a, generating the following training subsets: $\mathcal{D}_1$ 3.3b, $\mathcal{D}_2$ 3.3c and $\mathcal{D}_3$ 3.3d.

After the training dataset transformation, a binary classifier $\mathcal{C}_j(\mathbf{x})$ is generated using each training subset $\mathcal{D}_j$, obtaining a set of R classifiers defined by:

$$\mathcal{C}_{BR}(\mathbf{x}) = \{j : \mathcal{C}_j(\mathbf{x}) \in \{0, 1\}\}$$

Finally, the Multi-Label classification is obtained concatenating the predictions of each classifier in $\mathcal{C}_{BR}$.

The complexity of generating a Multi-Label classifier with BR method is $O(R\mathcal{C})$, since the generation of each binary classifier consumes time $O(\mathcal{C})$. Thus, applying this method when the number of labels is large, have a high computational cost. Another BR disadvantage, is that not consider the possible dependencies that exist between the labels because it builds independent binary classifiers for each label.

3.1.2 Chain Classifier

The Chain Classifier method (CC) is based on BR, but overcomes the independence labels assumption [RPHF11].

Let θ be an ordering on the labels, the training dataset transformation also creates R subsets denoted by $\mathcal{D}_{\theta_j}$. Every subset is composed of examples $(\mathbf{x}^i, \mathbf{y}_{\theta_1}^i, \dots, \mathbf{y}_{\theta_j}^i)$, where $\mathbf{y}_{\theta_1}^i, \dots, \mathbf{y}_{\theta_{j-1}}^i$ are part of the feature vector. The Figure 3.4 shows the transformation for a training dataset with three labels.

$\mathbf{x}$	y_{θ_1}
$\mathbf{x}^1$	$y_{\theta_1}^1$
$\mathbf{x}^2$	$y_{\theta_1}^2$
$\vdots$	$\vdots$
$\mathbf{x}^N$	$y_{\theta_1}^N$

(a)

$\mathbf{x}$	y_{θ_2}
$\{\mathbf{x}_1, y_{\theta_1}^1\}$	$y_{\theta_2}^1$
$\{\mathbf{x}_2, y_{\theta_1}^2\}$	$y_{\theta_2}^2$
$\vdots$	$\vdots$
$\{\mathbf{x}_N, y_{\theta_1}^N\}$	$y_{\theta_2}^N$

(b)

$\mathbf{x}$	y_{θ_3}
$\{\mathbf{x}_1, y_{\theta_1}^1, y_{\theta_2}^1\}$	$y_{\theta_3}^1$
$\{\mathbf{x}_2, y_{\theta_1}^2, y_{\theta_2}^2\}$	$y_{\theta_3}^2$
$\vdots$	$\vdots$
$\{\mathbf{x}_N, y_{\theta_1}^N, y_{\theta_2}^N\}$	$y_{\theta_3}^N$

(c)

Figure 3.4: Chain Classifier transformation on the training dataset with three labels in the Figure 3.3a, generating the following train subsets: $\mathcal{D}_{\theta_1}$ 3.4a, $\mathcal{D}_{\theta_2}$ 3.4b and $\mathcal{D}_{\theta_3}$ 3.4c.

Similar to BR, the Chain Classifier method learns a set of R Binary Classifiers, every $\mathcal{C}_{\theta_j}$, learned using the subset $\mathcal{D}_{\theta_j}$, subsequently adds the outputs of the previous classifiers $\{y_{\theta_1}, \dots, y_{\theta_{j-1}}\}$ as new features for the following predictions. It is important to note that the given label order θ is modeling the relations that might exist between labels in the training dataset. The final Multi-Label classification is given by:

$$\mathcal{C}_{cc}(\mathbf{x}_i, \mathbf{y}_i) = \{j : \mathcal{C}_j(\mathbf{x}, y_1, \dots, y_{j-1}) \in \{0, 1\}\} \quad (3.1)$$

3.1.3 Label Power-Set

The Label Power-Set method (LP) transforms the Multi-Label classification problem into a Multi-Class classification problem [CMM11]. The resulting set of labels in the MCC problem ($\mathbf{Y}_{MCC}$) is the set of all possible configurations for the labels in the original MLC problem.

$$\mathbf{Y}_{MCC} = \text{val}(\mathbf{Y}_{MLC}) \quad (3.2)$$

The LP transforms the training Multi-Label dataset $\mathcal{D}_{MLC}$ into an training Multi-Class dataset $\mathcal{D}_{MCC}$, mapping each feature vector $\mathbf{x}^i$ to the corresponding configuration of relevance labels on the original training dataset val ($\mathbf{Y}_{MLC}$). Since every label in the original MLC problem is binary, $|\mathbf{Y}_{MCC}| = 2^{R_{MLC}}$. The Figure 3.5 illustrates the LP training set transformation in a dataset with four labels.

$\mathbf{x}$	y_1	y_2	$\mathbf{x}$	00	01	10	11
$\mathbf{x}^1$	1	1	$\mathbf{x}^1$	0	0	0	1
$\mathbf{x}^2$	0	1	$\mathbf{x}^2$	0	1	0	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\mathbf{x}^N$	1	1	$\mathbf{x}^N$	0	0	0	1

(a)
(b)

Figure 3.5: Label Power-Set Transformation on a training Multi-Label dataset with three labels 3.5a into a training Multi-Class dataset 3.5b, then $\mathbf{Y}_{MLC} = \{Y_1, Y_2\}$ and $\mathbf{Y}_{MCC} = \{00, 01, 10, 11\}$

Although LP considers label dependence, when it is considered a large or even moderate number of labels, the Multi-Class learning task becomes very costly due to the exponential number of labels. Another important issue is the problem of *label imbalance*, which happens when there are labels on the training set represented by few examples.

3.1.4 Probabilistic Graphical Models

Probabilistic graphical model (PGM) use a graph-based representation as the basis for compactly encoding a complex distribution over a large number of RVs [KF09]. The Figure 3.6 illustrates an probabilistic model (Bayesian Network) example, representing the distribution over six RVs.

A PGM learned from the training dataset $\mathcal{D}$, can be used to predict the relevant labels by computation of the conditional probability of each label Y_j given the feature vector $\mathbf{x}$. Or computing the Most Probable Explanation of the labels $\mathbf{Y}$ given the feature vector $\mathbf{x}$.

It is clear that a PGM can be the base classifier for the BR, CC and LP methods. As well as directly perform the MLC by computation of the MPE on the model. Well-known and successful models for classification (Multi-label and Single-label) are, Bayesian Networks, and Markov Networks [CAMG14, ACMG13, FGG97, LMP01].

Figure 3.6: *An example of a probabilistic model, representing the distributions over six RVs.*

The Multi-Label Classifier based on the computation of the Most Probable Explanation on the model is given by the following equation:

$$\mathcal{C}_{MPE}(\mathbf{x}) = \underset{\mathbf{y}}{\operatorname{argmax}} P(\mathbf{y}, \mathbf{x}) \quad (3.3)$$

Chapter 4

Multi-Label Classification based on Sum-Product Networks

In this chapter, we will explain how to use SPN for Multi-Label Classification. There are several approaches for learning a Multi-Label classifier based on SPNs. For example adopting the Binary Relevance approach, for each label j , is learned a SPN $\mathcal{S}_j$ from the dataset $\mathcal{D}_j$ with examples $(\mathbf{x}^i, \mathbf{y}_j^i)$. A label j is then deemed relevant if:

$$\mathcal{P}_{\mathcal{S}_j}(y_j|\mathbf{x}) > 1/2. \quad (4.1)$$

The Figure 4.1 illustrates an example for construction and classification procedures of a Multi-Label classifier based on Sum-Product Networks following the Binary Relevance approach, obtained from a dataset with three labels.

Figure 4.1: Multi-label classifier based on SPN adopting Binary Relevance approach.

An alternative approach to BR is to adopt Classifier Chain, which begins by fixing an ordering for the labels $\theta_1, \dots, \theta_R$. Then, similar to BR, learns a SPN for each label as follows, $\mathcal{S}_{\theta_j}$ using the dataset $\mathcal{D}_{\theta_j}$ which contains examples $(\mathbf{x}^i, y_{\theta_1}^i, \dots, y_{\theta_j}^i)$. The label j is considered relevant if:

$$\mathcal{P}_{\mathcal{S}_{\theta_j}}(y_{\theta_j}|\mathbf{x}, y_{\theta_1}, \dots, y_{\theta_{j-1}}) > 1/2. \quad (4.2)$$

Figure 4.2: Multi-label classifier based on SPN adopting Classifier Chain approach.

As reviewed in section 2.5, SPNs learning is costly. Therefore, follow the BR and CC approaches scales poorly in the number of labels. In fact, in some preliminary results these approaches were not competitive.

We recommend to use the *Joint Distribution* approach, which learns a *single* SPN $\mathcal{S}$ over the set of variables $\mathbf{V}$ using the whole training set $\mathcal{D}$, where the scope of $\mathcal{S}$ is the feature vector and labels variables, $\mathbf{V} = \{\mathbf{X}, \mathbf{Y}\}$.

An approach for classification consists in maximizing the marginal probability of each label given the features, nevertheless, the resultant prediction may not be consistent with the data, which indicates that it may have lower joint probability on the model [LI13]. For example, consider the probability distributions for variables A and B in Figure 4.3, we want to compute the most likely configuration for A and B, maximizing the marginals for A and B $\text{argmax}_A \mathcal{P}(A) = 1$ and $\text{argmax}_B \mathcal{P}(B) = 1$ the configuration obtained is A=1 and B=1, in the other hand computing the max joint probability we obtain $\text{argmax}_{A,B} \mathcal{P}(A, B) = (0, 0)$.

A=0	A=1
0.4	0.6

(a)

	B=0	B=1
A=0	0.8	0.2
A=1	0.5	0.5

(b)

Figure 4.3: Probability distributions of variables A 4.3a and B 4.3b, where B depends on A.

In this work, we perform the classification by maximizing the join probability of the relevance label vector given the feature vector:

$$\mathcal{C}(\mathbf{x}) = \text{argmax}_{\mathbf{y}} \mathcal{P}_{\mathcal{S}}(\mathbf{y}|\mathbf{x}) \quad (4.3)$$

Note that the above equation selects the Most Probable Explanation (MPE) on $\mathcal{S}$. As already

mentioned in the Section 2.4, this problem is generally NP-hard.

We present some approximate algorithms for MPE to perform Multi-Label Classification, some of which are new.

4.1 Max-Prod Classification (MC)

Poon and Domingos suggested finding a MPE of an SPN $\mathcal{S}$ by (i) converting the network into a Max-Product Network $\mathcal{S}^m$ by replacing sum nodes with max nodes, then (ii) evaluating the network and finally (iii) backtracking nodes to find the corresponding configuration of the labels nodes [PD11]. The Max-Prod algorithm is described in more detail in section 2.4.

The Figure 4.4 illustrates an example for the Multi-Label classifier using the Max-Prod classification algorithm.

Figure 4.4: Multi-label classifier based on SPN computing the approximation of Most Probable Explanation configuration by Max-Prod Algorithm

The previous algorithm is efficient but inaccurate. We now propose some new algorithms for classification that approximate the most probable explanation .

4.2 Exhaustive Classification (EC)

The simplest and least effective algorithm to find $\mathcal{C}(\mathbf{x})$ is a brute-force approach that enumerates all possible relevance label vectors (2^R combinations of 0s and 1s), computes the probability for each one, by evaluation the SPN, and returns the configuration with the highest probability. Clearly, this algorithm is optimal but does not scale to many labels.

On the other hand, an efficient algorithm selects all distinct relevance label vectors in the training set, and then chooses the prediction with the highest probability as the final classification. However, our classifier loses generality by only predicting relevance label vectors showed in $\mathcal{D}$.

We propose the new algorithm, Exhaustive Classification, that fall between this two extrema. In order to reduce the number of relevance label vectors, selects the set of all distinct predictions on the training set $SV = \{\mathbf{y}^i | \mathbf{y}^i \in \mathcal{D}\}$ and then *optimizes* each prediction so as not to lose generality. Given an unlabeled example $\mathbf{x}$, and a relevance label vector $\mathbf{y}^i$ such that $\mathbf{y}^i \in SV$, EC optimizes the value of each label in $\mathbf{y}^i$ to maximizes its joint probability. As result of the optimization of each

prediction in SV obtains a new set of relevance labels vectors, that we call *candidates*. The Figure 4.5 shows an example of the optimization process.

Finally, selects the most likely candidate as the prediction associate to $\mathbf{x}$. In summary, Exhaustive

Figure 4.5: Example of Exhaustive classification optimization for a single label in a dataset with three labels

Classification predicts the relevance label vector for $\mathbf{x}$ by:

$$\mathcal{C}(\mathbf{x}) = \max_{\mathbf{y}^i \in SV} \operatorname{argmax}_{y_j^i} \mathcal{P}_S(y_1^i, \dots, Y_j^i = y_j^i, \dots y_R^i | \mathbf{x}). \quad (4.4)$$

The Algorithm 8 performs the optimization, first in Line 2, the method `getDistinctPredictions` gets all distinct predictions in $\mathcal{D}$, then obtains the set *candidates* by selecting the relevance for each label that maximizes the conditional probability for the prediction given the feature vector (PC method computes the conditional probability on the SPN).

Algorithm 8: CandidatesGeneration

Input: Feature vector: $\mathbf{x}$

Output: Distinct optimized relevance label vector SV'

```

1 candidates  $\leftarrow \{\}$ 
2  $SV \leftarrow \text{getDistinctPredictions}(\mathcal{D})$ 
3 for each  $y^i$  in  $SV$  do
4   for  $j \leftarrow 1$  to  $R$  do
5      $p_1 \leftarrow \text{PC}(y_1^i, \dots, Y_j^i = 1, \dots y_R^i | \mathbf{x})$ 
6      $p_0 \leftarrow \text{PC}(y_1^i, \dots, Y_j^i = 0, \dots y_R^i | \mathbf{x})$ 
7     if  $p_1 \geq p_0$  then
8        $Y_j^i = 1$ 
9     else
10       $Y_j^i = 0$ 
11    end
12  end
13  candidates  $\cup y^i$ 
14 end
15 return candidates

```

The Algorithm 9 selects the prediction with highest probability from the candidates set as the final classification (P method computes the marginal probability on the SPN). Finally, Figure 4.6 shows an Exhaustive Classification execution example.

Algorithm 9: Exhaustive Classification

Input: Feature vector $\mathbf{x}$
Output: Relevance label vector (prediction) $\mathbf{y}$

```

1  $\mathbf{y} \leftarrow \{\}$ 
2  $\text{candidates} \leftarrow \text{CandidatesGeneration}(\mathbf{x})$ 
3  $\text{max} \leftarrow -\infty$ 
4 for each  $\mathbf{y}^i$  in  $\text{candidates}$  do
5   if  $P(\mathbf{y}^i) > \text{max}$  then
6      $\text{max} \leftarrow P(\mathbf{y}^i)$ 
7      $\mathbf{y} \leftarrow \mathbf{y}^i$ 
8   end
9 end
10 return  $\mathbf{y}$ 

```

Figure 4.6: Example of Exhaustive Classification in a dataset with three labels, the *purple* arrows represent the procedure that obtains the candidates, and the *cyan* arrows represent the classification procedure.

4.3 Sequential Classification (SC)

The Sequential Classification algorithm is inspired by the Classifier Chain approach [RPHF11], however, learns a single network. Let θ be an ordering for the labels. We classify the θ_j th label by:

$$y_{\theta_j} = \operatorname{argmax}_{y_{\theta_j}} \mathcal{P}_S(y_{\theta_j} | \mathbf{x}, y_{\theta_1}, \dots, y_{\theta_{j-1}}) \quad (4.5)$$

The Algorithm 10 summarizes the Sequential Classification procedure, predicts each label by selecting the value that maximizes the conditional probability of each label relevance given the feature vector and the previous classifications in the ordering θ . The Figure 4.7 shows an example of SC, with a training set with three labels, note that the ordering θ is used only for the classification.

Algorithm 10: Sequential Classification**Input:** Feature vector $\mathbf{x}$, an ordering for the labels θ **Output:** Relevance labels vector (prediction) $\mathbf{y}$

```

1  $\mathbf{y} \leftarrow \{\}$ ;
2 for  $j \leftarrow 1$  to  $R$  do
3   if  $PC(Y_{\theta_j} = 1 | \mathbf{x}, y_{\theta_1}, \dots, y_{\theta_{j-1}}) \geq 1/2$  then
4      $Y_j^i = 1$ 
5   else
6      $Y_j^i = 0$ 
7   end
8    $\mathbf{y} \cup y_{\theta_j}$ 
9 end
10 return  $\mathbf{y}$ 

```

Figure 4.7: An example of sequential classification, with a training dataset with tree labels

Note that unlike CC, a single SPN is used to perform every classification. Like CC, the accuracy of the algorithm is very dependent on the label ordering adopted; also, selecting a good ordering is non trivial. We adopt two different greedy methods for selecting label orderings.

- **Static Best-First**

Orders labels by their probability $\mathcal{P}_{\mathcal{S}}(Y_j = 1 | \mathbf{x})$ such that Y_{θ_1} has the highest probability, followed by Y_{θ_2} , and so on.

- **Dynamic Best-First**

Selects an ordering during the classification. According to this method, the j th label to be selected is:

$$\theta_j = \arg \max_{0 < k \leq R} \mathcal{P}_{\mathcal{S}}(Y_k = 1 | \mathbf{x}, y_{\theta_1}, \dots, y_{\theta_{j-1}}), \quad (4.6)$$

where $y_{\theta_1}, \dots, y_{\theta_{j-1}}$ are the classifications performed by SC with the previously selected labels.

4.4 Pool of Classifications (PC)

The previous approaches try to solve the dependency on label ordering by greedily optimizing it. A common alternative approach to cope with sensitivity to model parameters is to consider ensembles of classifications. Let $CS = \{(y_1^i, \dots, y_R^i) : i = 1, \dots, k\}$ be a set of classifications, our method combine all classification on CS to obtain a single final prediction for the unlabeled example. The Algorithm 11 obtains a set CS of k classifications using the Classify method and then combine them using the method Combine to obtain the final prediction. The Figure 4.8 illustrates an example for PC with $k = 3$.

Algorithm 11: Pool of Classifications

Input: Feature vector $\mathbf{x}$, number of classifications k
Output: Relevance label vector (prediction) $\mathbf{y}$

```

1  $\mathbf{y} \leftarrow \{\}$ ;
2  $CS \leftarrow \{\}$ ;
3 for  $i \leftarrow 1$  to  $k$  do
4   |  $CS \cup \text{Classify}(\mathbf{x})$ 
5 end
6  $\mathbf{y} \leftarrow \text{Combine}(CS)$ ;
7 return  $\mathbf{y}$ 

```

Figure 4.8: An example of pool classification, with four labels and three relevance label vectors

We consider three different methods for producing a single classification from the set CS :

- **Majority voting:**

Selects labels by comparing weighted, where the weights are formed by votes, that is,

$$y_j = 1 \text{ iff } \frac{1}{k} \sum_{i=1}^k y_j^i \geq \frac{1}{2}. \quad (4.7)$$

- **Weighted average :**

Obtains the final label classification for each label by:

$$y_j = 1 \text{ iff } \frac{1}{k} \sum_{i=1}^k \mathcal{P}_S(Y_j^i = 1 | \mathbf{x}) \geq \frac{1}{2}, \quad (4.8)$$

where $\mathcal{P}_S(Y_j^i = 1 | \mathbf{x})$ is the probability of the label Y_j be relevant.

- **Max:**

It simply selects the ordering whose label achieves the highest joint probability (conditional on the features):

$$\mathbf{y} = \underset{\mathbf{y}^i}{\operatorname{argmax}} \mathcal{P}_S(\mathbf{y}^i | \mathbf{x}). \quad (4.9)$$

For example, consider the set of classification in the Figure 4.8: $\mathbf{y}^1 = [1, 0, 1, 1]$ $\mathbf{y}^2 = [0, 1, 1, 0]$ $\mathbf{y}^3 = [1, 1, 1, 0]$

- Combining with Majority voting method: $y_1 = 1$ ($2/3 \geq 1/2$), $y_2 = 1$ ($2/3 \geq 1/2$), $y_3 = 1$ ($3/3 \geq 1/2$), $y_4 = 0$ ($1/3 < 1/2$) and we obtain the final prediction $\mathbf{y} = [1, 1, 1, 0]$.
- Combining with Weighted average: Consider $\mathcal{P}_S(Y_1^1 = 1|\mathbf{x}) = 0.8$, $\mathcal{P}_S(Y_1^2 = 1|\mathbf{x}) = 0.4$, $\mathcal{P}_S(Y_3^1 = 1|\mathbf{x}) = 0.7$, $\mathcal{P}_S(Y_2^1 = 1|\mathbf{x}) = 0.1$, $\mathcal{P}_S(Y_2^2 = 1|\mathbf{x}) = 0.6$, $\mathcal{P}_S(Y_2^3 = 1|\mathbf{x}) = 0.7$, $\mathcal{P}_S(Y_3^1 = 1|\mathbf{x}) = 0.5$, $\mathcal{P}_S(Y_3^2 = 1|\mathbf{x}) = 0.9$, $\mathcal{P}_S(Y_3^3 = 1|\mathbf{x}) = 0.8$, $\mathcal{P}_S(Y_4^1 = 1|\mathbf{x}) = 0.9$, $\mathcal{P}_S(Y_4^2 = 1|\mathbf{x}) = 0.3$, $\mathcal{P}_S(Y_4^3 = 1|\mathbf{x}) = 0.2$.
Then $y_1 = 1$ ($1.9/3 \geq 1/2$), $y_2 = 0$ ($1.4/3 < 1/2$), $y_3 = 1$ ($2.3/3 \geq 1/2$), $y_4 = 0$ ($1.4/3 < 1/2$), and we obtain the final prediction $\mathbf{y} = [1, 0, 1, 0]$.
- Combining with Max: Consider $\mathcal{P}_S(\mathbf{y}^1) = 0.5$, $\mathcal{P}_S(\mathbf{y}^2) = 0.8$, $\mathcal{P}_S(\mathbf{y}^3) = 0.7$, then $\mathbf{y} = \mathbf{y}^2$ ($0.8 > 0.7 > 0.5$) and we obtain the final prediction $\mathbf{y} = [0, 1, 1, 0]$.

We can use several basis methods for classification, in this work we proposed use two methods previously described in this chapter.

Pool of Sequential Classification (PSC)

Consider a set of label orderings (obtained e.g. by randomly sampling orderings) $\theta^1, \dots, \theta^k$, the set CS be a set of classifications obtained from each ordering by using sequential classification.

To obtain the algorithm for PSC we need to add a new line on the Algorithm 11 between the lines (2-3) to generate randomly k orderings for the labels and, modify the line 4 to $CS \cup \text{SequentialClassification}(\mathbf{x}, \theta^i)$, therefore we obtain a set of classifications calling SC using distinct orderings. The Figure 4.9 shows an example of Pool Sequential Classification, using a training dataset with two labels.

Figure 4.9: An example of Pool Sequential Classification, using a training dataset with two labels

Pool of Exhaustive Classification (PEC)

Let *candidates* be the set obtained by EC optimization, described in the Section 4.2. The set *CS* is the set of k predictions with highest probability from *candidates*. If we use the combining method Max, described in the previous subsection, would obtain exactly the same relevance label vector that using only Exhaustive Classification.

To obtain the algorithm for PEC we only call the method *SetExhaustiveClassifications*($\mathbf{x}$), that be similar to the Algorithm 9, but instead of returns a single classification $\mathbf{y}$ returns the set of most likely k classification on the model. The Figure 4.10 shows an example of Pool Exhaustive Classification, using a training dataset with two labels.

Figure 4.10: An example of Pool Exhaustive Classification, using a training dataset with two labels.

4.5 Complexity Analysis

Let $|\mathcal{S}|$ be the number of nodes in $\mathcal{S}$. Exhaustive Classification takes time $O(RN|\mathcal{S}|)$, since it needs to optimize each label at most N relevance labels vectors and compute conditional probabilities in each of them from $\mathcal{S}$. The time complexity of Max-Prod Classification is $O(|\mathcal{S}|)$, since it requires two passes in the network $\mathcal{S}$, each taking linear time in $|\mathcal{S}|$. The time complexity of Sequential Classification depends on the method used to optimize the classification order. Static Best-First takes time $O(R|\mathcal{S}|)$ to rank the labels (as we need to compute conditional probabilities for each label). Dynamic Best-First takes time $O(R^2|\mathcal{S}|)$ to rank the labels, since at every classification we need to re-rank labels by their conditional probability. In either method, the time to produce classifications is $O(R|\mathcal{S}|)$. Thus, both approaches are linear in the size of the network; Static Best-First is also linear in the number of labels, while Dynamic Best-First is quadratic. In the case of Pool Classifications the complexity for Weighted Average, Voting and Max criteria is k times the complexity time of the basis classification algorithm. The Pool Sequential Classification takes time $O(kR|\mathcal{S}|)$, since it uses random orderings. The time complexity of Pool Exhaustive Classification is $O(kRN|\mathcal{S}|)$.

Chapter 5

Experiments

5.1 Datasets

We evaluated our proposed classifiers on 10 benchmark datasets ¹, these datasets were also used for Multi-Label Classification with CutNets [DMVE16].

Since the current implementations of learning algorithms for SPNs work only on binary data, we discretized the numeric features for each dataset by the *Label-Attribute Interdependence Maximization* (LAIM) [CLGV16].

Table 5.1 shows general characteristics of discretized datasets, such as domain, number of features (M), number of examples (N), number of labels (R), label cardinality $LC(\mathcal{D}) = \frac{1}{N} \sum_{i=1}^N |\mathbf{y}_i|$ and label density $LD(\mathcal{D}) = \frac{1}{N} \sum_{i=1}^N \frac{|\mathbf{y}_i|}{R}$, where $|\mathbf{y}|$ returns the number of ones in the binary vector $\mathbf{y}$.

Dataset	Domain	M	N	R	LC	LD
Arts-Yahoo	Text	500	7484	26	1.653	0.063
Business-Yahoo	Text	500	11214	30	1.598	0.053
CAL500	Music	68	502	174	26.043	0.149
Emotions	Music	72	593	6	1.868	0.311
Flags	Images	19	194	7	3.391	0.484
Health-Yahoo	Text	500	9205	32	1.644	0.051
Human	Biological	440	3106	14	1.185	0.084
Plant	Biological	440	978	12	1.078	0.089
Scene	Images	294	2407	6	1.073	0.178
Yeast	Biological	103	2417	14	4.237	0.301

Table 5.1: Multi-Label Datasets, their domains, size of their feature vector (M), number of instances (N), number of labels (R), label cardinality (LC) and label density (LD)

- **Yahoo Datasets:** The Arts-Yahoo, Business-Yahoo and Health-Yahoo datasets were obtained from the yahoo.com domain in order to categorize real Web page linked from the “Arts & Humanities”, “Business & Economy” and “Health” categories into a number of second-level subcategories [US03].
- **CAL500:** Music dataset used is a set of 500 “Western popular” songs associate to emotional content, genre, instrumentation, or vocal characterizations [TBTLO8]

¹ Available at <https://github.com/nicoladimauro/dcsn> and <http://meka.sourceforge.net>

- **Emotions:** The dataset consists of 100 songs from each of the following 7 different genres: Classical, Reggae, Rock, Pop, Hip-Hop, Techno and Jazz labeled with emotions like amazed-surprised or angry-fearful [TTKV08].
- **Flags** Contains details of some countries and their flags, and the goal is to predict some of the features [CLGV16].
- **Human:** This dataset is used to predict the sub-cellular locations of proteins according to their sequences on Human species [CLGV16].
- **Plant:** This dataset is used to predict the sub-cellular locations of proteins according to their sequences, for Plant species [CLGV16].
- **Scene:** Dataset of images used for categorize images into semantic classes such as beaches, sunsets or parties [BLSB04].
- **Yeast** The dataset is formed by micro-array expression data and phylogenetic profiles with 2417 genes dataset. Each gene is associated with a set of 14 functional classes like as Ionic Homeostasis or Cellular Biogenesis [EW02].

5.2 Metrics

To measure the performance of the proposed classifiers we adopt three commonly used metrics in MLC, each tailored for capturing different characteristics of the predictions [DWCH12, DMVE16].

5.2.1 Hamming Score (HS)

Rewards the percentage of correctly predicted labels, and is given by:

$$HS(\mathcal{D}, \mathcal{C}) = \frac{1}{NR} \sum_{i=1}^N \sum_{j=1}^R \mathbb{I}(y_{i,j} = \hat{y}_{i,j}). \quad (5.1)$$

HS does not distinguishes between correctly predicted relevance and irrelevance, and can be overoptimistic when the number of labels is high and label density is low.

5.2.2 Exact Match (EM)

Rewards classifications by the percentage of examples for which predictions are perfect: the relevant labels as predicted as relevant and the irrelevant one are predicted as absent. It is given by:

$$EM(\mathcal{D}, \mathcal{C}) = \frac{1}{N} \sum_{i=1}^N \mathbb{I}(\mathbf{y}_i = \hat{\mathbf{y}}_i). \quad (5.2)$$

EM can be over pessimistic, as the failure of a single relevance/irrelevance deems a classification incorrect.

5.2.3 Accuracy (Acc)

Rewards relevant predictions while discounting for irrelevant predictions, thus obtaining a compromise between HS and EM. It is computed by:

$$Acc(\mathcal{D}, \mathcal{C}) = \frac{1}{N} \sum_{i=1}^N \frac{|\mathbf{y}_i \wedge \hat{\mathbf{y}}_i|}{|\mathbf{y}_i \vee \hat{\mathbf{y}}_i|} \quad (5.3)$$

Where $\mathbb{I}(\cdot)$ is the indicator function, $\wedge \vee$ are logical operators (AND, OR), $\hat{y}_{i,j}$ is the predicted value of the label j for the example i in the $\mathcal{C}$ classifier and $y_{i,j}$ is the corresponding expected value in the dataset $\mathcal{D}$, $\hat{\mathbf{y}}_i$ is the predicted of the relevance labels vector for the example i in the $\mathcal{C}$ classifier and $\mathbf{y}_i$ is the corresponding expected relevance labels vector in the dataset $\mathcal{D}$.

5.3 Algorithms

For the experiments, we adopt the *Cross Validation* method to evaluate the generalization capability of our models, that splits the dataset in 5-folds, then uses 4 folds as training set and the remaining fold as test set, this process is executed 5 times by alternating the test set in a non-repeating manner. The experiments for each Multi-Label Classifiers (RSVM, RCNET and SPN-based) use exactly the same partitions at each execution of Cross Validation.

5.3.1 Multi-label Classifiers based on SPN

We obtain different SPN-based classifiers by varying the learning algorithm used (LL, LC or ID) as well as the classification algorithm (EC, MC, SC, P)². We denote each choice by the concatenations of the acronyms of the classification algorithm and learning algorithm. For example, EC+LL denotes the classifiers that uses LL as learning algorithm and EC for classification.

	LL	LC	ID
EC	EC+LL	EC+LC	EC+ID
MC	MC+LL	MC+LC	MC+ID
SC	SC+LL	SC+LC	SC+ID
PSC	PSC+LL	PSC+LC	PSC+ID
PEC	PEC+LL	PEC+LC	PEC+ID

Table 5.2: Multi-Label Classifiers based on Sum-Product Networks

Some classification algorithms require additional specifications. For example, SC uses either random, Static Best-First or Dynamic Best-First ordering. We randomly generated ten orderings when using Pool Sequential (PS) and selected ten vectors for Pool Exhaustive (PE), then applied the weighted average, majority voting and max methods. In the results Tables for SC, PS and PE, we only show the classifier with better performance using the ordering methods or the combination methods respectively.

We tuning the Sum-Product network learning algorithms, performing a grid-search on the likelihood to select the parameters. The algorithm limiting node splits and the algorithm with multivariate distributions as leaves, tuning G-test factor, Minimum instance number in a slice and smoothing probability factor³. While for the algorithm with direct and indirect variable interactions, we used the Libra toolkit [LR15], tuning the Per-split penalty, Max sum nodes cardinalities and Maximum number of node extensions.

²Available at <https://github.com/giulianavll/MLC-SPN>

³Source code is available at <http://www.di.uniba.it/~vergari/code/spyn.html>

5.3.2 State-Of-Art Multi-Label Classifiers

We compare our approaches against the state-of-the-art Multi-Label classifiers RCNET and RSVM.

RCNET

RCNET employs CutNets and adopts the exact MPE approach [DMVE16].⁴ Which was previously shown to outperform several other approaches such as Bayesian Chain Classifier, Binary relevance and the classifier chains methods with base classifiers Naive Bayes and Tree Augmented Naive Bayes.

RSVM

RSVM adopts the Random k-Labelsets for Multi-Label Classification (RaKel) approach [TKV11], where an ensemble of label power-set classifiers is learned. It uses as Multi-Class classifiers Support Vector Machines with polynomial kernel (using their openly implementation in MEKA⁵). Which shown competitive results compared with the classifiers in the experiments of LAIM⁶ (such as Dependent Binary Relevance, Ensemble of Classifier Chains and Hierarchy of Multi-label classifiers approaches with J48 as base classifier).

5.4 Results and Discussion for Multi-Label Classifiers based on SPN and State-of-art

Tables 5.3, 5.4 and 5.5 show the performance and ranking for Hamming Score, Exact Match, and Accuracy respectively for our proposed classifiers based on SPNs, the Multi-Label classifier based on CutsetNets (RCNET) and the Random k-labelsets approach using as basis classifier Support Vector Machines (RSVM). As we discussed in the previous chapter, the state-of-art classifiers chosen for the experiments (viz. RCNET and RSVM) was previously shown outperform several other approaches.

	Arts	Business	CAL500	Emotions	Flags	Health	Human	Plants	Scene	Yeast	AvgRnk
SC+LL	0.945(2)	0.977(1)	0.862(1)	0.793(8)	0.722(7)	0.968(8)	0.919(1)	0.915(1)	0.899(7)	0.784(2)	3.8
EC+ID	0.943(4)	0.977(1)	0.829(7)	0.808(2)	0.768(2)	0.969(2)	0.912(6)	0.904(5)	0.915(1)	0.774(4)	3.4
SC+ID	0.945(2)	0.976(2)	0.824(9)	0.8(6)	0.775(1)	0.969(2)	0.914(5)	0.909(3)	0.913(3)	0.77(7)	4
MC+ID	0.941(6)	0.976(2)	0.831(6)	0.811(1)	0.768(2)	0.969(2)	0.91(8)	0.903(6)	0.914(2)	0.769(9)	4.4
EC+LL	0.945(2)	0.977(1)	0.819(11)	0.808(2)	0.707(9)	0.968(8)	0.918(2)	0.911(2)	0.897(8)	0.77(7)	5.2
PEC+ID	0.943(4)	0.976(2)	0.827(8)	0.808(2)	0.768(2)	0.969(2)	0.911(7)	0.905(4)	0.91(4)	0.765(10)	4.5
PEC+LL	0.944(3)	0.977(1)	0.819(11)	0.808(2)	0.707(9)	0.968(8)	0.911(7)	0.911(2)	0.896(9)	0.771(6)	5.8
PEC+LC	0.945(2)	0.977(1)	0.845(4)	0.805(4)	0.707(9)	0.969(2)	0.909(9)	0.893(8)	0.885(11)	0.769(8)	5.8
PSC+LL	0.94(7)	0.977(1)	0.842(5)	0.785(11)	0.759(3)	0.968(8)	0.915(4)	0.896(7)	0.901(6)	0.752(11)	6.3
MC+LL	0.942(5)	0.976(2)	0.82(10)	0.808(2)	0.707(9)	0.961(15)	0.916(3)	0.904(5)	0.893(10)	0.769(8)	6.9
PSC+ID	0.932(9)	0.976(2)	0.812(13)	0.794(7)	0.754(5)	0.969(2)	0.897(10)	0.888(10)	0.915(1)	0.777(3)	6.2
EC+LC	0.945(2)	0.977(1)	0.814(12)	0.804(5)	0.707(9)	0.97(1)	0.909(9)	0.892(9)	0.885(11)	0.768(9)	6.8
SC+LC	0.944(3)	0.977(1)	0.756(14)	0.789(10)	0.729(6)	0.963(14)	0.738(14)	0.744(13)	0.863(13)	0.715(12)	10
PSC+LC	0.94(7)	0.977(1)	0.751(15)	0.806(3)	0.722(7)	0.947(16)	0.763(13)	0.761(12)	0.742(14)	0.588(13)	10.1
RSVM	0.948(1)	0.977(1)	0.851(3)	0.791(9)	0.756(4)	0.965(12)	0.89(12)	0.874(11)	0.908(5)	0.789(1)	5.9
RCNET	0.937(8)	0.973(3)	0.854(2)	0.783(12)	0.709(8)	0.965(12)	0.894(11)	0.892(9)	0.879(12)	0.773(5)	8.2

Table 5.3: Performance for the Hamming Score metric and in parenthesis the ranking of the algorithm.

The classifiers based on SPNs limiting the node splits with sequential classification (SC+LL), and SPNs with direct and indirect variable interactions using Exhaustive and Sequential classification (EC+ID and SC+ID) obtained the best average ranking for the Hamming Score metric. In the case of Exact Match metric, the best performances were obtained by Exhaustive, Max-Prod and Pool of Exhaustive classification algorithms on SPNs with direct and indirect interactions (viz.

⁴Source code is available at <https://github.com/nicoladimauro/dcsn>.

⁵Available at <http://meka.sourceforge.net>.

⁶Results available at <http://www.uco.es/grupos/kdis/wiki/MLdiscretization/>.

	Arts	Business	CAL500	Emotions	Flags	Health	Human	Plants	Scene	Yeast	Avg Rank
EC+ID	0.35(2)	0.586(5)	0(1)	0.361(6)	0.125(7)	0.525(2)	0.25(4)	0.236(7)	0.713(1)	0.2(2)	3.7
MC+ID	0.352(1)	0.577(8)	0(1)	0.353(7)	0.125(7)	0.524(3)	0.256(3)	0.241(6)	0.711(2)	0.2(2)	4
PEC+ID	0.35(2)	0.577(8)	0(1)	0.361(6)	0.125(7)	0.525(2)	0.257(2)	0.236(7)	0.685(4)	0.18(5)	4.4
PSC+ID	0.277(13)	0.577(8)	0(1)	0.398(5)	0.175(5)	0.525(2)	0.206(7)	0.245(5)	0.711(2)	0.215(1)	4.9
PEC+LL	0.311(7)	0.595(2)	0(1)	0.415(1)	0.205(4)	0.491(6)	0.257(2)	0.122(11)	0.591(9)	0.165(6)	4.9
SC+ID	0.329(3)	0.583(7)	0(1)	0.336(8)	0.125(7)	0.516(4)	0.241(5)	0.204(9)	0.705(3)	0.182(4)	5.1
EC+LC	0.297(11)	0.591(4)	0(1)	0.407(2)	0.205(4)	0.514(5)	0.196(8)	0.31(2)	0.591(9)	0.184(3)	4.9
PSC+LL	0.315(5)	0.595(2)	0(1)	0.297(10)	0.237(1)	0.474(8)	0.215(6)	0.298(3)	0.618(6)	0.122(12)	5.4
PEC+LC	0.297(11)	0.591(4)	0(1)	0.407(2)	0.205(4)	0.514(5)	0.196(8)	0.31(2)	0.554(11)	0.182(4)	5.2
SC+LL	0.3(9)	0.596(1)	0(1)	0.294(12)	0.205(4)	0.6(1)	0.147(10)	0.215(8)	0.593(8)	0.124(11)	6.5
EC+LL	0.299(10)	0.595(2)	0(1)	0.415(1)	0.205(4)	0.49(7)	0.121(12)	0.122(12)	0.598(7)	0.163(7)	6.3
MC+LL	0.325(4)	0.576(9)	0(1)	0.407(2)	0.205(4)	0.363(12)	0.135(11)	0.282(4)	0.589(10)	0.157(8)	6.5
PSC+LC	0.307(8)	0.592(3)	0(1)	0.407(2)	0.231(2)	0.402(10)	0.018(14)	0(14)	0.187(14)	0.008(14)	8.2
SC+LC	0.289(12)	0.592(3)	0(1)	0.361(6)	0.205(4)	0.456(9)	0.02(13)	0.067(13)	0.442(13)	0.072(13)	8.7
RSVM	0.226(14)	0.584(6)	0(1)	0.303(9)	0.211(3)	0.393(11)	0.185(9)	0.195(10)	0.64(5)	0.155(9)	7.7
RCNET	0.313(6)	0.567(10)	0(1)	0.295(11)	0.17(6)	0.456(9)	0.263(1)	0.344(1)	0.554(12)	0.147(10)	6.7

Table 5.4: Performance for the Exact Match metric and in parenthesis the ranking of the algorithm.

	Arts	Business	CAL500	Emotions	Flags	Health	Human	Plants	Scene	Yeast	AvgRank
PSC+ID	0.404(6)	0.722(9)	0.351(1)	0.609(5)	0.65(1)	0.634(1)	0.336(2)	0.302(5)	0.742(2)	0.502(3)	3.5
PSC+LL	0.425(4)	0.741(1)	0.319(3)	0.615(2)	0.621(6)	0.625(4)	0.257(5)	0.327(3)	0.702(6)	0.511(2)	3.6
PEC+ID	0.426(3)	0.739(2)	0.219(11)	0.607(6)	0.626(3)	0.634(1)	0.293(3)	0.241(8)	0.717(5)	0.5(4)	4.6
EC+ID	0.426(3)	0.738(3)	0.216(12)	0.607(6)	0.626(3)	0.634(1)	0.28(5)	0.241(8)	0.744(1)	0.499(5)	4.7
MC+ID	0.429(2)	0.733(6)	0.214(13)	0.592(7)	0.623(5)	0.632(2)	0.289(4)	0.246(7)	0.742(2)	0.497(6)	5.4
SC+ID	0.402(7)	0.734(5)	0.327(2)	0.591(8)	0.638(2)	0.626(3)	0.241(6)	0.214(11)	0.737(3)	0.483(9)	5.6
EC+LC	0.368(10)	0.739(2)	0.225(10)	0.611(4)	0.58(9)	0.634(1)	0.224(8)	0.325(4)	0.638(8)	0.491(7)	6.3
PEC+LC	0.368(10)	0.739(2)	0.249(7)	0.607(8)	0.58(9)	0.634(1)	0.224(8)	0.325(4)	0.628(10)	0.487(8)	6.7
PEC+LL	0.37(9)	0.739(2)	0.229(8)	0.609(5)	0.58(9)	0.61(5)	0.293(3)	0.124(12)	0.624(11)	0.481(10)	7.4
PSC+LC	0.417(5)	0.737(4)	0.279(4)	0.615(2)	0.604(7)	0.557(10)	0.227(7)	0.218(10)	0.474(13)	0.403(16)	7.8
EC+LL	0.367(11)	0.738(3)	0.229(8)	0.618(1)	0.58(9)	0.61(5)	0.136(12)	0.124(12)	0.631(9)	0.48(11)	8.1
SC+LL	0.359(12)	0.741(1)	0.276(5)	0.581(9)	0.594(8)	0.6(7)	0.166(10)	0.218(10)	0.628(10)	0.476(13)	8.5
SC+LC	0.352(13)	0.738(3)	0.263(6)	0.592(7)	0.594(8)	0.581(8)	0.216(9)	0.224(9)	0.484(12)	0.427(15)	9
MC+LL	0.396(8)	0.729(7)	0.226(9)	0.613(3)	0.58(9)	0.484(11)	0.154(11)	0.285(6)	0.624(11)	0.477(12)	8.7
RSVM	0.304(14)	0.738(3)	0.002(15)	0.561(10)	0.624(4)	0.569(9)	0.293(3)	0.33(2)	0.736(4)	0.526(1)	6.5
RCNET	0.432(1)	0.728(8)	0.203(14)	0.554(11)	0.563(10)	0.603(6)	0.361(1)	0.397(1)	0.669(7)	0.464(14)	7.3

Table 5.5: Performance for the Accuracy metric and in parenthesis the ranking of the algorithm.

EC+ID, MC+ID, and PEC+ID). Finally, the results for Accuracy metric show that Pool of Sequential classification on SPNs limiting node splits, Pools of Sequential and Exhaustive classifications on SPNs with direct and indirect variables interactions obtained highest performance (viz. PSC+LL, PEC+ID and PSC+ID).

These results reveal that in general, the proposed classifiers based on SPNs that use the learning algorithm with direct and indirect variables interactions (ID) outperforms the classifiers that learn with limit node splits (LL) or uses multivariate distributions as leaves (LC). Although, the complexity time of ID is higher compared with LL and LC, because it simultaneously learns two structures (SPN and Markov network). For the classifiers using Sequential classification, on average the best label ordering criteria are Static Best-First and Random. While using Pool classification the best criteria for combining the initial set of classifications are Weighted average and Majority voting.

According to our results, the best-proposed Multi-label classifiers ranks better than the state-of-art Multi-label classifiers evaluated in terms of Exact Match, Hamming Score, and Accuracy. RCNET ranks above 6 on average for all metrics. Finding the optimal classification (MPE) usually improved accuracy, especially with respect to Accuracy. This motivates the development of better algorithms for MPE in SPNs and suggests that SPNs are indeed competitive when exact inference is performed. RCNET only outperforms, in terms of Accuracy metric, our proposed classifier using Sum-Product Networks in three datasets (Arts, Human, and Plants).

The RaKel approach with Support Vector machines as basis multi-class classifier (RSVM) ranked above 5 on average for all metrics, and only shows better results for Accuracy metric in the datasets from the Biological domain (Human, Plants, and Yeast). While the proposed classifiers obtained better results in the others dataset, especially on Text, Music and Image domains where outper-

forms the state-of-art classifiers.

We will focus our discussion on the results obtained for Accuracy (see Table 5.5), as presented in previous sections it is one of the best measures for MLC. The proposed Multi-Label classifiers based on Sum-Product networks did not show the best performance for Plants, Human, Arts and Yeast dataset; according to our analysis, these datasets do not have any common characteristic, except that some of them have low label cardinality. In the other hand, our Multi-Label classifiers perform better in datasets with a large number of labels and a low number of training examples (viz. CAL500, Flags), in addition to the best results for Business, Emotions, Health and Scene.

5.4.1 Comparing classifiers with Wilcoxon signed-rank test

The Wilcoxon signed-rank test is a non-parametric statistical hypothesis test (null hypothesis significance test) used when comparing two paired samples [Dem06]. Then, it can be used to compare the performance of two classifiers on a large collection of datasets (greater than ten datasets) for a specific metric. Given a significance level α (normally set to $\alpha = 0.05$), if the result of the test, p-value, is less than α , indicates that a classifier has a statistically significant difference with the other, otherwise that is not enough evidence to assume any conclusion.

We use the Wilcoxon signed-rank test to compare RSVM and the performance of our best performed classifier for each metric, according with the Tables 5.3, 5.4 and 5.5.

Metric	Compared Classifiers	p-value
Hamming Score	SC+LL vs RSMV	0.6833
Exact Match	EC+ID vs RSVM	0.0469
Accuracy	PSC+ID vs RSVM	0.0745

Table 5.6: *P-value obtained from the Wilcoxon signed-rank test on the Compared classifiers for each Metric*

The results obtained for the classifiers comparisons of Hamming Score and Accuracy metrics, indicating that is not enough evidence to affirm that the compared classifiers have statistically significant difference. Therefore, the obtained results are not conclusive and may have been affected by the number of dataset considered in our experiments (10 datasets).

5.4.2 Comparing classifiers with Bayesian signed-rank test

Bayesian tests can accept the null hypotheses, calculating the posterior probability of the null and the alternative hypotheses. While the null-hypothesis significance tests can only reject the null hypothesis. The Bayesian signed-rank test returns probabilities that, based on the measured performance, one classifier is better than another or vice versa or they are within the region of practical equivalence (rope) [BMC⁺14], [BCDZ17].

Figures 5.1, 5.2 and 5.3 shows the results obtained for the Bayesian signed-rank test (Considering rope=0.01) on pairwise evaluations for RSVM, RCNET and our proposed classifiers for HS, EM and Acc respectively (According with the Tables 5.3, 5.4 and 5.5). Darker cells represent greater probability of "row classifier" being better than "column classifier", this probability is also show on the cell. For example, in the Figure 5.1, $P(\text{PSC+ID} > \text{RSVM}) = 0.898$ (dark blue), $P(\text{RSVM} > \text{PSC+ID}) = 0.102$ (light blue) and $P(\text{PSC+ID rope RSVM}) = 1 - 0.898 - 0.0102 = 0$ (not showed in the figure). Note that, the probability of the best rank classifiers based on SPN been better than the state-of-art (RSVM and RCNET) is highest, consequently these cells are the darkest.

	PSC+ID	PSC+LL	PEC+ID	EC+ID	MC+ID	SC+ID	EC+LC	PEC+LC	PEC+LL	PSC+LC	EC+LL	SC+LL	SC+LC	MC+LL	RSVM	RCNET
PSC+ID	-	0.658	0.874	0.739	0.816	0.864	0.94	0.94	0.999	0.998	0.998	1.0	1.0	0.979	0.967	0.898
PSC+LL	0.129	-	0.326	0.372	0.557	0.637	0.959	0.959	0.989	0.99	0.996	1.0	1.0	1.0	0.813	0.849
PEC+ID	0.006	0.082	-	0.0	0.0	0.647	0.713	0.776	0.902	0.952	0.992	0.986	0.994	0.971	0.778	0.801
EC+ID	0.01	0.14	0.025	-	0.0	0.747	0.739	0.78	0.913	0.952	0.982	0.985	0.992	0.959	0.783	0.797
MC+ID	0.011	0.122	0.016	0.0	-	0.48	0.789	0.796	0.908	0.956	0.982	0.979	0.993	0.967	0.777	0.766
SC+ID	0.0	0.023	0.156	0.101	0.108	-	0.772	0.763	0.943	0.942	0.989	0.97	0.994	0.93	0.692	0.7
EC+LC	0.01	0.0	0.056	0.064	0.1	0.126	-	0.0	0.325	0.823	0.429	0.857	0.944	0.71	0.575	0.403
PEC+LC	0.009	0.0	0.124	0.148	0.154	0.13	0.008	-	0.321	0.82	0.556	0.788	0.902	0.808	0.558	0.381
PSC+LL	0.0	0.005	0.0	0.002	0.01	0.022	0.067	0.069	-	0.635	0.035	0.322	0.804	0.283	0.495	0.27
PSC+LC	0.001	0.0	0.019	0.019	0.035	0.009	0.15	0.151	0.356	-	0.635	0.375	0.319	0.578	0.269	0.113
EC+LL	0.0	0.0	0.001	0.001	0.007	0.002	0.0	0.0	0.0	0.357	-	0.044	0.553	0.067	0.297	0.268
SC+LL	0.0	0.0	0.014	0.014	0.017	0.0	0.048	0.012	0.27	0.499	0.498	-	0.441	0.454	0.285	0.276
SC+LC	0.0	0.0	0.003	0.005	0.004	0.0	0.016	0.002	0.136	0.054	0.407	0.063	-	0.318	0.207	0.072
MC+LL	0.0	0.0	0.01	0.015	0.025	0.02	0.007	0.007	0.227	0.414	0.261	0.411	0.675	-	0.232	0.092
RSVM	0.025	0.104	0.144	0.121	0.128	0.283	0.415	0.433	0.497	0.727	0.701	0.714	0.788	0.767	-	0.202
RCNET	0.102	0.147	0.193	0.196	0.216	0.299	0.596	0.617	0.722	0.883	0.725	0.715	0.928	0.899	0.793	-

Figure 5.1: Probabilities of each classifier being better than the others for Accuracy metric according to Bayesian signed-rank test ($rope=0.01$)

	EC+ID	MC+ID	PEC+ID	PSC+ID	PEC+LL	SC+ID	EC+LC	PSC+LL	PEC+LC	SC+LL	EC+LL	MC+LL	PSC+LC	SC+LC	RSVM	RCNET
EC+ID	-	0.0	0.152	0.268	0.873	0.612	0.509	0.862	0.512	0.914	0.951	0.848	0.975	0.979	0.873	0.982
MC+ID	0.0	-	0.081	0.263	0.803	0.517	0.557	0.869	0.555	0.905	0.916	0.846	0.972	0.984	0.866	0.986
PEC+ID	0.0	0.0	-	0.243	0.751	0.308	0.454	0.824	0.477	0.882	0.897	0.793	0.973	0.983	0.879	0.979
PSC+ID	0.249	0.218	0.637	-	0.653	0.698	0.269	0.762	0.266	0.859	0.906	0.81	0.944	0.985	0.742	0.994
PEC+LL	0.099	0.172	0.168	0.313	-	0.308	0.079	0.448	0.235	0.506	0.041	0.339	0.93	0.994	0.883	0.881
SC+ID	0.0	0.0	0.0	0.125	0.563	-	0.367	0.728	0.386	0.747	0.851	0.734	0.965	0.975	0.732	0.952
EC+LC	0.436	0.394	0.454	0.361	0.179	0.518	-	0.627	0.036	0.742	0.487	0.781	0.942	0.966	0.894	0.944
PSC+LL	0.132	0.127	0.171	0.223	0.379	0.26	0.225	-	0.293	0.749	0.701	0.783	0.92	0.985	0.514	0.924
PEC+LC	0.433	0.397	0.439	0.365	0.188	0.51	0.0	0.585	-	0.742	0.522	0.797	0.942	0.965	0.802	0.928
SC+LL	0.082	0.092	0.114	0.137	0.218	0.241	0.051	0.082	0.146	-	0.5	0.224	0.935	0.947	0.518	0.442
EC+LL	0.044	0.08	0.09	0.08	0.0	0.132	0.0	0.211	0.035	0.213	-	0.114	0.931	0.976	0.692	0.607
MC+LL	0.15	0.148	0.201	0.16	0.107	0.237	0.015	0.148	0.065	0.671	0.193	-	0.87	0.975	0.46	0.614
PSC+LC	0.021	0.026	0.026	0.047	0.005	0.029	0.012	0.019	0.012	0.042	0.005	0.072	-	0.106	0.075	0.148
SC+LC	0.006	0.009	0.007	0.011	0.0	0.022	0.0	0.011	0.0	0.01	0.0	0.016	0.812	-	0.104	0.154
RSVM	0.116	0.116	0.106	0.235	0.068	0.247	0.099	0.322	0.144	0.447	0.293	0.498	0.917	0.89	-	0.782
RCNET	0.015	0.012	0.017	0.002	0.078	0.032	0.014	0.039	0.021	0.316	0.296	0.282	0.824	0.815	0.166	-

Figure 5.2: Probabilities of each classifier being better than the others for Exact Match metric according to Bayesian signed-rank test ($rope=0.01$)

	SC+LL	EC+ID	SC+ID	MC+ID	EC+LL	PEC+ID	PEC+LL	PEC+LC	PSC+LL	MC+LL	PSC+ID	EC+LC	SC+LC	PSC+LC	RSVM	RCNET
SC+LL	-	0.032	0.06	0.055	0.057	0.132	0.08	0.291	0.244	0.168	0.387	0.456	0.881	0.968	0.207	0.721
EC+ID	0.064	-	0.0	0.0	0.064	0.0	0.089	0.175	0.159	0.151	0.179	0.273	0.985	0.993	0.182	0.671
SC+ID	0.058	0.0	-	0.0	0.049	0.0	0.056	0.255	0.102	0.125	0.229	0.268	0.978	0.991	0.227	0.775
MC+ID	0.073	0.0	0.0	-	0.062	0.0	0.064	0.177	0.084	0.168	0.148	0.271	0.992	0.994	0.182	0.569
EC+LL	0.0	0.0	0.0	0.0	-	0.0	0.0	0.002	0.088	0.0	0.192	0.006	0.965	0.967	0.148	0.471
PEC+ID	0.088	0.0	0.0	0.0	0.047	-	0.048	0.191	0.033	0.055	0.182	0.245	0.984	0.993	0.21	0.655
PEC+LL	0.0	0.0	0.0	0.0	0.0	0.0	-	0.002	0.036	0.0	0.124	0.004	0.953	0.968	0.117	0.358
PEC+LC	0.0	0.0	0.016	0.0	0.011	0.001	0.02	-	0.025	0.008	0.104	0.037	0.953	0.969	0.015	0.027
PSC+LL	0.024	0.0	0.0	0.0	0.161	0.0	0.145	0.076	-	0.157	0.046	0.234	0.967	0.996	0.02	0.332
MC+LL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.022	-	0.055	0.0	0.941	0.917	0.109	0.192
PSC+ID	0.019	0.0	0.0	0.0	0.112	0.0	0.117	0.132	0.014	0.128	-	0.169	0.966	0.991	0.001	0.208
EC+LC	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.007	0.0	0.007	-	0.953	0.968	0.02	0.038
SC+LC	0.0	0.0	0.0	0.0	0.003	0.0	0.003	0.003	0.0	0.006	0.0	0.003	-	0.403	0.0	0.007
PSC+LC	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.002	0.0	0.0	0.0	0.045	-	0.0	0.007
RSVM	0.038	0.005	0.026	0.012	0.296	0.064	0.284	0.233	0.023	0.435	0.063	0.457	0.968	0.985	-	0.302
RCNET	0.0	0.006	0.016	0.002	0.019	0.013	0.015	0.0	0.001	0.041	0.04	0.044	0.81	0.957	0.001	-

Figure 5.3: Probabilities of each classifier being better than the others for Hamming Score metric according to Bayesian signed-rank test ($rope=0.01$)

In addition, the Figure 5.4 reports the samples from the posteriors (represents as points), the simplex (the large orange triangle) and three regions (in orange). For instance, the region at the bottom-left of the triangle is relative to the case where "left classifier" is more probable than "rope" and "right classifier" together; the region at the top of the triangle represents the case where "rope" is more probable and the region bottom-right the "right classifier" is more probable.

Figure 5.4: (a) Reports the posterior for *PSC+ID* vs. *RVSM* for *Accuracy Metric*, (b) Reports the posterior for *EC+ID* vs. *RVSM* for *Exact Match Metric* and (c) Reports the posterior for *SC+LL* vs. *RVSM* for *Hamming Score Metric* for the Bayesian sign-rank test ($\text{rope}=0.01$).

For the three posterior at the Figure 5.4, the probabilities for the "left classifiers" (based on SPN) been better than the "right classifier" (*RVSM*) is greater than the opposite case. In the case of Hamming Score metric, the posterior shows that the classifiers are practical equivalents or *SC+LL* is better than *RVSM* with high probability.

Chapter 6

Conclusions

Multi-Label Classification (MLC) generalize traditional classification by associating every example with a set of relevant labels. MLC has been shown to be much more challenging than traditional (i.e., single-label) classification. In this work, we investigated the use of Sum-Product Networks (SPN) for Multi-Label Classification. We exploited several approaches varying either the algorithm used for learning the network or the algorithm used for issuing classifications. We compared our proposed approaches against two state-of-the-art Multi-Label classifiers on a set of benchmark datasets.

The results showed that our approaches are competitive of the state-of-the-art methods (viz. RCNET and Rakel with SVM). The proposed classifiers based on Sum-Product Networks outperformed the other classifiers in terms of Accuracy, Hamming Score and Exact Match metrics. Especially a dataset with a very high number of relevant labels, our approaches clearly outperformed the other approaches. This suggests that SPNs might better capture the intricate dependences among labels, which might be crucial in domains with a high number of interdependent labels. Although, further experiments are need to verify this claim.

Learning more expressive SPNs using the Indirect and Direct learning algorithm [RL14] resulted in highest accuracy, but also in longest learning time, which might be a problem for domains with very large number of labels. SPN classifiers learned using the method described in [VDME15] performed slightly worse than those learned using the ID algorithm with much smaller training times.

If the main concern is the model learning time, we recommend use Pool of Sequential classification on SPNs limiting node splits, which average rank was five for the three evaluated metrics. While if the main concern is the classification time, the Max-Prod classification on SPN with direct and indirect variable interactions is the best option, that is the second best average rank.

6.1 Suggestions for Future Research

In future work, we intent to investigate the use SPNs within the Random k-Label sets (RaKel) approach. Propose new algorithms for approximate the Most Probable Explanation inspired on several approach for Multi-Label Classification, such as Hierarchy Of Multi-Label classifiERs (HOMER) and RaKel.

Also, would like to investigate the performance of the proposed classifiers using another methods for learning an Sum-Product Networks.

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