Concise and interpretable multi-label rule sets

Martino Ciaperoni
Department of Computer Science
Aalto University
Espoo, Finland
martino.ciaperoni@aalto.fi

Han Xiao
Department of Computer Science
Aalto University
Espoo, Finland
han.xiao@aalto.fi

Aristides Gionis
Division of Theoretical Computer Science
KTH Royal Institute of Technology
Stockholm, Sweden
argioni@kth.se

Abstract—**Multi-label classification is becoming increasingly ubiquitous, but not much attention has been paid to interpretability. In this paper, we develop a multi-label classifier that can be represented as a concise set of simple "if-then" rules, and thus, it offers better interpretability compared to black-box models. Notably, our method is able to find a small set of relevant patterns that lead to accurate multi-label classification, while existing rule-based classifiers are myopic and wasteful in searching rules, requiring a large number of rules to achieve high accuracy. In particular, we formulate the problem of choosing multi-label rules to maximize a target function, which considers not only discrimination ability with respect to labels, but also diversity. Accounting for diversity helps to avoid redundancy, and thus, to control the number of rules in the solution set. To tackle the said maximization problem we propose a 2-approximation algorithm, which relies on a novel technique to sample high-quality rules. In addition to our theoretical analysis, we provide a thorough experimental evaluation, which indicates that our approach offers a trade-off between predictive performance and interpretability that is unmatched in previous work.**

I. INTRODUCTION

Machine-learning algorithms are nowadays being used in almost every domain. While such algorithms are known to perform well in many tasks, they are often used as "black-boxes," i.e., the decision processes involved are too complex for humans to interpret. The lack of interpretability limits considerably the level of trust humans put in machine-learning algorithms and thus, poses a barrier for the wide adoption of machine-learning techniques in the real world. In an attempt to overcome this barrier, interpretable and explainable machine learning have recently emerged as increasingly prominent topics. In the standard classification setting, the goal is to learn a classifier that accurately maps data points to two or more *mutually exclusive* classes.

In this paper, we focus on a different setting, namely, *multi-label classification*. In contrast to the standard setting, in multi-label classification, a point can be associated with more than one class at the same time. Though multi-label classification has been extensively studied, the main focus is still on improving predictive performance [24]. Significantly less attention has been paid to interpretability aspects.

Classification rules, due to their simple structure, are gaining popularity in interpretable multi-label classification literature. In rule-based approaches, the goal is to learn a set of rules that captures the most prominent patterns between features and labels in the data. A rule usually takes the form "{set of predicates} → {set of labels}." For a given data point, a rule would predict the associated labels to be present, if all the predicates in the rule evaluate to true. Due to the structural simplicity of rules, classifiers based on a set of rules are generally considered more interpretable than other types of classifiers, such as neural networks or even decision trees.

The research question that we bring forward is whether we can design rule-based multi-label classification methods that are both accurate and interpretable. BOOMER [19], [20], a recently-proposed rule-based classifier based on gradient boosting, gives promising results in accuracy. However, despite being a rule-based approach, its interpretability is limited due to producing a set of rules that is both *too large* and *redundant*.

In this work, we propose CORSET, a rule-based method that significantly improves over the state-of-the-art BOOMER. The improvement is due to (1) reducing rule redundancy, which is achieved by incorporating a term in our objective that penalizes for rule overlap, and (2) explicitly limiting the complexity of rules via a suite of novel sampling schemes. As a result, our method produces a concise set of interpretable rules. An illustration of the concept of our approach is given in Fig. 1.

Example. To illustrate the improvement of CORSET over BOOMER, we consider as an example the bibtex dataset, where each data point represents a scientific article, with bag-of-words as features and topics as labels. We first consider predictive performance as a function of the number of rules. In Fig. 2, we show the (micro-averaged) balanced F_1 scores, a popular measure for multi-label classification used throughout this paper, for both CORSET and BOOMER. Due to the conciseness of its learned rules, CORSET achieves a score close to 0.36 with about 100 rules, whereas BOOMER needs over 800 rules to achieve similar performance. Note that CORSET's performance starts to drop after about 100 rules, as there are no more good rules to learn. The drop indicates overfitting, which can be addressed by standard methods, e.g., cross validation. In addition, Fig. 3 demonstrates the conciseness of the rules found by CORSET vs. the ones by BOOMER. Here, we show a subset of rules as a bipartite graph, where nodes at the top represent labels and nodes at the bottom represent the predicates (features). Rules are represented by colors and two nodes are connected if they are part of the same rule. CORSET uses fewer rules than BOOMER and rules tend to contain fewer predicates, resulting in a sparser graph.
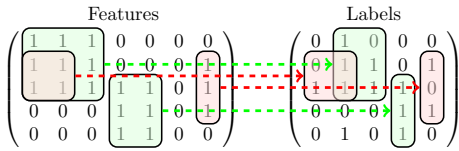
Fig. 1: Illustration of the concept of our approach for multi-label rule selection. A toy dataset is visualized as a feature matrix and a label matrix. Four rules are shown as colored regions. Regions covered by the same rule are connected by a dashed arrow. The rules in green are chosen because of accuracy, generality, and diversity. The rules in red are discarded.
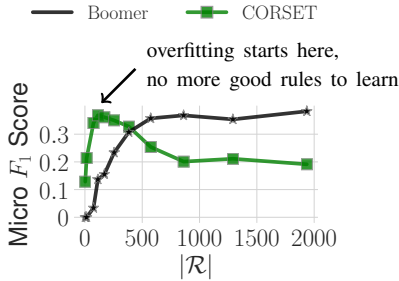

Fig. 2: Micro F_1, as a function of number of rules for CORSET vs. BOOMER in the bibtex dataset.
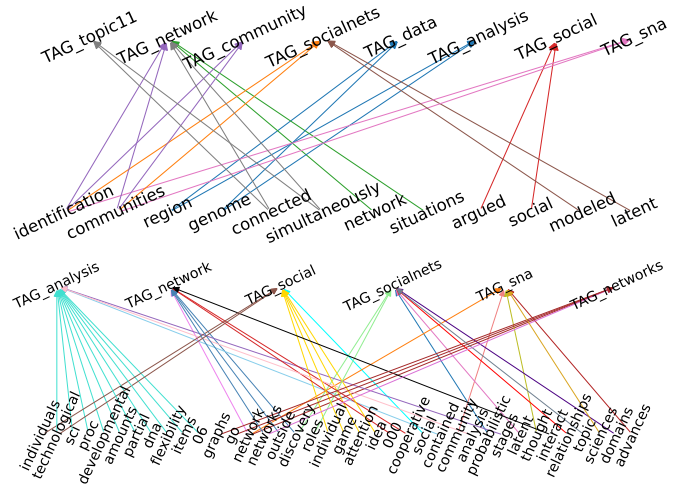

Fig. 3: An example set of rules returned by our algorithm (top) and BOOMER (bottom) on the bibtex dataset. We depict all rules for the set of labels {SNA, socialnets, social, networks, analysis}.

Concretely, in this work we make the following contributions.

- We frame the problem of learning concise rule sets as an optimization problem. The problem is **NP**-hard and our proposed algorithm CORSET, given a set of rule candidates, achieves an approximation ratio of 2.
- The performance of CORSET depends on the quality of the candidate rules. To find good rules efficiently, we design a suite of fast sampling algorithms with probabilistic guarantees as well as an effective heuristic.
- Our experiments show that CORSET achieves competitive predictive performance compared to the state-of-the-art, while offering significantly better interpretability.

The rest of this paper is organized as follows. Section II discusses related work. Section III formalizes the problem we consider. Section IV illustrates CORSET, omitting the details of the rule-sampling algorithms it relies on, which are described in Section V and VI. Afterwards, Section VII analyses the complexity of CORSET and finally Section VIII presents a thorough experimental evaluation of CORSET.

II. RELATED WORK

Multi-label classification. In multi-label classification the goal is to learn a function that maps input points to one or more predefined categories. For instance, a song can be associated with multiple music genres. A plethora of algorithms have been proposed for this problem; interested readers may refer to a recent survey [24]. The simplest approaches for multi-label classification are the so-called transformation methods, which convert the original problem into multiple single-label classification problems. The main drawback of these approaches

is that they fail to capture label correlations. To overcome this issue, label power-set approaches map each distinct set of labels to a unique meta-label, which serves as target label for a single-label classifier. Clearly, these approaches do not scale with the number of labels and the pruned problem transformation method [21] has been proposed as a remedy. Another line of research focuses on designing ad-hoc multi-label classification methods by extending existing single-label algorithms. Examples include adaption from support vector machines [7], k-nearest neighbor classifiers [28], and perceptrons [6].

Interpretable machine learning. There is no agreed formal definition of interpretability, but it can be loosely defined as the degree to which a human can understand the cause of a decision [16]. Broadly speaking, interpretability in machine learning can be achieved by constraining the complexity of algorithms so that the process behind the decision of the algorithm is understandable to humans. A related topic is explainable machine learning, where the goal is to provide explanations to the predictions of black-box models.

Rule-based approaches to single-label classification. Research in interpretable machine learning has boomed in the last years. Rule-based (or associative) approaches have shown promising potential, because decisions are driven by a simple set of "if-then" rules. Liu et al. [15] are among the first to investigate association rule mining for single-label classification tasks, followed by extensions such as MCAR [22] and ADA [25]. These approaches are conceptually similar, but differ in their methodologies for rule learning, ranking, pruning, and prediction.

Concise rule sets. Our work pursues for the first time the goal of designing a multi-label associative classifier for achieving a given classification performance with the smallest possible num-

ber of rules. A similar objective has been recently considered in the context of single-label classification. In particular, Zhang et al. [26] frame the problem of learning a set of classification rules as an optimization problem with an objective function combining rule quality and diversity. A 2-approximation algorithm is then proposed to solve this problem, which relies on existing frameworks for max-sum diversification and pattern sampling. In this paper, we investigate how to extend these ideas to the multi-label classification setting. The problem of controlling the number of rules has also been studied for rule boosting, where learned rules are combined additively [3]. An extension to multi-label classification represents a possible direction of future work. In addition to the number of rules, conciseness of a rule set, and thus interpretability, has been defined in terms of number of conditions [10] as well as of the Minimum Description Length principle [8].

Rule-based approaches to multi-label classification. In general, adaptation from the single-label to the multi-label setting is not trivial and while single-label associative classification has been studied extensively, relatively few attempts have been made for associative multi-label classification. In an early work, Thabtah et al. [23] propose a label ranking-based assignment method. More recently new approaches have been developed, and SeCo [12] and Boomer [20] are state-of-the-art in the current literature of rule-based multi-label classification. The main limitation of the existing works, addressed in our paper, is that they use a very large set of highly redundant rules, which hinders interpretability. We compare our method against SeCo [12] and Boomer [20] in Section VIII.

Pattern sampling. Association pattern discovery is challenging due to the prohibitive size of the pattern space. This challenge is inherited by rule-based classifiers. To avoid exhaustively searching the pattern space, efficient pattern-sampling methods have been proposed [1], [2]. In this work we extend these sampling methods to efficiently find high-quality candidate multi-label rules, as discussed in detail in Section V.

III. PROBLEM STATEMENT

At a high level, our objective is to capture the relevant patterns in the data that best discriminate a set of labels and are as concise as possible. Next we formally define the problem.

A. Preliminaries

We denote sets and multisets by uppercase letters e.g., X. For a finite X, we denote by $\mathcal{P}(X)$ its power set. We consider a binary *dataset* $\mathcal{D}$ over a *feature set* $\mathcal{F}$ and a *label set* $\mathcal{L}$. The dataset $\mathcal{D}$ is a set of *data records*, $D_1, \ldots, D_n$. A data record $D = (F, L)$ consists of a set of features $F \subseteq \mathcal{F}$ and a set of labels $L \subseteq \mathcal{L}$. We denote by F_D and L_D the feature set and label set of D, respectively. Furthermore, we denote by $|\mathcal{F}|$ and $|\mathcal{L}|$ the dimensions of the feature and label space, respectively, and we denote by $|\mathcal{D}|$ the total number of data records. We use $\|\mathcal{F}\|$ and $\|\mathcal{L}\|$ to refer to the total number of feature and label occurrences over all data records.

In multi-label classification, the goal is to learn a function mapping as accurately as possible the features F_D to one or more labels L_D. We use mappings consisting of *conjunctive rules*. A conjunctive rule $R = (H \to T)$ consists of a non-empty feature set H (called *head*) and a non-empty label set T (called *tail*). The head H can be viewed as a predicate $H : \{0, 1\}^{|\mathcal{F}|} \to \{\text{true}, \text{false}\}$, which states whether an instance F contains all the features in H. If the predicate evaluates to true for some instance, the tail T of R specifies that labels T should be predicted as present.

We say that a head H *matches* a data record D if $H \subseteq F_D$. Similarly, a tail T matches D if $T \subseteq L_D$. We say that a rule R *covers* a data record D if $H_R \subseteq F_D$ and similarly R matches a data record D if both H_R and T_R match D. For a dataset $\mathcal{D}$, we denote the *support set* of $X \in \{H, T, R\}$ by:

$$\mathcal{D}[X] = \{D \in \mathcal{D} \mid X \text{ matches } D\}.$$

The *space of all possible rules* we consider is $\mathcal{U} = \mathcal{P}(\mathcal{F}) \times \mathcal{P}(\mathcal{L})$, i.e., the Cartesian product of the power set of the feature set and the power set of the label set.

B. Problem formulation

We want to discover rules that are accurate and general, but also sufficiently different from each other. To capture this trade-off, we design an objective function that consists of a *quality term* $q : \mathcal{U} \to \mathbb{R}$ measuring the accuracy and generality of a single rule, and a *diversity term* $d : \mathcal{U} \times \mathcal{U} \to \mathbb{R}$ measuring the distance between pairs of rules.

Quality term. Given a rule R and a set of rules $\mathcal{R}$, the quality $q(R; \mathcal{R})$ of R with respect to $\mathcal{R}$ is the product of two values: the *uncovered area* $\text{area}(R; \mathcal{R})$, capturing the generality of R with respect to $\mathcal{R}$, and its *adjusted accuracy* $a(R)$,

$$q(R; \mathcal{R}) = \text{area}(R; \mathcal{R}) \cdot a(R).$$

Next we describe these two functions. To capture generality, we first define the *coverage* of R as:

$$\text{cov}(R) = \{(i, k) \mid R \text{ matches } D_i \in \mathcal{D} \text{ and } k \in T\}. \quad (1)$$

In other words, the coverage of a rule is the set of label occurrences it matches in a dataset. To incorporate what is already covered by a set of selected rules $\mathcal{R}$, we define *uncovered area* of R with respect to $\mathcal{R}$ as

$$\text{area}(R; \mathcal{R}) = \left| \text{cov}(R) \setminus \bigcup_{R \in \mathcal{R}} \text{cov}(R) \right|, \quad (2)$$

that is, the size of covered label occurrences by R after excluding those already covered by $\mathcal{R}$. Thus, a rule R is considered general with respect to $\mathcal{R}$ if $\text{area}(R; \mathcal{R})$ is large.

Before introducing the adjusted-accuracy function, we need some additional notation. Data records whose labels contain T are said to be positive with respect to T, whilst the remaining ones are negative. More formally, a tail T bi-partitions a dataset $\mathcal{D}$ into two disjoint sets: a set of *positive data records* $\mathcal{D}_T^+ = \{D \in \mathcal{D} \mid T \subseteq L_D\}$ and a set of *negative data records* $\mathcal{D}_T^- = \{D \in \mathcal{D} \mid T \nsubseteq L_D\}$. Given a rule R, let $P_{\mathcal{D}[R]} = \frac{|\mathcal{D}[R]|}{|\mathcal{D}[H]|}$ be the *precision* of R and $P_{\mathcal{D}} = \frac{|\mathcal{D}[T]|}{|\mathcal{D}|}$ is the *base rate* of

T in $\mathcal{D}$. We denote the corresponding binomial distributions as $\mathrm{Bin}\big(P_{\mathcal{D}[R]}\big)$ and $\mathrm{Bin}(P_{\mathcal{D}})$, respectively. Then the *adjusted accuracy* of R is defined as:

$$a\left(R\right) = I(R) \cdot D_{\mathrm{KL}}\big(\mathrm{Bin}\big(P_{\mathcal{D}[R]}\big) \,||\, \mathrm{Bin}(P_{\mathcal{D}})\big), \qquad (3)$$

where $I(R)$ is 1 if $P_{\mathcal{D}[R]} > P_{\mathcal{D}}$ and 0 otherwise, and $D_{\mathrm{KL}}(\cdot \,||\, \cdot)$ is the KL divergence between two probability distributions. The underlying intuition is that if the precision of a rule is below its base rate, it is useless, and receives a zero score. If instead the precision of a rule is larger than the base rate, the higher the precision is, the larger the score.

Diversity term. We measure the distance between two rules by how much their coverages overlap. Formally, given two rules R_1 and R_2, their distance is defined as

$$d\left(R_1, R_2\right) = 1 - \frac{|\mathrm{cov}(R_1) \cap \mathrm{cov}(R_2)|}{|\mathrm{cov}(R_1) \cup \mathrm{cov}(R_2)|},$$

which is the *Jaccard distance* between $\mathrm{cov}(R_1)$ and $\mathrm{cov}(R_2)$.

Problem definition. We frame the learning problem as a combinatorial optimization problem with budget constraint, where we set a budget on the maximum number of rules to discover, and rules should be selected to maximize a linear combination of the quality and diversity term.

Problem 1: Given a dataset $\mathcal{D} = \{D_i\}_{i=1}^{n}$, a budget $B \in \mathbb{Z}_+$, a space of rules $\mathcal{S} \subseteq \mathcal{U}$, and a parameter $\lambda \in \mathbb{R}_+$, find a set of B rules $\mathcal{R} = \{R_1, \dots, R_B\} \subseteq \mathcal{S}$, to maximize the following objective

$$f\left(\mathcal{R}\right) = \sum_{R \in \mathcal{R}} q\left(R; \mathcal{R} \setminus \{R\}\right) + \lambda \sum_{R_i, R_j \in \mathcal{R}, i \neq j} d(R_i, R_j). \quad (4)$$

This problem is known to be NP-hard [4]. In the next section, we present a greedy algorithm which finds a solution to Problem 1 with an approximation factor of 2, provided that the space of rules $\mathcal{S}$ can be visited in polynomial time.

IV. CORSET LEARNING ALGORITHM

In this section, we present a meta algorithm named CORSET (*concise rule set*) for Problem 1. CORSET greedily picks one rule at a time from a pool of candidate rules, so as to maximize the marginal gain for the objective in (4), i.e.,

$$f\left(\mathcal{R} \cup \{R\}\right) - f\left(\mathcal{R}\right) = q\left(R; \mathcal{R}\right) + \lambda \sum_{R_j \in \mathcal{R}} d(R, R_j).$$

The candidate rules are generated by a procedure called GEN-CANDRULES. The effectiveness of GENCANDRULES heavily affects the predictive performance of the classifier. The goal is to sample high-quality rules in terms of generality, diversity and accuracy. This is a challenging goal since the size of rule space is exponential [9] and GENCANDRULES should therefore avoid exploring the whole space. We defer the description of the candidate generation to Sections V and VI.

For now, we focus on the description of the main algorithm. CORSET maintains a set of selected rules, $\mathcal{R}$, which is initially empty. At each iteration, CORSET considers a pool of candidate rules generated by GENCANDRULES. Within this pool, the rule R^* maximizing the marginal gain of (4) with respect to

---

Algorithm 1: The CORSET algorithm.

Data: data $\mathcal{D}$, tolerance τ
Result: a set of multi-label classification rules $\mathcal{R}$.

1   $\mathcal{R}, \mathcal{R}' \leftarrow \emptyset, \mathcal{C}_R \leftarrow \emptyset$;
2   **while** $c > \tau$ **do**
3     $\mathcal{C} \leftarrow \text{GENCANDRULES}(\mathcal{R})$;
4     $\mathcal{C}_R \leftarrow \mathcal{C}_R \cup \mathcal{C}$;
5     $R^* \leftarrow \arg\max_{R \in \mathcal{C}} [f\left(\mathcal{R} \cup \{R\}\right) - f\left(\mathcal{R}\right)]$;
6     $c \leftarrow \frac{\sum_{D \text{ matched by } R^*} |L_D \cap T_{R^*} \setminus \cup_{R \in \mathcal{R} | R \text{ matches } D} T_R|}{\|\mathcal{L}\|}$;
7     $\mathcal{R} \leftarrow \mathcal{R} \cup R^*$;
8   **end**
9   **for** $i = 1, .. |\mathcal{R}|$ **do**
10    $R^* \leftarrow \arg\max_{R \in \mathcal{C}_R} \left[f\left(\mathcal{R}' \cup \{R\}\right) - f\left(\mathcal{R}'\right)\right]$;
11    $\mathcal{R}' \leftarrow \mathcal{R}' \cup R^*$;
12   **end**
13   **if** $f(\mathcal{R}') > f(\mathcal{R})$ **then return** $\mathcal{R}'$;
14   **else return** $\mathcal{R}$;

$\mathcal{R}$ is selected and added to $\mathcal{R}$. The process stops when the proportion of labels in $\mathcal{L}$ predicted by $\mathcal{R} \cup R^*$ and not by $\mathcal{R}$ falls below a user-specified tolerance level τ.

To ensure the aforementioned approximation guarantee, we need to obtain a new set of rules $\mathcal{R}'$ by repeating the greedy procedure a second time, over the full set of candidates rules, because using a different candidate set at each iteration does not offer a guarantee. As in practice $\mathcal{R}'$ is not necessarily better than $\mathcal{R}$, we return as solution the set that yields the largest objective function value, between the two.

The pseudocode of CORSET is shown in Algorithm 1. Note that GENCANDRULES receives as input the current rule set $\mathcal{R}$, so as to generate rules different from $\mathcal{R}$. The solution is guaranteed to be within a constant factor of the optimal solution.

Proposition 1: For a fixed pool of candidate rules, CORSET is a 2-approximation algorithm for Problem 1.

As shown by Borodin et al. [4], the approximation factor is guaranteed by the properties of the objective function, namely by the *submodularity* of the quality function and the fact that the Jaccard distance is a *metric*. Proof is given in Appendix.

Prediction. At prediction time, given the set of selected rules $\mathcal{R}$, we return the set of predicted labels for an instance F as $\bigcup_{R \in \mathcal{R} | H_R \subseteq F} T_R$, that is, the union of tails of rules such that F evaluates to true for the head predicate.

V. RULE SAMPLING

In the next two sections, we present the main contribution of our work, a suite of rule-sampling algorithms used by GENCANDRULES. In this section, we first describe the technical basis of our proposal, then we formulate our sampling problem, and present our algorithms for it. In the next section, we discuss some important limitations of the proposed sampling method and describe practical enhancements.

A. Background: Two-stage pattern sampling

Our sampling scheme builds on the pattern-sampling algorithms proposed by Boley et al. [1], [2]. These algorithms allow us to sample patterns according to a target distribution over the pattern space, without the need of exhaustive enumeration. The target distribution reflects a measure of interestingness for the patterns. Example measures include support, area, and, if the data are labelled, discriminativity. Sampling algorithms for a variety of measures share a two-stage structure, whilst the details depend on the measure under consideration.

The key insight brought by Boley et al. [1], [2] is that *random experiments reveal frequent events*. We use sampling by support and area for illustration. Consider a dataset $\mathcal{D} = \{D_1, \ldots, D_n\}$ over a finite ground set $\mathcal{E}$, with $D \subseteq \mathcal{E}$ for each $D \in \mathcal{D}$. Consider the problem of sampling an itemset (pattern) $F \subseteq \mathcal{E}$ with probability proportional to its *support* $q_{\text{supp}}(F) = |D\,[F]|$.

For each $D \in \mathcal{D}$, the set of itemsets including D in their support is $\mathcal{P}(D)$. It can be shown that sampling an itemset F uniformly from $\biguplus_{D \in \mathcal{D}} \mathcal{P}(D)$, where $\biguplus$ denotes the union operator of multi-sets, is the same as sampling F according to $|D[F]|$. To avoid materializing $\biguplus_{D \in \mathcal{D}} \mathcal{P}(D)$, Boley et al. use a two-step procedure:

1. sample a data record D with probability proportional to the weight $w(D) = \sum_{F \in \mathcal{P}(D)} 1 = 2^{|D|}$.
2. sample an itemset F uniformly from $\mathcal{P}(D)$.

To sample from the "area" distribution $q_{\text{area}}(F) = |F||D\,[F]|$, the above procedure is changed as follows: $w(D) = \sum_{F \in \mathcal{P}(D)} F = |D| 2^{|D|-1}$, and then sample F with weight $|F|$ from $\mathcal{P}(D)$.

The two-stage sampling idea can be generalized to a number of other measures. Some of them, such as discriminativity, which we use later, require sampling tuples of data records rather than a single one in the first stage.

Next we describe two sampling distributions and the corresponding sampling algorithms for our objective. The first distribution is a generalization of the area function (not discussed by Boley et al. [1], [2]) and is used for tail sampling. The second distribution is discriminativity and is used for head sampling. For the latter, we propose an improved sampling algorithm, which is faster than the original version [2].

B. Sampling objectives

Our rule sampling objective is a product of two values, reflecting the generality of a rule $R = (H \rightarrow T)$ given the current set of rules $\mathcal{R}$, and its discriminative power:

$$\Pr(H, T) \propto w(H, T; \mathcal{R}) = q_a(H; T) \cdot \text{area}(T; \mathcal{R}). \quad (5)$$

Note that the uncovered area function in 2 generalizes to tails, i.e., $\text{area}(T; \mathcal{R}) = \left| \text{cov}(T) \setminus \bigcup_{T' \in \mathcal{R}} \text{cov}(T') \right|$ and $\text{cov}(T) = \{(i, k) \mid T \text{ matches } D_i \in \mathcal{D} \text{ and } k \in T\}$.

For q_a we choose the discriminativity measure studied by Boley et al. [1], which permits sampling in polynomial time. Given a tail $T \subseteq \mathcal{L}$, the *discriminativity* of H is defined as

$$q_{\text{disc}}(H; T) = \left| \mathcal{D}_T^+[H] \right| \left| \mathcal{D}_T^- \setminus \mathcal{D}_T^-[H] \right|. \quad (6)$$

The goal is to sample heads that have as large support as possible in $\mathcal{D}_T^+$ and as small support as possible in $\mathcal{D}_T^-$.

To sample from distribution (5), we use the following steps:

1. sample T with probability proportional to $\text{area}(T; \mathcal{R})$;
2. sample H with probability proportional to $q_a(H; T)$.

We explain each sampling step next.

C. Tail sampling

To sample from $\text{area}(T; \mathcal{R})$, we apply a similar two-step sampling procedure as in Boley et al. [1]: we first sample a data record D with probability proportional to its weight $w(D; \mathcal{R})$ and then sample T from D. The function $\text{area}(T; \mathcal{R})$ is a generalization of the area function considered in Boley et al. [1]. Adapting the original algorithm to our case requires to design a weight function $w(\cdot; \mathcal{R})$ appropriate for our target. To define $w(\cdot; \mathcal{R})$, a few new definitions are needed. Given a rule R and a data record D, the *D-specific coverage* of R is defined to be

$$\text{cov}_D(R) = \begin{cases} L_D \cap T_R, & \text{if } R \text{ matches } D, \\ \emptyset, & \text{otherwise.} \end{cases} \quad (7)$$

Extending D-specific coverage to a rule set $\mathcal{R}$, we have:

$$\text{cov}_D(\mathcal{R}) = \bigcup_{R \in \mathcal{R}} \text{cov}_D(R). \quad (8)$$

Given a label set T, its *marginal coverage* with respect to $\mathcal{R}$ is

$$\text{cov}_D(T; \mathcal{R}) = (L_D \cap T) \setminus \text{cov}_D(\mathcal{R}), \quad (9)$$

that is, the covered label occurrences in D by T, excluding those by $\mathcal{R}$. As a shortcut, we define $\overline{\text{cov}}_D(\mathcal{R}) = \text{cov}_D(L_D; \mathcal{R})$, i.e., the set of label occurrences in D not covered by $\mathcal{R}$.

The weight of a label set T on a data record D is:

$$w(T, D; \mathcal{R}) = |\text{cov}_D(T; \mathcal{R})|. \quad (10)$$

We give a small example to illustrate these definitions:

$$D : F_D = \{0, 1, 2, 3\}, \ L_D = \{a, b, c\}$$
$$R_1 : \{0, 1\} \rightarrow \{a\}$$
$$R_2 : \{1, 2\} \rightarrow \{a, b\} \quad \mathcal{R} = \{R_1, R_2, R_3\}$$
$$R_3 : \{2, 3\} \rightarrow \{a, c\} \quad T = \{b, c\}$$

For R_1, R_2, R_3, the sets $\text{cov}_D(\cdot)$ are $\{a\}, \{a, b\}, \emptyset$, respectively. Therefore, $\text{cov}_D(T; \mathcal{R}) = \{c\}$ and $w(T, D; \mathcal{R}) = 1$.

The intuition of the definition of $w(T, D; \mathcal{R})$ is that T has large weight on D if it contains many label occurrences not covered by $\mathcal{R}$. Therefore, the weight of any data record D is simply the summation of the weights over all possible tails:

$$w(D; \mathcal{R}) = \sum_{T \subseteq L_D} w(T, D; \mathcal{R}) = |\overline{\text{cov}}_D(\mathcal{R})| \, 2^{|L_D|-1}, \quad (11)$$

where the second equality can be shown by simple algebra. Using these weights, we adapt the sampling algorithm of Boley et al. [1], [2] as per Algorithm 2.

By a similar proof technique as in Boley et al. [1], we have:

Algorithm 2: Two-stage tail sampling.

Data: a dataset $\mathcal{D}$, weights $w(D;\mathcal{R})$ (as in 11).
Result: a tail $T \subseteq \mathcal{L}$ with $T \sim \text{area}(T;\mathcal{R})$.
1 draw $D \sim w(D;\mathcal{R})$;
2 **return** $T \sim w(T, D;\mathcal{R})$

Proposition 2: Algorithm 2 returns $T \sim \text{area}(T;\mathcal{R})$.

The proof is provided in Appendix.

D. Head sampling

After a tail T is sampled, we sample H according to $q_a(H;T) = q_{\text{disc}}(H;T)$, from (6). The two-stage sampling scheme by Boley et al. can be applied for this case. In contrast to the previous cases, the weight function is defined on *pairs* of data records:

$$w(D^+, D^-) = 2^{|D^+|} - 2^{|D^+ \cap D^-|} - |D^+ \setminus D^-|, \quad (12)$$

where $D^+ \in \mathcal{D}_T^+$ and $D^- \in \mathcal{D}_T^-$, and $|D^+|$ (resp. $|D^-|$) denotes the number of features present in D^+ (resp. D^-). Thus, pre-computing the weights leads to *quadratic* space complexity in $|\mathcal{D}|$, which limits the practicality of the sampling procedure.

The above limitation is addressed by Boley et al. [2] using the technique of *coupling from the past* (CFTP), which leads to *linear* space complexity. Unlike many Markov chain Monte Carlo (MCMC) methods, CFTP can guarantee that samples are generated according to the target distribution. It operates by simulating the Markov chain *backwards* by sampling from a proposal distribution, until all states coalesce to the same unique state. The main challenge of using CFTP is the design of the proposal distribution and the efficient monitoring of coalescence condition.

The proposal distribution should be (i) efficient to sample from; and (ii) an appropriate approximation to the target distribution to obtain fast convergence. Boley et al. [2] devise a "general-purpose" proposal distribution, which works for all target distributions they consider. For the case of discriminativity, the proposal distribution is defined as

$$\overline{w}(D^+, D^-) = \sqrt{w_1(D^+) \cdot w_2(D^-)}, \quad (13)$$

where $w_1(D^+) = 2^{|D^+|} - |D^+| - 1$ and $w_2(D^-) = 2^{|\mathcal{F}|} - 2^{|D^-|} - |D^-| - 1$. Sampling from $\overline{w}(\cdot, \cdot)$ can be done efficiently by sampling separately from $w_1(\cdot)$ and $w_2(\cdot)$. However, we argue that the choice of $\overline{w}(\cdot, \cdot)$ is not a good approximation of the target, and therefore it suffers from slow convergence. The reason is that when a data record is high-dimensional but sparse, as is often the case in multi-label classification, $w_2(D^-)$ and hence $\overline{w}(D^+, D^-)$ grow exponentially with the number of features, making the acceptance probability extremely low and, as a consequence, convergence is extremely slow.

To overcome the convergence issue, we use a different proposal distribution better suited for our setting. Our proposal is the same as in (13), except that w_2 is defined as a uniform function, $w_2(D^-) = 1$ for all $D^- \in \mathcal{D}_T^-$ and the square root is removed. An appealing property is that the new choice is a *tight*

Algorithm 3: Two-stage head sampling.

Data: a dataset $\mathcal{D}$, a tail T, weights $w_1(\cdot)$ and $w_2(\cdot)$.
Result: a head $H \in \mathcal{F}$ with $H \sim q_a(H;T)$.
1 initialize $i \leftarrow 1$, $\mathbf{D} \leftarrow \perp$;
2 **while** $\mathbf{D} = \perp$ **do**
3     $i \leftarrow i + 1$;
4   **for** $t = 2^i, \ldots, 0$ **do**
5   draw $u_t \sim u([0,1])$ and $\mathbf{C}_t \sim \overline{w}(\mathbf{C}_t)$;
6   **if** $u_t \leq \frac{\overline{w}(\mathbf{D})w(\mathbf{C}_t)}{w(\mathbf{D})\overline{w}(\mathbf{C}_t)}$ **then** $\mathbf{D} \leftarrow \mathbf{C}_t$;
7   **end**
8 **end**
9 draw
   $H_1 \sim u(\mathcal{P}(D^+ \setminus D^-) \setminus \emptyset), H_2 \sim u(\mathcal{P}(D^+ \cap D^-))$;
10 **return** $H = H_1 \cup H_2$

---

upper bound of 12, therefore providing a better approximation to the original version. Further, we empirically verify that using our proposal gives much faster convergence than using the one by Boley et al [2].

Head sampling is summarized in Algorithm 3. We first use CFTP (lines 1-7) to sample a pair (D^+, D^-). Then we sample a head in line 9. We denote $u(\cdot)$ as the uniform distribution over a set. For brevity, we use a boldface letter to denote a pair of records, e.g., $\mathbf{D}$. We denote an empty pair by $\perp$, and define $\overline{w}(\perp)/w(\perp) = 1$.

VI. ENHANCEMENTS TO THE SAMPLING SCHEME

A. Limitations of the two-stage pattern-sampling framework

While theoretically sound, in our setting, the two-stage sampling framework [1], [2] suffers from two limitations, as can be verified empirically. First, we observe that most of the sampled rules are very specific, with very low support. Second, rule interpretability is not explicitly considered.

Heavy-hitter problem for tail sampling. Consider the tail sampling part. Notice that the weight of a data record D in (11) is exponential in L_D. If there is a data record $D \in \mathcal{D}$ whose $|L_D|$ is moderately larger than the rest, its weight dominates, making it very likely to be sampled in the first sampling step. We refer to this issue as *the heavy-hitter problem*. For instance in bibtex, the largest label set of a data record D^* contains 28 labels while the second largest contains 16. The probability of D^* being sampled is 99.97%. A tail sampled from D^* has an expected length of 14.5. Empirically, tails of about this length match only a few data records. Thus, most of the sampled tails have low support, hampering the goal of sampling general rules.

Heavy-hitter problem for head sampling. A similar issue arises in head sampling. The weight function in (12) grows exponentially with $|D^+|$, so that CFTP most likely returns the positive data records with the highest number of present features. Therefore, sampled heads tend to be very long and have small support (often 1). Thus, they may have high discriminativity but cannot generalize to unseen data.

Algorithm 4: Tail sampling under $\mathcal{S}^-$ according to uncovered area.

Data: a dataset $\mathcal{D}$, sample space $\mathcal{S}^-$, and a rule set $\mathcal{R}$
Result: a tail $T \in \mathcal{S}^-$ with $T \sim \text{area}(T; \mathcal{R})$.
1 let $I[D] \leftarrow \{S \in \mathcal{S}^- \mid S \subseteq L_D\}$, for each $D \in \mathcal{D}$;
2 let $w(D) \leftarrow \sum_{S \in I[D]} |S \setminus \text{cov}_D(\mathcal{R})|$ for each $D \in \mathcal{D}$;
3 draw $D \sim w(D)$;
4 draw $T \in I[D] \sim |T|$;
5 **return** T

Tail interpretability. Interpretability of tails is a central focus in our work. Nonetheless, in the original pattern-sampling algorithms [1], [2] all elements in $\mathcal{P}(L)$ are considered possible tails, regardless of whether they are interpretable or not. Some tails are sampled simply because labels in them co-occur frequently, rather than because they are truly interpretable.

The root of the above limitations is the enormous sample space under consideration, which we address next.

B. Tail sampling under interpretable label space

We propose to restrict the label sample space to a much smaller sample space $\mathcal{S}^- \subseteq \mathcal{P}(\mathcal{L})$ designed to contain only interpretable label sets so as to mitigate the heavy-hitter problem. We call $\mathcal{S}^-$ the *interpretable label space*. Before describing the construction of $\mathcal{S}^-$, we notice that pattern sampling under any subspace of $\mathcal{P}(\mathcal{L})$ is a slight generalization of the original sampling setting. Most importantly, the original sampling algorithms can be adapted to different sample spaces, such as $\mathcal{S}^-$, while preserving probabilistic guarantees.

In Algorithm 4, we describe a procedure for sampling by uncovered area under $\mathcal{S}^-$. The algorithm can be easily adapted for other sampling objectives e.g., discriminativity. Compared to sampling under $\mathcal{P}(\mathcal{L})$, we require the extra step of determining the set $I[D]$ of patterns in $\mathcal{S}^-$ contained by $D \in \mathcal{D}$ and computing the weight for D accordingly.

Constructing $\mathcal{S}^-$. To construct the interpretable label space, we first define interpretability in our setting. Humans like to think in an associative manner [17]. To accommodate such tendency, we argue that a label set is interpretable if the corresponding labels are sufficiently associated. The problem of constructing $\mathcal{S}^-$ is then framed as finding sufficiently associated label sets.

We rely on a graph-based approach whereby we construct a suitable label graph and extract its dense subgraphs. Specifically, we construct a directed weighted graph $\mathcal{G} = (V, E, p)$. Each node represents a label. A node pair (u, v) is an edge in E if $\mathcal{D}[\{u\}] \cap \mathcal{D}[\{v\}] \neq \emptyset$. The corresponding weight is defined as $p(u, v) = \frac{|\mathcal{D}[\{u\}] \cap \mathcal{D}[\{v\}]|}{|\mathcal{D}[\{u\}]|}$, which can be interpreted as the conditional probability that label v occurs given that label u occurs. The need of a directed graph arises because in real-world multi-label datasets, association of labels is asymmetric.

Finally, probabilistic interpretation of the edge weights suggests that $\mathcal{G}$ can be viewed as a *probabilistic graph* [29]. Under such point of view, our problem can be seen as finding

highly probable cliques in $\mathcal{G}$ [18], whose probability of forming is above pre-specified threshold. To solve this problem, we adapt a depth-first search (DFS) procedure similar to the one proposed by Mukherjee et al. [18].

Efficient preprocessing. Execution of line 1 in Algorithm 4 can be done efficiently by framing the problem appropriately. In this problem, we are given a set of subsets $\mathcal{S}^-$ and we are asked to find, for each $D \in \mathcal{D}$, the subsets in $\mathcal{S}^-$ that are contained in L_D. A naive solution checks the containment relations for all pairs of L_D and $\mathcal{S}^-$, and in practice can take hours for many datasets. However, the problem is an instance of the *the set containment problem*, extensively studied by the database community. Among several efficient solutions proposed for this problem, we resort to one well-established algorithm, PRETTI [11], built upon the idea of inverted index and prefix trees. The running time is effectively brought down to a few seconds.

C. Improved head sampling

To alleviate the heavy-hitter problem during head sampling, we consider two approaches. The first approach is based on reduced sample space, but may have scalability issues. The second is a greedy heuristic, which explicitly maximizes a modified version of discriminativity.

1. Using reduced sample space. We adapt a similar idea as in tail sampling (Section VI-B) and use a reduced sample space $\mathcal{S}^-$ for head sampling. However, when the feature matrix is dense, a scalability issue arises. The DFS procedure may take exponential time. For sufficiently sparse graphs this is not a concern in practice, whereas in denser graphs, constructing $\mathcal{S}^-$ becomes a bottleneck.

2. A greedy heuristic. To address the above scalability issue, we propose a greedy heuristic, which drops the probabilistic guarantee, but is highly effective in practice. We use CFTP as in Algorithm 3 to sample a tuple (D^+, D^-). Then we greedily select features in $D^+ \setminus D^-$ to maximize a modified version of discriminativity: for any H, we define the measure

$$\phi(H) = \left| \mathcal{D}[H] \cap \mathcal{D}_T^+ \right| - \gamma \left| \mathcal{D}[H] \cap \mathcal{D}_T^- \right|, \qquad (14)$$

where γ weighs the importance of positive and negative support, so smaller values of γ lead to more general but more error-prone heads. Further, we use early stopping (controlled by ϵ) when $|\mathcal{D}[H]|$ is too small.

The algorithm is described in Algorithm 5. It iteratively picks a feature $h \in F_{D^+} \cup F_{D^-}$, which maximizes the marginal gain of ϕ. The best feature h^* is added to H and the support is updated accordingly. Finally, a linear sweep over H finds the head with the highest objective value (in (14)). In practice, we use a pre-computed inverted index to allow for efficient intersection of supports. Variations of Algorithm 5 have been investigated in which the input is deterministic, the difference in line 4 is normalized by $\mathcal{D}[\{h\}]$ and the support is replaced by support not covered by previously chosen rules.

Summary. The second approach scales better for dense feature matrices than the first approach. However, the first approach has

Algorithm 5: A greedy heuristic for head sampling.

Data: a dataset $\mathcal{D}$, sets $\mathcal{D}_T^+$, $\mathcal{D}_T^-$, parameters γ and ϵ.
Result: a head $H \in \mathcal{F}$.

1 let $F' \leftarrow F_{D^+} \setminus F_{D^-}$;
2 initialize $H \leftarrow$ an empty list, $Q_{\text{disc}} \leftarrow$ an empty list;
3 **while** $|H| < |F'|$ **do**
4 $\quad h^* \leftarrow \arg\max_{h \in F'} [\phi(H \cup \{h\}) - \phi(H)]$;
5 $\quad$ add h^* to H, add $\phi(H)$ to Q_{disc} ;
6 $\quad F' \leftarrow F' \setminus h^*$;
7 $\quad$ **if** $|\mathcal{D}[H]| < \epsilon\, |\mathcal{D}_T^+|$ **then** break;
8 **end**
9 $i^* \leftarrow \arg\max_{i=1,\dots,|H|} Q_{\text{disc}}[i]$;
10 **return** $H[1 : i^*]$

---

the following advantages: (1) head sampling has probabilistic guarantees, (2) it is much faster to run when the feature matrices are sparse. In the sequel, we use CORSET-SURS to denote the version where the first approach is used for head sampling, and CORSET-GH when the second approach is used.

VII. COMPLEXITY ANALYSIS

Time complexity. Let T_f be the time complexity of evaluating the quality and diversity function. T_f is bounded by $|\mathcal{D}|(|\mathcal{F}| + |\mathcal{L}|)$. Let $\mathcal{S}_{\mathcal{L}}^-$ be the interpretable sample space for tail sampling and $\mathcal{S}_{\mathcal{F}}^-$ be the reduced sample space for head sampling. The pre-processing times $T_S^{\mathcal{L}}$ and $T_S^{\mathcal{F}}$ to construct $\mathcal{S}_{\mathcal{L}}^-$ and $\mathcal{S}_{\mathcal{F}}^-$ are exponential in the worst case. It follows that the time complexity of CORSET is $\mathcal{O}(B|\mathcal{C}_R|T_f + T_S^{\mathcal{L}} + T_S^{\mathcal{F}})$. If $\mathcal{F}$ is sufficiently sparse, the exponential complexity is not a concern in practice. When $\mathcal{F}$ is dense, it is appropriate to use CORSET-GH, for which the time complexity is $\mathcal{O}(B|\mathcal{C}_R|T_f + T_S^{\mathcal{L}})$.

Space complexity. Space $S_R = \mathcal{O}(|\mathcal{D}| + |\mathcal{F}| + |\mathcal{L}|)$ is required to keep a single rule, as we store head, tail, and coverage. Let S_S denote the space complexity of sampling. In both tail and (owing to CFTP) head sampling, we only need to store a single weight value for each data record. Building $\mathcal{S}_{\mathcal{L}}^-$ and $\mathcal{S}_{\mathcal{F}}^-$ requires space $\mathcal{O}(|\mathcal{F}|^2)$ and $\mathcal{O}(|\mathcal{L}|^2)$, respectively. Furthermore, storing samples from $\mathcal{S}_{\mathcal{L}}^-$ ($\mathcal{S}_{\mathcal{F}}^-$) takes space $\mathcal{O}(|\mathcal{D}||\mathcal{S}_{\mathcal{L}}^-|)$ ($\mathcal{O}(|\mathcal{D}||\mathcal{S}_{\mathcal{F}}^-|)$). Despite this theoretical complexity, the graphs are very sparse in practice. Combining the above, we have that $S_S = \mathcal{O}(|\mathcal{L}|^2 + |\mathcal{F}|^2 + |\mathcal{D}||\mathcal{S}_{\mathcal{L}}^-| + |\mathcal{D}||\mathcal{S}_{\mathcal{F}}^-|)$ and the space complexity of CORSET is $\mathcal{O}(||\mathcal{F}|| + ||\mathcal{L}|| + |\mathcal{C}_R|S_R + S_S)$. When CORSET-GH is used, the greedy head sampler only takes space $\mathcal{O}(|\mathcal{F}|)$ and hence S_S reduces to $S_{S+} = \mathcal{O}(|\mathcal{L}|^2 + |\mathcal{D}||\mathcal{S}_{\mathcal{L}}^-| + |\mathcal{F}|)$ so that the space complexity of CORSET-GH is $\mathcal{O}(||\mathcal{F}|| + ||\mathcal{L}|| + |\mathcal{C}_R|S_R + S_{S+})$.

VIII. EXPERIMENTAL EVALUATION

The main goal in this section is to empirically show that CORSET (and in particular its two implementations CORSET-SURS and CORSET-GH) deliver a concise set of rules while still providing competitive performance in multi-label classification. We first present the experimental setup and then the results.

TABLE I: Summary statistics of the datasets used in the experimental evaluation. The last two columns refer to the average number of labels per example, and the total number of distinct label sets.

Dataset	Instances	Attributes	Labels	Cardinality	Distinct
mediamill	43 907	120	101	4.38	6 555
Yelp	10 810	671	5	1.64	32
corel-5k	5 000	499	374	3.52	3 175
bibtex	7 395	1 836	159	2.40	2 856
enron	1 702	1 001	53	3.38	753
medical	978	1 449	45	1.24	94
birds	645	260	19	1.01	133
emotions	593	72	6	1.87	27
CAL500	502	68	174	26.04	502

A. Experimental setup

Datasets. We use both synthetic and real-world datasets.

We use synthetic datasets to better understand the behavior of the methods with respect to different parameters. Data are obtained from a set of generating rules, and as a consequence, a notion of ground truth is available. For each generating rule, we sample its support either (i) uniformly at random, or (ii) from a skewed distribution where a small subset of rules covers a large portion of the data, mimicking the typical behaviour of real-world data. All generating rules have the same number of attributes and labels. Thus, to obtain the synthetic dataset, we start with a feature and label matrices in which all entries are identically 0. Then, for each rule, once its support is sampled, we set to 1 its attributes and labels over its support.

For real-world data, we use heterogeneous benchmark datasets for multi-label classifications[1]. Summary statistics of the datasets are shown in Table I. Categorical and numerical features are converted to binary form. For simplicity, we convert numerical features into binary ones by setting to 0 all values lower than a given percentile p (90-th percentile by default) and by setting to 1 the rest of the values. A more refined pre-processing is advisable to improve performance.

Metrics. To measure the quality of a classifier, we use the popular balanced F_1 score, which micro-averages precision and recall. To monitor rule diversity, we report the average pairwise intersection between the coverage of different rules. To assess interpretability we report the number of rules $\mathcal{R}$.

Baselines. We compare our classifier with three baselines.

SECO [13] is a rule-based classifier, which extracts new rules iteratively and discards the associated covered examples from the training data if enough of their labels are predicted by already learned rules. Given a rule head, SECO searches for the best possible tail according to a metric, while pruning the search space by exploiting properties of the metric, and introducing bias towards tails with multiple labels.

BOOMER [3], [20] utilizes the gradient-boosting framework to learn ensembles of single-label or multi-label classification

---

[1]http://mulan.sourceforge.net, https://www.uco.es/kdis/mllresources/

rules that are combined additively to minimize the empirical risk with respect to a suitable loss function.

SVM-BR [5], [27] is a linear support vector machine classifier based on the binary relevance approach, whereby each label is treated independently. This classifier is not rule-based, and serves as a black-box baseline.

In general, BOOMER takes advantage of a large number of rules, which are then combined to generate the final scores from which the predictions are derived. In this way, it achieves state-of-the-art performance in associative multi-label classification. In addition, it controls the number of rules in the ensemble with a single parameter. Thus, it is the most important baseline. For the synthetic datasets, we focus on comparing our approach with BOOMER for increasing number of rules, whereas for the real-world datasets we consider all baselines.

Parameter setting. For the experiments with synthetic data, we explore the scalability of our algorithm with respect to the number of attributes and labels, as well as robustness with respect to noise. We vary the level of noise (proportion of flipped entries in the feature and label matrix), and the number of attributes and labels by a geometric progression of ratio 1.5. When not varied, the number of attributes and labels are fixed to 100, and the noise level to 0.01. When the noise is varied there are 10 ground truth rules, otherwise the number of generating rules increases with the size of the data and it is given by $\lfloor \frac{\min(|\mathcal{F}|, |\mathcal{L}|)}{3} \rfloor$.

For the experiments with real-world data, we tune the hyper-parameters of all methods via random search to minimize micro-averaged F_1 on a validation set. The size of each sampled pool of rules $\mathcal{C}$ does not need to be tuned. Larger $\mathcal{C}$ improves performance at the cost of increased runtime. While tuning we fix $\mathcal{C} = 150$, otherwise $\mathcal{C}$ is set to 500 by default. All hyper-parameters are searched in the range $(0, 1)$, except for λ that is searched in $(10^{-2}, 10^2)$. We also investigate the impact of λ on the the diversity of the set of chosen rules $\mathcal{R}$, by varying it in a geometric progression of ratio 10. All experiments results are obtained as average over 10 repetitions to account for randomness.

Implementation. Experiments are executed on a machine with 2×10 core Xeon E5 2680 v2 2.80 GHz processor and 256 GB memory. Our implementation is available online[2]. To speed-up and facilitate hyper-parameter tuning for CORSET we have implemented two practical changes. First, we run only the first round of greedy selection in Algorithm 1. The second round guarantees the approximation factor, but often offers a modest increase in performance, not worth the increase in running time. Second, we pass as input to CORSET the number of rules to be returned (at most 150) instead of the tolerance parameter (c in Algorithm 1) to reduce variability and simplify hyperparameter optimization.
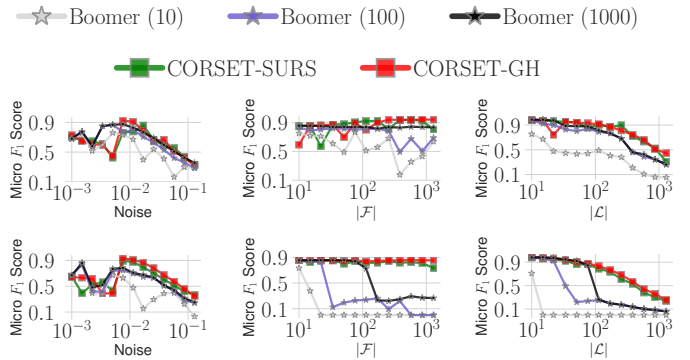

Fig. 4: Synthetic datasets generated from rules with uniform (top) and skewed (bottom) coverage. Micro-averaged F_1 score against proportion of noise (left), number of attributes (middle) and labels (right). The x-axis is in log scale.

B. Results

Synthetic datasets. Results on synthetic datasets, both for data generated from rules with uniform and skewed coverage, are shown in Fig. 4. The number of rules retrieved by CORSET is at most the number of generating rules, 33. On the other hand, BOOMER based on 10 rules consistently offers poor performance. The classification accuracy of BOOMER increases when the number of rules increases, but even with 1000 rules, our method outperforms BOOMER while using a very concise set of rules. Unlike BOOMER, CORSET seeks to uncover the true set of generating rules and only use those for classification. Thus, the experiments with synthetic datasets clearly show the advantage of our approach. Also note that the performance of CORSET, unlike that of BOOMER, does not significantly deteriorate when $|\mathcal{F}|$ increases.

Real datasets: classification performance and interpretability. Results on real datasets, for classification performance and interpretability, are shown in Table II. In some cases, SECO does not terminate within a time interval of 12 hours, in such cases we report NA in the corresponding table entry. Table II shows that BOOMER requires a very large number of rules to achieve competitive performance. Thus, it does not offer high interpretability. Similarly, SVM-BR performs well but it is not interpretable. Instead, CORSET extracts a small set of rules, guaranteeing ease of interpretation, and yet it is consistently competitive with the baselines on all the datasets. CORSET always requires fewer rules than rule-based alternatives to attain the same performance in multi-label classification, and it is never drastically worse than BOOMER with 1000 rules or even SVM-BR, suggesting that the *price of interpretability*, if there is one, is small when CORSET is used. Finally, note that CORSET-GH often outperforms CORSET-SURS but using a larger set of rules.

Real datasets: diversity and impact of λ. A fundamental characteristic of CORSET is that it allows to control the degree

---

[2]https://github.com/DiverseMultiLabelClassificationRules/CORSET

TABLE II: Micro-averaged F_1-scores on real datasets achieved by CORSET-SURS , CORSET-GH, SECO, BOOMER with increasing number of rules, and SVM-BR. The last three columns show the number of rules for CORSET-SURS , CORSET-GH, and SECO.

| Dataset	CORSET-SURS	CORSET-GH	SECO	Boomer (10)	Boomer (100)	Boomer (1000)	BR-SVM	$\|\mathcal{R}\|$ CORSET-SURS	$\|\mathcal{R}\|$ CORSET-GH	$\|\mathcal{R}\|$ SECO
mediamill	0.44	0.51	NA	0.43	0.44	0.50	0.50	150	150	NA
Yelp	0.66	0.64	NA	0.47	0.63	0.75	0.70	67	82	NA
corel-5k	0.18	0.18	NA	0.00	0.00	0.03	0.16	142	150	NA
bibtex	0.36	0.40	NA	0.00	0.13	0.36	0.41	74	150	NA
enron	0.55	0.53	NA	0.39	0.47	0.54	0.52	41	48	NA
medical	0.81	0.83	0.63	0.00	0.50	0.91	0.99	27	88	199
birds	0.37	0.42	0.39	0.00	0.34	0.46	0.42	42	48	122
emotions	0.53	0.54	0.53	0.17	0.49	0.54	0.56	42	68	199
CAL500	0.29	0.32	NA	0.31	0.31	0.33	0.53	150	150	NA
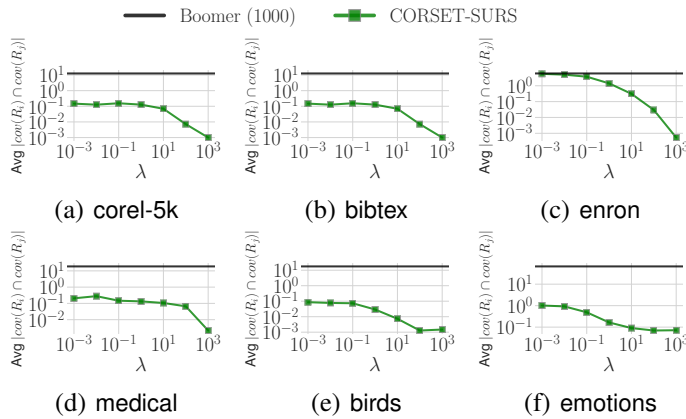
Fig. 5: Real datasets. Average coverage overlap between pairs of rules as a function of λ (lower values indicate higher diversity). Both axes are in log scale.

of diversity in the set of recovered rules via a single tunable parameter λ. In Fig. 5, we show for a subset of datasets that the shared coverage within rules is lower for CORSET than for BOOMER, and moreover that increasing the value of λ is very effective in reducing overlap between rules. In practice λ must be carefully tuned to optimize the performance of CORSET. As the impact of λ is not significantly different in CORSET-SURS and CORSET-GH, we only show results for the former.

IX. CONCLUSION

We propose a novel rule-based classifier, CORSET, for multi-label classification tasks. Our training objective explicitly penalizes rule redundancy, encouraging the algorithm to learn a concise set of rules. Furthermore, we design a suite of fast sampling algorithms, which can generate rules with good accuracy and interpretability. We show that CORSET achieves competitive performance comparable to strong baselines, while offering better interpretability.

Our work opens interesting questions for future research. Can we design training objectives that reflect popular multi-label classification metrics, while producing concise rule sets? Can

we use the techniques in this work to address the interpretability issue of existing rule-based classifiers?

REFERENCES

[1] M. Boley, C. Lucchese, D. Paurat, and T. Gärtner. Direct local pattern sampling by efficient two-step random procedures. In *Proceedings of the 17th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 582–590, 2011.

[2] M. Boley, S. Moens, and T. Gärtner. Linear space direct pattern sampling using coupling from the past. In *Proceedings of the 18th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 69–77, 2012.

[3] M. Boley, S. Teshuva, P. L. Bodic, and G. I. Webb. Better short than greedy: Interpretable models through optimal rule boosting. In *Proceedings of the 2021 SIAM International Conference on Data Mining (SDM)*, pages 351–359, 2021.

[4] A. Borodin, H. C. Lee, and Y. Ye. Max-sum diversification, monotone submodular functions and dynamic updates. In *Proceedings of the 31st ACM SIGMOD Symposium on Principles of Database Systems*, pages 155–166, 2012.

[5] C. Cortes and V. Vapnik. Support-vector networks. *Machine learning*, 20(3):273–297, 1995.

[6] K. Crammer and Y. Singer. A family of additive online algorithms for category ranking. *Journal of Machine Learning Research*, 3:1025–1058, 2003.

[7] A. Elisseeff and J. Weston. A kernel method for multi-labelled classification. *Advances in neural information processing systems*, 14:681–687, 2001.

[8] J. Fischer and J. Vreeken. Sets of robust rules, and how to find them. In *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*, pages 38–54. Springer, 2019.

[9] J. Fürnkranz, D. Gamberger, and N. Lavrač. *Foundations of rule learning*. Springer Science & Business Media, 2012.

[10] B. Ghosh, D. Malioutov, and K. S. Meel. Efficient learning of interpretable classification rules. *arXiv preprint arXiv:2205.06936*, 2022.

[11] R. Jampani and V. Pudi. Using prefix-trees for efficiently computing set joins. In *International Conference on Database Systems for Advanced Applications*, pages 761–772, 2005.

[12] Y. Klein, M. Rapp, and E. Loza Mencía. Efficient discovery of expressive multi-label rules using relaxed pruning. In P. Kralj Novak, T. Šmuc, and S. Džeroski, editors, *Discovery Science*, pages 367–382. Springer International Publishing, Oct. 2019. Best Student Paper Award.

[13] Y. Klein, M. Rapp, and E. Loza Mencía. Efficient discovery of expressive multi-label rules using relaxed pruning. In *International Conference on Discovery Science*, pages 367–382. Springer, 2019.

[14] S. Kosub. A note on the triangle inequality for the jaccard distance. *Pattern Recognition Letters*, 120:36–38, 2019.

[15] B. Liu, W. Hsu, Y. Ma, et al. Integrating classification and association rule mining. In *Kdd*, volume 98, pages 80–86, 1998.

[16] T. Miller. Explanation in artificial intelligence: Insights from the social sciences. *Artificial intelligence*, 267:1–38, 2019.

[17] C. K. Morewedge and D. Kahneman. Associative processes in intuitive judgment. *Trends in cognitive sciences*, 14(10):435–440, 2010.

[18] A. P. Mukherjee, P. Xu, and S. Tirthapura. Mining maximal cliques from an uncertain graph. In *2015 IEEE 31st International Conference on Data Engineering*, pages 243–254. IEEE, 2015.

[19] M. Rapp, E. L. Mencía, J. Fürnkranz, and E. Hüllermeier. Gradient-based label binning in multi-label classification. *arXiv preprint arXiv:2106.11690*, 2021.

[20] M. Rapp, E. L. Mencía, J. Fürnkranz, V.-L. Nguyen, and E. Hüllermeier. Learning gradient boosted multi-label classification rules. *arXiv preprint arXiv:2006.13346*, 2020.

[21] J. Read. A pruned problem transformation method for multi-label classification. In *New Zealand Computer Science Research Student Conference*, page 41, 2008.

[22] F. Thabtah, P. Cowling, and Y. Peng. Mcar: multi-class classification based on association rule. In *The 3rd ACS/IEEE International Conference onComputer Systems and Applications, 2005.*, page 33, 2005.

[23] F. A. Thabtah, P. Cowling, and Y. Peng. Mmac: A new multi-class, multi-label associative classification approach. In *Fourth IEEE International Conference on Data Mining (ICDM'04)*, pages 217–224, 2004.

[24] V. Tidake and S. Sane. Multi-label classification: a survey. *International Journal of Engineering and Technology*, 7(4.19):1045–1054, 2018.

[25] X. Wang, K. Yue, W. Niu, and Z. Shi. An approach for adaptive associative classification. *Expert Systems with Applications*, 38(9):11873–11883, 2011.

[26] G. Zhang and A. Gionis. Diverse rule sets. In *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 1532–1541, 2020.

[27] M.-L. Zhang, Y.-K. Li, X.-Y. Liu, and X. Geng. Binary relevance for multi-label learning: an overview. *Frontiers of Computer Science*, 12(2):191–202, 2018.

[28] M.-L. Zhang and Z.-H. Zhou. Ml-knn: A lazy learning approach to multi-label learning. *Pattern recognition*, 40(7):2038–2048, 2007.

[29] Z. Zou, J. Li, H. Gao, and S. Zhang. Mining frequent subgraph patterns from uncertain graph data. *IEEE Transactions on Knowledge and Data Engineering*, 22(9):1203–1218, 2010.

APPENDIX

PROOF OF PROPOSITION 1

To show that CORSET is a 2-approximation algorithm for Problem 1, we need to show that in the objective function:

$$f(\mathcal{R}) = \sum_{R \in \mathcal{R}} q(R; \mathcal{R} \setminus \{R\}) + \lambda \sum_{R_i, R_j \in \mathcal{R}, i \neq j} d(R_i, R_j)$$

the first term (quality function) is monotone and submodular and the distance junction, namely the Jaccard distance, is a metric.

First, the quality function is a sum of non-negative terms, and hence it is monotone non-decreasing. It is straightforward to prove that the function is additionally submodular. Consider two rule sets $\mathcal{R}'$ and $\mathcal{R}''$ such that $\mathcal{R}' \subseteq \mathcal{R}''$.

Given a new rule R^* marginal gain in $q(R^*; \mathcal{R}')$ is:

$$\Delta' = a(R^*) \times \left| \text{cov}(R^*) \setminus \bigcup_{R \in \mathcal{R}'} \text{cov}(R) \right|.$$

Similarly, the marginal gain in $q(R^*; \mathcal{R}'')$ is:

$$\Delta'' = a(R^*) \times \left| \text{cov}(R^*) \setminus \bigcup_{R \in \mathcal{R}'} \text{cov}(R) \right|$$

$$= a(R^*) \times \left| \text{cov}(R) \setminus \bigcup_{R \in \mathcal{R}'} \text{cov}(R) \setminus \bigcup_{R \in \mathcal{R}'' \setminus \mathcal{R}'} \text{cov}(R) \right|.$$

Since

$$\left| \text{cov}(R^*) \setminus \bigcup_{R \in \mathcal{R}'} \text{cov}(R) \right|$$

$$\geq \left| \text{cov}(R) \setminus \bigcup_{R \in \mathcal{R}'} \text{cov}(R) \setminus \bigcup_{R \in \mathcal{R}'' \setminus \mathcal{R}'} \text{cov}(R) \right|,$$

it immediately follows that $\Delta' \geq \Delta''$. Therefore, we conclude that the quality function is submodular.

As concerns the Jaccard distance, first notice that:

$$d(R, R) = 1 - \frac{|\text{cov}(R) \cap \text{cov}(R)|}{|\text{cov}(R) \cup \text{cov}(R)|} = 0.$$

Furthermore, the Jaccard distance is symmetric:

$$d(R_1, R_2) = d(R_2, R_1) = 1 - \frac{|\text{cov}(R_1) \cap \text{cov}(R_2)|}{|\text{cov}(R_1) \cup \text{cov}(R_2)|}$$

$$= 1 - \frac{|\text{cov}(R_2) \cap \text{cov}(R_1)|}{|\text{cov}(R_2) \cup \text{cov}(R_1)|}.$$

Finally,to prove that the Jaccard distance is a metric, it is left to prove that it satisfies the triangle inequality. Several proofs that the triangle inequality holds for the Jaccard distance exist [14].

Borodin et al. [4] show that the properties we have proved for the quality and distance function in $f(\mathcal{R})$ guarantee that CORSET is a 2-approximation algorithm for Problem 1.

PROOF OF PROPOSITION 2

We prove that Algorithm 2 returns $T \sim \text{area}(T; \mathcal{R})$.

$$Pr(T \text{ is drawn}) = \sum_{D \in \mathcal{D}} Pr(T \text{ is drawn and } D \text{ is drawn})$$

$$= \sum_{D \in \mathcal{D}} Pr(D \text{ is drawn}) Pr(T \text{ is drawn from } \mathcal{P}(L_D))$$

$$= \sum_{D \in \mathcal{D}[T]} Pr(D \text{ is drawn}) Pr(T \text{ is drawn from } \mathcal{P}(L_D))$$

$$\propto \sum_{D \in \mathcal{D}[T]} w(D; \mathcal{R}) \times \frac{w(T, D; \mathcal{R})}{w(D; \mathcal{R})}$$

$$= \sum_{D \in \mathcal{D}[T]} w(T, D; \mathcal{R}) = \sum_{D \in \mathcal{D}[T]} |\text{cov}_D(T; \mathcal{R})| = \text{area}(T; \mathcal{R}).$$

The first and second equalities follow from the law of total probability, and the chain rule of probabilities, respectively. The third equality is guaranteed because T can only be sampled from $D \in \mathcal{D}[T]$. If D is not in $\mathcal{D}[T]$, it has null probability of generating T. In the fourth equality, we have used:

$$\sum_{T \subseteq L_D} w(T, D; \mathcal{R}) = w(D; \mathcal{R}).$$

Finally, the last equality follows since $\text{area}(T; \mathcal{R})$ can be obtained by summing the marginal coverage $|\text{cov}_D(T; \mathcal{R})|$ of T on D, given $\mathcal{R}$, over all data records $D \in \mathcal{D}[T]$.