Learning sparse optimal rule fit by safe screening

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Abstract

In this paper, we consider linear prediction models in the form of a sparse linear combination of rules, where a rule is an indicator function defined over a hyperrectangle in the input space. Since the number of all possible rules generated from the training dataset becomes extremely large, it has been difficult to consider all of them when fitting a sparse model. In this paper, we propose Safe Optimal Rule Fit (SORF) as an approach to resolve this problem, which is formulated as a convex optimization problem with sparse regularization. The proposed SORF method utilizes the fact that the set of all possible rules can be represented as a tree. By extending a recently popularized convex optimization technique called safe screening, we develop a novel method for pruning the tree such that pruned nodes are guaranteed to be irrelevant to the prediction model. This approach allows us to efficiently learn a prediction model constructed from an exponentially large number of all possible rules. We demonstrate the usefulness of the proposed method by numerical experiments using several benchmark datasets.

1 Introduction

In this paper, we consider prediction models in the form of a sparse linear combination of rules, where each rule is represented as an indicator function defined over a hyperrectangle in the input space \( [1, 2, 3, 4, 5] \). An example of a rule is a function that returns 1 if a subject’s age is between 20 and 29 and his/her weight is between 70 kg and 80 kg, and 0 otherwise (see Fig. 1). More generally, each rule is defined over a hyperrectangle in the space of the input (original) variables, and returns 1 if a sample is in the hyperrectangle or 0 otherwise. The goal of this paper is to develop a learning algorithm that can find the optimal sparse linear combination of rules from among the extremely large number of all possible rules (see Fig. 2). An advantage of using rules in prediction models is their interpretability. For example, when predicting the risk of a certain disease, if the prediction function is represented by a linear combination of rules, it is easy for healthcare providers to advise people what actions are effective to reduce the risk of contracting the disease (e.g., losing weight, quitting smoking). To learn prediction models with rules, however, we have to consider the set of all possible rules; if we have \( d \) input features and the \( j \)th feature has \( s_j \) distinct values (\( j \in \{1, 2, \ldots, d\} \)), the

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Samples
| Age (years) | Height (cm) | Weight (kg) | Rule 1 | Rule 2 | Rule 3 | Rule 4 | Rule 5 |
|------------|-------------|-------------|--------|--------|--------|--------|--------|
| 25         | 171.4       | 56.1        |        |        |        |        |        |
| 36         | 178.3       | 79.4        |        |        |        |        |        |
| 22         | 160.8       | 61.3        |        |        |        |        |        |

Rules
| Age (years) | Rule 1 | Rule 2 | Rule 3 | Rule 4 | Rule 5 |
|-------------|--------|--------|--------|--------|--------|
| [20, 29]    |        |        |        |        |        |
| [20, 39]    |        |        |        |        |        |
| [20, 39]    |        |        |        |        |        |
| [20, 39]    |        |        |        |        |        |
| [50, 60]    |        |        |        |        |        |

Samples with rules being incorporated as features
| Age (years) | Height (cm) | Weight (kg) | Rule 1 | Rule 2 | Rule 3 | Rule 4 | Rule 5 |
|-------------|-------------|-------------|--------|--------|--------|--------|--------|
| 25          | 171.4       | 56.1        | 1      | 0      | 1      | 1      | 1      |
| 36          | 176.3       | 79.4        | 0      | 1      | 1      | 1      | 0      |
| 22          | 160.8       | 61.3        | 1      | 0      | 1      | 0      | 0      |

Figure 1: An illustrative example of using rules as binary features in prediction models. Given a dataset (top-left table), we consider learning a sparse prediction model from the table below.

Figure 2: Outline of the proposed SORF method.

The number of all possible rules is \( \prod_{j=1}^{d} s_j (s_j + 1)/2 \). This number grows exponentially with \( d \): even for \( s_1 = s_2 = \cdots = s_d = 10 \), the number of rules is \( 55^d \), which is as large as \( 2.5 \times 10^{17} \) for \( d = 10 \) and \( 6.4 \times 10^{34} \) for \( d = 20 \). We therefore need to introduce efficient algorithms for obtaining the optimal combination of rules. The problem of learning predictive models in the form of a linear combination of rules has been studied before, e.g. [1, 2, 3, 4, 6], but these approaches are not optimal in the sense that they do not consider all possible rules. A typical heuristic for finding rule candidates is to employ decision trees, as seen in the random forest [6] and RuleFit [3] algorithms. Recently, a learning method that can in principle consider all possible rules, called Rule-Enhanced Penalized Regression (REPR), was proposed [5]. REPR constructs a prediction model by iteratively finding and adding the most useful rule for the current model. The key feature of REPR is that, at each iteration, it can efficiently find the most useful rule using the column generation and the branch-and-bound method. To the best of our knowledge, REPR is the first algorithm that can potentially consider all possible rules in the prediction model learning. However, in practice, it is quite time-consuming to conduct column generation and a branch-and-bound search in a tree every time a rule is added. Moreover, REPR is specific to regression problems; and is not generally applicable to classification problems. In this paper we propose a method called Safe Optimal Rule Fit (SORF) for learning prediction models with rules, which is formulated as a convex optimization problem with sparse regularization. Different from REPR, SORF is formulated for both regression and classification problems. The main advantage of the proposed SORF method is that it can find a superset of the optimal set of rules with one search of a tree. To this end, we extend the recently popularized convex optimization technique, called safe screening, for learning prediction models with the optimal set of rules. Safe screening is a methodology for reducing the number of features to be optimized before and/or during the optimization, without losing the optimality of the fitted model (neither probabilistic nor heuristic). Recently, safe screening methods for sparse optimization or similar problems have been proposed [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. Here, we extend the basic idea of using safe screening for pattern mining [18] in the SORF algorithm, although a non-trivial extension is required to adapt it for application to sets of rules.

Related works and our contributions Here we discuss existing methods for constructing prediction models with rules. First, we note that each node of a decision tree represents the condition of classifying samples, e.g., “Value of feature \( j \) is larger than \( H \)”, and is thus interpreted as a rule.
Random forest [6] first generates multiple training datasets by resampling the original training dataset, and then builds a decision tree for each of these datasets. RuleFit [3] uses random forests for generating the candidate sets of rules, where paths not only from the root to a leaf but also from the root to an internal node are considered as candidates. From the candidate sets of rules, the most useful sets for predictive models are selected via \( |\mathbf{L}| \)-penalized empirical risk minimization (Section 2.2). A disadvantage of these decision-tree-based methods is that they cannot consider all possible rules. This indicates that their results are suboptimal in the sense that some optimal set of rules might not be included in the candidate sets of rules. The existing REPR method [5] and the proposed SORF method can solve this difficulty by efficiently searching over the entire tree. As stated above, a disadvantage of REPR is its high computational cost for searching a tree for many times (the number of rules to retrieve). In fact, in the experiment of [5], they stopped the optimization before convergence by setting a relaxed stopping criterion. On the other hand, SORF needs to search a tree only once by using novel pruning conditions derived from safe screening techniques.

Notations We use the following notations in the rest of this paper. For any natural number \( n \), \([n] := \{1, \ldots, n\}\). For \( n \times d \) matrix \( \mathbf{A} \), \( \mathbf{A}_i \) \( (i \in [n]) \), \( \mathbf{A}_j \) \( (j \in [d]) \) and \( a_{ij} \) represent the \( i \)-th row vector, \( j \)-th column vector and \((i, j)\) element of \( \mathbf{A} \) respectively. For any \( d \)-dimensional vector \( \mathbf{v} \), let \( L_1 \) norm and \( L_2 \) norm be \( \|\mathbf{v}\|_1 := |v_1| + \cdots + |v_d| \) and \( \|\mathbf{v}\|_2 := \sqrt{|v_1|^2 + \cdots + |v_d|^2} \) respectively. The indicator function is written as \( I(\cdot) \), i.e., \( I(u) = 1 \) if \( u \) is true, or \( I(u) = 0 \) otherwise. For any function \( f \), \( \text{dom} f \) represents the feasible domain of \( f \).

2 Problem Formulation

Consider a labeled (supervised) training dataset of \( n \) samples and \( d \) features, denoted by \( \{(\mathbf{x}_i, y_i)\}_{i \in [n]} \), where \( \mathbf{x}_i \in \mathbb{R}^d \) is a \( d \)-dimensional sample vector and \( y_i \) is its label \( (y_i \in \mathbb{R} \text{ for regression problems, and } y_i \in \{-1, +1\} \text{ for binary classification problems}) \). We define the matrix consisting of all sample vectors by \( \mathbf{X} := [\mathbf{x}_1, \ldots, \mathbf{x}_n]^\top \). For \( k \)-way categorical features \((k \geq 3)\), let us compose \( k-1 \) dummy features (at most one of them is 1 and the rest are 0). In this paper, since we interpret rules as new features in the prediction model, for clarity, we call the original features the input features.

2.1 Representation of rules

First, we formally define the “rule” stated in Section 1. We assume that rules are defined for integral features with a bounded domain. Therefore, if \( \mathbf{X} \) has continuous input features, we compute their discretized values \( \mathbf{\bar{X}} \) beforehand, and we use these values instead of \( \mathbf{X} \) when we consider rules. Here, \( \mathbf{\bar{x}} \) and \( \bar{x}_{ij} \) are defined as corresponding parts of \( \mathbf{\bar{X}} \). For simplicity, we assume that \( \bar{x}_{ij} \in \{0, 1, \ldots, s_j - 1\} \) \( (s_j \in \{1, 2, \ldots\} \ \forall j \in [d]) \). We define \( \mathcal{S} \) as the set of all possible discretized samples, that is, \( \mathcal{S} = \{0, 1, \ldots, s_1 - 1\} \times \{0, 1, \ldots, s_2 - 1\} \times \cdots \times \{0, 1, \ldots, s_d - 1\} \). Examples of discretization methods are shown in Appendix [B].

Given \( \ell, \mathbf{u} \in \mathcal{S} \) such that \( \ell_j = u_j \ \forall j \in [d] \), the rule with segment \( \ell, \mathbf{u} \), denoted by \( r_{(\ell, \mathbf{u})} : \mathcal{S} \rightarrow \{0, 1\} \), is a function of the (discretized) sample \( \mathbf{\bar{x}} \in \mathcal{S} \), and returns a binary value determined by:

\[
r_{(\ell, \mathbf{u})}(\mathbf{\bar{x}}) := \prod_{j \in [d]} I(\ell_j \leq \bar{x}_j \leq u_j).
\]

\(r_{(\ell, \mathbf{u})}(\mathbf{\bar{x}})\) becomes 1 if \( \mathbf{\bar{x}} \) is in the hyperrectangle composed by \( \ell \) and \( \mathbf{u} \), or 0 otherwise. We call a pair \( (\ell, \mathbf{u}) \) a rule segment if it forms a non-empty rule (i.e. \( 0 \leq \ell_j \leq u_j \leq s_j - 1 \ \forall j \in [d] \)). We define \( \mathcal{R} \) as the set of all rule segments except \((0, s - 1)\) (i.e., the rule which returns 1 for any sample), where \( s := [s_1, \ldots, s_d]^\top \), \( 0 := [0, \ldots, 0]^\top \) and \( \mathbf{1} := [1, \ldots, 1]^\top \). The number of possible segments for the \( j \)-th input feature \((\ell_j, u_j)\) is \( s_j(s_j + 1)/2 \), and therefore

\[
|\mathcal{S}| = \prod_{j \in [d]} \frac{s_j(s_j + 1)}{2} , \quad |\mathcal{R}| = |\mathcal{S}| - 1 = \prod_{j \in [d]} \frac{s_j(s_j + 1)}{2} - 1 .
\]

2.2 Sparse learning with input-space segmentation

In this paper, we aim to learn the following regression or classification function that can include any number of rules:

\[
f(\mathbf{x}) := b + \mathbf{x}^\top \eta + \sum_{k \in \mathcal{R}} \zeta_k r_k(\mathbf{\bar{x}}),
\]
We apply Lemma 2 to Lemma 1 to detect inactive features without knowing the optimal dual solution

We can also compute (6) and (7) analytically:

where

In Lemma 1, that is, Lemma (Theorem 3 in [14])

inactive features) before the exact problem vector sparse, i.e., most of the elements will be zero. In this problem, since the set of all possible rules is enormous, we expect the L₁ penalty to only extract rules that are useful for prediction. The formulation (3) and (4) is obtained by setting \( \phi(u) := \frac{1}{2}u^2 \), \( \bar{\alpha}_i := \bar{y}_i \bar{x}_i \), \( \bar{\alpha}_i := \max \left[ \begin{array}{c} 0, 1 \end{array} \right] - \bar{y}_i \bar{x}_i \), \( \bar{\beta}_i := \bar{y}_i \), \( \gamma_i := 0 \), \( \forall i \in [n] \). Then, let us consider the dual problem of (3) and (4):

\[
\theta^* := \max_{\theta \in \mathbb{R}^d} D_{P,\lambda}(\theta) := -\frac{1}{2}\|\theta\|_2^2 + \delta^\top \theta,
\]

where \( \delta := y \), \( \varepsilon := -\infty \) in the regression and \( \delta := 1 \), \( \varepsilon := 0 \) for the classification. Using the above definitions, for any \( j \in [d] \) and \( k \in \mathcal{R} \), we can prove the following relationships exist between the primal solution \( \eta^* \) and \( \zeta^* \) and the dual solution \( \theta^* \):

**Lemma 1.** For an input feature \( j \in [d] \) and rule \( k \in \mathcal{R} \),

\[
\left| \sum_{i \in [n]} \bar{\alpha}_{ij} \theta_i^* \right| < \rho \Rightarrow \eta_j^* = 0, \quad \left| \sum_{i \in [n]} \bar{\alpha}_{ik} \theta_i^* \right| < \lambda \Rightarrow \zeta_k^* = 0.
\]

The proof of Lemma 1 is shown in Appendix A.1.

### 2.3 Safe feature screening

In this section, we show how to construct the safe screening scheme outlined in Section 1. As stated in Section 2.2, we expect many of \( \eta^* \) and \( \zeta^* \) to be zero with the L₁ penalty. The safe screening methods [11] [14] detect \( j \in [d] \) and \( k \in \mathcal{R} \) such that \( \eta_j^* = 0 \) and/or \( \zeta_k^* = 0 \) (which we call inactive features) before the exact \( \eta^* \) and \( \zeta^* \) are computed. This can be achieved with the following relationship:

**Lemma 2** (Theorem 3 in [14]). Let \( \langle \tilde{\eta}, \tilde{\zeta}, \tilde{b} \rangle \in \text{dom} P_{\rho,\lambda}(\eta, \zeta, b) \) and \( \tilde{\theta} \in \text{dom} D_{\rho,\lambda}(\theta) \) be arbitrary feasible solutions of the primal and dual problems, respectively. Then, the optimal solution of the dual problem \( \theta^* \) is always within the following hypersphere in the dual solution space \( \theta \in \mathbb{R}^n \):

\[
\Theta_{\theta^*} := \{ \theta \mid \| \theta - \theta^* \|_2 \leq R_{\rho,\lambda} \},
\]

where \( R_{\rho,\lambda} := \sqrt{2\left( P_{\rho,\lambda}(\tilde{\eta}, \tilde{\zeta}, \tilde{b}) - D_{\rho,\lambda}(\tilde{\theta}) \right)} \).

We apply Lemma 2 to Lemma 1 to detect inactive features without knowing the optimal dual solution \( \theta^* \). To do this, we compute upper bounds of \( \| \sum_{i \in [n]} \bar{\alpha}_{ij} \theta_i^* \|, \forall j \in [d] \) and \( \| \sum_{i \in [n]} \bar{\alpha}_{ik} \theta_i^* \|, \forall k \in \mathcal{R} \) in Lemma 1 that is,

\[
\text{UB}(j) := \max_{\theta \in \mathbb{R}^n} \left| \sum_{i \in [n]} \bar{\alpha}_{ij} \theta_i \right| \quad \text{s.t.} \quad \| \theta - \tilde{\theta} \|_2 \leq \sqrt{2\left( P_{\rho,\lambda}(\tilde{\eta}, \tilde{\zeta}, \tilde{b}) - D_{\rho,\lambda}(\tilde{\theta}) \right)}, \quad \beta^\top \theta = 0.
\]

\[
\text{UB}(k) := \max_{\theta \in \mathbb{R}^n} \left| \sum_{i \in [n]} \bar{\alpha}_{ik} \theta_i \right| \quad \text{s.t.} \quad \| \theta - \tilde{\theta} \|_2 \leq \sqrt{2\left( P_{\rho,\lambda}(\tilde{\eta}, \tilde{\zeta}, \tilde{b}) - D_{\rho,\lambda}(\tilde{\theta}) \right)}, \quad \beta^\top \theta = 0.
\]

We can also compute (6) and (7) analytically:
Lemma 3. The solutions of the optimization problems (8) and (9) are given as follows:

\[ UB(j) = \left| \sum_{i \in [n]} \hat{a}_{ij} \hat{b}_i \right| + R_{p, \lambda} \sqrt{\sum_{i \in [n]} \hat{a}_{ij}^2 - \frac{(\sum_{i \in [n]} \hat{a}_{ij} \hat{b}_i)^2}{\| \beta \|^2}}, \]  

(8)

\[ UB(k) = \left| \sum_{i \in [n]} \hat{a}_{ik} \hat{b}_i \right| + R_{p, \lambda} \sqrt{\sum_{i \in [n]} \hat{a}_{ik}^2 - \frac{(\sum_{i \in [n]} \hat{a}_{ik} \hat{b}_i)^2}{\| \beta \|^2}}. \]  

(9)

The proofs of (8) and (9) are shown in Appendix A.2. From Lemmas 1 and 3 we have

\[ UB(j) < \rho \Rightarrow \eta^* = 0, \quad UB(k) < \lambda \Rightarrow \zeta^* = 0. \]  

(10)

The conditions (10) can be used to detect inactive features without knowing the optimal solutions \( \eta^* \), \( \zeta^* \), \( b^* \) or \( \theta^* \). This helps ensure the optimization is efficient. Note that, however, only applying the relationships above is not sufficient to obtain the optimal solution with the reasonable computational cost since the number of all possible rules grows exponentially with \( d \) (equation (1)). To tackle this problem, we developed safe feature screening techniques based on properties of the rules.

3 Proposed method

In this section, we introduce a new safe screening method for rules, named Safe Optimal Rule Fit (SORF). In this method, we enumerate all possible rules as a search tree, in which each node represents a rule. With this tree, we derive a condition to prune the search space, that is, to detect nodes whose descendants are all inactive. With this condition (in addition to the ordinary feature-wise screening condition (10)), we can obtain optimal solutions efficiently.

3.1 Tree representation of input-space segmentation

First, we show how to represent all rules as a tree. A simple approach is to build a tree with itemsets, according to whether a rule is included or not. However, this will result in an excessive number of possible combinations. We first construct a tree that enumerates all rules without duplication or omissions according to Theorem 1.

Theorem 1. The following procedure can enumerate all rule segments \( (\ell, u) \in \mathcal{R} \cup \{ (0, s - 1) \} \) as a tree \( T \) (each tree node represents a rule segment) without duplication or omission:

- Initialize a tree \( T \) with only one root node \( (0, s - 1) \).
- Do the following for any leaf node \( (\ell', u') \) in \( T \) until no further child nodes can be added:
  - For all \( j' \in \{ \tau, \tau + 1, \ldots, d \} \), where \( \tau = \max_{j \in [d], (\ell, u) \neq (0, s - 1)} j \).
  - \( \ell' < u'_j \Rightarrow \text{add a child node } ((\ell'_1, \ldots, \ell'_{j-1}, \ell'_j + 1, \ell'_{j+1}, \ldots, \ell'_d), u') \text{ under } (\ell', u') \). \]  
  (11)
  - \( \ell'_j = 0 < u'_j \Rightarrow \text{add a child node } ((\ell'_1, u'_1, \ldots, u'_{j-1}, u'_j - 1, u'_{j+1}, \ldots, u'_d)) \text{ under } (\ell', u') \).  
  (12)

The proof of the above theorem, the complete algorithm for building the tree and an example of a tree are shown in Appendix A.3.

3.2 Safe Optimal Rule Fit (SORF)

In this section, given the tree of all rules presented in Section 3.1, we show how to remove inactive rules from the tree. For the optimal solution of (2), we denote the set of active rules in the optimal solution by \( \mathcal{R}^* := \{ k \mid k \in \mathcal{R}, \hat{\zeta}_k \neq 0 \} \). Then, the proposed SORF method computes the candidates for the active rules \( \hat{\mathcal{R}} \) (i.e., \( \mathcal{R}^* \subseteq \hat{\mathcal{R}} \subseteq \mathcal{R} \)). This reduces the number of rules from \( |\mathcal{R}| \) to \( |\hat{\mathcal{R}}| \) and makes the optimization more efficient. First, we confirm that it is sufficient to solve (2) with respect to \( \hat{\mathcal{R}} \) rather than to \( \mathcal{R} \) to compute the optimal solution of (2).

Lemma 4. Let \( \hat{\mathcal{R}} \) be a set such that \( \mathcal{R}^* \subseteq \hat{\mathcal{R}} \subseteq \mathcal{R} \), and \( P_{p, \lambda}(\eta, \zeta, b) \) be the objective function of (2) in which \( \zeta_{\hat{\mathcal{R}} \setminus \hat{\mathcal{R}}} = 0 \) as follows:

\[ P_{p, \lambda}^\hat{\mathcal{R}}(\eta, \zeta, b) := \sum_{i \in [n]} \phi(\alpha_i^T \eta + \alpha_i^T \hat{\zeta} + \beta_i b + \gamma_i) + \rho \| \eta \|_1 + \lambda \| \zeta_{\hat{\mathcal{R}}} \|_1, \]
where \( \tilde{\alpha}_{ik,R} := \{ \tilde{\alpha}_{ik} \}_{k \in R}, \tilde{\zeta}_{R} := \{ \zeta_k \}_{k \in R}, \tilde{\zeta}_{R \setminus R} := \{ \zeta_k \}_{k \in R \setminus R} \). Then, the optimal solution of the original problem \([2]\) is given by

\[
(\eta^*, \zeta_R^*, b^*) = \arg\min_{\eta \in \mathbb{R}^d, \zeta_R \in \mathbb{R}^{|R|}, b \in \mathbb{R}} P_{\rho, \lambda}^R(\eta, \zeta_R, b), \quad \zeta_{R \setminus R}^* = 0. \tag{14}
\]

Then, we show how to prune rules from \( R \) to obtain \( \hat{R} \). For a rule \( k \in R \), we denote by \( R_{\text{sub}}(k) \subseteq R \) the set of rules that are the descendants of \( k \) in the tree, including \( k \) itself. Then, we derived the safe screening condition where all rules in \( R_{\text{sub}}(k) \) are inactive as in Theorem \([2]\). The theorem is proved with a similar idea to that in the safe screening method for search trees for predictive pattern mining \([18]\).

**Theorem 2.** Given an arbitrary pair of primal and dual feasible solution \((\tilde{\eta}, \tilde{\zeta}, \tilde{b}) \in \text{dom} P_{\rho, \lambda}(\eta, \zeta, b), \tilde{\theta} \in \text{dom} D_{\rho, \lambda}(\theta)\) and \( R_{\rho, \lambda} = \sqrt{2(P_{\rho, \lambda}(\tilde{\eta}, \tilde{\zeta}, \tilde{b}) - D_{\rho, \lambda}(\tilde{\theta}))} \), for any node \( k '\in R_{\text{sub}}(k) \) in the tree, the following relationship holds:

\[
\text{SRPC}(k) := u_k + R_{\rho, \lambda} \sqrt{|k|} < \lambda \Rightarrow \zeta_k^* = 0,
\]

where \( u_k := \max\left\{ \sum_{i, \beta_i \geq 0} \tilde{\alpha}_{ik} \beta_i, -\sum_{i, \beta_i < 0} \tilde{\alpha}_{ik} \beta_i \right\}, \quad v_k := \sum_{r \in [n]} \tilde{\alpha}_{ik}^2 \quad \forall k \in R. \)

The proof of this theorem is shown in Appendix \([A,4]\). The main technique for deriving this condition uses the relationship between a node \( k \) and its descendant \( k \):

\[
\forall k \in R, k' \in R_{\text{sub}}(k) : \quad r_k(x) = 0 \Rightarrow r_{k'}(x) = 0, \quad r_{k'}(x) = 1 \Rightarrow r_k(x) = 1. \tag{15}
\]

By \([15]\), it is clear that the number of samples satisfying the rule \( k \) is at least that of \( k' \in R_{\text{sub}}(k) \). The condition for determining whether to prune a part of a tree, \( \text{SRPC}(k) < \lambda \), states that for all nodes \( k' \in R_{\text{sub}}(k) \) the condition of inactiveness must hold \([10]\). Moreover, from \([15]\) we have the following corollary:

**Corollary 1.** For any node \( k' \in R_{\text{sub}}(k) \), \( \text{SRPC}(k) \geq \text{SRPC}(k') \) holds.

The corollary states that, the deeper into the tree we search, the easier the pruning will be. The proofs of Corollary \([1]\) and Theorem \([2]\) are shown in Appendix \([A,5]\).

### 4 Experiments

#### 4.1 Experimental setting

In this section, we demonstrate the usefulness of the proposed method through three numerical experiments. We present the datasets we used in Table \([4]\). In all of the experiments, we consider only one regularization parameter by setting \( \rho = \lambda \). The optimization procedure in SORF was implemented with the coordinate gradient descent method \([20]\), and the computation terminates when duality gap \( < 10^{-6} \) \( (P_{\rho, \lambda}(\tilde{\eta}, \tilde{\zeta}, \tilde{b}) - D_{\rho, \lambda}(\tilde{\theta})) \) in Lemma \([2]\), where the measure for optimality is always non-negative. To check if the safe screening condition was satisfied, we used two types of feasible solutions: One is the solution on the way of the optimization; we check the condition for every 10-th iteration of the optimization. The other is the previous solution in the regularization path: since we compute multiple solutions for different \( \lambda \)'s for speeding up and/or controlling the number of active rules, we use the solution for the previous \( \lambda \) as the feasible solution of the current \( \lambda \). Details are shown in Appendix \([C]\). All of the computations were conducted on 12 cores of an Intel(R) Xeon(R) CPU E5-2687W v4 (3.00GHz) with 256 GB of memory.

#### 4.2 Experiment 1: Effect of incorporating rules

In Experiment 1, to demonstrate the usefulness of incorporating rules into the prediction model, we compared the predictive performance of our method with LASSO in the regression experiment and \( L_1 \)-penalized squared hinge SVM in the classification experiment. The discretization of SORF is based on quantiles points (see, Appendix \([B,2]\), and the number of discretizations \( M \) is set to \( M \in \{5, 8, 10\} \). The dataset was divided into \#training:\#validation:\#test, with a ratio of 1:1:1, and the regularization parameter \( \lambda \) was determined from \( \lambda \in \{2^{-1}, \ldots, 2^4\} \) by 2-fold cross validation using the training and validation datasets. After that, we learned the model using the selected \( \lambda \).
Table 1: Datasets used in this experiment.Datasets marked † are from [21], while others are from [22]. Before the computation, we normalized every input feature and label (only for the regression problem) in the datasets to have mean zero and variance one.

| Datasets for regression | n  | d  | Datasets for classification | n  | d  |
|------------------------|----|----|----------------------------|----|----|
| SERVO                  | 167| 10 | FOURCLASS†                 | 862| 2  |
| YACHT                  | 308| 6  | HABERMAN                   | 306| 3  |
| COOL (Energy Efficiency)| 768| 8  | LIVER (liver-disorders)†    | 145| 5  |
| HEAT (Energy Efficiency)| 768| 8  | MAMMOGRAPHIC               | 830| 9  |

Table 2: Results of Experiment 1 (regression)

| Dataset  | $M = 5$ MSE | $|R|$ | $M = 8$ MSE | $|R|$ | $M = 10$ MSE | $|R|$ | LASSO MSE |
|----------|-------------|------|-------------|------|--------------|------|----------|
| SERVO    | 0.04366 9.8e05 | 0.04366 9.8e05 | 0.04366 9.8e05 | 0.54355 |
| YACHT    | 0.10955 7.6e06 | 0.04937 5.5e08 | 0.02723 5.0e09 | 0.27376 |
| COOL     | 0.02508 1.5e08 | 0.02626 2.3e09 | 0.02588 5.3e09 | 0.11428 |
| HEAT     | 0.00215 1.5e08 | 0.00223 2.3e09 | 0.00219 5.3e09 | 0.07802 |

Table 3: Results of Experiment 1 (classification)

| Dataset       | $M = 5$ Accuracy | $|R|$ | $M = 8$ Accuracy | $|R|$ | $M = 10$ Accuracy | $|R|$ | SVM Accuracy |
|---------------|------------------|------|------------------|------|-------------------|------|--------------|
| FOURCLASS     | 0.92014 2.2e02   | 0.98264 1.3e03 | 0.96528 3.0e03 | 0.76042 |
| HABERMAN      | 0.76471 2.2e02   | 0.74510 1.3e03 | 0.7431 3.0e03 | 0.72549 |
| LIVER         | 0.75510 7.6e05   | 0.79592 6.0e07 | 0.77551 5.0e08 | 0.71429 |
| MAMMOGRAPHIC  | 0.83813 3.3e05   | 0.82734 7.9e05 | 0.82734 1.2e06 | 0.82014 |

and evaluated the predictive performance of the test dataset. In the training computation, we set the regularization path as 1,000 divisions of $\lambda_{\text{max}}$ to $\lambda \in \{2^{-1}, \ldots, 2^4\}$ on a logarithmic scale. We evaluated the predictive performance using the mean squared error (MSE) in the regression experiments and the classification accuracy in the classification experiments. In Experiment 1, we imposed constraints on the number of types of input features included in each rule, which are 2 for COOL and HEAT, and 5 for MAMMOGRAPHIC. The results are shown in Tables 2 and 3. From these results, it was confirmed that the proposed method that incorporates the rules into the model has high predictive accuracy rates even for datasets which simple linear models such as LASSO and linear SVM cannot provide high accuracy rates.

### 4.3 Experiment 2: Optimal rule retrieval by existing method

In Experiment 2, we conducted experiments to evaluate how similar the rules obtained by the existing methods (random forest, RuleFit) were to those retrieved by the optimal model obtained by SORF. We compared the similarity of the sets of rules retrieved by the proposed SORF algorithm and existing methods when each of them retrieved 100 rules. First, we note that since we have to determine the discretization before applying SORF but not random forest and RuleFit, we impose the constraint that the threshold for partitioning in random forest and RuleFit must be chosen from the results of the discretization. Moreover, since we do not need the test dataset in Experiment 2, all samples in the dataset are used for training. We compared the similarity of the two sets of rules with the Jaccard-coefficient-based measure, where the Jaccard coefficient between two discrete sets $A$, $B$ is defined as $\text{Jac}(A, B) := |A \cap B| / |A \cup B|$. Given a rule $k \in R$, we define its volume $V_k := \{s \mid s \in S, r_k(s) = 1\}$. Then, given the sets of rules retrieved by random forest (RuleFit) $R_1 = \{r_1, r_2, \ldots, r_N\}$ and SORF $R_2 = \{r^*_1, r^*_2, \ldots, r^*_N\}$, their similarity $\text{Sim}(R_1, R_2)$ is defined by the average of the highest Jaccard coefficients for each of $R_1$ to $R_2$, that is, $\text{Sim}(R_1, R_2) := \frac{1}{N} \sum_{s \leq |N|} \max_{s \in |N|} \text{Jac}(V_k, V^*_k)$. (Note: This similarity measure is nonsymmetric.) To generate sets of 100 rules, random forest used 10 different decision trees with at most 10 leaves (10 rules) each. For RuleFit, first we created a random forest of 10 different decision trees with at most 100 leaves.
Table 4: Results of Experiments 2. For small datasets where it was difficult to obtain 100 rules (FOURCLASS and HABERMAN), we only retrieved 50 rules.

| Dataset | Regression | Classification |
|---------|------------|----------------|
|         | random forest | RuleFit       | Dataset | random forest | RuleFit       |
| SERVO   | 0.383       | 0.368         | LIVER   | 0.301       | 0.272         |
| YACHT   | 0.424       | 0.523         | MAMMOGRAPHIC | 0.255       | 0.210         |
| COOL    | 0.154       | 0.154         | FOURCLASS | 0.651       | 0.950         |
| HEAT    | 0.130       | 0.119         | HABERMAN | 0.686       | 0.816         |

Table 5: Results of Experiment 3: computational costs for retrieving 100 rules. Bold results indicate the lowest costs. Since Table 1 in [5] provides the computation times per rule by REPR, in this table we show 100 times of them for the comparison. Here, $\delta$ is the discretization parameter (Appendix B.1).

| Dataset | $\delta$ | $|R|$ | SORF | REPR |
|---------|----------|-----|------|------|
|         |          |     | #Search nodes | Time (sec) | #Search nodes | Time (sec) |
| SERVO   | 0        | 9.8e05 | $8.2e03$  | 7       | 3.6e04       | 11         |
| YACHT   | 0        | 2.6e10 | 9.9e04   | 39      | 5.3e04       | 36         |
| COOL    | 0.005    | 1.1e10 | $9.0e04$  | 30      | 3.7e05       | 288        |
| HEAT    | 0.005    | 1.1e10 | $8.7e04$  | 32      | 3.9e05       | 222        |

(198 rules) each, then we reduce the forests to approximately 100 rules as follows. To adjust the number of rules for SORF and RuleFit, both of which uses LASSO to reduce the number of rules used, we took the regularization path with small interval, and then selected the results whose number of active rules is the closest to 100. The number of discretizations is 5 for each input feature. The results are shown in Table 4. We find that the results of these methods differ greatly from the optimal results obtained by SORF unless the number of input features is small (FOURCLASS, HABERMAN). This implies that the existing methods considered here cannot examine all possible rules effectively when the number of possible combinations of rules is large.

### 4.4 Experiment 3: Comparison with REPR

In Experiment 3, we compared the computational costs of SORF and REPR, which have similar optimality in their obtained results. Since the paper describing REPR [5] presents the computation times and the numbers of searched tree nodes used to retrieve 100 rules, we compared these with the time taken to retrieve 100 rules by SORF.[2] As no implementation of REPR is publically available, we conducted the following computations with SORF: First, for all four regression datasets in Table 1 (which are all also used in [5]), we discretized the input features of the datasets in the same manner as for REPR (Appendix B.1). Then, we divided each dataset into test:training, where the ratio of the sizes was 1:4, at random and computed 100 rules for the training dataset. We took the average for 10 random seeds. We add that these experimental results with REPR may not be fully optimized since they use heuristics to end the computation before it has found the optimal solution (Section 5 in [5]). In addition, the computation times are for parallel computations. SORF does not introduce similar schemes in the following results, that is, SORF is computed under more difficult conditions. The results are shown in Table 5. SORF is computationally less expensive than REPR for three out of four datasets, and for the other dataset (YACHT), comparable results are obtained, although we conducted the experiment under more difficult conditions for SORF. We consider that, compared to conducting a computationally expensive search for each rule in REPR, the strategy of SORF of searching a tree only once to retrieve all rules was very effective.

[1] Random forest uses rules at tree leaves, while RuleFit uses rules at all nodes except the root (Section 4).

[2] The method for retrieving 100 rules is almost the same as in Experiment 2, however, to make sure we run SORF under stricter conditions, we stop the computation when we retrieve 100 or more rules (not “closest to 100”).
5 Conclusion

In this paper, we proposed a new safe screening method for efficiently learning the optimal model by identifying the set of rules that provide the most accurate predictions, from all possible sets of rules. Our method expressed an extremely large number of rules as a tree structure, and enabled efficient learning while guaranteeing the optimality of the obtained model by searching the tree only once. Furthermore, we demonstrated the usefulness of our method through numerical experiments for regression and classification problems using several benchmark datasets.

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A Proofs

A.1 Proof of Lemma 1

Proof. From the KKT condition (see, e.g., [23]) for the primal problem (2) and the dual problem (5),

\[
\sum_{i \in [n]} \hat{\alpha}_{ij} \theta_i^* \in \begin{cases} 
\rho \text{sign} \left( \eta_j^* \right) & \text{if } \eta_j^* \neq 0, \forall j \in [d], \\
[-\rho, \rho] & \text{if } \eta_j^* = 0, \forall j \in [d], 
\end{cases}
\]

\[
\sum_{i \in [n]} \tilde{\alpha}_{ik} \theta_i^* \in \begin{cases} 
\lambda \text{sign} \left( \zeta_k^* \right) & \text{if } \zeta_k^* \neq 0, \forall k \in \mathcal{R}, \\
[-\lambda, \lambda] & \text{if } \zeta_k^* = 0, \forall k \in \mathcal{R}, 
\end{cases}
\]

This suggests that

\[
\left| \sum_{i \in [n]} \hat{\alpha}_{ij} \theta_i^* \right| < \rho \Rightarrow \eta_j^* = 0, \forall j \in [d], \quad \left| \sum_{i \in [n]} \tilde{\alpha}_{ik} \theta_i^* \right| < \lambda \Rightarrow \zeta_k^* = 0, \forall k \in \mathcal{R}.
\]

\[\square\]

A.2 Proof of Lemma 3

The proof of (8) and (9) are almost the same. Here, we show only the proof for (9).

Proof. Let \(\hat{\alpha}_{ik} := [\hat{\alpha}_{1k}, \ldots, \hat{\alpha}_{nk}]^\top, k \in \mathcal{R}\). First, the objective function of the convex optimization problem (7) can be rewritten as follows:

\[
\max_{\theta \in \mathbb{R}^n} \hat{\alpha}_k^\top \theta \quad \Leftrightarrow \max_{\theta} \max \left\{ \hat{\alpha}_k^\top \theta, -\hat{\alpha}_k^\top \theta \right\} \quad \Leftrightarrow \max \left\{ -\min_{\theta} (-\hat{\alpha}_k)^\top \theta, -\min_{\theta} \hat{\alpha}_k^\top \theta \right\}. \tag{16}
\]

Thus, we consider the following convex optimization problem:

\[
\min_{\theta} \hat{\alpha}_k^\top \theta \quad \text{s.t.} \quad \|\theta - \tilde{\theta}\|_2^2 \leq R_{p,\lambda}^2, \quad \beta^\top \theta = 0. \tag{17}
\]

Here, we rewrite the optimization problem (17) using the Lagrange function \(L(\theta, \mu, \nu)\) as

\[
\min_{\theta} \max_{\mu \geq 0, \nu} L(\theta, \mu, \nu), \quad \text{where} \quad L(\theta, \mu, \nu) := \hat{\alpha}_k^\top \theta + \mu (\|\theta - \tilde{\theta}\|_2^2 - R_{p,\lambda}^2) + \nu \beta^\top \theta. \tag{18}
\]

The KKT conditions for (18) are as follows:

\[
\mu > 0, \\
\|\theta - \tilde{\theta}\|_2^2 - R_{p,\lambda}^2 \leq 0, \\
\beta^\top \theta = 0, \tag{19}
\]

\[
\mu (\|\theta - \tilde{\theta}\|_2^2 - R_{p,\lambda}^2) = 0. \tag{20}
\]

In this case, we set \(\mu > 0\) because there exists a minimum for this optimization problem only when \(\mu > 0\). Differentiating the Lagrange function w.r.t. \(\theta\) and using the fact that it takes its minimum at zero,

\[
\theta = \tilde{\theta} - \frac{1}{2\mu} (\hat{\alpha}_k + \nu \beta). \tag{21}
\]

By substituting (21) into (18) and rearranging,

\[
\max_{\mu \geq 0, \nu} \frac{1}{4\mu} \|\hat{\alpha}_k + \nu \beta\|_2^2 + (\hat{\alpha}_k + \nu \beta)^\top \tilde{\theta} - \mu R_{p,\lambda}^2.
\]
Since the objective function is a quadratic concave function w.r.t. $\nu$, we obtain the following by using (19):

$$\nu = -\frac{\hat{\alpha}_k^\top \beta}{\|\beta\|^2_2}.$$  

By substituting this into (21),

$$\theta = \hat{\theta} - \frac{1}{2\mu} \left( \hat{\alpha}_k - \frac{\hat{\alpha}_k^\top \beta}{\|\beta\|^2_2} \beta \right).$$  

(22)

Since $\mu > 0$ and (20) indicates $\|\theta - \hat{\theta}\|^2_2 - R_{\rho,\lambda}^2 = 0$, by substituting (22) into this equality, we obtain the following identity:

$$\mu = \frac{1}{2\|\beta\|^2_2 R_{\rho,\lambda}} \sqrt{\|\hat{\alpha}_k\|^2_2 \|\beta\|^2_2 - (\hat{\alpha}_k^\top \beta)^2}.$$  

Then, from (22), the solution of (17) is given as

$$\theta = \hat{\theta} - \frac{\|\beta\|^2_2 R_{\rho,\lambda}}{\|\hat{\alpha}_k\|^2_2 \|\beta\|^2_2 - (\hat{\alpha}_k^\top \beta)^2} \left( \hat{\alpha}_k - \frac{\hat{\alpha}_k^\top \beta}{\|\beta\|^2_2} \beta \right),$$  

and the minimum of the objective function (17) is

$$\hat{\alpha}_k^\top \hat{\theta} - R_{\rho,\lambda} \sqrt{\|\hat{\alpha}_k\|^2_2 - (\hat{\alpha}_k^\top \beta)^2/\|\beta\|^2_2}.$$  

(23)

Then, substituting (23) into (16), the optimal objective value of (9) is given as

$$\left| \hat{\alpha}_k^\top \hat{\theta} \right| + R_{\rho,\lambda} \sqrt{\|\hat{\alpha}_k\|^2_2 - (\hat{\alpha}_k^\top \beta)^2/\|\beta\|^2_2}.$$  

A.3 Proof of Theorem 2 and its pseudocode

Proof. To shrink a rule segment $(\ell, u)$, first we choose $j \in [d]$, $\ell_j < u_j$ and then compute either $\ell_j \leftarrow \ell_j + 1$ or $u_j \leftarrow u_j - 1$. Therefore, replacing (11) with “$\tau \leftarrow 1$” and replacing (13) with “$\ell_j' < u_j'$ . . . enumerates all rule segments, although this procedure will contain duplicates (generating a directed acyclic graph rather than a tree). To avoid these duplications, we set the priority of these operations as follows: (i) progressing from smaller input feature IDs to larger IDs, (ii) considering upper bounds then lower bounds. In the algorithm above, the order (i) is achieved by (11), while (ii) by (12) and (13). This assures no duplication occurs in the enumeration.

The pseudocode of Theorem 1 is presented in Algorithm 1. An example of the tree is shown in Fig. 3.

A.4 Proof of Theorem 2

To prove Theorem 2, it is sufficient to show the following lemma:

Lemma 5. For any $k' \in R_{\text{sub}}(k)$,

$$\text{UB}(k') = \sum_{i \in [n]} \alpha_{ik'} \hat{\theta}_i + R_{\rho,\lambda} \sqrt{\sum_{i \in [n]} \alpha_{ik'}^2 - \left( \sum_{i \in [n]} \alpha_{ik'}/\beta_i \right)^2/\|\beta\|^2_2} \leq u_k + R_{\rho,\lambda} \sqrt{v_k} = \text{SRPC}(k).$$

To prove Lemma 5, we use the following lemma.

Lemma 6. Given an arbitrary $n$ dimensional vector $c \in \mathbb{R}^n$, for any rule $k \in R$, the following relationship holds:

$$\max \left\{ \sum_{i : c_i > 0} c_i r_k(\bar{x}_i), - \sum_{i : c_i < 0} c_i r_k(\bar{x}_i) \right\} \geq \sum_{i \in [n]} c_i r_k(\bar{x}_i), \quad \forall k' \in R_{\text{sub}}(k).$$
Algorithm 1 Algorithm for constructing the tree structure in Theorem 1

Input: \( \{ s_j \}_{j \in [d]} \)

```
RootNode.Rule ← (Head = 0, Tail = s - 1).

RootNode.ChildNodes ← [].

MAKESUBTREE(RootNode)
```

function MAKESUBTREE(Node)

\( \tau \leftarrow \max_{j \in [d], (\ell_j, n_j) \neq (0, s_j - 1)} j. \)

for \( j \leftarrow \tau, \tau + 1, \ldots, d \) do

if NewNode.Rule.Head[\( j' \)] < NewNode.Rule.Tail[\( j' \)] then

if Node.Rule[\( j' \)].Head = 0 then

NewNode.Rule ← (copy of Node.Rule).

NewNode.Rule.Tail[\( j' \)] ← NewNode.Rule.Tail[\( j' \)] - 1

NewNode.ChildNodes ← [].

Node.ChildNodes.append(NewNode)

MAKESUBTREE(NewNode)

end if

NewNode.Rule ← (copy of Node.Rule).

NewNode.Rule.Head[\( j' \)] ← NewNode.Rule.Head[\( j' \)] + 1

NewNode.ChildNodes ← [].

Node.ChildNodes.append(NewNode)

MAKESUBTREE(NewNode)

end if

end for

end function

Therefore, using this equation and (15), the following relationship holds:

\[
\max \left\{ \sum_{i \in [n]} c_i r_{k'}(\bar{x}_i), - \sum_{i \in [n]} c_i r_{k}(\bar{x}_i) \right\} \geq \left| \sum_{i \in [n]} c_i r_{k'}(\bar{x}_i) \right|.
\]

Figure 3: An example of the tree structure constructed under Theorem 1 for \( d = 2, s_1 = s_2 = 3 \). Blue and red blocks denote the rule segments of input features \( j = 1 \) and \( j = 2 \), respectively. The colors of the edges represent which input feature (\( j' \) in (11)) is shrunk. Nodes with yellow backgrounds denote \( \tau = 2 \), that is, the segment for feature \( j = 1 \) cannot be shrunk further. Dotted edges represent the segments shrunk following (13) (others by (12)).

**Proof of Lemma**

First the following relationship holds:

\[
\sum_{i \in [n]} c_i r_{k'}(\bar{x}_i) = \sum_{\ell_i, n_i > 0} c_i r_{k'}(\bar{x}_i) + \sum_{\ell_i, n_i < 0} c_i r_{k'}(\bar{x}_i).
\]

Using this equation and (15), the following relationship holds:

\[
\sum_{\ell_i, n_i < 0} c_i r_{k'}(\bar{x}_i) \leq \sum_{\ell_i, n_i < 0} c_i r_{k}(\bar{x}_i) \leq \sum_{i \in [n]} c_i r_{k'}(\bar{x}_i) \leq \sum_{\ell_i, n_i > 0} c_i r_{k'}(\bar{x}_i) \leq \sum_{\ell_i, n_i > 0} c_i r_{k}(\bar{x}_i).
\]

Therefore,

\[
\max \left\{ \sum_{\ell_i, n_i > 0} c_i r_{k}(\bar{x}_i), - \sum_{\ell_i, n_i < 0} c_i r_{k}(\bar{x}_i) \right\} \geq \left| \sum_{i \in [n]} c_i r_{k'}(\bar{x}_i) \right|.
\]
Proof of Lemma\[5\] First, from Lemma \[6\]
\[
\left| \sum_{i \in [n]} \tilde{\alpha}_{ik} \tilde{\beta}_i \right| \leq \max \left\{ \sum_{i: \beta_i > 0} \tilde{\alpha}_{ik} \tilde{\beta}_i \left| r_k (\bar{x}_i) \right| - \sum_{i: \beta_i < 0} \tilde{\alpha}_{ik} \tilde{\beta}_i \right\} := u_k.
\]

Further, it is clear that
\[
\sum_{i \in [n]} \tilde{\alpha}_{ik}^2 - \frac{(\sum_{i \in [n]} \tilde{\alpha}_{ik} \beta_i)^2}{\| \beta \|^2} \leq \sum_{i \in [n]} \tilde{\alpha}_{ik}^2 \leq \sum_{i \in [n]} \tilde{\alpha}_{ik}^2 := v_k.
\]

From these results,
\[
\left| \sum_{i \in [n]} \tilde{\alpha}_{ik} \tilde{\beta}_i \right| + R_{p, \lambda} \sqrt{\sum_{i \in [n]} \tilde{\alpha}_{ik}^2 - \frac{(\sum_{i \in [n]} \tilde{\alpha}_{ik} \beta_i)^2}{\| \beta \|^2}} \leq u_k + R_{p, \lambda} \sqrt{v_k}.
\]

Proof of Theorem\[2\] From Lemmas\[2\],[3] and \[5\] the following relationship holds:
\[
\left| \sum_{i \in [n]} \tilde{\alpha}_{ik'} \theta_i^* \right| \leq UB(k') \leq SRPC(k'), \forall k' \in R_{sub}(k).
\]

Applying Lemma\[1\] and equation \[24\], we obtain Theorem\[2\].

A.5 Proof of Corollary\[1\]

Proof. For any pair of nodes $k \in \mathcal{R}$ and $k' \in \mathcal{R}_{sub}(k)$,
\[
\sum_{i: \beta_i > 0} \tilde{\alpha}_{ik} \tilde{\beta}_i = \sum_{i: \beta_i > 0} \beta_i \tilde{\beta}_i r_k (\bar{x}_i) \geq \sum_{i: \beta_i > 0} \beta_i \tilde{\beta}_i r_{k'} (\bar{x}_i) = \sum_{i: \beta_i > 0} \tilde{\alpha}_{ik} \tilde{\beta}_i, \quad \text{(25)}
\]
\[
\sum_{i: \beta_i < 0} \tilde{\alpha}_{ik} \tilde{\beta}_i = \sum_{i: \beta_i < 0} \beta_i \tilde{\beta}_i r_k (\bar{x}_i) \leq \sum_{i: \beta_i < 0} \beta_i \tilde{\beta}_i r_{k'} (\bar{x}_i) = \sum_{i: \beta_i < 0} \tilde{\alpha}_{ik} \tilde{\beta}_i, \quad \text{(26)}
\]
where both inequalities are proved by \[15\], while all equalities are proved by the definitions of $\tilde{\alpha}_{ik}$ and $\beta_i$ for \[3\] and \[4\]. Since $u_k$ is defined as $u_k := \max\{\sum_{i: \beta_i > 0} \tilde{\alpha}_{ik} \tilde{\beta}_i, -\sum_{i: \beta_i < 0} \tilde{\alpha}_{ik} \tilde{\beta}_i\}$ (Theorem\[3\]), we examine for all four cases which value is larger for $u_k$ and $u_{k'}$.

- If $u_k = \sum_{i: \beta_i > 0} \tilde{\alpha}_{ik} \tilde{\beta}_i$ and $u_{k'} = \sum_{i: \beta_i > 0} \tilde{\alpha}_{ik} \tilde{\beta}_i$, $u_k \geq u_{k'}$ holds due to \[25\].
- If $u_k = \sum_{i: \beta_i > 0} \tilde{\alpha}_{ik} \tilde{\beta}_i$ and $u_{k'} = -\sum_{i: \beta_i < 0} \tilde{\alpha}_{ik} \tilde{\beta}_i$, $u_k \geq u_{k'}$ holds since
  \[
u_k \geq -\sum_{i: \beta_i < 0} \tilde{\alpha}_{ik} \tilde{\beta}_i \geq u_{k'},
\]
  where the first inequality is from the definition of $u_k$, and the last inequality is from \[26\].
- If $u_k = -\sum_{i: \beta_i < 0} \tilde{\alpha}_{ik} \tilde{\beta}_i$ and $u_{k'} = \sum_{i: \beta_i > 0} \tilde{\alpha}_{ik} \tilde{\beta}_i$, $u_k \geq u_{k'}$ holds since
  \[
u_k \geq \sum_{i: \beta_i > 0} \tilde{\alpha}_{ik} \tilde{\beta}_i \geq u_{k'},
\]
  where the first inequality is from the definition of $u_k$, and the last inequality is from \[25\].
- If $u_k = -\sum_{i: \beta_i < 0} \tilde{\alpha}_{ik} \tilde{\beta}_i$ and $u_{k'} = -\sum_{i: \beta_i < 0} \tilde{\alpha}_{ik} \tilde{\beta}_i$, $u_k \geq u_{k'}$ holds due to \[26\].

This proves the corollary. □
After we retrieve the rule as a segment of the discretized values, let us consider how to represent the
rule. As stated in Section 2.1, we have to obtain the discretized values \( \{ x_{ij} \} \) (\( \forall i \in [n], j \in [d] \)). \( x_{ij} \in \{ 0, 1, \ldots, s_j - 1 \} \). In the experiment, we discretized the data in the
following manner. Let \( \omega^{(j)} \) \( ( j \in [d] ) \) be a permutation of \( [n] \) such that \( x_{1, j}, x_{2, j}, \ldots, x_{n, j} \) is
sorted in ascending order.

Throughout this paper, we consider the case where there is a gap larger than \( \delta \).

### B.1 Discretization by interval

This method for discretization is also used in REPR [5]. Set a threshold parameter \( \delta \in (0, 1) \). Then, for each input feature \( j \in [d] \), if \( x_{ij} < \delta ( \max_{i \in [d]} x_{ij} - \min_{i \in [d]} x_{ij} ) \), assign different values to \( x_{ij} \) and \( x_{ij} \), that is, \( x_{ij} = x_{ij} + 1 \). Otherwise assign the same value to both. An example is shown in Figure 4.

### B.2 Discretization by quantiles

Set a division parameter \( M \in \{ 2, 3, \ldots \} \). Let \( q_m = 1 + ( n - 1 ) m / M \) (\( m \in [ M - 1 ] \)) be the index of the \( m \)-th \( M \)-quantiles out of \( n \). Then, for each input feature \( j \in [d] \) and \( m \in [M - 1] \),

- If \( x_{\omega^{(j)} \omega^{(j)}} \) and \( x_{\omega^{(j)} \omega^{(j)}} \) are different, then assign different values to \( x_{\omega^{(j)} \omega^{(j)}} \) and \( x_{\omega^{(j)} \omega^{(j)}} \).
- Otherwise, assign different values to \( x_{\omega^{(j)} \omega^{(j)}} \) and \( x_{\omega^{(j)} \omega^{(j)}} \), where
  - \( q' := \max \{ o \mid x_{\omega^{(j)} \omega^{(j)}} < x_{\omega^{(j)} \omega^{(j)}} \} \) if \( q_m \leq \min \{ o \mid x_{\omega^{(j)} \omega^{(j)}} = x_{\omega^{(j)} \omega^{(j)}} \} + \max \{ o \mid x_{\omega^{(j)} \omega^{(j)}} = x_{\omega^{(j)} \omega^{(j)}} \} / 2 \),
  - \( q' := \min \{ o \mid x_{\omega^{(j)} \omega^{(j)}} > x_{\omega^{(j)} \omega^{(j)}} \} \) otherwise.

Note that, the \( j \)-th input feature is discretized to at most \( M \) distinct values, not always \( M \) (i.e., \( s_j \leq M \)). Such a case can occur, for example, when \( x_{\omega^{(j)} \omega^{(j)}} = x_{\omega^{(j)} \omega^{(j)} + 1} \).

### B.3 Discretized space to the original space

After we retrieve the rule as a segment of the discretized values, let us consider how to represent the
segment in the original space. This process is needed when we make a prediction for the test samples
that are unknown at the time of the discretization. In the experiments in this paper, when a training
dataset \( X \) is discretized as \( \hat{X} \), we define that a discretized sample \( \hat{x}' \in \hat{X} \) represents the segment
[\( u, v \)] in the original space \( ( u, v ) \in \mathbb{R}^d, u_j \leq v_j \forall j \in [d] \) defined as follows for each \( j \in [d] \):

- If \( 0 < x'_j < s_j - 1 \), then \( u_j = ( Z_j[x'_j - 1] + Z_j[x'_j] ) / 2 \) and \( v_j = ( Z_j[x'_j] + Z_j[x'_j + 1] ) / 2 \),
- If \( x'_j = 0 \), then \( u_j = -\infty \) and \( v_j = ( Z_j[0] + Z_j[1] ) / 2 \), or
- If \( x'_j = s_j - 1 \), then \( u_j = ( Z_j[s_j - 2] + Z_j[s_j - 1] ) / 2 \) and \( v_j = +\infty \),

Figure 4: An example of discretization by intervals.
Algorithm 2 Regularization path computation algorithm (When $\rho = \lambda$)

Input: $\{(x_i, y_i)\}_{i \in [n]}$
- Discretize $X$ into $\tilde{X}$ and make $\mathcal{R}$.
- $\lambda_0 \leftarrow \max \left\{ \max_{j \in [d]} \left| \sum_{i \in [n]} x_{ij} (y_i - \bar{y}) \right|, \max_{k \in \mathcal{R}} \left| \sum_{i \in [n]} r_k (\bar{x}_i) (y_i - \bar{y}) \right| \right\}$
- Initialize $\{(\eta^{(\lambda_0)}, \zeta^{(\lambda_0)}, \hat{\eta}^{(\lambda_0)}, \hat{\zeta}^{(\lambda_0)}, \theta^{(\lambda_0)})\}$

for $t = 1, \ldots, T$
- $\{(\eta^{(\lambda_t)}, \zeta^{(\lambda_t)}, \hat{\eta}^{(\lambda_t)}, \hat{\zeta}^{(\lambda_t)})\} \leftarrow \{(\eta^{(\lambda_{t-1})}, \zeta^{(\lambda_{t-1})}, \hat{\eta}^{(\lambda_{t-1})}, \hat{\zeta}^{(\lambda_{t-1})})\}$
- Calculate $\mathcal{R}(\lambda_t)$ by searching tree by SORF with $\{(\eta^{(\lambda_t)}, \zeta^{(\lambda_t)}, \hat{\eta}^{(\lambda_t)}, \hat{\zeta}^{(\lambda_t)})\}$ as feasible solutions.
- Solve (14) with $\mathcal{R} = \mathcal{R}(\lambda_t)$ and obtain $\{(\eta^{(\lambda_t)}, \zeta^{(\lambda_t)}, \hat{\eta}^{(\lambda_t)}, \hat{\zeta}^{(\lambda_t)}, \theta^{(\lambda_t)})\}$.

end for

Output: $\{(\eta^{(\lambda_t)}, \zeta^{(\lambda_t)}, \hat{\eta}^{(\lambda_t)}, \hat{\zeta}^{(\lambda_t)}, \theta^{(\lambda_t)})\}_{t \in [T]}$

where $Z_j[s] := \min_{i \in [n], \tilde{x}_{ij} = s} x_{ij}$ and $\overline{Z}_j[s] := \max_{i \in [n], \tilde{x}_{ij} = s} x_{ij}$ are the smallest and the largest original values, respectively, in $X_j$ whose discretized result is $s$. This means that the thresholds in the original space to assign the discretized values are taken at midpoints for each feature (see the lower panel in Fig. 4). This result can also be used for predicting test samples; if the test sample is in $[u, v]$, it is discretized as in $\tilde{x}'$ above.

C Regularization path of SORF

In this section, for simplicity, we consider the situation where $\rho = \lambda$, i.e., we determine only one regularization parameter. In order for the pruning to work well, it is better to derive small $R_{\rho, \lambda}$ in Theorem[2] As discussed after presenting Theorem[2] it is advantageous to know another solution close to the one being computed. Thus, when we compute the optimization for multiple $\lambda$ as $\lambda_0 > \lambda_1 > \cdots > \lambda_T$ (e.g., model selections), first we compute the solution for the largest $\lambda_0$, then compute the solution for the next largest $\lambda_1$ after the features are safely screened by the solutions for $\lambda_0$. In this paper, we take $\lambda_{\max}$ as $\lambda_0$, where $\lambda_{\max}$ is the smallest $\lambda$ when $\eta^* = 0$ and $\zeta^* = 0$ holds (i.e., all features are inactive). This can be computed in [18]:

$$\lambda_{\max} := \max \left\{ \max_{j \in [d]} \left| \sum_{i \in [n]} x_{ij} (y_i - \bar{y}) \right|, \max_{k \in \mathcal{R}} \left| \sum_{i \in [n]} r_k (\bar{x}_i) (y_i - \bar{y}) \right| \right\},$$

where $\bar{y}$ is the sample mean of $\{y_i\}_{i \in [n]}$. Its upper bound can be easily computed as follows. The following relationship is derived from [15].

$$\left| \sum_{i \in [n]} r_k (\bar{x}_i) (y_i - \bar{y}) \right| \leq \max \left\{ \sum_{i : y_i - \bar{y} > 0} r_k (\bar{x}_i) (y_i - \bar{y}), - \sum_{i : y_i - \bar{y} < 0} r_k (\bar{x}_i) (y_i - \bar{y}) \right\}.$$

The regularization path computation algorithm of SORF is shown in Algorithm[2]