Safe Feature Pruning for Sparse High-Order Interaction Models

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Abstract

Taking into account high-order interactions among covariates is valuable in many practical regression problems. This is, however, computationally challenging task because the number of high-order interaction features to be considered would be extremely large unless the number of covariates is sufficiently small. In this paper, we propose a novel efficient algorithm for LASSO-based sparse learning of such high-order interaction models. Our basic strategy for reducing the number of features is to employ the idea of recently proposed safe feature screening (SFS) rule. An SFS rule has a property that, if a feature satisfies the rule, then the feature is guaranteed to be non-active in the LASSO solution, meaning that it can be safely screened-out prior to the LASSO training process. If a large number of features can be screened-out before training the LASSO, the computational cost and the memory requirement can be dramatically reduced. However, applying such an SFS rule to each of the extremely large number of high-order interaction features would be computationally infeasible. Our key idea for solving this computational issue is to exploit the underlying tree structure among high-order interaction features. Specifically, we introduce a pruning condition called safe feature pruning (SFP) rule which has a property that, if the rule is satisfied in a certain node of the tree, then all the high-order interaction features corresponding to its descendant nodes can be guaranteed to be non-active at the optimal solution. Our algorithm is extremely efficient, making it possible to work, e.g., with 3rd order interactions of 10,000 original covariates, where the number of possible high-order interaction features is greater than $10^{12}$.

Keywords: Machine Learning, Sparse Modeling, Safe Screening, High-Order Interaction Model
1 Introduction

Sparse learning of high-dimensional models has been actively studied in the past decades [1]. Among many approaches, LASSO [2] is one of the most widely used methods, and its statistical and computational properties have been intensively investigated. The main task in LASSO training is to identify the set of active features whose coefficients turn out to be nonzero at the optimal solution. In case we know which features would be active, the solution trained only with those active features is guaranteed to be optimal. This observation suggests so-called feature screening approaches, where we first screen-out a subset of features which would be non-active at the optimal solution, and then train a LASSO only with the remaining features. The LASSO training can be highly efficient if a majority of non-active features could be screened out a priori.

Existing screening approaches are categorized into two types. In the first type of approaches called non-safe feature screening, a subset of features which are predicted to be non-active at the optimal solution are first identified, and then a LASSO is trained after screening out those features. Since the predictions might be incorrect, the obtained LASSO solution is used for checking if all the screened-out features are really non-active. Unless all of them are confirmed to be truly non-active, some of those features must be brought back into the working feature set, and a LASSO is trained again with the updated working feature set. In non-safe screening approaches, such a trial-and-error process must be repeated until all the optimality conditions are satisfied.

Another type of approaches called safe feature screening (SFS) was recently introduced by El Ghaoui et al. [3]. The advantage of SFS is that the screened-out features are guaranteed to be non-active at the optimal solution, meaning that the iterative trial-and-error process is not necessary. The safe feature screening approach has been receiving an increasing attention in the literature, and several extensions have been recently studied [3, 4, 5, 6]. SFS is especially useful when the number of features is extremely large and the entire data set cannot be stored in the memory. Once a subset of features are screened-out by SFS, those features can be completely removed from the memory because they would never be accessed during the following LASSO training process.

In this paper, we study sparse learning problems for high-order interaction models. Let us denote the original training set by \( \{(z^i, y^i)\}_{i \in [n]} \), where \( n \) is the number of training instances, \( z^i := [z^i_1 \ldots z^i_d]^T \) is the \( d \)-dimensional original covariates, and \( y^i \) is the scalar response. In high-order interaction models up to order \( r \), we have \( D = \sum_{\kappa \in [r]} \binom{d}{\kappa} \) features. Thus, the expanded \( n \times D \) design matrix \( X \) has the form:

\[
X := \begin{bmatrix}
    z^1_1 & \ldots & z^1_d & z^2_1 z^1_2 & \ldots & z^2_1 z^{d-1}_d & \ldots & z^1_1 z^1_2 \ldots z^1_r & \ldots & z^1_1 z^1_2 \ldots z^{d-r+1}_d z^{d-r+2}_d \ldots z^1_d \\
    \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\
    z^n_1 & \ldots & z^n_d & z^n_1 z^n_2 & \ldots & z^n_1 z^{d-1}_d & \ldots & z^n_1 z^n_2 \ldots z^n_r & \ldots & z^n_1 z^n_2 \ldots z^{d-r+1}_d z^{d-r+2}_d \ldots z^n_d
\end{bmatrix}.
\] (1)
Figure 1: The underlying tree structure among high-order interaction features ($d = 4$ and $r = 3$).

Then, we consider LASSO problem

$$
\beta^* := \arg\min_{\beta \in \mathbb{R}^D} \frac{1}{2} \| y - X\beta \|^2_2 + \lambda \| \beta \|_1,
$$

(2)

where $y := [y^1 \ldots y^n]^\top \in \mathbb{R}^n$ and $\lambda > 0$ is the regularization parameter which makes a balance between the first loss term and the second regularization term. Unless the original input dimension $d$ is fairly small, the number of features $D$ would be extremely large. For example, when $d = 10,000$ and $r = 3$, we have $D > 10^{12}$ features. Although a variety of LASSO training algorithms have been proposed, it is still computationally infeasible to solve such a high-dimensional LASSO problem. Furthermore, it would also be difficult to load the entire (expanded) data set in the memory, making it hard to use existing LASSO solvers.

Our basic strategy is to develop an SFS method particularly suited for high-order interaction models, and screen-out majority of non-active features before actually training the model by the LASSO. Unfortunately, any existing SFS methods cannot be used for our problem because it is impossible to evaluate each SFS rule for each of the extremely large $D$ features. Our key idea for overcoming this computational difficulty is to exploit the underlying tree structure among high-order interaction features as depicted in Figure 1.

We propose, what we call, safe feature pruning (SFP), a novel safe feature screening method for high-order interaction models. Our SFP rule is a condition defined in each node of the tree such that, if the condition is satisfied in a certain node, then all the high-order interaction features corresponding to its descendant nodes are guaranteed to be non-active at the optimal solution. It allows us to safely screen-out a large number of high-order interaction features.

2 LASSO for high-order interaction models

2.1 Problem setup

In this paper we study sparse learning of high-order interaction models. Throughout the paper, we assume that $z^i_j, (i,j) \in [n] \times [d]$ is standardized to $[0,1]$. As mentioned in the previous section, the training set
in the original covariate domain is denoted as \{(z^i, y^i)\}_{i\in[n]} where \(z^i \in [0,1]^d\) and \(y^i \in \mathbb{R}\). In addition, we also denote the training set in the expanded feature domain as \{(x^i, y^i)\}_{i\in[n]} where \(x^i \in [0,1]^D\) is the expanded feature vector of the \(i\)th training instance, i.e., the \(i\)th row of the design matrix \(X\) in (1). Note that high-order interaction features \(x^i_j, (i, j) \in [n] \times [D]\) is also defined in \([0,1]\). Furthermore, we denote the \(j\)th column of the wide design matrix \(X\) as \(x_j, j \in [D]\). The problem we consider here is to find a sparse solution \(\beta^* = [\beta^*_1, \ldots, \beta^*_D]^\top\) by solving the LASSO problem in (2).

2.2 Preliminaries and basic idea

When the penalty parameter \(\lambda\) is sufficiently large, only a small portion of the \(D\) coefficients \(\{\beta_j^*\}_{j \in D}\) would be non-zero. We denote the index set of the active features as

\[ \mathcal{A}^* := \{ j \in [D] : \beta^*_j \neq 0 \}. \]

In convex optimization literature, it is well-known that the optimal solution does not depend on non-active variables, which is formally stated as follows.

Lemma 1. Let \(\mathcal{A}\) be an index set such that \(\mathcal{A}^* \subseteq \mathcal{A} \subseteq [D]\). Then, the solution of the LASSO problem (2) is given as

\[ \beta^*_\mathcal{A} = \arg\min_{\beta \in \mathbb{R}^{\lvert \mathcal{A} \rvert}} \frac{1}{2} \| y - X_{\mathcal{A}} \beta \|_2^2 + \lambda \| \beta \|_1, \quad \beta^*_\bar{\mathcal{A}} = 0, \quad (3) \]

where \(\beta^*_\mathcal{A}\) and \(\beta^*_\bar{\mathcal{A}}\) are the subvectors of \(\beta^*\) with the components in \(\mathcal{A}\) and \(\bar{\mathcal{A}} := [D] \setminus \mathcal{A}\), respectively, and \(X_{\mathcal{A}} \in [0,1]^{n \times |\mathcal{A}|}\) is a submatrix of \(X\) which only has columns indexed by \(\mathcal{A}\).

Lemma 1 indicates that, if we have an index set \(\mathcal{A} \supseteq \mathcal{A}^*\), the optimal solution \(\beta^*\) in (2) could be efficiently obtained by solving a smaller optimization problem that does not depend on all the \(D\) features but only on a subset of features in \(|\mathcal{A}|\).

Safe screening In order to find an index set \(\mathcal{A} \supseteq \mathcal{A}^*\), we employ recently introduced technique called safe feature screening (SFS) [3]. SFS enables us to find a subset of non-active features without actually solving the optimization problem. Roughly speaking, SFS algorithm for LASSO problem is based on its primal-dual relationship. The dual problem of the LASSO problem in (2) is written as

\[ \min_{\{\theta_i\}_{i \in [n]}} \frac{1}{2} \sum_{i \in [n]} (\theta_i - \frac{1}{\lambda} y^i)^2 \quad \text{subject to} \quad \sum_{i \in [n]} x^i_j \theta_i \leq 1 \quad \forall j \in [D], \quad (4) \]

where \(\{\theta_i\}_{i \in [n]}\) are the dual variables. Then, using the standard convex optimization theory (e.g., see [7]), we have the following lemma (see [3] for the proof).

Lemma 2. Let \(\{\theta_i^*\}_{i \in [n]}\) be the optimal dual solutions of the LASSO dual problem in (4). Then,

\[ \left| \sum_{i \in [n]} x^i_j \theta_i^* \right| < 1 \Rightarrow \beta^*_j = 0, \quad j \in [D]. \quad (5) \]
The key idea of SFS is to efficiently compute an upper bound $U_j$ for each $j \in [D]$ without actually solving the dual problem such that

$$U_j \geq \left| \sum_{i \in [n]} x^j_i \theta^*_i \right|$$

(6)

Lemma 2 indicates

$$U_j < 1 \Rightarrow \beta^*_j = 0,$$

meaning that a non-active coefficient $\beta^*_j$ might be identified before solving the optimization problem. After the seminal work of El Ghaoui et al [3], several approaches for efficiently computing such an upper bound have been proposed [4, 5, 6, 8]. In this paper, we particularly use an idea of using variational inequality for computing upper bounds, which was recently proposed by Liu et al. [5].

Safe screening has been used when a sequence of LASSO solutions for various values of $\lambda$ are computed (c.f., regularization path [9]). When we compute a sequence of solutions, we start from $\lambda_{\text{max}}$ where a LASSO solution for any $\lambda > \lambda_{\text{max}}$ is $\beta^* = 0$. Then, we compute a sequence of LASSO solutions for a decreasing sequence of $\lambda$ by using the previous solution as the initial warm-start solution. Upper bounds $\{U_j\}_{j \in [D]}$ in (6) can be constructed by using the optimal solution of the LASSO for another regularization parameter $\tilde{\lambda} > \lambda$, which should have been already obtained in the above context.

Tree structure and pruning rule

Unfortunately, SFS alone is not sufficient for our problem because it is intractable to compute an upper bound $U_j$ for each of the exponentially large number of features. For handling such extremely large number of features in the expanded feature domain, we exploit the underlying tree structure. We consider a simple tree structure as depicted in Figure 1. We denote each node of the tree by an index $j \in [D]$. For any node $j$ in the tree, let $D_e(j)$ be a set of its descendant nodes. Our main contribution in this paper is to develop a novel SFS method particularly designed for fitting sparse high-order interaction models. Specifically, in each node of the tree, we derive a condition called safe feature pruning (SFP) rule. Our SFP rule has the following nice property:

$$\text{SFP rule for a node } j \text{ is satisfied } \Rightarrow \left| \sum_{i \in [n]} x^j_i \theta^*_i \right| < 1 \text{ for all } j' \in D_e(j).$$

(7)

This property indicates that, if the SFP rule in a certain node $j$ of the tree is satisfied, then we can guarantee that all the high-order interaction terms corresponding to its descendant nodes can be safely screened-out.

2.3 Related works

Before presenting our main contribution, let us briefly review related works in the literature. Fitting high-order interaction models has long been desired in many regression problems. In biomedical studies, for example, many complex diseases such as cancer are known to be the consequences of high-order interaction
effects of multiple genetic factors [10] [11] [12] [13]. In the past decade, several authors proposed extensions of
the LASSO for incorporating interaction effects, and studied their statistical properties [14] [15] [16]. However,
one of these works have sufficient computational mechanisms for handling exponentially large number
of high-order interaction features. Most of these works thus focus only on 2\textsuperscript{nd}-order interaction features
for moderate number of original covariates \( d \). One commonly used heuristic for reducing the number of
interaction features is to introduce so-called strong heredity assumption [14] [15] [16], where, e.g., an interaction
term \( z_1 z_2 \) would be selected only when both of \( z_1 \) and \( z_2 \) are selected. However, such a heuristic assumption
eliminates a chance to find out novel high-order interaction features when there are no strong associations in
their marginal main effects. To the best of our knowledge, an only exceptional approach that can be applied
to high-order interaction modeling for sufficiently large data sets is itemset boosting (IB) algorithm presented
in [17]. IB algorithm is a boosting-type algorithm, where a single feature is added and the model is updated
in each step. In a nutshell, IB algorithm manages its working feature set by exploiting the underlying tree
structure as we do. However, since the working feature set in IB algorithm is non-safe (no guarantee to be
active or non-active), aforementioned trial-and-error process is necessary. We compare our approach with IB
algorithm in [14] and demonstrate that the former is computationally more efficient than the latter. Another
line of related studies is about the statistical issue such as feature selection consistency [18, 19] for high-
order interaction models. We have been studying how to apply post-selection inference framework recently
introduced in [20] to statistical inferences on high-order interaction models in [21].

\section{Safe feature pruning for high-order interaction models}

In this section we present our main result. The proposed safe feature pruning (SFP) is used when we
compute a sequence of LASSO solutions for a decreasing sequence of the regularization parameter \( \lambda \). Let
\( \lambda_{\text{max}} > \lambda_1 > \ldots > \lambda_T \) be a sequence of regularization parameter values at each of which we want to compute
the LASSO solution, where \( \lambda_{\text{max}} := \max_{j \in [D]} |x_j^\top y| \). Furthermore, we denote the optimal LASSO solutions
for those sequence of regularization parameters as \( \beta^*(\lambda_t) := [\beta_1^t(\lambda_t), \ldots, \beta_D^t(\lambda_t)]^\top \in \mathbb{R}^D \) for \( t \in [T] \).

The outline of the algorithm for computing the sequence of solutions is summarized in Algorithm \ref{alg:safe}
In line 1, we initialize \( \lambda_0 \) and \( \beta^*(\lambda_0) \) by \( \lambda_{\text{max}} \) and its corresponding solution \( \beta^*(\lambda_{\text{max}}) = \mathbf{0} \). Line 3 is the core
of our algorithm, where we find a superset \( \mathcal{A}(\lambda_t) \) of \( \mathcal{A}^*(\lambda_t) := \{ j \in [D] : \beta_j^t(\lambda_t) \neq 0 \} \) by the proposed SFP
method (see Theorem \ref{thm:superset}). In line 4, the LASSO problem is solved for obtaining \( \beta^*(\lambda_t) \) by using any LASSO
solver only with a set of features in \( \mathcal{A}(\lambda_t) \).

The following theorem is used in line 3 of the Algorithm \ref{alg:safe} Given the optimal LASSO solution \( \beta^*(\lambda_{t-1}) \)
for a regularization parameter \( \lambda_{t-1} \), for any \( \lambda_t \in (0, \lambda_{t-1}) \), we can develop a SFP rule such that, if the
\footnote{The largest regularization parameter \( \lambda_{t-1} \) can be efficiently computed again by exploiting the tree structure among
features. Specifically, for any node \( j \) and its arbitrary descendant node \( j' \), by noting that \( 0 \leq x_j^i \leq x_j^i \) for any \( i \in [n] \), we have
\( |x_j^i y| \leq \max(\sum_{i \in [n] \mid y > 0} x_j^i y | \sum_{i \in [n] \mid y > 0} x_j^i y |, \sum_{i \in [n] \mid y < 0} x_j^i y | | \sum_{i \in [n] \mid y < 0} x_j^i y | \). Using this relationship,
we can efficiently find the maximum \( |x_j^i y| \) by searching over the tree with pruning.}
Algorithm 1 An outline for computing a sequence of LASSO solutions with safe feature pruning

**Input:** \{(z^i, y^i)\}_{i \in [n]}, \{r\}, \{\lambda_t\}_{t \in [T]}

1. \(\lambda_0 \leftarrow \max_{j \in [d]} |x^\top_j y|\) and \(\beta^*(\lambda_0) \leftarrow 0\)
2. for \(t = 1, \ldots, T\) do
3. Find \(A(\lambda_t) \supseteq A^*(\lambda_t)\) by safe feature pruning (SFP) method with \((\lambda_{t-1}, \beta^*(\lambda_{t-1}))\)
4. Compute the LASSO solution \(\beta^*(\lambda_t)\) by using only a subset of features in \(A(\lambda_t)\)
5. end for

**Output:** \{\(\beta^*(\lambda_t)\)\}_{t \in [T]}

Theorem 3 (safe feature pruning with \((\lambda_{t-1}, \beta^*(\lambda_{t-1}))\)). Suppose that the optimal LASSO solution \(\beta^*(\lambda_{t-1})\) is available for a regularization parameter \(\lambda_{t-1}\). In addition, for any \(\lambda_t \in (0, \lambda_{t-1})\), define

\[
P_1 := \frac{1}{2} \left( ||x_j||_2 \|b\|_2 + \sum_{i : c_i > 0} c_i x^j_i \right), \quad P_2 := \frac{1}{2} \left( ||x_j||_2 \|b - \frac{a^\top b}{\|a\|_2} a\|_2 + \sum_{i : d_i > 0} d_i x^j_i \right),
\]

\[
M_1 := \frac{1}{2} \left( ||x_j||_2 \|b\|_2 - \sum_{i : c_i < 0} c_i x^j_i \right), \quad M_2 := \frac{1}{2} \left( ||x_j||_2 \|b - \frac{a^\top b}{\|a\|_2} a\|_2 - \sum_{i : d_i < 0} d_i x^j_i \right),
\]

where

\[
a := \frac{1}{\lambda_{t-1}} \sum_{j \in [d] : \beta^*_j(\lambda_{t-1}) \neq 0} x_j \beta^*_j(\lambda_{t-1}), \quad b := \left( \frac{1}{\lambda_t} - \frac{1}{\lambda_{t-1}} \right) y + a,
\]

\[
c := \left( \frac{1}{\lambda_t} + \frac{1}{\lambda_{t-1}} \right) y - \frac{\lambda_{t-1}}{\lambda_t} a, \quad d := c - \frac{a^\top b}{\|a\|_2} a.
\]

Then, for any node \(j\) in the tree such that \(x_j \neq 0\),

\[
\max\{U^+_j, U^-_j\} < 1 \quad \Rightarrow \quad \beta^*_j(\lambda_t) = 0 \quad \text{for all} \quad j' \in De(j), \quad (8)
\]

where, when \(\lambda_{t-1} = \lambda_{\max} = \max_{j \in [d]} |x^\top_j y|\),

\[
U^+_j := P_1, \quad U^-_j := M_1,
\]

while, when \(\lambda_{t-1} < \lambda_{\max}\),

\[
U^+_j := \max\{P_1, P_2\}, \quad U^-_j := \max\{M_1, M_2\}.
\]

Furthermore, when the original covariates \(z^i_j \in \{0, 1\}\) for \(i \in [n]\) and \(j \in [d]\), then

\[
U^+_j := \begin{cases} P_2 & \text{if } - \sum_{i \in [n] : a_{i} < 0} a_{i} x^i_j < \frac{a^\top b}{\|b\|_2} \\ \max\{P_1, P_2\} & \text{otherwise} \end{cases},
\]

\[
U^-_j := \begin{cases} M_2 & \text{if } \sum_{i \in [n] : a_{i} > 0} a_{i} x^i_j < \frac{a^\top b}{\|b\|_2} \\ \max\{M_1, M_2\} & \text{otherwise} \end{cases}.
\]
The proof of Theorem 3 is presented in supplementary appendix A. In the depth-first search in the tree, if we encounter a node with $x_j = 0$, then we can, of course, guarantee that its descendant nodes would be non-active. Note that the SFP condition in (8) can be computed by using the sparse previous solution $\beta^*(\lambda_{t-1})$ and a set of information available in the node $j$. It means that, if the SFP rule is satisfied at a certain node $j$ in the tree, we can stop searching over the tree and all its descendant nodes can be screened-out.

Our pruning approach relies on the fact that original covariates are defined in $[0, 1]$. For example, it is easy to note that

$$x_j^i \leq x_j^i \forall (j', j) \in [D]^2 \text{ such that } j' \in De(j).$$

Such diminishing monotonicity properties on the high-order interaction features indicate that higher-order interaction features which correspond to deep nodes in the tree are more likely to be non-active than those corresponding to shallow nodes. For example, if the original covariates are defined in binary domain, i.e., $x_j \in \{0, 1\}$, then the features would be more sparse as we consider higher-order interactions. As we see in the following experiment section, when the original covariates are sparse, our pruning approach works quite well.

For covariates defined in binary domain, where values 1 and 0 respectively indicate the existence and the non-existence of a certain property, it is easy to interpret interaction effects because they simply indicate co-existence of multiple properties. On the other hand, for continuous covariates, the interpretation of an interaction effect would depend on its coding. If each covariate is defined in $[0, 1]$ domain, and the value represents the “degree” of an existence of a certain property, then an interaction effect can be similarly understood as the “degree” of co-existence of multiple properties.

4 Experiments

In this section, we demonstrate the effectiveness of the proposed safe feature pruning (SFP) approach through numerical experiments.

4.1 Experimental setup

In the experiments, we computed a sequence of LASSO solutions at a decreasing sequence of regularization parameters $\lambda$. Specifically, we started from $\lambda_0 = \lambda_{\max} := \max_{j \in [D]} |x_j^T y|$, and considered a sequence $\lambda_t = (1 - 0.1/\sqrt{t})\lambda_{t-1}$ for $t = 1, 2, \ldots$ until $\lambda_t/\lambda_{\max} < 0.01$. We considered interaction model up to $r = 3^{rd}$ order. As the LASSO solver, we used shooting algorithm. All the codes were implemented by ourselves in C++, and all the experiments were conducted by HP workstation Z800 (Xeon(R) CPU X5675 (3.07GHz), 48GB MEM).
4.2 Synthetic data experiments

First, we investigated the advantage of the proposed pruning scheme by comparing the computational costs with and without the safe feature pruning (SFP) on small synthetic data sets. The synthetic data were generated from

\[ y = X\beta + \varepsilon, \varepsilon \sim N(0, \sigma^2 I), \]

where \( y \in \mathbb{R}^n \) is the response vector, \( X \in \mathbb{R}^{n \times D} \) is the input design matrix, \( \beta \in \mathbb{R}^D \) is the coefficient vector, and \( \varepsilon \in \mathbb{R}^n \) is the Gaussian noise vector. Here, we did not actually compute the extremely wide design matrix \( X \) because it has exponentially large number of columns. Instead, we generated a random binary matrix \( Z \in \{0, 1\}^{n \times d} \) and each expanded high-order interaction feature \( x^i_j \) was generated from the \( i^{th} \) row of \( Z \) only when it was needed. For simplicity and computational efficiency, we assumed that the covariates (hence interaction features as well) are binary, and the sparsity \( \eta \in [0, 1] \) (the fraction of 0s in the entries of \( Z \)) was changed among 95%, 90%, 85%, 80% to see how sparsity can be exploited for efficient computation. We set \( \beta = 0, \sigma = 0.1, n = 1,000 \) and \( d = 1,000 \). The total computation time in seconds and the average pruning rates are shown in Table 1. The results indicate that SFP is fairly effective for computational efficiency. Furthermore, as the data set gets sparse, the advantage of SFP increases.

4.3 Benchmark data experiments

Next, we compared the proposed SFP approach with itemset boosting (IB) algorithm presented in [17]. IB algorithm is a variant of working set method, where a set of working features and a LASSO solution trained only with the working feature set are maintained in each step. IB algorithm updates the working set by adding a feature that most violates the current optimality condition. The core of IB algorithm is that it can efficiently find the most violating feature by exploiting the underlying tree structure and anti-monotonicity property. Since there is no guarantee that all the features not in the working set are truly non-active in IB algorithm, one must repeat trial-and-error process until all the optimality conditions are satisfied.

We used seven benchmark datasets in libsvm dataset repository [22] as listed in Table 2. In each dataset, we restrict the maximum numbers of instances \( n \) and covariates \( d \) to be 10,000. Although some of these datasets are for binary classifications, we regarded the response \( \{y_i\}_{i \in [n]} \) be real variables, and standardized them so that they have the mean zero and the variance one. As we discussed in §3, we only considered

![Table 1: Computation time in seconds for computing a sequence of LASSO solutions.](image)
Table 2: Total computation time for computing a sequence of LASSO solutions in high order interaction models (seconds) for various benchmark datasets.

| Data     | n    | d    | \(\delta = 1.5\)         | \(\delta = 2.0\)         |
|----------|------|------|---------------------------|---------------------------|
|          |      |      | IB       | SFP       | IB       | SFP       |
| usps     | 7,291| 256  | 10514.81 | 4506.82   | 1373.21  | 1907.21   |
| madelon  | 2,000| 500  | 6685.99  | 1865.42   | 982.69   | 358.08    |
| protein  | 10,000| 357  | 33320.01 | 1975.00   | 20593.55 | 1297.30   |
| mnist    | 10,000| 780  | 47985.89 | 10047.49  | 7418.59  | 4009.85   |
| r1v1_bin | 10,000| 10,000| 1707.81  | 734.60    | 2893.67  | 826.56    |
| real-sim | 10,000| 10,000| 11122.02 | 3583.31   | 15101.93 | 3473.46   |
| news20   | 10,000| 10,000| > 100K   | 34988.51  | > 100K   | 28568.94  |

binary original covariates. For a continuous covariate in the original data set, we first standardized it to have the mean zero and the variance one, and then represented the covariate by two binary variables, each of which indicates whether the value is greater than \(\delta\) or the value is smaller than \(-\delta\), where \(\delta \in \{1.5, 2.0\}\). The computation time in seconds are shown in Table 2. We see in the table that the proposed SFP is faster than IB algorithm in almost all cases. Figure 2 shows the results on usps, protein and mnist data sets (same figures for other datasets are presented in supplementary Appendix B). For each data set, (a) computation time in seconds, (b) the number of traverse nodes, and (c) the number of active features are plotted for each regularization parameter values. We first see in (a) and (b) that the computation time is roughly proportional to the number of traverse nodes. Comparing SFP and IB algorithm in (a) and (b), the former is faster than the latter especially when \(\lambda\) is small. Furthermore, the computational costs of IB algorithm in (a) and (b) seems to be positively correlated with the number of active features in (c). A possible explanation of these observations is that, when \(\lambda\) is small, IB algorithm must repeatedly search over the tree for finding out which feature would be coming into the working set since there are many active features that newly enters to the working set. On the other hand, the computational cost of the proposed SFP did not increase as IB algorithm because SFP approach can screen-out large number of features at the same time. The plots in (c) suggests that, when \(\lambda\) is small, many high-order interaction features (2nd and 3rd order interaction features are shown in green and blue, respectively) become active, indicating the potential advantage of considering high-order interaction features.

5 Conclusion

We proposed a safe feature screening rules called *safe feature pruning (SFP)* for high-order interaction models. A key advantage of SFP is that, by exploiting the underlying tree structure among high-order
interaction features and its anti-monotonicity property, a large number of high-order interaction features can be simultaneously screened out by evaluating a few simple conditions on the tree. As long as the original covariates are sufficiently sparse, our algorithm can be used for high-order interaction models with the number of features \( D > 10^{12} \). Our next future work would be to extend this idea to classification setups.

A Proof of Theorem 3

In this section we prove Theorem 3. To prove the theorem, we use a recent results on safe feature screening developed in [5]. Our technical contribution in the following proof is in bounding the screening condition of a feature in a node based only on the information available in its ancestor node, which is the crucial property of the proposed safe feature pruning.

Although the notations and formulations are different, the following proposition is essentially identical
with the recent result in \cite{5}.

**Proposition 4** \cite{5}. Consider a pair of regularization parameters $\lambda_1$ and $\lambda_2$ for the LASSO problem in \cite{4} such that $\max_{j \in [D]} |x_j^* y| \geq \lambda_1 > \lambda_2 > 0$, and denote the optimal dual variable vectors for these two problems as $\theta_1^*$ and $\theta_2^*$, respectively. In addition, define

$$a := \frac{y}{\lambda_1} - \theta_1^*, \quad b := \frac{y}{\lambda_2} - \theta_1^*, \quad c := \frac{y}{\lambda_2} + \theta_1^*.$$ 

Furthermore, for each $j \in [D]$, define

$$u_j^+ := \begin{cases} \frac{1}{2}(x_j^T c + \|x_j\|_2\|b\|_2) & \text{if } \frac{b^T a}{\|b\|_2} \leq -\frac{x_j^T a}{\|x_j\|_2} \\ \frac{1}{2}(x_j^T c + \|x_j\|_2\|b\|_2) & \text{otherwise.} \end{cases} \quad (9)$$

$$u_j^- := \begin{cases} \frac{1}{2}(-x_j^T c + \|x_j\|_2\|b\|_2) & \text{if } \frac{b^T a}{\|b\|_2} \leq \frac{x_j^T a}{\|x_j\|_2} \\ \frac{1}{2}(-x_j^T c + \|x_j\|_2\|b\|_2) & \text{otherwise.} \end{cases} \quad (10)$$

Then, for $j \in [D],

$$\max\{u_j^+, u_j^-\} < 1 \quad \Rightarrow \quad |x_j^T \theta_2^*| < 1,$$

i.e., the $j^{th}$ feature is non-active in the optimal solution of LASSO with the regularization parameter $\lambda_2$.

For the proof of this proposition, see \cite{5}.

**Proof of Theorem** \cite{4} Remember that, for a feature indexed by $j$, a feature indexed by $j'$ represent a feature corresponding to one of its descendant nodes, i.e., $j' \in De(j)$. To prove the theorem, using the result of Proposition 3 it is suffice to show that

$$U_j^+ < 1 \quad \Rightarrow \quad u_{j'}^+ < 1 \quad \text{and} \quad U_j^- < 1 \quad \Rightarrow \quad u_{j'}^- < 1. \quad (11)$$

First, we prove the case with $\lambda_{t-1} = \lambda_{\max} = \max_{j \in [D]} |x_j^T y|$. In this case, from the primal-dual relationship of the optimal LASSO solution, the optimal dual solution at $\lambda_{t-1}$ is written as $\theta_{t-1}^* = \frac{y}{\lambda_{t-1}}$. Since it means $a = 0$, from (9) and (10),

$$u_j^+ = \frac{1}{2}(x_j^T c + \|x_j\|_2\|b\|_2), \quad u_j^- = \frac{1}{2}(-x_j^T c + \|x_j\|_2\|b\|_2).$$

Using the fact that

$$x_j^T c = \sum_{i; c_i > 0} c_i x_j^i + \sum_{i; c_i < 0} c_i x_j^i \leq \sum_{i; c_i > 0} c_i x_j^i \leq \sum_{i; c_i > 0} c_i x_j^i \quad (12)$$

and

$$\|x_j\|_2 \leq \|x_{j'}\|_2,$$
we have

\[ u^+_j = \frac{1}{2}(x^+_j c + \|x^+_j\|_2 \|b\|_2) \leq \frac{1}{2} \left( \sum_{i : c_i > 0} c_i x^+_i + \|x^+_j\|_2 \|b\|_2 \right) = P_1, \]  

(13)

\[ u^-_j = \frac{1}{2}(-x^-_j c + \|x^-_j\|_2 \|b\|_2) \leq \frac{1}{2} \left( -\sum_{i : c_i < 0} c_i x^-_i + \|x^-_j\|_2 \|b\|_2 \right) = M_1, \]  

(14)

which proves the theorem when \( \lambda_t = \lambda_{\max} \).

Next, we consider \( \lambda_t < \lambda_{\max} \). In this case, we cannot decide which of the two cases in (9) and (10) are applied. In the first case of (9) and (10) are applied, we can show that

\[ u^+_j \leq P_1 \quad \text{and} \quad u^-_j \leq M_1 \]

in the same way as (13) and (14). On the other hand, when the second case of (9) is applied, we can show that

\[ u^+_j = \frac{1}{2}(x^+_j c + \|x^+_j\|_2 \|b\|_2) \leq \frac{1}{2} \left( \sum_{i : d_i > 0} d_i x^+_i + \sum_{i : d_i < 0} d_i x^-_i \right) \leq \sum_{i : d_i > 0} d_i x^+_i \leq \sum_{i : d_i > 0} d_i x^-_i \]

where we used

\[ x^+_j d = \sum_{i : d_i > 0} d_i x^+_i + \sum_{i : d_i < 0} d_i x^-_i \leq \sum_{i : d_i > 0} d_i x^+_i \]

and

\[ \|x^+_j - \frac{x^+_j a}{\|a\|_2^2} a\|_2 \leq \sqrt{\|x^+_j\|_2^2 - \left( \frac{x^+_j a}{\|a\|_2^2} \right)^2} \leq \|x^+_j\|_2 \]

When the second case of (14) is applied, we can show the following in the same way as above:

\[ u^-_j = \frac{1}{2}(-x^-_j c + \|x^-_j\|_2 \|b\|_2) \leq \frac{1}{2} \left( -\sum_{i : d_i < 0} d_i x^-_i + \sum_{i : d_i > 0} d_i x^+_i \right) \leq \sum_{i : d_i < 0} d_i x^-_i \]

Finally, when the original covariates \( z^+_i \) is binary, we can judge which of the two cases in (13) and (14) are applied by using the information available at the node \( j \), and a slightly tighter bounds can be obtained (the proof of how one can make this judgment is omitted, but it can be shown in a similar manner as above).

\[ \blacksquare \]

B Additional Experimental Results

In this section, we show the results on several benchmark datasets. For each dataset, (a) Computation time in seconds, (b) The number of traverse nodes, (c) The number of active features, (d) The number of solving
LASSO in IB, (e) The number of non-screened out features and total active features, (f) Computation total time in seconds are plotted in the following figures with $\delta = 1.5$ (left) and $\delta = 2.0$ (right).

B.1 Results on usps

(a) Computation time in seconds

(b) The number of traverse nodes

(c) The number of active features
(d) The number of solving LASSO in IB

(e) The number of non-screened out features and total active features

(f) Computation total time in seconds
B.2 Results on madelon

(a) Computation time in seconds

(b) The number of traverse nodes

(c) The number of active features
(d) The number of solving LASSO in IB

(e) The number of non-screened out features and total active features

(f) Computation total time in seconds
B.3 Results on protein

(a) Computation time in seconds

(b) The number of traverse nodes

(c) The number of active features
(d) The number of solving LASSO in IB

(e) The number of non-screened out features and total active features

(f) Computation total time in seconds
B.4 Results on mnist

(a) Computation time in seconds

(b) The number of traverse nodes

(c) The number of active features
(d) The number of solving LASSO in IB

(e) The number of non-screened out features and total active features

(f) Computation total time in seconds
B.5 Results on rcv1_binary

(a) Computation time in seconds

(b) The number of traverse nodes

(c) The number of active features
(d) The number of solving LASSO in IB

(e) The number of non-screened out features and total active features

(f) Computation total time in seconds
B.6 Results on real-sim

(a) Computation time in seconds

(b) The number of traverse nodes

(c) The number of active features
(d) The number of solving LASSO in IB

(e) The number of non-screened out features and total active features

(f) Computation total time in seconds
B.7 Results on news20

(a) Computation time in seconds

(b) The number of traverse nodes

(c) The number of active features
(d) The number of solving LASSO in IB

(e) The number of non-screened out features and total active features

(f) Computation total time in seconds
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