Abstract

Since the seminal paper by Breiman in 2001, who pointed out a potential harm of prediction multiplicities from the view of explainable AI, global analysis of a collection of all good models, also known as a “Rashomon set,” has been attracted much attention for the last years. Since finding such a set of good models is a hard computational problem, there have been only a few algorithms for the problem so far, most of which are either approximate or incomplete. To overcome this difficulty, we study efficient enumeration of all good models for a subclass of interpretable models, called rule lists. Based on a state-of-the-art optimal rule list learner, CORELS, proposed by Angelino et al. in 2017, we present an efficient enumeration algorithm CorelsEnum for exactly computing a set of all good models using polynomial space in input size, given a dataset and a error tolerance from an optimal model. By experiments with the COMPAS dataset on recidivism prediction, our algorithm CorelsEnum successfully enumerated all of several tens of thousands of good rule lists of length at most $\ell = 3$ in around 1,000 seconds, while a state-of-the-art top-$K$ rule list learner based on Lawler’s method combined with CORELS, proposed by Hara and Ishihata in 2018, found only 40 models until the timeout of 6,000 seconds. For global analysis, we conducted experiments for characterizing the Rashomon set, and observed large diversity of models in predictive multiplicity and fairness of models.

1 Introduction

In applications of machine learning models to critical decision-making tasks, such as judicial decisions and loan approvals, there have been increasing concerns about the interpretability of the models [8, 17]. If the decisions based on their predictions might have a significant impact on individuals, decision-makers must provide the reason of the decisions to assure users of their correctness [17]. Consequently, learning interpretable models, such as decision trees, rule sets, and rule lists, has attracted considerable attention in recent years [2, 8, 11, 13]. Because these models are expressed as combinations of simple “if-then” rules as shown in Table 1, it is easy for humans to understand and validate how the models make predictions [8].
Table 1: An example of a pair of competing rule lists of length $\ell = 3$ with similar accuracies, 62.5% and 60.9%, for predicting two-year recidivism on the COMPAS dataset. Although two rule lists have similar accuracy (Acc), they have quite different values of discrimination measures, namely, demographic parity (DP) and equal opportunity (EO), whose definitions can be found in Sec. 4.2. They also have a large discrepancy value 0.325 (the relative Hamming distance between their prediction vectors).

| Acc  | DP  | EO  | Rule list models                                      |
|------|-----|-----|-------------------------------------------------------|
| 0.625 | 0.083 | 0.061 | if juvenile-felonies $> 0$ & current-charge-degree=Felony, then Yes |
|      |     |     | else if juvenile-misdemeanors=0 & priors>3, then Yes |
|      |     |     | else predict No                                        |
| 0.609 | 0.052 | 0.042 | if sex=Male & juvenile-crimes $> 0$, then Yes |
|      |     |     | else if age=18-20 & priors=0, then Yes |
|      |     |     | else predict No                                        |

Recently, for interpretable models, there has been another concern about the situation where there exist multiple models that are approximately equally accurate by relying on different features [10,16,18]. In the seminal paper, Breiman [4] has named such phenomenon “Rashomon effect”. By showing examples of feature importance, he explained how different models with similar accuracy can generate different explanations for prediction tasks. From this view, he argues that it is unreliable to use explanations derived from a single predictive model for the class of interpretable models such as decision trees and rule lists. By introducing the notion of prediction multiplicities, Marx et al. [16] showed how a prediction problem can show multiplicities, and how we can measure the diversity of a set of good models.

For example, we show in Table 1 a part of results of experiments in Sec. 5 on the COMPAS dataset [3] for the task of predicting two-year recidivism. The table contains a pair of competing rule lists which was found by our algorithm CorelsEnum, associated with the values of the accuracy (Acc), and two major discrimination measures, namely, demographic parity (DP) [5] and equal opportunity (EO) [12] (see Sec. 4.2). Although two rule lists have similar accuracies of 62.5% and 60.9%, respectively, they have quite different characteristics in DO and EO. Moreover, we observed that there were some rule list which was only 1% less accurate than an optimal rule list, while it made different predictions on 11% of training data from the optimal one made. This type of prediction multiplicity is called discrepancy [16], and will be discussed later in Sec. 5.2.3.

The central notion in the studies mentioned above is the collection of good models within a given model class $\mathcal{H}$ that have similar accuracy as an optimal model on a given dataset, which is also called a “Rashomon set”, and has been discussed by several authors [16,18]. Here, we assume to measure the goodness of a model $h$ by the empirical risk $L(h)$ on dataset $S$, which is the proportion of the data that the model makes incorrect predictions. Then, the notion of Rashomon sets is captured by the following definition, due to Fisher, Rudin, and Dominici [7]: the Rashomon set with error tolerance $\varepsilon > 0$ is defined as the set $\mathcal{R}_\varepsilon$ of all models $h$ whose empirical risk $L(h)$ is at most larger than that of optimal model $h_*$ within...
tolerance $\varepsilon > 0$, that is, given by:

$$R_{\varepsilon} := \{ h \in \mathcal{H} \mid L(h) \leq L(h^*) + \varepsilon \}.$$ 

Although all models in $R_{\varepsilon}$ achieve similar accuracy, they often differ markedly in their predictions for individual inputs and thus may have different properties \cite{10,16,17}. Consequently, characterizing the set $R_{\varepsilon}$ plays an important role in validating the reliability of $\mathcal{H}$ on a specific prediction problem \cite{16}.

To characterize the Rashomon set $R_{\varepsilon}$ by existing criteria, one often needs to compute the set $R_{\varepsilon}$ for a certain model class $\mathcal{H}$ on a given dataset. However, since $R_{\varepsilon}$ can contain exponentially many models in the input size, exact computation of $R_{\varepsilon}$ still remains challenging \cite{17}. Although there are only a few existing methods for the task \cite{11,18}, they can only provide a subset of $R_{\varepsilon}$ randomly or approximately. Therefore, no one has exactly computed the Rashomon set $R_{\varepsilon}$ for the class of interpretable models on real datasets and measured the existing criteria to characterize the set $R_{\varepsilon}$ \cite{17}.

In this paper, we focus on the class of rule lists \cite{2,11}, and study an exact computation of all the rule lists in the Rashomon set $R_{\varepsilon}$. For that purpose, we extend CORELS \cite{2}, which is a state-of-the-art optimal rule list learner, and propose an efficient algorithm for exactly computing the set $R_{\varepsilon}$ on a given dataset and the best-achievable empirical risk. Based on $R_{\varepsilon}$, we then measure the following prediction multiplicity scores \cite{16}: the ambiguity $\alpha_{\varepsilon}$ is the proportion of data that has at least one model with conflicting prediction from $h_0$, while the discrepancy $\delta_{\varepsilon}$ is the maximum proportion of data that a model can make different prediction from $h_0$ over all good models (see Sec. 4.2).

Our contributions are summarized as follows:

- We propose an exact algorithm CorelsEnum for computing the Rashomon set for the class of rule lists. Based on CORELS \cite{2}, our algorithm can efficiently enumerate all good rule lists with length at most $K$ and within error tolerance $\varepsilon$. Unlike the previous method \cite{11}, CorelsEnum uses only polynomial working space to compute the whole set.
- By experiments on the COMPAS dataset \cite{3}, with a large value of $\varepsilon = 15\%$, our CorelsEnum successfully computed the Rashomon set $R_{\varepsilon}$ of around 23,354 all good rule lists of length at most $\ell = 3$ in 1,000 seconds, while the previous one for top-$K$ rule lists, Corelslawler \cite{11}, listed only top-40 rule lists before the timeout of 6,000 seconds.
- Based on the computed Rashomon sets $R_{\varepsilon}$, we analyzed the diversity of a set of good models in terms of predictive multiplicity \cite{16} and unfairness range \cite{1,6}. We found that the Rashomon set $R_{\varepsilon}$ with small error tolerance $\varepsilon = 1\%$ had large prediction multiplicities $\alpha_{\varepsilon} = 29\%$ and $\delta_{\varepsilon} = 11\%$. For discrimination scores, we observed a trade-off between the score and the empirical risk, and the existence of a few clusters of good models with similar scores.

As consequences, our results revealed that real datasets such as COMPAS could have the large diversity of models that cannot be ignored in explanability. Thus, we need further researches for efficient methods to integrate competitive rules to apply existing model explanation methods.
1.1 Related Work

Rule models, such as decision trees, rule sets, and rule lists, are popular interpretable models [2,8,14,17]. Among them, rule lists and their variants [2,11,20] have been widely studied from the view of global optimization. Angelino et al. [2] proposed an algorithm CORELS that finds a single optimal rule list that exactly minimizes the size-penalized empirical risk by branch-and-bound search. In this paper, we extended CORELS for computing the complete set of all almost-accurate rule lists using enumeration and data mining techniques [9].

Computation of the Rashomon set $R_{\varepsilon}$ has been attracting increasing attention in recent years [17] from various perspectives, such as interpretability [7,18], predictive multiplicity [16], and fairness [1,6]. However, exact computation of $R_{\varepsilon}$ with a small memory footprint still remains challenging [17]. Particularly, Semenova et al. [18] described a procedure for randomly sampling a subset of $R_{\varepsilon}$ for decision trees of bounded size. Hara and Ishihata [11] have proposed an efficient top-$K$ rule list learner, called CorelsLawler here, based on empirical risk using the well-known Lawler’s method [11]. We remark that neither of the above methods did not achieve as goals exact computation of the whole $R_{\varepsilon}$ and polynomial working space. In contrast, our algorithm achieved both of these requirements.

2 Preliminaries

In this section, we give basic definitions and notation, which will be necessary in the following sections. We also introduce our problem of computing the collection of all good models for a class of models. For the notions that are not found here, please consult appropriate textbooks such as [13].

2.1 Notation

For a predicate $\psi$, $I[\psi]$ denotes the indicator of $\psi$; that is, $I[\psi] = 1$ if $\psi$ is true, and $I[\psi] = 0$ otherwise. Throughout this paper, we consider the binary classification problem as our prediction problem, and assume Boolean features as in most studies on learning rule models [2,14]. Then, the input and output domains are $X = \{0,1\}^J$ and $Y = \{0,1\}$, respectively, where $J \in \mathbb{N}$ is the number of features. An example is a tuple $(x, y) = (x_1, \ldots, x_J) \in X$ and a prediction label (or a label) $y \in \mathcal{Y}$, and a dataset is a sequence $S = \{(x_n, y_n)\}_{n=1}^N$ of $N$ examples, where $S \in (X \times \mathcal{Y})^N$. For a given classifier, or a prediction model, $h: X \rightarrow \mathcal{Y}$ and dataset $S$, the empirical risk of $h$ is defined as $L(h \mid S) := \frac{1}{N} \sum_{n=1}^N l(y_n, h(x_n)) \in [0,1]$, where $l: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_{\geq 0}$ is a loss function that measures the difference between the prediction $h(x)$ and the true label $y$. In this paper, we assume the 0-1 loss $l(y, \hat{y}) = I[y \neq \hat{y}]$. The number of misclassifications by $h$ on $S$ is defined as $\#Err(h \mid S) := \sum_{n=1}^N l(y_n, h(x_n)) \in [0..N]$. Note that the empirical risk is given by $L(h \mid S) = \frac{1}{N} \#Err(h \mid S)$.

2.2 Rule List

In this study, we focus on the class of classifiers, called rule lists [2,11], defined as follows. Let $X = \{0,1\}^J$ be an input domain of $J$ Boolean features. Let $\mathcal{T}$ be a set, called a vocabulary,
which consists of terms over a set of $J$ Boolean features $x_1, \ldots, x_J$ over $\{0, 1\}$. Each term $t$ in $T$ is a conjunction $t = (x_{i_1} \land \cdots \land x_{i_k})$ of Boolean features, and represents a Boolean assertion $t: X \to \{0, 1\}$ such that $t$ evaluates true on an input vector $x \in X$ if $x_{i_j} = 1$ for all $1 \leq j \leq k$, and false otherwise. For example, (‘age = 18 - 20’) $\land$ (‘sex = Male’) is a term used in experiments of Sec. 5. As with previous studies [2, 14], we assume that $T$ includes the constant 1 (true), and that $T$ is pre-mined by frequent itemset mining algorithms (e.g., FP-growth [9] or LCM [19]).

Let $\mathcal{Y}$ be a set of prediction labels. A rule over $\mathcal{T}$ and $\mathcal{Y}$ is a pair $(t \to y)$ of a term $t \in \mathcal{T}$ and a label $y \in \mathcal{Y}$, which corresponds to the conditional statement “if $t$, then $y$.” A rule list of length $\ell \geq 1$ over $\mathcal{T}$ and $\mathcal{Y}$ is a tuple $d = (r_1, \ldots, r_\ell)$ of $\ell$ rules, where (i) $r_i = (t_i \to y_i)$ is a rule for every $1 \leq i \leq \ell$, and (ii) the last rule $r_\ell$ always has constant test $t_\ell = 1$, and is called the default rule. In Table 1 we show an example of a rule list. We denote by $\circ$ the concatenation operation for rule sequences. A rule list $d = ((t_i \to y_i))_{i=1}^\ell$ naturally defines a prediction model $h_d: \mathcal{X} \to \mathcal{Y}$ such that given an input $x$ in $\mathcal{X}$, the prediction $y = h_d(x)$ in $\mathcal{Y}$ is computed by the code below:

\[
\text{if } t_1(x) \text{ then predict } y_1, \text{ else if } t_2(x) \text{ then predict } y_2, \ldots, \text{ else if } t_{\ell-1}(x) \text{ then predict } y_{\ell-1}, \text{ else predict } y_\ell.
\]

In the above code, whenever the label $y_i$ is predicted, the condition $t_1(x) = 0 \land \cdots \land t_{i-1}(x) = 0$ and $t_i(x) = 1$ must hold. Then, we say that $x$ falls into the $i$-th rule $r_i$. For a given dataset $S \in (\mathcal{X} \times \mathcal{Y})^N$, regularization parameter $\lambda \geq 0$, and a set $\mathcal{T}$ of candidate terms, the task of learning a rule list is formulated as:

\[
h_d^* = \arg\min_{h_d \in \mathcal{H}} R_\lambda(h_d \mid S) := L(h_d \mid S) + \lambda \cdot |d|.
\]

Although finding an optimal solution of the problem (1) is a hard combinatorial optimization, it can be efficiently solved by recent branch-and-bound optimization algorithms such as CORELS [2] in many practical instances.

### 2.3 Computation of Rashomon Sets

To characterize the set of good models, the Rashomon set has been introduced as a set of models that achieve near-optimal accuracy [17]. For a prediction problem $(\mathcal{X}, \mathcal{Y})$, let $\mathcal{H}$ be a set of classifiers $h: \mathcal{X} \to \mathcal{Y}$, which we call a model class. Following previous studies [16, 18], we define the Rashomon set as a subset of classifiers that achieve accuracy close to a given reference classifier $h_0 \in \mathcal{H}$ with respect to a certain loss function $l$ and a given error tolerance $\varepsilon \geq 0$.

**Definition 1** Given a model class $\mathcal{H}$, reference classifier $h_0 \in \mathcal{H}$, dataset $S$, and error tolerance $\varepsilon \geq 0$, the Rashomon set $\mathcal{R}_\varepsilon(h_0 \mid S)$ is defined as follows:

\[
\mathcal{R}_\varepsilon(h_0 \mid S) := \{ h \in \mathcal{H} \mid L(h \mid S) \leq L(h_0 \mid S) + \varepsilon \}.
\]

As with existing studies [16, 18], we assume the reference classifier $h_0$ to be an optimal rule list $h_d^*$ for the learning problem (1), which can be obtained using CORELS [2]. Note that the choice of $h_0$ is independent of our results. Now, we formally define our problem as follows:
Problem 1 Given a dataset $S$, a set of terms $T$, a reference rule list $h_0$, an error tolerance $\varepsilon \geq 0$, and $\ell \geq 0$, compute the Rashomon set $R_\varepsilon(h_0 \mid S)$ for the class of rule lists of length at most $\ell$.

By solving Problem 1 we can obtain the Rashomon set $R_\varepsilon(h_0 \mid S)$ of rule lists of length $\leq \ell$, and can analyze the properties of $R_\varepsilon(h_0 \mid S)$ from various perspectives described in Sec. 4.

2.4 Optimal Rule List Learner CORELS

Our algorithm is designed based on the recent branch-and-bound optimization algorithm CORELS for learning a single optimal rule list, proposed by Angelino et al. [2]. Here, we will briefly review CORELS, and discuss how we can extend CORELS to exact computation of the Rashomon set.

The inputs to the CORELS algorithm are a set $T$ of terms, a set $\mathcal{Y}$ of labels, a training dataset $S$, and numbers $\ell \geq 1$ and $\lambda > 0$. Invoked as Corels$(T, \mathcal{Y}, \ell, \lambda, S)$ with input parameters, CORELS finds an optimal rule list $d_*$ with length $\leq \ell$ that minimizes the objective $R(d_*)$ in eq. (1) by traversing the hypothesis space of prefixes of rule lists as follows. For every $1 \leq k \leq \ell$, let $d_k := r_1 \circ \cdots \circ r_k$ is called a $k$-prefix, where $r_i = (t_i \rightarrow y_i)$ and $\circ$ is the concatenation. Then, CORELS starts with the empty prefix () and by recursively expanding the current $(k-1)$-prefix $\pi$ to $k$-prefix $\pi' = \pi \circ r_k$, $0 \leq k \leq \ell$, by appending a new rule $r_k \in T \times \mathcal{Y}$. The CORELS algorithm employs sophisticated pruning strategies using constraints such as maximum rule length $L$, and the estimate of a lower bound of the objective.

If $M_{\text{corels}} \leq |\mathcal{Y}|^\ell |T|^{\ell-1}$ is the number of candidate prefixes for CORELS to visit, CORELS runs in $t_{\text{corels}} = O(M_{\text{corels}}|S|)$ time and $s_{\text{corels}} = O(L + |S| + |T|)$ space in the worst case using stack of length at most $L$.

3 Methods for finding good models

In this section, we study efficient methods for finding a set of good models on a given training dataset. Firstly, in Sec. 3.1 we briefly review an existing algorithm, referred to as CorelsLawler in this paper, for Top-$K$ enumeration of good rule lists using CORELS algorithm as a black-box function, proposed by Hara and Ishihata [11]. Next, in Sec. 3.2 we propose our algorithm CorelsEnum that efficiently enumerate all the rule lists of length $\leq K$ in the Rashomon set on a given dataset.

3.1 Lawler’s method combined with Corels algorithm

Lawler’s method [13] is a well-known framework for top-$K$ enumeration using a black-box optimization function. In Algorithm 1 we show the pseudo-code for Hara and Ishihata’s algorithm [11], called CorelsLawler here, for finding top-$K$ rule lists using Lawler’s method. This algorithm iteratively calls CORELS [2], to find one of the optimal rule lists within the
Algorithm 1 Lawler’s method with CORELS for finding Top-$K$ rule lists with respect to prediction error (score).

**Input:** A set $\mathcal{T}$ of all terms, a label set $\mathcal{Y}$, $\ell \geq 0$, $\lambda > 0$, and a dataset $S$.

**Output:** A list $\text{Answers}$ of top-$K$ rule lists in prediction error.

**Procedure CorelsLawler**

1: $\text{Answers} \leftarrow \emptyset$
2: $(\text{score}, \text{Rule}) \leftarrow \text{Corels}(\mathcal{T}, \mathcal{Y}, \ell, \lambda, S)$
3: Queue $\leftarrow \{(\text{score}, (\text{Rule}, \mathcal{T}, \emptyset))\}$  \quad \triangleright A priority queue of $(\text{Rule}, T, F)$ with score as key, where Rule is a rule set, $T$ and $F$ are include and exclude sets of features.
4: while Queue $\neq \emptyset$ and $|\text{Answers}| < K$ do
5: $(\text{score}, (\text{Rule}, T, F)) \leftarrow \text{Queue}.\text{deletemin}()$  \quad \triangleright An entry with minimum score
6: $\text{Terms} \leftarrow \text{Rule}.\text{Terms}()$
7: if $\text{Terms} \notin F$ then  \quad \triangleright Terms is the set of all terms used in Rule
8: $\text{Answers} \leftarrow \text{Answers} \cup \{(\text{score}, \text{Rule})\}$
9: $F \leftarrow F \cup \{\text{Terms}\}$
10: for each $f \in \text{Terms}$ do
11: $(\text{score}', \text{Rule}') \leftarrow \text{Corels}((\mathcal{T}\{f\}), \mathcal{Y}, \ell, \lambda, S)$
12: $\text{Queue} \leftarrow \text{Queue} \cup \{(\text{score}', (\text{Rule}', (\mathcal{T}\{f\}), F \cup \{f\})\}$
13: return $\text{Answers}$

subspace of hypothesis. During the search, It removes some terms appearing in a discovered rule list $\text{Rule}$ from $\mathcal{T}$ to efficiently search the hypothesis space of good models, where $\text{Rule.\text{Terms}()}$ is the set of terms appearing in $\text{Rule}$.

If $K$ is the number of good models to output, we can show that the time and space complexity of $\text{CorelsLawler}$ is at most $t_{\text{lawler}} = O(t_{\text{corels}} \cdot K \ell)$ time and $s_{\text{lawler}} = O(s_{\text{corels}} + K \ell)$ space. A major disadvantage of $\text{CorelsLawler}$ is its exponential space complexity since it must keep the set $F$ of all terms found so far for the membership test at Line 7. Since $|F| \leq K \leq M_{\text{corels}} \leq |\mathcal{T}|^{\ell-1}|\mathcal{Y}|^\ell$, $|F|$ becomes exponential in $\ell$ in the worst case.

### 3.2 The Proposed Algorithm CorelsEnum

By extending CORELS, we devised our algorithm $\text{CorelsEnum}$ for computing the Rashomon set of rule lists in polynomial space in $\ell$ and other inputs. In Algorithm 2, we show the pseudocode of the $\text{CorelsEnum}$ algorithm. Given a vocabulary $\mathcal{T}$, a label set $\mathcal{Y}$, the maximum length parameter $\ell \geq 0$, a dataset $S$ of $N$ example, and the empirical risk $L(h_{d_0} \mid S)$ of a reference rule list $d_0$, $\text{CorelsEnum}$ traverses the space of rule lists in depth-first manner from a shorter prefix to longer one, starting from the empty prefix ($\lambda$).

At each iteration with a candidate prefix $d_p = (r_1, \ldots, r_k)$, $0 \leq k \leq \ell$, the algorithm either builds a rule list $d$ from the current prefix $d_p$, or makes branching with children $d_p' = d_p \circ (t \rightarrow y)$ for all possible combinations of a term $t$ in $\mathcal{T}$ and a label $y$ in $\mathcal{Y}$.

Invoked with as arguments $d_p = ()$, $k$, $L_\ast = L(h_{d_0} \mid S) + \varepsilon$, $\mathcal{T}$, $\mathcal{Y}$, $\ell$, and $S$, the recursive procedure $\text{CorelsEnum}$ computes the Rashomon set of all rule lists with length $\leq \ell$ on a dataset $S$ at each iteration as follows:
Algorithm 2 A basic algorithm CorelsEnum for computing the Rashomon set $\mathcal{R}_e(h_0 \mid S)$ consisting of all rule lists $h_d$ with length $\leq \ell$ such that $L(h_d \mid S) \leq L(h_{d_0} \mid S) + \varepsilon$, with respect to a reference rule list $h_{d_0}$.

Procedure CorelsEnum($dp, k, L_*, \mathcal{T}, \mathcal{Y}, \ell, S$):

Input: A candidate prefix $dp = (r_1, \ldots, r_k)$, its length $k \geq 0$, a non-empty set of terms $\mathcal{T}$, a label set $\mathcal{Y}$, $\ell \geq 0$, $\lambda > 0$, $L_* \in [0, 1]$, and a dataset $S \in (\mathcal{X} \times \mathcal{Y})^N$.

Output: The subset of $\mathcal{R}_e(h_0 \mid S)$ consisting of all rule lists with prefix $dp$.

1: for label $y \in \mathcal{Y}$ do \hspace{1em} \triangleright Step 1: Processing a rule list $d$ with default label $y$
2: \hspace{1em} $d \leftarrow (dp \circ (1 \rightarrow y))$; $L \leftarrow L(h_d \mid S)$
3: if $L \leq L_*$ then \hspace{1em} \triangleright A solution is found
4: \hspace{2em} Output $(d, L)$ as a solution
5: if $k \geq \ell$ then return \hspace{1em} \triangleright Pruning by the maximum length
6: for term $t \in \mathcal{T}$ do \hspace{1em} \triangleright Step 2: Generating children of a parent prefix $dp$
7: \hspace{1em} for label $y \in \mathcal{Y}$ do
8: \hspace{2em} $dp' \leftarrow (dp \circ (t \rightarrow y))$
9: \hspace{2em} if $LB(dp', S) \leq L_*$ then \hspace{1em} \triangleright Pruning by a lowerbound of $L$
10: \hspace{3em} CorelsEnum($dp', k+1, L_*, \mathcal{T} \setminus \{t\}, \mathcal{Y}, \ell, S$) \hspace{1em} \triangleright Recursive call
11: return

- Receive the current candidate prefix $dp$ of length $0 \leq k \leq \ell$ over $\mathcal{T}$.
- For each label $y$ in $\mathcal{Y}$, test if the rule list $d = dp \circ (1 \rightarrow y)$ and its empirical risk $L = L(h_d \mid S)$ satisfies that $L < L_*$. If the test succeeds, output the pair $(d, L)$ as a solution.
- For each $t \in \mathcal{T}$ and $y \in \mathcal{Y}$, do: First, generate the child prefix $dp' = dp \circ (t \rightarrow y)$ of length $k+1$ from $dp$ by appending a new rule $(t \rightarrow y)$, make a recursive call with $dp'$, and updating $\mathcal{T}'$ by removing $t$ to avoid duplicates.

In our algorithm, we employ some pruning techniques of CORELS in a similar way to prune search of unnecessary subspaces as follows, where we attach comments to the corresponding part of Algorithm 2:

1) **Pruning based on minimum support**: it asserts that each rule must capture enough number of examples for the reliability of prediction.
2) **Pruning based on estimated lower bounds**: When invoking recursive call for a child $dp'$, if the lower bound function $LB$ does not satisfy $LB(dp', S) \leq L_*$, prune all computation for $dp'$ and all of its descendants. We use the lower bound function $LB(d, S)$ that is same to the empirical risk $L(h_d \mid S)$ except that all data that fall in the default rule are ignored [2] as in CORELS.
3) **Pruning based on symmetry**: If a range of consecutive rules $r_i, r_{i+1}, \ldots, r_j$ in a rule list $d$, $1 \leq i < j \leq k$, have the same labels $y_i = y_{i+1} = \cdots = y_j$, any permutation of them does not change the prediction by $h_d$. Thus, we can keep some $r_\sigma$, $1 \leq \sigma \leq j$, and discard the rest of them.
effectively prune the unnecessary subspaces of candidates. Let $M_{\text{enum}} \leq |Y|^{\ell-1}|T|$ be the number of candidate prefixes for CorelsEnum to visit. We show the following theorem.

**Theorem 1** CorelsEnum of Algorithm 2 enumerates all good rules with length $\leq \ell$ on a data set $S \in (X \times Y)^N$ in $t_{\text{enum}} = O(M_{\text{enum}}|S|)$ time and $s_{\text{enum}} = O(|S| + |T| + \ell^2)$ space.

**Proof:** The time complexity follows that CorelsEnum requires $O(|S|)$ time at each iteration to compute the objectives. The space complexity follows that the algorithm only keep at most $\ell$ rule lists with length $\leq \ell$ on any branch of the search tree. □

A major advantage of CorelsEnum is that CorelsEnum has the polynomial space complexity in all inputs including $\ell$ independent of the number of solutions $K \leq |T|^{\ell-1}|Y|^{\ell}$, while CorelsLawler requires the space proportional to $K$, which may be exponential in $\ell$ in the worst case. CorelsEnum has amortized polynomial delay complexity, that is, it lists candidates in $O(|S|)$ time per candidate. We remark that if the pruning strategy for CORELS effectively cuts candidates earlier on an input, it is possible that CorelsLawler runs much faster than CorelsEnum since the search space of the former is narrower than the latter.

### 4 Evaluation Criteria for Characterizing Rashomon Sets

In this section, we introduce model criteria for analyzing the Rashomon set from the views of prediction multiplicity [16], and fairness of prediction [12].

Several useful criteria have been proposed for characterizing some properties of a certain model class, such as interpretability [7], multiplicity [16], and fairness [1][6], through the lens of the Rashomon set. In particular, we focus on the **predictive multiplicity** and **unfairness range** described below. Note that these criteria can be easily computed once the Rashomon set $R_\varepsilon(h_0 \mid S)$ is obtained.

#### 4.1 Predictive Multiplicity

Marx et al. [16] have introduced the **predictive multiplicity** as the ability of a prediction problem to admit competing models that assign conflicting predictions. Given a reference classifier $h_0$, the predictive multiplicity is exhibited over the Rashomon set $R_\varepsilon(h_0 \mid S)$ if there exists a classifier $h \in R_\varepsilon(h_0 \mid S)$ such that $h(x) \neq h_0(x)$ for some $x$ in the dataset $S$. To measure the predictive multiplicity, **ambiguity** and **discrepancy** have been proposed [16].

**Ambiguity.**

Ambiguity represents the number of predictions by the reference classifier $h_0$ that can change over the set of competing classifiers $h \in R_\varepsilon(h_0 \mid S)$. Formally, the ambiguity $\alpha_\varepsilon(h_0 \mid S)$ is defined by

$$
\alpha_\varepsilon(h_0 \mid S) := \frac{1}{N} \sum_{n=1}^{N} \max_{h \in R_\varepsilon(h_0 \mid S)} \mathbb{I}[h(x_n) \neq h_0(x_n)] \in [0, 1].
$$

(2)
The ambiguity $\alpha_z(h_0 \mid S)$ reflects the number of individuals $x$ who could contest their assigned prediction $h_0(x)$ by the deployed model $h_0$ since their predictions are determined depending on the model choice by the decision-makers [16].

### 4.1.2 Discrepancy.

Discrepancy represents the maximum number of predictions that can change if we switch the reference classifier $h_0$ with a competing classifier $h \in R_e(h_0 \mid S)$. Formally, the discrepancy $\delta_z(h_0 \mid S)$ is defined by

\[
\delta_z(h_0 \mid S) := \max_{h \in R_e(h_0 \mid S)} \text{DistHum}(h, h_0 \mid S) \in [0, 1],
\]

where $\text{DistHum}(h, h_0 \mid S) := \frac{1}{N} \sum_{n=1}^{N} \mathbb{I}[h(x_n) \neq h_0(x_n)] \in [0, 1]$ is the normalized Hamming distance between the vectors of the predictions by $h$ and $h_0$. Compared to the ambiguity, the discrepancy $\delta_z(h_0 \mid S)$ reflects the number of the conflicting predictions $h(x_n) \neq h_0(x_n)$ by a single competing model $h \in R_e(h_0 \mid S)$ [16].

### 4.2 Discrimination Scores and Unfairness Ranges

While Coston et al. [6] have proposed a framework that evaluate the fairness of the classifiers over the Rashomon set, Aïvodji et al. [1] have pointed out that the Rashomon effect corresponds to the risk of fairwashing, which is a malicious attack that rationales unfair complex models by interpretable and fair surrogate models [4]. By motivating these studies, we introduce the unfairness range to evaluate the fairness over the Rashomon set $R_e(h_0 \mid S)$.

Let $z_n \in \{0, 1\}$ be a sensitive attribute (e.g., gender or race) with respect to the $n$-th example $(x_n, y_n)$ in a dataset $S$. To evaluate the fairness of a classifier $h$ with respect to the sensitive attribute $z$, we focus on demographic parity (DP) [5] and equal opportunity (EO) [12], which are major discrimination criteria based on statistical parity. The DP and EO scores of $h$ on $S$ are defined as: $DP(h \mid S) := \hat{P}(h(x) = 1 \mid z = 1) - \hat{P}(h(x) = 1 \mid z = 0), \quad \text{EO}(h \mid S) := \hat{P}(h(x) = 1 \mid y = 1, z = 1) - \hat{P}(h(x) = 1 \mid y = 1, z = 0)$, where $\hat{P}$ is the empirical probability over the joint distribution on $y$, $z$, and $h(x)$ of $S$.

Let $D \in \{\text{DP, EO}\}$ be any discrimination score. We introduce the unfairness range of the Rashomon set $R_e(h_0 \mid S)$, denoted $\gamma_{\text{DP}}^D$, as an approximation of the distribution of $D$ for the models in $R_e$. Formally, the unfairness range is the interval $\gamma_{\text{DP}}^D(h_0 \mid S) := [\min_h D(h \mid S), \max_h D(h \mid S)] \subseteq [-1, +1]$, where $h$ ranges over $R_e(h_0 \mid S)$. Since we can exactly compute the Rashomon set $\mathcal{R} := R_e(h_0 \mid S)$ in $t_{\text{enum}}$ by using CorelsEnum proposed in Sec. 3.2, now we can compute the range $\gamma_{\text{DP}}^D(h_0 \mid S)$ in linear time in $t_{\text{enum}} + |\mathcal{R}|$ by scanning $\mathcal{R}$.

### 5 Experiments

In this section, we analyze the class of rule lists on the COMPAS dataset [3] through the lens of the Rashomon effect using our proposed algorithm.
Figure 1: Cumulative histogram of the number of the models in the Rashomon set for each value of the error tolerance $\varepsilon$ from 1\% to 15\%.

Table 2: Results of execution time and the number of models found on COMPAS dataset by the existing method (CorelsLawler) and our proposed method (CorelsEnum) within around 6,000 seconds. The existing method was stopped at $K = 40$ by timeout.

|                  | Existing method | Proposed method |
|------------------|-----------------|-----------------|
| Run time (s)     | 6021            | 1058            |
| Memory (MB)      | 209.3           | 202.4           |
| Number of models | 40              | 23354           |

5.1 Experimental Setting

Datasets. We used COMPAS dataset for the task of criminal decision, which comprises 20 categorical attributes of individual people, relating their criminal history, with a total of 6,489 training examples (90\%) $S$ and 721 test examples (10\%) $S'$. The task is binary classification, where the positive category $y = 1$ indicates that the individual recidivates within two years. The sensitive attributes $z$ represent the race of the individuals. Programs. We implemented CorelsLawler and CorelsEnum (Sec.3) in Python 3.7 with numpy package. All the experiments were conducted on 64-bit macOS Big Sur 11.2.3 with Intel Core i9 2.4GHz CPU and 32GB Memory. We used the libraries: pandas for preprocessing, and matplotlib, pyplot.violinplot for charts.

Setting. Throughout this paper, we used the following setting for model parameters. A label set is $Y = \{Yes, No\}$, and the maximum length of rule lists is $\ell = 3$. We used the vocabulary $\mathcal{T} \subseteq \mathcal{T}_{\text{corels}}$ of 64 terms selected from the set $\mathcal{T}_{\text{corels}}$ of all 155 terms in the github repository of CORELS so that a term $t$ is selected if and only if it evaluates true on at least half of the positive examples as with previous studies. Consequently, we obtain a candidate space of size $M = |\mathcal{T}|^{\ell-1}|Y|^\ell = 64^22^3 = 32,798$. We first obtained a reference classifier $h_0$ by CORELS on the training dataset $S$, and then computed the Rashomon set $\mathcal{R}_\varepsilon = \mathcal{R}_\varepsilon(h_0 \mid S)$ by CorelsEnum. We computed $\mathcal{R}_\varepsilon$ by varying the error tolerance $\varepsilon$ from 1\% to 15\%, and analyzed its properties for each $\varepsilon$.

\[1\] This was because we were interested in characterizing the positive category as in [11].
Figure 2: The objective value (training error plus $\lambda$ times the rule list length) against the rank $k$ of a rule list on the COMPAS dataset for existing and proposed methods.

Figure 3: Predictive multiplicity of discovered rule lists in the Rashomon set on the COMPAS dataset. The violin plots (above) show the distribution of discrepancy and the line plots (below) show the ambiguity of rule lists over the Rashomon set.

5.2 Experimental Results

5.2.1 The Numbers of Good Rule Lists by Varying the Error Tolerance

In Fig. 1, we show the number of the models in the Rashomon set by varying the error tolerance $\varepsilon$ from 1% to 15%. In the figure, the reference model $h_0$ locates at $\varepsilon = 1\%$, which amounts to training error 34.8%, while the baseline model $h_*$, which is such a constant rule list that always outputs $y = 0$ for any input $x$, locates at $\varepsilon = 10\%$, which amounts to the training error 44.8%, i.e., the ratio of the examples with $y = 0$ in the training dataset $S$. From Fig. 1, we can see that the total number of models in $R_\varepsilon(h_0 | S)$ increases rapidly between the error tolerance $\varepsilon$ of 9% and 10%, and almost saturates after $\varepsilon$ exceeds 10%. For example, the Rashomon set with $\varepsilon = 9\%$ (resp. $\varepsilon = 10\%$) contained 5679 (resp. 11446) rule lists. This is because the Rashomon sets with $\varepsilon \geq 10\%$ included exponentially many rule lists as accurate as the baseline model $h_*$ in the number of candidate terms in $T$. 
Figure 4: The histograms of the discrepancies $\delta_\varepsilon$ of discovered rule lists in the Rashomon set with error tolerance $\varepsilon = 1\%$ on the COMPAS dataset, where the blue and yellow histograms show the frequencies in the training and test data sets, respectively.

Figure 5: Distributions of discrimination scores with respect to demographic parity (DP, upper) and equal opportunity (EO, lower) on the COMPAS dataset. Here, the violin plots show the frequencies of models with a certain score, while the error bar shows the unfairness range with DP and EO. The score for the base model is shown in red dashed lines).

5.2.2 Comparison of the Existing and the Proposed Algorithms

Next, we compared the existing method (CorelsLawler) in Sec. 3.1 and our proposed method (CorelsEnum) in Sec. 3.2 in terms of running time and memory. We ran experiments for finding good rule lists in the objective function $R_\lambda$ with parameter $\lambda = 0.015$ for both algorithms within around 6,000 seconds.

Table 2 shows the comparison of the running time and memory usage of both algorithms within 6,000 seconds. We see that without limit of the error tolerance $\varepsilon$, the proposed algorithm CorelsEnum enumerated all 23354 models including all good models for any $\varepsilon \geq 0$, while the existing method was stopped at $K = 40$ by timeout of 6,000 seconds after finding top-40 good models. From these results, we observed that the proposed CorelsEnum was about 5.7 times faster than the existing CorelsLawler. Fig. 2 shows the objective function value against the rank of the models. For the top-40 models, we confirmed that both algorithms successfully found models with the same value of the objective function.
5.2.3 Predictive Multiplicity

Next, we examine the predictive multiplicity of the Rashomon set on the COMPAS dataset. Fig. 3 shows the results on the discrepancy \( \delta_\varepsilon(h_0 \mid S) \) and ambiguity \( \alpha_\varepsilon(h_0 \mid S) \) of the Rashomon set \( \mathcal{R}_\varepsilon = \mathcal{R}_\varepsilon(h_0 \mid S) \) on the training dataset \( S \) for each \( \varepsilon \). From Fig. 3, we observed that the values of \( \delta_\varepsilon \) and \( \alpha_\varepsilon \) monotonically increased as \( \varepsilon \) increased. For example, the value of discrepancy (resp. ambiguity) with \( \varepsilon = 1\% \) was \( \delta_\varepsilon = 11\% \) (resp. \( \alpha_\varepsilon = 29\% \)). These results imply that 11\% of predictions can be changed by switching the reference classifier \( h_0 \) with a classifier \( h \in \mathcal{R}_\varepsilon \) that is only 1\% less accurate, and that 29\% of individuals are assigned conflicting predictions by at least one classifier \( h \in \mathcal{R}_\varepsilon \) with the error tolerance 1\%. We also measured \( \delta_\varepsilon \) for all good rule lists \( h \in \mathcal{R}_\varepsilon \). Fig. 4 shows the histogram of these values with \( \varepsilon = 1\% \) on the training dataset \( S \) and test dataset \( S' \). From Fig. 4, we can see that there were rule lists that achieved lower discrepancy than that of the reference classifier \( h_0 \). It suggests that we can obtain another reference classifier with lower discrepancy than \( h_0 \) by exhaustive search of the Rashomon set \( \mathcal{R}_\varepsilon \).

5.2.4 Unfairness Range

Finally, Fig. 5 shows the distribution of discrimination scores demographic parity (DP) and equal opportunity (EO) on rule lists in the Rashomon set. In the figure, we can clearly see the trade-off between the empirical risk \( L(h \mid S') \) and the minimum discrimination scores by the lower ends of violin plots, which is consistent with existing theoretical results \[12\]. For example, we have a higher discrimination value of \( \text{DP} = 0.10 \) in the higher accuracy case with error tolerance \( \varepsilon = 1\% \), while we can have a lower and better value of \( \text{DP} = 0.02 \) in the lower accuracy case with error tolerance \( \varepsilon = 7\% \). After error tolerance \( \varepsilon \geq 10\% \) of the trivial, constant learner, we see that the distribution becomes stable, and most rule lists in the population hold the lowest \( \text{DP} = 0.02 \). Furthermore, we can see that the rule lists are concentrated to a few clusters, in the violin plots for \( \varepsilon \) from 1\% to 8\%, indicating existence of a few subgroups of good rule lists that behave similarly in their syntax and predictions.

6 Conclusion

In this paper, we studied efficient computation of all good models in the Rashomon set for the class of rule lists. By extending a state-of-the-art algorithm \textsc{CORELS} for a globally optimal rule list, we proposed an exact algorithm \textsc{CorelsEnum} for enumerating all the rule lists in the Rashomon set. To evaluate the usefulness of \textsc{CorelsEnum}, we conducted experiments on the COMPAS dataset, and analyzed the computed Rashomon set of the rule lists from the perspectives of predictive multiplicity and fairness.

In future work, we plan to conduct experiments on other real datasets and with larger values of \( \ell \geq 4 \). It is also interesting to extend our algorithm to other rule models, such as decision trees of bounded size.

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References

[1] Aivodji, U., Arai, H., Gambs, S., Hara, S.: Characterizing the risk of fairwashing. In: Proc. NeurIPS 2021, to appear (2021)

[2] Angelino, E., Larus-Stone, N., Alabi, D., Seltzer, M., Rudin, C.: Learning certifiably optimal rule lists. In: Proc. KDD 2017. p. 35–44 (2017)

[3] Angwin, J., Larson, J., Mattu, S., Kirchner, L.: Machine Bias. ProPublica (2016)

[4] Breiman, L.: Statistical Modeling: The Two Cultures (with comments and a rejoinder by the author). Stat. Sci. 16(3), 199 – 231 (2001)

[5] Calders, T., Kamiran, F., Pechenizkiy, M.: Building classifiers with independency constraints. In: Proc. ICDM Workshops 2009. pp. 13–18 (2009)

[6] Coston, A., Rambachan, A., Chouldechova, A.: Characterizing fairness over the set of good models under selective labels. In: Proc. ICML 2021. pp. 2144–2155 (2021)

[7] Fisher, A., Rudin, C., Dominici, F.: All models are wrong, but many are useful: Learning a variable’s importance by studying an entire class of prediction models simultaneously. J. Mach. Learn. Res. 20(177), 1–81 (2019)

[8] Guidotti, R., Monreale, A., Ruggieri, S., Turini, F., Giannotti, F., Pedreschi, D.: A survey of methods for explaining black box models. CSUR. 51(5), 1–42 (2018)

[9] Han, J., Kamber, M., Pei, J.: Data Mining: Concepts and Techniques. Morgan Kaufmann, 3rd edn. (2011)

[10] Hancox-Li, L.: Robustness in machine learning explanations: Does it matter? In: Proc. FAT* 2020. pp. 640–647 (2020)

[11] Hara, S., Ishihata, M.: Approximate and exact enumeration of rule models. In: Proc. AAAI 2018. pp. 3157–3164 (2018)

[12] Hardt, M., Price, E., Srebro, N.: Equality of opportunity in supervised learning. In: Proc. NeurIPS 2016. pp. 3323–3331 (2016)

[13] Hastie, T., Tibshirani, R., Friedman, J.: The Elements of Statistical Learning. Springer Series in Statistics, Springer (2001)

[14] Lakkaraju, H., Bach, S.H., Leskovec, J.: Interpretable decision sets: A joint framework for description and prediction. In: Proc. KDD 2016. pp. 1675–1684 (2016)

[15] Lawler, E.L.: A procedure for computing the $k$ best solutions to discrete optimization problems and its application to the shortest path problem. Manag. Sci. 18(7), 401–405 (1972)

[16] Marx, C., Calmon, F., Ustun, B.: Predictive multiplicity in classification. In: Proc. ICML 2020. pp. 6765–6774 (2020)
[17] Rudin, C.: Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. Nat. Mach. Intell. 1, 206–215 (2019)

[18] Semenova, L., Rudin, C., Parr, R.: A study in rashomon curves and volumes: A new perspective on generalization and model simplicity in machine learning. arXiv preprint, arXiv:1908.01755 (2019)

[19] Uno, T., Kiyomi, M., Arimura, H., et al.: Lcm ver. 2: Efficient mining algorithms for frequent/closed/maximal itemsets. In: Proc. FIMI 2004 (2004)

[20] Wang, F., Rudin, C.: Falling Rule Lists. In: Proc. AISTATS 2015. pp. 1013–1022 (2015)