Learning Hierarchical Interactions at Scale: A Convex Optimization Approach

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Abstract

In many learning settings, it is beneficial to augment the main features with pairwise interactions. Such interaction models can be often enhanced by performing variable selection under the so-called strong hierarchy constraint: an interaction is non-zero only if its associated main features are non-zero. Existing convex optimization based algorithms face difficulties in handling problems where the number of main features \( p \sim 10^3 \) (with total number of features \( \sim p^2 \)). In this paper, we study a convex relaxation which enforces strong hierarchy and develop a scalable algorithm for solving it. Our proposed algorithm employs a proximal gradient method along with a novel active-set strategy, specialized screening rules, and decomposition rules towards verifying optimality conditions. Our framework can handle problems having dense design matrices, with \( p = 50,000 \) (\( \sim 10^9 \) interactions)—instances that are much larger than current state of the art. Experiments on real and synthetic data suggest that our toolkit hierScale outperforms the state of the art in terms of prediction and variable selection and can achieve over a 1000x speed-up.

1 Introduction

In many machine learning applications, augmenting main effects with pairwise interactions can lead to better statistical models [5]. Given a response vector \( y \in \mathbb{R}^n \) and data matrix \( X = [X_1, X_2, \ldots, X_p] \in \mathbb{R}^{n \times p} \) we consider a linear model of the form:

\[
y = \beta_0 + X\beta + \sum_{i<j} \theta_{ij}X_i \times X_j + \epsilon,
\]

where \( \times \) denotes element-wise multiplication and \( \epsilon \) is a noise vector (with small \( \ell_2 \)-norm). Above, \( \beta_0 \) is the intercept, \( X\beta \) corresponds to the main effects and \( \sum_{i<j} \theta_{ij}X_i \times X_j \) denotes the interaction effects. The goal here is to learn the coefficients \( \beta, \theta \). For small \( n \), this quickly leads to an ill-posed

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problem as the total number of coefficients: \( p + \binom{p}{2} \) can far exceed \( n \). Thus, imposing sparsity can be beneficial from both the statistical and computational viewpoints. While vanilla sparsity-inducing regularization methods (e.g., using \( \ell_0 \) or \( \ell_1 \) norm) can help, structured sparsity can be much more effective in this setting. Particularly, we consider the strong hierarchy (SH) property \([17, 5]\) which states that an interaction term should be non-zero only if its corresponding main effect terms are both non-zero, i.e.,

**Strong Hierarchy (SH):** \( \theta_{ij} \neq 0 \implies \beta_i \neq 0 \) and \( \beta_j \neq 0 \)

SH is a natural property that is widely used in high-dimensional statistics \([5]\): it leads to interpretable models with good predictive performance.

The problem of variable selection under strong hierarchy has been widely studied in the literature. For example, Wu et al. \([25]\), Hao and Zhang \([12]\) developed heuristic (greedy) approaches. Choi et al. \([8]\), Bien et al. \([5]\), Lim and Hastie \([16]\), She et al. \([21]\) introduced more principled regularization-based formulations and corresponding algorithms. While the results of the regularization-based formulations are impressive, two main issues are present (i) the choice of regularization (or penalty) the authors make are somewhat adhoc and (ii) the algorithms can have difficulty scaling to large \( p \) (e.g., 50,000). In this paper, we tackle these two issues. For (i), we propose a formulation that is transparently derived from the convex relaxation of a natural mixed integer program (MIP) that enforces SH. To address (ii), we develop a novel scalable algorithm that effectively exploits the sparse group structure of the problem. Our algorithm combines a proximal method with efficient screening, novel decomposition rules for verifying optimality (in parallel) and identifying sub-optimal variables and groups (to be used in further optimization). We also propose a new method designed to avoid costly gradient evaluations and a safe screening rule to detect zero variables a-priori. Our algorithm is available through our open-source toolkit \textit{hierScale}.

**Problem Formulation:** In what follows, we denote the interaction column \( X_i \ast X_j \) by \( \tilde{X}_{ij} \).

Performing variable selection under the strong hierarchy constraint for model \((1)\) can be naturally expressed using \( \ell_0 \) regularization:

\[
\begin{align*}
\min_{\beta, \theta} \quad & f(\beta, \theta) + \alpha_1 \|\beta\|_0 + \alpha_2 \|\theta\|_0 \\
\text{s.t.} \quad & \theta_{ij} \neq 0 \implies \beta_i \neq 0 \text{ and } \beta_j \neq 0
\end{align*}
\]  

where, \( f(\beta, \theta) = \frac{1}{2} \| y - X\beta - \sum_{i<j} \tilde{X}_{ij} \theta_{ij} \|_2^2 \), and \( \| u \|_0 \) denotes the number of non-zeros in the vector \( u \). The regularization parameters \( \alpha_1 \) and \( \alpha_2 \) control the number of non-zeros in \( \beta \) and \( \theta \), respectively. Note that we ignore the intercept term to simplify the presentation. Problem \((2)\) can

\footnote{The toolkit will be available on Github soon.}
be modelled using the following mixed integer formulation

$$\min_{\beta, \theta, z} f(\beta, \theta) + \alpha_1 \sum_i z_i + \alpha_2 \sum_{i<j} z_{ij}$$

s.t. 
- $|\beta_i| \leq Mz_i, \ \forall \ i \in [p]$ 
- $|\theta_{ij}| \leq Mz_{ij}, \ \forall \ i < j$ 
- $z_i \geq z_{ij}, \ z_j \geq z_{ij}, \ \forall \ i < j$ 
- $z_i \in \{0, 1\} \ \forall \ i, \ z_{ij} \in \{0, 1\} \ \forall \ i < j$

(3)

where $M$ is a large constant chosen such that any optimal solution $\beta^*, \theta^*$ to (2) satisfies $\|\beta, \theta\|_\infty \leq M$. Here $z_i = 0$ implies $\beta_i = 0$ and similarly $z_{ij} = 0$ implies $\theta_{ij} = 0$. Problem (3) is known to be NP-Hard [18] and can be very difficult to scale. Thus, our focus will be on solving its convex relaxation—see Lemma 1. For easier presentation we introduce some notation. For every $i \in \{1, 2, \ldots, p\}$, we define $G_i$ as the set of all interaction indices corresponding to main effect $i$, i.e.,

$$G_i \equiv \{(1, i), (2, i), \ldots, (i - 1, i), (i, i + 1), \ldots, (i, p)\}.$$

We use the notation $\theta_{G_i}$ to refer to the vector of $\theta_{ij}$’s whose indices are in $G_i$ and the notation $\theta$ to refer to the vector of all the $\theta_{ij}$’s in the model. The following lemma presents a convex relaxation of the MIP in Problem (3):

**Lemma 1.** A convex relaxation of Problem (3) is:

$$\min_{\beta, \theta} F(\beta, \theta) \equiv f(\beta, \theta) + \Omega(\beta, \theta)$$

(4)

s.t. $\|\beta\|_\infty \leq M, \|\theta\|_\infty \leq M$

where, $\Omega(\beta, \theta) \equiv \lambda_1 \sum_{i=1}^p \max\{|\beta_i|, \|\theta_{G_i}\|_\infty\} + \lambda_2 \|\theta\|_1$ and $\lambda_1 \equiv \alpha_1 / M, \lambda_2 \equiv \alpha_2 / M$.

The focus of the paper will be on solving (4). Note that if an upper bound $M$ is not known, we can always set $M = \infty$. It can be shown [5] that a solution to (4) satisfies SH with probability one, when $y$ is absolutely continuous with respect to the Lebesgue measure.

The following remark establishes a conceptual link between a Lasso solution and a solution to Problem (4).

**Remark 1.** If we apply a vanilla Lasso to the interactions problem (i.e., solve $\min_{\beta, \theta} f(\beta, \theta) + \lambda \|\beta\|_1 + \lambda \|\theta\|_1$), then it need not satisfy SH. However, if a Lasso solution satisfies (i) SH and (ii) $|\beta_i| \geq \|\theta_{G_i}\|_\infty$ for all $i$; then it is optimal for Problem (4) with $M = \infty$ and $\lambda_1 = \lambda_2 = \lambda$.

**Prior Work:** A very popular approach in the literature is the Hierarchical Lasso [5], which enforces SH by solving the following convex problem

$$\min_{\beta, \theta} f(\beta, \theta) + \lambda \sum_{i=1}^p \max\{|\beta_i|, \|\theta_{G_i}\|_1\} + \lambda \|\theta\|_1$$

(5)
Lemma 2 presents a MIP formulation corresponding to the Hierarchical Lasso. This sheds light onto its undesirable statistical properties when compared to our relaxation (4).

**Lemma 2.** The Hierarchical Lasso is a relaxation of the following MIP formulation with $\alpha = \lambda M$:

$$
\begin{align*}
\min_{\beta, \theta, z} & f(\beta, \theta) + \alpha \sum_i z_i + \alpha \sum_{i<j} z_{ij} \\
\text{s.t.} & |\beta_i| \leq Mz_i, \quad \forall \ i \in [p] \\
& |\theta_{ij}| \leq Mz_{ij}, \quad \forall \ i < j \\
& z_i \geq \sum_j z_{ij} \quad \forall i \\
& z_i \in \{0, 1\} \quad \forall \ i, z_{ij} \in \{0, 1\} \quad \forall \ i < j.
\end{align*}
$$

The MIP formulation in (6) limits the number of non-zero interactions corresponding to any main effect to at most 1, e.g., we cannot have $\theta_{12} \neq 0$ and $\theta_{13} \neq 0$. This observation suggests that the Hierarchical Lasso will overly shrink the interaction terms, which can hurt its variable selection.

In addition to the Hierarchical Lasso, many methods for enforcing SH exist in the literature. The methods can be broadly categorized into multi-step methods (e.g., Wu et al. [25], Hao and Zhang [12], Bayesian and probabilistic methods (e.g., Chipman [7], Thanei et al. [22]), and regularization/optimization based methods. We will present some of the methods in the latter category as they share the most similarity with our work. Choi et al. [8] re-parameterize the interactions problem so that $\theta_{ij} = \gamma_{ij} \beta_i \beta_j$ (where $\gamma_{ij}$ is an optimization variable) and enforces sparsity by adding an $\ell_1$ norm regularization on $\beta$ and $\theta$. However, the latter approach leads to a non-convex objective, which is difficult to solve and scale. Radchenko and James [20] enforce SH by using $\ell_2$ regularization on the predictions made by every group and develop a corresponding algorithm. Lim and Hastie [16] use an overlapped group Lasso formulation to enforce SH and solve the problem by using a variant of the FISTA algorithm [2] along with strong screening rules [23] for eliminating zero variables prior to optimization. Their toolkit glinternet is the fastest toolkit for learning sparse interactions we are aware of. More recently, She et al. [21] present prediction error bounds and an algorithm for solving a formulation similar to (4), but with the $\ell_\infty$ norm replaced with $\ell_2$ norm. Unfortunately, prior work cannot easily scale beyond $p$ in the hundreds to few thousands. A main reason is that the commonly used optimization sub-routines (e.g., FISTA and ADMM) are limited by full gradient evaluations – particularly, $\nabla f(\beta, \theta)$ requires $O(np^2)$ operations and a single such evaluation can be costly (when $p \sim 50,000$). It is worth mentioning that Jenatton et al. [14] consider the problem of sparse learning under hierarchical tree structures and develop a very scalable algorithm. One of their formulations combines $\ell_\infty$ group norm and $\ell_1$ norm regularization (similar to our relaxation). However, their tree structure cannot model our formulation and so their algorithm is not applicable here.

**Contributions:** The main contribution of our work is developing an algorithm that goes well
beyond the current computational landscape. Our algorithm carefully mitigates costly full gradient evaluations (i.e., $\nabla f(\beta, \theta)$). It has four key components: (i) Proximal-gradient updates with a new screening method that can identify most of the zero variables/groups in one pass (see Section 2) (ii) Optimality decomposition rules, which allow for checking the optimality conditions in parallel and pinpointing the violating variables/groups, thus allowing us to develop problem-specific active-set updates (see Section 3) (iii) A novel method for avoiding full gradient evaluations by reusing pre-computed quantities (allowing to certify the optimality of any solution by evaluating only a small subset of $\nabla f(\beta, \theta)$) (see Section 4.1), and (iv) A new safe screening rule to identify zero variables a-priori (see Section 4.2). Finally, we note that our implementation supports multi-core processing, which can significantly speed up computation.

**Notation, etc:** We use the notation $[p]$ to refer to the set $\{1, 2, \ldots, p\}$. We denote the complement of a set $A$ by $A^c$. For a set $A \subseteq [p]$, $\beta_A$ refers to the sub-vector of $\beta$ restricted to coordinates in $A$. We use $\nabla_{\beta_A, \theta_B} f(\beta, \theta)$ to refer to the components of $\nabla f(\beta, \theta)$ corresponding to the vectors $\beta_A$ and $\theta_B$. For any scalar $a$, we define $[a]_+ = \max\{a, 0\}$; and $\text{sign}(a) = a/|a|$ if $a \neq 0$ and $\text{sign}(0) \in [-1, 1]$. A function $u \mapsto g(u)$ is said to be Lipschitz with parameter $L$ if $\|g(u) - g(v)\| \leq L\|u - v\|$ for all $u, v$ (where, $\|\cdot\|$ is the usual $\ell_2$-norm). Proofs of all lemmas and theorems are in the appendix.

## 2 Proximal Updates and Dual Reformulation

In this section, we develop an algorithm for solving the convex relaxation defined in (4). Before proceeding, we note that the algorithm we introduce here is meant to generate quick solutions for problems with relatively small $p$ (e.g., $p \leq 10^3$) – the ideas developed in subsequent sections build upon this algorithm to scale it to much larger problems. The groups $G_i, i = 1, \ldots, p$, which appear in the $\|\cdot\|_\infty$ terms in (4) are all overlapping – particularly, $G_i \cap G_j \neq \emptyset$ for all $i, j \in [p]$. This structure restricts us to algorithms that can handle overlap in the non-smooth part of the objective (for example, coordinate descent cannot be directly applied here). We propose tackling the problem using proximal gradient descent (PGD) [19, 2] which has proven effective for solving non-smooth minimization problems. PGD is an iterative algorithm, where at every iteration (i.e., proximal update), it minimizes an upper bound on the objective. We present the algorithm below.

**Algorithm 1: Proximal Gradient Descent**

- Initialize $\beta^0, \theta^0$; let $L$ be Lipschitz parameter of the gradient map $(\beta, \theta) \mapsto \nabla f(\beta, \theta)$.
- For $k \geq 0$ repeat the following till convergence:

$$
\begin{align*}
\hat{\beta} &\leftarrow \beta^k - \frac{1}{L} \nabla_{\beta} f(\beta^k, \theta^k), \\
\hat{\theta} &\leftarrow \theta^k - \frac{1}{L} \nabla_{\theta} f(\beta^k, \theta^k) \\
\beta^{k+1} &\leftarrow \arg\min_{\|\beta\|_\infty \leq M} \left\| \begin{bmatrix} \beta - \hat{\beta} \\ \theta - \hat{\theta} \end{bmatrix} \right\|_2^2 + \Omega(\beta, \theta)
\end{align*}
$$

(7)
The sequence of iterates $\beta^k$ generated by Algorithm 1 is guaranteed to converge to an optimal solution $\beta^*, \theta^*$ \[1\]. The convergence rate is $O(1/k)$ – this can be improved to $O(1/k^2)$ by using accelerated PGD \[19, 1\]. Unfortunately, there is no closed-form expression for the proximal update in (7) – this is due to the tight coupling between the different groups of variables in $\Omega(\beta, \theta)$. However, many of the groups that are zero in the optimal solution to (7) can be easily identified as we present in the next lemma, which appears to be a new result.

**Lemma 3. (Proximal Screening)** Let $\beta^*, \theta^*$ be an optimal solution to Problem (7). Then, for every $i$:

$$\sum_j [\tilde{\theta}_{ij} - \frac{\lambda_2}{L}]_+ \leq \frac{\lambda_1}{L} - |\tilde{\beta}_i| \implies \beta^*_i, \theta^*_G_i = 0; \quad (8)$$

and for every $i, j$, we have: $|\tilde{\theta}_{ij}| \leq \lambda_2/L \implies \theta^*_{ij} = 0$.

In practice, the proximal screening above identifies the majority of the zero variables. However, we still need to perform minimization over the variables that do not satisfy the conditions of Lemma 1. To this end, in Theorem 1, we present a dual reformulation of Problem (7), which is computationally more tractable. Before stating the theorem, we introduce some necessary notation. We define the boxed soft-thresholding operator as follows:

$$S_{\gamma,M}(\tilde{v}) = \begin{cases} 
0 & \text{if } |\tilde{v}| - \gamma \leq 0 \\
(|\tilde{v}| - \gamma) \text{sign}(\tilde{v}) & \text{if } 0 \leq |\tilde{v}| - \gamma \leq M \\
M \text{sign}(\tilde{v}) & \text{o.w.}
\end{cases}$$

We associate every $\beta^i$ with a dual variable $u^i \in \mathbb{R}$, and every $\theta_{ij}$ with two dual variables: $w^i_j \in \mathbb{R}$ and $w^j_i \in \mathbb{R}$. Moreover, we use the notation $w^i \in \mathbb{R}^{p-1}$ to refer to the vector composed of $w^i_j$ for all $j$ such that $j \neq i$.

**Theorem 1. (Dual formulation)** A dual of Problem (7) is:

$$\max_{u, w} q(u, w) \quad s.t. \quad \|(u^i, w^i)\|_1 \leq 1 \quad \forall \ i \quad (9)$$

where $q(u, w)$ is a continuously differentiable function with a Lipschitz continuous gradient, where:

$$\nabla u^i q(u, w) = \lambda_1 S_{0,M}(\tilde{\beta}^i - \frac{\lambda_1}{L} u^i) \quad \text{and} \quad \nabla w^i_j q(u, w) = \nabla w^i_j q(u, w)$$

$$\nabla w^i_j q(u, w) = \lambda_1 S_{\frac{\lambda_2}{L},M}(\tilde{\theta}_{ij} - \frac{\lambda_1}{L}(w^i_j + w^j_i)) \quad (\text{o.w.})$$

If $u^*, w^*$ is a solution to (9), then a solution to (7) is:

$$\beta^*_i = \frac{\nabla u^i q(u^*, w^*)}{\lambda_1} \quad \text{and} \quad \theta^*_{ij} = \frac{\nabla w^i_j q(u^*, w^*)}{\lambda_1}. \quad (10)$$

In problem (9), the separability of the feasible set across the $(u^i, w^i)$’s and the smoothness of $q(u, w)$ make the problem well-suited for the application of block coordinate ascent (BCA) \[4, 24\], which
optimizes with respect to a single block at a time. When updating a particular block in BCA, we perform inexact maximization by taking a step in the direction of the gradient of the block and projecting the resultant vector onto the feasible set, i.e., the $\ell_1$ ball. Before running BCA, we performing a screening pass to identify the zero groups as described in Lemma 3. We present the algorithm more formally below.

**Algorithm 2: BCA with Screening for Solving (7)**

- Initialize with $u, w$ and take step size $\alpha_i, i \in [p].$
- Use the screening rules of Lemma 3 to identify the zero groups and variables in the primal. Let $Z$ be the set of zero groups, i.e., $Z = \{i \mid i \text{satisfies (8)}\}.$
- Remove unnecessary dual variables: if $\theta_{ij}$ was identified to be zero by the screening rules, remove the variables $w^i_j$ and $w^j_i$ from $w^i$ and $w^j$, respectively.
- For all $i \in Z^c$ perform updates (till convergence):
  \[
  \begin{bmatrix}
  u^i \\
  w^i
  \end{bmatrix} \leftarrow P_{\|\cdot\|_1 \leq 1} \left( \begin{bmatrix}
  u^i \\
  w^i
  \end{bmatrix} + \alpha_i \nabla_{u^i,w^i} q(u,w) \right)
  \]
  where, for a vector $a$, $P_{\|\cdot\|_1 \leq 1}(a)$ denotes projection of $a$ onto the unit $\ell_1$-ball.
- For the variables not set to zero by screening, use (10) to compute their optimal values.

Note that the iterative updates in the algorithm are only applied to the blocks in $Z^c$, i.e., those that have not passed the screening test in (8). In the worst case (if no variables are removed from $w^i$), updating block $i$ requires $O(p)$ operations as this is the time complexity of projecting on the $\ell_1$ ball (e.g., see Duchi et al. [9]) and that of computing the gradient $\nabla_{u^i,w^i} q(u,w)$. Thus, the average time complexity per coordinate is $O(1)$.

If $k_i$ is the number of variables in $w^i$ (after removing unnecessary variables as described in the algorithm), then the Lipschitz parameter of $\nabla_{u^i,w^i} q(u,w)$ is given by $L_i = (k_i + 1)\frac{\lambda_2^2}{L}$ (this follows by observing that each component of $\nabla_{u^i,w^i} q(u,w)$ is a piece-wise linear function with a maximal slope of $\frac{\lambda_2^2}{L}$). Thus, by standard results on block coordinate descent (e.g., Beck and Tetruashvili [3], Bertsekas [4]), Algorithm 2 with step size $\alpha_i = \frac{1}{L_i}$ converges at a rate of $O(\frac{1}{t})$ (where $t$ is the iteration counter). In practice, the algorithm converges in few full passes – especially when active set updates and screening rules are employed, as we describe in the next two sections.

### 3 Decomposition Rules

Running Algorithms 1 and 2 on the full data can become computationally expensive when $p$ is in the order of thousands. The reason is that every evaluation of $\nabla f(\beta, \theta)$ requires $O(np^2)$ operations, which can take several minutes on a modern machine when $p \sim 50,000$. To minimize the number of costly gradient evaluations, we propose running Algorithm 1 on a subset of the variables, i.e., an active set. After obtaining the optimal solution restricted to the active set, we augment the
active set with the variables that violate the optimality conditions (if any) and resolve the problem on the new active set. The success of this method relies on the effectiveness of the algorithm used for choosing the active set. Ideally we want the initial active set to include the support of the optimal solution, which leads to a single evaluation of $\nabla f(\beta, \theta)$ (required to check the optimality of the resulting active-set solution). Below, we introduce a new effective method to decompose and parallelize the search for violating variables and groups outside the active set.

We first provide a concrete definition of our active set and active-set algorithm. The active set is defined by the sets $A \subseteq [p]$ and $T_i \subseteq G_i$ for every $i \in A$. The set $A$ contains the indices of the $\beta_i$’s to include in the model, and each $T_i$ contains the indices of the $\theta_{ij}$s to include. Denote the set of all indices in the active set, corresponding to interaction-effects by $T$, i.e., $T \overset{\text{def}}{=} \cup_i T_i$. We always choose our active set to obey SH, i.e., if $(i, j) \in T_i$ then $i \in A$ and $j \in A$. Moreover, we ensure that if $(i, j) \in T_i$ then $(i, j) \in T_j$. Given $A$ and the $T_i$s, our active-set algorithm solves the following problem using Algorithm 1 and Algorithm 2:

$$\beta^*, \theta^* \in \arg \min_{\beta_{Tc}=0, \theta_{Gc}=0, \|\beta\|_\infty \leq M, \|\theta\|_\infty \leq M} f(\beta, \theta) + \Omega(\beta, \theta) \quad (11)$$

In what follows, we will characterize the optimality of the active set solution $\beta^*, \theta^*$. Particularly, we will answer the following questions. Is the active set solution optimal for Problem (1)? If not, how can we determine which blocks of variables violate the optimality conditions? It turns out that the blocks of variables that (potentially) violate optimality are related to the connected components of a graph that we will introduce in the next definition.

**Definition 1.** (Connected Components) Let $\beta^*, \theta^*$ be an optimal solution to (11). Define the simple undirected graph $G = (V, E)$ with vertex and edge sets given by:

$$V = \left\{ i \in [p] \mid \beta^*_i, \theta^*_{Gi} = 0 \right\}$$

$$E = \left\{ \{i, j\} \mid |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| > \lambda_2, i \in V, j \in V, i \neq j \right\}.$$

Let the $k$ connected components of $G$ be denoted by $\{G_l\}_{l=1}^k$ where, $G_l = (V_l, E_l)$, $l \in [k]$. We say that a component $G_l$ is isolated if it is composed of a single vertex.

Theorem 2 characterizes the optimality of the active-set solution $\beta^*, \theta^*$. Before stating the theorem, we provide some intuition. We say that a solution is coordinate-wise optimal if optimizing with respect to every variable (with all others being fixed) does not improve the objective. In simple regularization schemes, say using the standard Lasso, coordinate-wise optimality implies global optimality. This observation allows checking the optimality of the Lasso solution in parallel, which typically leads to significant speed-ups. However, in group-based regularization, such as the one used in our objective function, coordinate-wise optimality does not generally imply global optimality. This can complicate the check of the optimality conditions. Fortunately, the next theorem presents a way to decompose the optimality conditions – particularly, we show that a
form of “block-wise optimality” implies global optimality, which allows for checking the optimality conditions of the different blocks in parallel.

**Theorem 2. (Optimality Decomposition)** Let $\beta^*, \theta^*$ be an optimal solution to (11) and define $\mathcal{W} = \{(i, j) \mid \theta^*_{ij} = 0, i \notin \mathcal{V}, j \notin \mathcal{V}\}$. Then, $\beta^*, \theta^*$ is optimal for Problem (11) if and only if $|\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| \leq \lambda_2 \forall \ i, j \in \mathcal{W}$ and

$$0 \in \arg \min_{\beta_{Vl}, \theta_{El}} F(\beta, \theta) \text{ s.t. } \beta_{Vl}, \theta_{El} = \beta^*_{Vl}, \theta^*_{El}, \forall l$$

(12)

*Condition (12) can be rewritten as:*

- **If** $\mathcal{G}_l$ **is isolated**, i.e., $\mathcal{V}_l = \{i\}$, then, condition (12) holds if and only if $|\nabla_{\beta_i} f(\beta^*, \theta^*)| \leq \lambda_1$.

- **If** $\mathcal{G}_l$ **is not isolated**, for every $\{i, j\} \in \mathcal{E}_l$ we define the following variables: $\mu^i_j \in \mathbb{R}_{\geq 0}$ if $i \in \mathcal{V}_l$ and $\mu^j_i \in \mathbb{R}_{\geq 0}$ if $j \in \mathcal{V}_l$. Moreover, let $c_{ij} \overset{\text{def}}{=} |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)|/\lambda_1 - \lambda_2/\lambda_1$. Then, condition (12) holds if and only if the following linear system is feasible in $\mu$:

$$\sum_{j \mid \{i, j\} \in \mathcal{E}_l} \mu^i_j \leq 1 - |\nabla_{\beta_i} f(\beta^*, \theta^*)|/\lambda_1, \forall i \in \mathcal{V}_l$$

(13a)

$$\mu^i_j + \mu^j_i = c_{ij} \quad \text{if } \{i, j\} \in \mathcal{E}_l, i \in \mathcal{V}_l, j \in \mathcal{V}_l$$

(13b)

$$\mu^i_j = c_{ij} \quad \text{if } \{i, j\} \in \mathcal{E}_l, i \in \mathcal{V}_l, j \notin \mathcal{V}_l$$

(13c)

$$\mu^j_i = c_{ij} \quad \text{if } \{i, j\} \in \mathcal{E}_l, j \in \mathcal{V}_l, i \notin \mathcal{V}_l$$

(13d)

Theorem 2 suggests that optimality checks can be done in parallel by considering the optimality of each connected component (as in (12)) independently. In practice, the connected components have small sizes (in the order of tens to hundreds) implying that the LPs needed to check optimality (i.e., those in (13)) have a small number of variables and can be solved quickly using standard LP solvers.

We now present an algorithm to update the active set if there are violations to the optimality conditions (see Theorem 2). A direct adaption of active-set methods will involve a full pass (iteration) of the optimization algorithm (PGD in our case) over all variables, and then augment the current active set with additional variables [10]. However, one pass of PGD over all the variables can be very costly because of Algorithm 2. We thus avoid this approach and propose a new algorithm by appealing to Theorem 2.

Suppose we have obtained a solution $\beta^*, \theta^*$ based on the active set defined by $\mathcal{A}$ and $\mathcal{T}$ (as described in (11)). By checking the conditions of Theorem 2 in parallel, we can quickly ascertain whether the solution is optimal or not. Suppose the solution is not optimal. Based on Theorem 2, if $|\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| > \lambda_2$ for some $i, j \in \mathcal{W}$, then we augment $\mathcal{T}$ with $(i, j)$. This ensures that in the next time Problem (11) is solved over the augmented active set, the variable $\theta_{ij}$ cannot violate
the optimality conditions. Similarly, if condition (12) is not satisfied for some isolated \( G_l \), then we augment \( A \) with \( V_l \) (which contains a single index in this case). However, if condition (12) is not satisfied for some non-isolated \( G_l \), then it is not clear which variables should be added to the active set. In this case, we find the variables with the largest violations to feasibility. Particularly, we add a slack variable \( \xi_{ij} \in \mathbb{R}_{\geq 0} \) to the constraints (13b), (13c), (13d), and solve the following linear program:

\[
\min_{\mu \geq 0, \xi \geq 0} \| \xi \|_1 \quad \text{(14)}
\]

s.t. \[
\sum_{j|\{i,j\} \in E_l} \mu_{ij}^l \leq 1 - |\nabla f(\beta^*, \theta^*)|/\lambda_1, \quad \forall i \in V_l
\]
\[
\mu_{ij}^l + \mu_{ji}^l = c_{ij} - \xi_{ij} \quad \text{if } \{i,j\} \in \mathcal{E}_l, i \in V_l, j \in V_l
\]
\[
\mu_{ij}^l = c_{ij} - \xi_{ij} \quad \text{if } \{i,j\} \in \mathcal{E}_l, i \in V_l, j \notin V_l
\]
\[
\mu_{ji}^l = c_{ij} - \xi_{ij} \quad \text{if } \{i,j\} \in \mathcal{E}_l, j \in V_l, i \notin V_l
\]

Let \( \xi^* \) be the optimal solution to (14). If we remove all the constraints corresponding to \( \xi_{ij}^* > 0 \), then we end up with a feasible system. Thus, it is natural in this case to add the indices \((i,j)\) corresponding to \( \xi_{ij}^* > 0 \) (or potentially a subset of them) to \( T \). Note that in this case, if \((i,j)\) is added to \( T \), we add \( i \) and \( j \) to the set \( A \) (if either is not already in \( A \)). Next, we present Algorithm 3, in which we formally describe the process of solving Problem (4) by incrementally augmenting the active set.

---

**Algorithm 3: Active-set Algorithm for Problem (4)**

- Initialize with \( \beta^*, \theta^* \); and output an optimal solution to (4). Let \( A \leftarrow \text{Supp}(\beta^*) \) and \( T \leftarrow \text{Supp}(\theta^*) \). Repeat Steps 1–4 till optimality conditions of Theorem 2 are met:

  1. Update \( \beta^*, \theta^* \) via (11) using Algorithms 1 and 2.
  2. Compute \( \nabla f(\beta^*, \theta^*) \), construct the graph \( G \) and find its connected components \( G_l, l \in [k] \) (see Definition 1).
  3. Let \( \mathcal{W} = \{(i,j) \mid \theta^*_{ij} = 0, i \notin V, j \notin V\} \) and update:

\[
\mathcal{T} \leftarrow \mathcal{T} \cup \{(i,j) \in \mathcal{W} \mid |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| > \lambda_2\}
\]

  4. For every \( G_l \) (in parallel):

- If \( G_l \) is isolated and \( |\nabla \beta_i f(\beta^*, \theta^*)| > \lambda_1 \): then \( A \leftarrow A \cup \{i\} \).
- If \( G_l \) is not isolated, solve (14) to get \( \xi^* \). For every \((i,j)\) with \( \xi_{ij}^* > 0 \):

\[
\mathcal{T} \leftarrow \mathcal{T} \cup (i,j) \text{ and } A \leftarrow A \cup \{i,j\}.
\]
4 Advanced Screening Rules

In this section, we introduce two screening rules for reducing the computation in Algorithm 3. We note that our rules are not heuristic, i.e., they guarantee that the final solution is optimal for Problem (4). The rule in Section 4.1 allows for running Algorithm 3 while only evaluating a part of the gradient. The safe rule in Section 4.2 presents a way to discard \( \theta_{ij} \)'s that are zero in an optimal solution, prior to running Algorithm 3.

4.1 Avoiding Full Gradient Evaluations?

As discussed earlier, computing \( \nabla f(\beta, \theta) \) is a major bottleneck. While Algorithm 3 can mitigate this problem by typically requiring a small number of gradient evaluations, it requires at least one such evaluation to certify the optimality of the active-set solution–this can also be computationally demanding. Here we propose a novel screening method, which can make use of pre-computed quantities and certify optimality of the active-set solution without additional evaluations of the full gradient.

Note that in Algorithm 3, Step 2 involves computing \( \nabla f(\beta^*, \theta^*) \). Observe that the gradients of the \( \theta_{ij} \)'s with \( |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| \leq \lambda_2 \) are never used by the algorithm (and neither are those of non-zero \( \theta_{ij} \)'s). Thus, the algorithm requires access to the gradients of the \( \theta_{ij} \)'s in the following critical set

\[
S = \{(i, j) \mid |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| > \lambda_2, \theta^*_{ij} = 0\}. \tag{15}
\]

Suppose an oracle reveals to us \( S \). Then, by having access to \( S \), we can replace \( \nabla f(\beta^*, \theta^*) \) with \( \nabla_{\beta, \theta} f(\beta^*, \theta^*) \) in Step 2 of the algorithm. This reduces the gradient computation cost from \( O(np^2) \) (cost of computing \( \nabla f(\beta^*, \theta^*) \)) to \( O(n(p + |S|)) \). Typically, \( S \) represents a very small fraction of the variables; and hence promises significant computational gains. Unfortunately, such an oracle to construct \( S \) (exactly) is not available–so we propose to obtain a set \( \hat{S} \supseteq S \)–we can then perform step 2 in Algorithm 3 by only evaluating \( \nabla_{\beta, \theta} f(\beta^*, \theta^*) \). If \( |\hat{S}| \) is not much larger than \( |S| \), then we can significantly reduce the computational cost – this is indeed what we see in our experiments.

The next lemma, presents a way to construct \( \hat{S} \) by using the gradient of a solution \( \beta^w, \theta^w \) that was obtained prior to \( \beta^*, \theta^* \) (e.g., from a warm start or a previous iteration of Algorithm 3).

**Lemma 4.** Let \( (\beta^w, \theta^w) \) and \( (\beta^*, \theta^*) \) be two feasible solutions to Problem (4). Let \( \gamma = (X\beta^w + \tilde{X}\theta^w) - (X\beta^* + \tilde{X}\theta^*) \) and \( C \defeq \max_{i,j} \|\tilde{X}_{ij}\|_2 \). Then, the following holds:

\[
S \subset \hat{S} \defeq \{(i, j) \mid |\nabla_{\theta_{ij}} f(\beta^w, \theta^w)| > \lambda_2 - C\|\gamma\|_2\}
\]

where, \( S \) is the critical set defined in (15).

Next, we describe a procedure, based on Lemma 4, to avoid full gradient evaluations in Algorithm 3. During the course of Algorithm 3, we always maintain a solution \( \beta^w, \theta^w \) for which we store
∇f(β^w, θ^w). We replace Step 2 in Algorithm 3 with the following:

1. Compute ˆS defined in Lemma 4.
2. Compute \( \nabla_{\beta, \theta} f(\beta^*, \theta^*) \); construct the graph \( G \) and its connected components \{G_l\}_1^k \) (see Definition 1).
3. If \(|\hat{S}|\) is large (e.g., exceeds 10^5), compute \( \nabla f(\beta^*, \theta^*) \), set \((\beta^w, \theta^w) \leftarrow (\beta^*, \theta^*)\) and store \( \nabla f(\beta^w, \theta^w) \).

Note that \( \hat{S} \) (Step 1, above) can be efficiently constructed in \( O(|\hat{S}| + \log(p)) \) by using a variant of binary search on the sorted \( |\nabla f(\beta^w, \theta^w)| \) (the latter can be sorted once with cost \( O(\log p) \) and stored). Step 3 above, ensures that \( \beta^w, \theta^w \) is updated when it needs to be re-estimated (i.e., \(|\hat{S}|\) is too large). This screening procedure works well when the predictions made by the solutions \( \beta^w, \theta^w \) and \( \beta^*, \theta^* \) are close (i.e., \( \gamma \) defined in Lemma 4 is sufficiently small, making \( \hat{S} \) close to \( S \)). The initial \( \beta^w, \theta^w \) can be obtained from the previous solution in the regularization path. Predictions across consecutive solutions in the path are usually similar, explaining the multi-fold speedups we empirically observe in our experiments.

### 4.2 Safe Screening Rule

Here we introduce a safe screening rule \[11\] which can identify a subset of the zero interaction coefficients in any optimal solution to Problem (4). This subset of variables can be safely discarded prior to running Algorithm 3. The rule is given in the next lemma:

**Lemma 5.** Let \( \beta^*, \theta^* \) be any optimal solution to Problem (4). For every \( i < j \), define

\[
t_{ij} = |\hat{X}_{ij}^T y| + \|\hat{X}_{ij}\|^2 \|y\| \left(1 - \lambda_2/\|\hat{X}^T y\|_{\infty}\right)
\]

then, \( t_{ij} < \lambda_2 \implies \theta^*_{ij} = 0 \).

Our safe rule matches that in Ghaoui et al. \[11\] for the standard Lasso applied to the matrix \( \hat{X} \) with regularization parameter \( \lambda_2 \). Other safe rules that can potentially eliminate more variables (by exploiting the hierarchical structure) are also possible – however, such rules would require solving quadratic programs to identify zero groups, which can make them less effective than Lemma 5 (see the proof of Lemma 5 for insights). Empirically, we found Lemma 5 to work well for large values of \( \lambda_2 \) (i.e., corresponding to a small number of interaction effects).

### 5 Experiments

We study the empirical performance of our proposed algorithm on both real and synthetic datasets. We compare against two popular toolkits for learning interactions under the SH constraint: hierNet \[5\] and glinternet \[16\]. Following Lim and Hastie \[16\], we also compare to boosting with trees of depth 2 using XGBoost, a popular tool to learn interactions (though, boosting does not strictly
lead to models obeying SH).

**Our Toolkit hierScale:** We implemented our proposed algorithm in an open-source toolkit, written in Python with critical code sections compiled into machine code using Numba [15]. hierScale has a low memory footprint (it generates interaction columns on the fly) and supports multi-core computation (with load balancing).

**Synthetic Data Generation:** We generate \( X_{n \times p} \) to be an iid standard Gaussian ensemble; and form \( y = X\beta^0 + \tilde{X}\theta^0 + \epsilon \), where \( \epsilon \sim \text{iid} \ N(0, \sigma^2) \) is independent of \( X \). For \( \beta^0 \) and \( \theta^0 \), we consider three settings: (I) Hierarchical Truth: \( \beta^0 \) and \( \theta^0 \) satisfy SH, (II) Anti-Hierarchical Truth: \( \theta^0_{ij} \neq 0 \Rightarrow \beta^0_i = 0, \beta^0_j = 0 \), and (III) Main-Only Truth: All interaction-effects are zero. In (I)–(III), all non-zero coefficients are set to 1. For (I) and (II), we set \( \|\theta^0\|_0 = \|\beta^0\|_0 \). We take \( \sigma^2 \) such that the signal-to-noise-ratio (SNR) = \( \text{Var}(X\beta^0 + \tilde{X}\theta^0)/\sigma^2 \) = 10.

**Timings:** We compare the running time of hierScale versus two popular and publicly available toolkits: hierNet and glinternet, on both synthetic and real datasets. We generate the synthetic data under hierarchical truth with \( n = 1000 \) and \( \|\beta^0\|_0 = \|\theta^0\|_0 = 5 \) and take \( p \) between 500 and 50,000 (~1.25 \times 10^9 interaction effects). Among real data, we consider the Amazon Reviews dataset [13] which uses (TF/IDF transformed) text data to predict review helpfulness. We use two variants of the dataset: Amazon-1 (\( p = 10160 \) and \( n = 1000 \)) and Amazon-2 (\( p = 5000 \) and \( n = 1000 \)). We also consider the dataset from CoEPrA 2006 (Regression Problem 1) (\( p = 5786, n = 89 \)) and the Riboflavin dataset (\( p = 4088, n = 71 \)) [6]. For all toolkits, we set the tolerance level to \( 10^{-6} \), \( \lambda_{\text{min}} = 0.05\lambda_{\text{max}} \) and generate a path with 100 solutions. For hierScale, we set \( \lambda_2 = 2\lambda_1 \). In order to ensure a fair comparison, we do not use the safe screening rule of Section 4.2 as other toolkits can be adapted to use it (further speedups to hierScale are possible with this method). Computations are carried out on a machine with a 12-core Intel Xeon E5 @ 2.7 GHz and 64GB of RAM.

The results are in Table 1. We see that hierScale achieves over a 4900x speed-up compared to hierNet and a 690x speed-up compared to glinternet (e.g., on the Amazon Reviews dataset glinternet cannot terminate in a week)—whereas, hierScale can handle problems with \( p = 50,000 \) in a few minutes! Finally, we note that She et al. [21] recently proposed an algorithm for a problem similar to ours, but have not provided a public toolkit—the largest problem reported in their paper is for \( p = 1000 \): In the best case, their method takes \( \sim 51 \) seconds per solution, whereas hierScale takes only 0.2 seconds; and is significantly faster.

**Variable Selection:** Following Lim and Hastie [16], we compare the False Discovery Rate (FDR) of different methods at different sparsity levels. We generate synthetic data with \( n = 100, p = 200, \) and \( \|\beta\|_0 = 10 \) and report the FDR averaged over 100 datasets, in Figure 1. Under hierarchical truth, all the methods perform roughly similarly. However, under anti-hierarchy or main-only truth, our method can perform significantly better.

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2Available at [http://www.coepra.org](http://www.coepra.org)
Table 1: Average time (s) for obtaining a solution in the regularization path. The symbols * and ** indicate that the toolkit does not terminate in 3 days and 1 week, respectively. The dash (-) indicates a crash due to memory management issues.

| Toolkit   | Synthetic datasets | Real datasets |
|-----------|--------------------|---------------|
|           | p=500 1000 2000 5000 15000 50000 | Ribo. Coepra Amazon-1 Amazon-2 |
|           | (p=4088) (p=5786) (p=5000) (p=10160) |
| hierScale | 0.1 0.2 0.5 3.2 26.6 730 | 2.2 3.3 1.7 8.7 |
| glinternet | 0.3 1 3.8 24.4 226.9 * | 2.7 7.8 * ** |
| hierNet   | 490 - - - - - | - - - - - |

**Prediction Tasks:** We now compare the prediction performance of hierScale with competing methods on both synthetic and real datasets.

**Synthetic data:** We use the same dataset as for variable selection (above). We tune on a separate validation set and report the prediction MSE on the testing data (training, validation and test sets are of the same size). For hierNet and glinternet we tune over 50 parameter values. For hierScale we use 50 \( \lambda_1 \)-values and \( \lambda_2 \in \{ \lambda_1, 2\lambda_1 \} \). For XGBoost we use 50 tree-sizes (between 20 and 1000) and learning rates \( \in \{0.01, 0.1\} \). Results across 20-runs (for Main Only Truth) are presented in Figure 2. Our method shows significant improvements in prediction accuracy. The results for hierarchical and anti-hierarchical truth are in the appendix, with results across methods being comparable.

**Real data:** We consider the Riboflavin dataset (here, \( n = 71, p = 4088 \)) [6] for predicting Vitamin B\(_2\) production from gene expression levels. We train on 50 randomly chosen samples and compute the test RMSE on the remaining 21 samples. We repeat this training/testing procedure 30 times and report the average RMSE. We plot the RMSE versus the sparsity level in Figure 3. hierScale considers \( \lambda_2 \in \{ \lambda_1, 10\lambda_1, 100\lambda_1 \} \) and for XGBoost, we vary learning rate \( \in \{0.01, 0.1, 1\} \). Figure 3 reports results with best MSE. We see that the SH methods (hierScale and glinternet) can be more effective than boosting at low/moderate sparsity levels (note \( n = 71 \) is small), which is desirable for interpretable learning. On this dataset, hierScale shows marginal improvement in RMSE over glinternet.
Figure 1: False Discovery Rate (FDR) for different methods that enforce SH, under 3 settings (I) Hierarchical Truth, (II) Anti-Hierarchical Truth and (III) Main Only Truth (top to bottom). hierScale-1 and hierScale-2 refer to our proposed method with $\lambda_2 = \lambda_1$ and $\lambda_2 = 2\lambda_1$, respectively.

Figure 2: Mean-squared Error (MSE) on the test data for synthetic data (Main only truth). XGBoost is limited to depth 2 trees.
Figure 3: RMSE on the Riboflavin dataset with $n = 50$ and $p = 4088$ gene expressions. XGBoost is limited to depth 2 trees.

6 Conclusion

We studied the problem of learning sparse interactions under the strong hierarchy constraint. We introduced a transparent convex relaxation for the problem and developed a scalable algorithm for solving it. Our algorithm exploits the sparse group structure in the objective function through decomposing the optimality conditions and utilizing specialized screening rules. Experiments on real and synthetic data show that our method enjoys significant speed-ups over the current state of the art and more robust variable selection.

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Appendices

A  Proofs

A.1 Proof of Lemma 1

Suppose the $z_i$s and $z_{ij}$s are relaxed to $[0, 1]$ and fix some feasible solution $\beta, \theta$. Let us (partially) minimize the objective function with respect to $z$, while keeping $\beta, \theta$ fixed, to obtain a solution $z^*$. Then, $z^*$ must satisfy $z_i^* = \max\{\frac{|\beta|}{\lambda}, \max_{k, j \in G_i} z_{kj}\}$ for every $i$ (since this choice is the smallest feasible $z_i$). Moreover, $z_{ij}^* = \frac{|\theta_{ij}|}{\lambda}$ for every $i < j$ (by the same reasoning). Substituting the optimal values $z_i^*$ and $z_{ij}^*$ leads to the result of the lemma.

A.2 Proof of Lemma 2

Same reasoning as Lemma 1.

A.3 Proof of Lemma 3

The lemma can be established by writing down the optimality conditions of the problem. We present a simpler argument which uses Theorem 1 and the convergence of BCA (i.e., Algorithm 2 without the initial screening phase). Suppose $\sum_j \max\{\tilde{\theta}_{ij} - \frac{\lambda_2}{\lambda_1}, 0\} \leq \frac{\lambda_1}{\lambda} - |\tilde{\beta}_i|$ is satisfied for some $i$. Let $u, w$ be some feasible solution to the dual (e.g., solution of all zeros). Now update $u, w$ so that the following is satisfied

$$u^i = \frac{L}{\lambda_1} \tilde{\beta}_i$$

and for every $j$ such that $j \neq i$:

$$w^i_j = \max\left\{\frac{L}{\lambda_1}|\tilde{\theta}_{ij}| - \frac{\lambda_2}{\lambda_1}, 0\right\} \text{sign}(\tilde{\theta}_{ij}) \quad \text{and} \quad w^j_i = 0$$

Note that $u, w$ is still feasible after this update and it can be readily verified that $\nabla_{u^i, w^i} q(u, w) = 0$ and $\nabla_{w^i_j} q(u, w) = 0$ for every $j$. Thus, BCA will never change $u^i, w^i$, or $w^j_i$ (for any $j$) in subsequent iterations. Since BCA is guaranteed to converge to an optimal solution, we conclude that the values in (16) and (17) (which correspond to $\beta_i^*, \theta_{Gi}^* = 0$) are optimal.

For the case when $|\tilde{\theta}_{ij}| \leq \frac{\lambda_2}{\lambda_1}$, if we set $w^i_j = w^j_i = 0$, then BCA will never change $w^i_j$ or $w^j_i$, which leads to $\theta_{ij}^* = 0$. 

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Finally, since the solution $\beta$ follows:

$$w^i \text{ and } w^j \text{ written as } \sum w^i \beta_i + \langle w^i, \theta_{G_i} \rangle \text{ s.t. } \|(u^i, w^i)\|_1 \leq 1$$ (18)

Plugging the above into the proximal problem and switching the order of the min and max (which is justified by strong duality), we arrive to the dual of the proximal problem:

$$\max_{u,w} \min_{\beta, \theta} \frac{L}{2} \left\| \begin{bmatrix} \beta - \tilde{\beta} \\ \theta - \tilde{\theta} \end{bmatrix} \right\|^2 + \lambda_1 \sum_i (u^i \beta_i + \langle w^i, \theta_{G_i} \rangle) + \lambda_2 \|\theta\|_1 \quad \text{s.t. } \|\beta\|_\infty \leq M, \quad \|\theta\|_\infty \leq M, \quad \|(u^i, w^i)\|_1 \leq 1, \forall i \in [p]$$ (19)

Note that each dual variable $u^i$ is a scalar which corresponds to the primal variable $\beta^i$. Similarly, the dual vector $w^i \in \mathbb{R}^{p-1}$ corresponds to $\theta_{G_i}$. The term $\sum_i (u^i \beta_i + \langle w^i, \theta_{G_i} \rangle)$ in (19) can be written as $\sum_i u^i \beta_i + \sum_{i < j} \theta_{ij} (w^i_j + w^j_i)$, where $w^i$ and $w^j$ are the components of the vectors $w^i$ and $w^j$, respectively, corresponding to $\theta_{ij}$. Using this notation, we can rewrite Problem (19) as follows:

$$\max_{u,w} \min_{\beta, \theta} \sum_i h(\beta_i, u^i; \tilde{\beta_i}) + \sum_{i < j} g(\theta_{ij}, w^i_j, w^j_i; \tilde{\theta_{ij}}) \quad \text{s.t. } \|\beta\|_\infty \leq M, \quad \|\theta\|_\infty \leq M, \quad \|(u^i, w^i)\|_1 \leq 1, \forall i \in [p]$$ (20)

where

$$h(a, b; \tilde{a}) \overset{\text{def}}{=} \frac{L}{2} (a - \tilde{a})^2 + \lambda_1 a b \quad \text{and} \quad g(a, b; \tilde{a}) \overset{\text{def}}{=} \frac{L}{2} (a - \tilde{a})^2 + \lambda_1 a (b + c) + \lambda_2 |a|$$

The optimal solution of the inner minimization in (20) is (uniquely) given by:

$$\beta^*_i \overset{\text{def}}{=} \arg \min_{|\beta_i| \leq M} h(\beta_i, u^i; \tilde{\beta_i}) = S_{0, M} \left( \tilde{\beta_i} - \frac{\lambda_1}{L} u^i \right)$$

$$\theta^*_{ij} \overset{\text{def}}{=} \arg \min_{|\theta_{ij}| \leq M} g(\theta_{ij}, w^i_j, w^j_i; \tilde{\theta_{ij}}) = S_{\frac{\lambda_2}{L}, M} \left( \tilde{\theta_{ij}} - \frac{\lambda_1}{L} (w^i_j + w^j_i) \right)$$ (21)

Therefore, the dual problem can equivalently written as:

$$\max_{u,w} \sum_i h(\beta^*_i, u^i; \tilde{\beta_i}) + \sum_{i < j} g(\theta^*_{ij}, w^i_j, w^j_i; \tilde{\theta_{ij}}) \quad \text{s.t. } \|(u^i, w^i)\|_1 \leq 1 \quad \forall i$$ (22)

Finally, since the solution $\beta^*, \theta^*$ is defined in (21) is unique, Danskin's theorem implies that the
dual objective function \(q(u, w)\) is continuously differentiable and that

\[
\nabla_u q(u, w) = \lambda_1 \beta_i^* \quad \text{and} \quad \nabla_{w^i} q(u, w) = \nabla_{w^j} q(u, w) = \lambda_1 \theta_{ij}^*.
\]

(23)

A.5 Proof of Theorem 2

Define \(c = \frac{\lambda_2}{\lambda_1}\). Let \(Z = \{i, j \mid \theta_{ij}^* = 0, i \in \mathcal{V} \text{ or } j \in \mathcal{V}\}\). We split the proof into the following 3 parts:

• Part 1: We prove that \(\beta^*, \theta^*\) is optimal if and only if

\[
0 \in \partial_{\beta^*, \theta^*} F(\beta^*, \theta^*) \quad \forall i, j \in \mathcal{W}
\]

and

\[
0 \in \partial_{\beta^*, \theta^*} F(\beta^*, \theta^*) \quad \forall i, j \in \mathcal{V}\]

Before proceeding, we recall the following facts about the subgradients of the \(\ell_\infty\) and \(\ell_1\) norms.

For an arbitrary vector \(v \in \mathbb{R}^p\) such that \(v \neq 0\), we have:

\[
\partial_{v_i} \|v\|_\infty = \begin{cases} 
0 & \text{if } |v_i| < \|v\|_\infty \\
\alpha_i \text{sign}(v_i) & \text{if } |v_i| = \|v\|_\infty
\end{cases}
\]

(24)

where \(\alpha_i \geq 0\) and \(\sum_i \alpha_i = 1\). Otherwise, if \(v = 0\), then

\[
\partial \|v\|_\infty = \{u \in \mathbb{R}^p \mid \|u\|_1 \leq 1\} \quad \text{and} \quad \partial \|v\|_1 = [-1, 1]^p
\]

(25)

Part 1. Since the problem is convex subject to only box constraints, the necessary and sufficient optimality condition can be stated as there exists a subgradient \(h \in \partial F(\beta^*, \theta^*)\) such that for every variable \(v\) (i.e., \(v = \beta_i\) or \(v = \theta_{ij}\))

\[
\begin{align*}
  h_v &= 0 \quad \text{if } |v_i^*| < M \\
  h_v &\leq 0 \quad \text{if } v_i^* = M \\
  h_v &\geq 0 \quad \text{if } v_i^* = -M
\end{align*}
\]

(26)

where \(h_v\) is the component of \(h\) corresponding to variable \(v\).

Let \(S = \{i, j | \theta_{ij}^* \neq 0\}\). Note that the sets \(S, W,\) and \(Z\) (in the statement of the lemma) form a partition of \(G\). Then, it can be readily seen that the subdifferential \(\partial F(\beta^*, \theta^*)\) can be decomposed...
as:

$$
\partial F(\beta^*, \theta^*) = \partial_{\beta V, \theta S} F(\beta^*, \theta^*) \times \prod_{i,j \in \mathcal{W}} \partial_{\theta_{ij}} F(\beta^*, \theta^*) \times \partial_{\beta V, \theta z} F(\beta^*, \theta^*)
$$

(27)

Since $\beta^*_V, \theta^*_S$ are part of the optimal solution to Problem (11), then we know that there exists a subgradient $h_{\beta V, \theta S} \in \partial_{\beta V, \theta S} F(\beta^*, \theta^*)$ which satisfies (26) for every variable $v$ in $\beta_V$ and $\theta_S$. Let us augment $h_{\beta V, \theta S}$ with zeros (so that any variable $v$ outside $\beta_V, \theta_S$ has $h_v = 0$). The vector $h$ satisfies the optimality conditions in (26), by construction. Thus, $\beta^*, \theta^*$ is optimal if and only if $h \in \partial F(\beta^*, \theta^*)$. But (27) implies that $h \in \partial F(\beta^*, \theta^*)$ is equivalent to:

$$
\begin{align*}
& h_{\beta V, \theta S} \in \partial_{\beta V, \theta S} F(\beta^*, \theta^*) \\
& 0 \in \partial_{\theta_{ij}} F(\beta^*, \theta^*) \quad \forall i, j \in \mathcal{W} \\
& 0 \in \partial_{\beta V, \theta z} F(\beta^*, \theta^*)
\end{align*}
$$

(28)

(29)

(30)

But (28) holds by construction. Thus, $h \in \partial F(\beta^*, \theta^*)$ (or equivalently $\beta^*, \theta^*$ is optimal) if and only if (29) and (30) hold.

Part 2. Next, we will derive the equivalent conditions under which $0 \in \partial_{\beta V, \theta z} F(\beta^*, \theta^*)$ holds. The latter condition holds if and only if there exists subgradients $d^i, s^i \in \partial_{\beta_i, \theta_{G_i}} \max\{||\beta^*_i||, ||\theta^*_G||_\infty\}$ for every $i$ and subgradient $l \in \partial_{\theta z} ||\beta||_1$ such that

$$
\begin{align*}
& \nabla_{\theta_{ij}} f(\beta^*, \theta^*) + \lambda_1(s^i_j + s^i_j) + \lambda_2 l_{ij} = 0 \quad \forall i, j \in \mathcal{Z} \\
& \nabla_{\beta_i} f(\beta^*, \theta^*) + \lambda_1 d^i = 0 \quad \forall i \in \mathcal{V}
\end{align*}
$$

(31)

(32)

where $s^i_j$ denotes the component of $s^i$ corresponding to the variable $\theta_{ij}$, and similarly $l_{ij}$ denotes the component of $l$ corresponding to $\theta_{ij}$.

Suppose $i, j \in \mathcal{Z}$. The definition of $\mathcal{Z}$ allows for the possibility that either $i$ or $j$ is not $\mathcal{V}$. If $i \notin \mathcal{V}$, then $\beta^*_i, \theta^*_G_i \neq 0$, which by (24) implies that $s^i_j = 0$. Similarly, if $j \notin \mathcal{V}_l, s^i_j = 0$. Thus, (31) can be equivalently written as (after rearrangement of the terms):

$$
\begin{align*}
& s^i_j + s^i_j = -\nabla_{\theta_{ij}} f(\beta^*, \theta^*) / \lambda_1 - c_{ij} \quad \forall i < j \text{ s.t. } i \in \mathcal{V}_l, j \in \mathcal{V}_l \\
& s^i_j = -\nabla_{\theta_{ij}} f(\beta^*, \theta^*) / \lambda_1 - c_{ij} \quad \forall i < j \text{ s.t. } i \in \mathcal{V}_l, j \notin \mathcal{V}_l \\
& s^i_j = -\nabla_{\theta_{ij}} f(\beta^*, \theta^*) / \lambda_1 - c_{ij} \quad \forall i < j \text{ s.t. } j \in \mathcal{V}_l, i \notin \mathcal{V}_l
\end{align*}
$$

(33)

Note that our current system, which is composed of (32) and (33), only involves the subgradients $d^i, s^i \in \partial_{\beta_i, \theta_{G_i}} \max\{||\beta^*_i||, ||\theta^*_G||_\infty\}$ for every $i \in \mathcal{V}$ and $l$. By using (25), the latter subgradients can
be written equivalently as:

\[
|d_i| + \sum_{j \neq i} |x_j^i| \leq 1 \quad \forall i \in \mathcal{V}
\]

\[
|l_{ij}| \leq 1 \quad \forall i, j \in \mathcal{I}
\]  \hspace{1cm} (34)

Therefore, \(0 \in \partial_{\beta, \theta} F(\beta^*, \theta^*)\) is equivalent to saying that the linear system composed of (32), (33), (34) is feasible, i.e., the following system is feasible:

\[
|d_i| + \sum_{j \neq i} |x_j^i| \leq 1 \quad \forall i \in \mathcal{V}
\]

\[
\nabla_{\beta_i} f(\beta^*, \theta^*) + \lambda_1 d_i = 0 \quad \forall i \in \mathcal{V}
\]

\[
s_j^i + s_i^j = -\nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1 - c_{ij} \quad \forall i < j \text{ s.t. } i \in \mathcal{V}_l, j \in \mathcal{V}_l
\]

\[
s_i^j = -\nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1 - c_{ij} \quad \forall i < j \text{ s.t. } i \in \mathcal{V}_l, j \notin \mathcal{V}_l
\]

\[
s_j^i = -\nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1 - c_{ij} \quad \forall i < j \text{ s.t. } j \in \mathcal{V}_l, i \notin \mathcal{V}_l
\]

\[
|l_{ij}| \leq 1 \quad \forall i, j \in \mathcal{I}
\]

The variables \(d_i\) and \(l_{ij}\) in the above system can be eliminated to get the following equivalent system:

\[
\sum_{j \neq i} |x_j^i| \leq 1 - |\nabla_{\beta_i} f(\beta^*, \theta^*)|/\lambda_1 \quad \forall i \in \mathcal{V}
\]

\[
|s_j^i + s_i^j + \nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1| \leq c \quad \forall i < j \text{ s.t. } i \in \mathcal{V}_l, j \in \mathcal{V}_l
\]

\[
|s_j^i + \nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1| \leq c \quad \forall i < j \text{ s.t. } i \in \mathcal{V}_l, j \notin \mathcal{V}_l
\]

\[
|s_i^j + \nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1| \leq c \quad \forall i < j \text{ s.t. } j \in \mathcal{V}_l, i \notin \mathcal{V}_l
\]  \hspace{1cm} (36)

When \(|\nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1| \leq c\), we can always set \(s_j^i = s_i^j = 0\) without affecting feasibility. Substituting \(s_{ij} = 0\) whenever \(|\nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1| \leq c\) (i.e., whenever \(\{i, j\} \notin \mathcal{E}_l\)) in (36), leads to the following equivalent system:

\[
\sum_{j \neq i} |x_j^i| \leq 1 - |\nabla_{\beta_i} f(\beta^*, \theta^*)|/\lambda_1 \quad \forall i \in \mathcal{V}
\]

\[
|s_j^i + s_i^j + \nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1| \leq c \quad \forall \{i, j\} \in \mathcal{E}, i \in \mathcal{V}, j \in \mathcal{V}
\]

\[
|s_j^i + \nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1| \leq c \quad \forall \{i, j\} \in \mathcal{E}, i \in \mathcal{V}, j \notin \mathcal{V}
\]

\[
|s_i^j + \nabla_{\theta_{ij}} f(\beta^*, \theta^*)/\lambda_1| \leq c \quad \forall \{i, j\} \in \mathcal{E}, j \in \mathcal{V}, i \notin \mathcal{V}
\]  \hspace{1cm} (37a-d)
The above system is feasible if and only if for every \( l \) the following system is feasible:

\[
\sum_{j \mid (i,j) \in \mathcal{E}_l} |s_{ij}^l| \leq 1 - |\nabla_{\beta_i} f(\beta^*, \theta^*)| / \lambda_1 \quad \forall i \in \mathcal{V}_l \quad (38a)
\]

\[
|s_{ij}^l + s_{ij}^l + \nabla_{\theta_{ij}} f(\beta^*, \theta^*)| / \lambda_1 \leq c \quad \forall \{i,j\} \in \mathcal{E}_l, i \in \mathcal{V}_l, j \in \mathcal{V}_l \quad (38b)
\]

\[
|s_{ij}^l + \nabla_{\theta_{ij}} f(\beta^*, \theta^*)| / \lambda_1 \leq c \quad \forall \{i,j\} \in \mathcal{E}_l, i \in \mathcal{V}_l, j \notin \mathcal{V}_l \quad (38c)
\]

\[
|s_{ij}^l + \nabla_{\theta_{ij}} f(\beta^*, \theta^*)| / \lambda_1 \leq c \quad \forall \{i,j\} \in \mathcal{E}_l, j \in \mathcal{V}_l, i \notin \mathcal{V}_l \quad (38d)
\]

But the feasibility of the above system with respect to \( l \) is equivalent to saying that \( 0 \in \partial_{\beta_{ij}, \theta_{ij}} F(\beta^*, \theta^*) \) for every \( l \) (this follows by using same argument we used to show that \( 0 \in \partial_{\beta_{ij}, \theta_{ij}} F(\beta^*, \theta^*) \) is equivalent to system (36) being feasible). This establishes the first part of the lemma. In what follows, we simplify the system (38).

If \( \mathcal{G}_i \) is isolated then \( \mathcal{E}_l \) is empty, and thus (38) becomes equivalent to \( |\nabla_{\beta_i} f(\beta^*, \theta^*)| \leq \lambda_1 \). Now let us assume that \( \mathcal{G}_i \) is not isolated. In (38), we have \( |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| / \lambda_1 > c \) (by definition of the set \( \mathcal{E}_l \)). Thus, if (38) is feasible, it can be readily seen that we can always construct a feasible solution where the inequalities of (38b) satisfy:

\[
s_{ij}^l + s_{ij}^l = -\text{sign}(\nabla_{\theta_{ij}} f(\beta^*, \theta^*))(|\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| / \lambda - c) \quad (39)
\]

\[
\text{sign} s_{ij}^l \in \{-\text{sign}(\nabla_{\theta_{ij}} f(\beta^*, \theta^*)), 0\}
\]

\[
\text{sign} s_{ij}^l \in \{-\text{sign}(\nabla_{\theta_{ij}} f(\beta^*, \theta^*)), 0\}
\]

Multiplying (39) by \(-\text{sign}(\nabla_{\theta_{ij}} f(\beta^*, \theta^*))\), we arrive to \( |s_{ij}^l| + |s_{ij}^l| = |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| / \lambda_1 - c \), and the latter constraint can be used in place of (37b) without affecting feasibility. By a similar reasoning, we can replace (37c) and (37d) with \( |s_{ij}^l| = |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| / \lambda_1 - c \) and \( |s_{ij}^l| = |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| / \lambda_1 - c \), respectively. Thus, the new linear system only involves terms of the form \( |s_{ij}^l| \) and \( |s_{ij}^l| \). Replacing the latter two terms with \( \mu_{ij}^l \in \mathbb{R}_{\geq 0} \) and \( \mu_{ij}^l \in \mathbb{R}_{\geq 0} \), we arrive to the result of the lemma.

Part 3. The condition \( 0 \in \partial_{\theta_{ij}} F(\beta^*, \theta^*) \) where \( i, j \in \mathcal{W} \) is equivalent to saying that there exists subderivatives \( s_{ij}^l \in \partial_{\theta_{ij}} \max\{|\beta_i^*|, \|\theta_{G_i}^*\|\infty\} \), \( s_{ij}^l \in \partial_{\theta_{ij}} \max\{|\beta_j^*|, \|\theta_{G_j}^*\|\infty\} \), and \( l_{ij} \in \partial_{\theta_{ij}} \|\theta^*\|_1 \) such that

\[
\nabla_{\theta_{ij}} f(\beta^*, \theta^*) + \lambda_1 (s_{ij}^l + s_{ij}^l) + \lambda_2 l_{ij} = 0 \quad (40)
\]

Since \( i, j \in \mathcal{W} \), we have \( \beta_i^*, \theta_{G_i}^* \neq 0 \) and \( \beta_j^*, \theta_{G_j}^* \neq 0 \). Thus, by (24), \( s_{ij}^l = s_{ij}^l = 0 \), and therefore, (40) becomes: \( \nabla_{\theta_{ij}} f(\beta^*, \theta^*) + \lambda_2 l_{ij} = 0 \). But, since \( \theta_{ij}^* = 0 \), \( l_{ij} \) \in \partial_{\theta_{ij}} \|\theta^*\|_1 \) is equivalent to \( |l_{ij}| \leq 1 \). Thus, we conclude that \( \nabla_{\theta_{ij}} f(\beta^*, \theta^*) + \lambda_2 l_{ij} = 0 \) is equivalent to \( |\nabla_{\theta_{ij}} f(\beta^*, \theta^*)| \leq \lambda_2 \).
A.6 Proof of Lemma 4

Let $i, j \in S$. By the triangle inequality:

$$|\nabla_{\theta f} (\beta^*, \theta^*)| \leq |\nabla_{\theta f} (\beta^w, \theta^w)| + |\nabla_{\theta f} (\beta^*, \theta^*) - \nabla_{\theta f} (\beta^w, \theta^w)|$$  \hspace{1cm} (41)

But

$$|\nabla_{\theta f} (\beta^*, \theta^*) - \nabla_{\theta f} (\beta^w, \theta^w)| = |\tilde{X}^T(y - X\beta^* + \tilde{X}\theta^*) - \tilde{X}^T(y - X\beta^w + \tilde{X}\theta^w)|$$

$$\leq \|\tilde{X}\|_2 \|(X\beta^* + \tilde{X}\theta^*) - (X\beta^w + \tilde{X}\theta^w)\|_2$$

$$\leq C\|\gamma\|_2$$

Plugging the upper bound above into (41), we get

$$|\nabla_{\theta f} (\beta^*, \theta^*)| \leq |\nabla_{\theta f} (\beta^w, \theta^w)| + C\|\gamma\|_2.$$  \hspace{1cm} (42)

Therefore, if $(i, j) \in S$, i.e., $|\nabla_{\theta f} (\beta^*, \theta^*)| > \lambda_2$ then $|\nabla_{\theta f} (\beta^w, \theta^w)| + C\|\gamma\|_2 > \lambda_2$, implying that $(i, j) \in \hat{S}$.

A.7 Proof of Lemma 5

The proof is based on that of [11] for the standard Lasso. Let $c$ be a constant such that $c \leq F(\beta^*, \theta^*)$.

First, note that Problem (4) can be equivalently written as:

$$\min_{\beta, \theta, m, u, v} \frac{1}{2}\|m\|_2^2 + \lambda_1 \sum_i \|u_i, v_{G_i}\|_\infty + \lambda_2 \|\theta\|_1$$  \hspace{1cm} (42)

$$m = y - X\beta + \tilde{X}\theta, \quad u^i = \beta_i \forall i, \quad v^i_{G_i} = \theta_{G_i} \forall i, \quad \|u^i, v^i_{G_i}\|_\infty \leq M \forall i.$$  \hspace{1cm} (43)

Dualizing all the constraints in the above, we arrive to the following dual of the problem:

$$\max_{\rho, \alpha, \gamma, \xi} -\frac{1}{2}\|\rho\|_2^2 - \rho^Ty - M \sum_i \xi^i$$  \hspace{1cm} (44)

$$\|\alpha^i, \gamma^i\|_1 - \xi^i \leq \lambda_1, \forall i$$  \hspace{1cm} (45)

$$|\tilde{X}^T\rho - (\gamma^j + \gamma^j_i)| \leq \lambda_2 \forall i < j$$  \hspace{1cm} (46)

$$X^T\rho - \alpha = 0$$  \hspace{1cm} (47)

$$\xi \geq 0$$  \hspace{1cm} (48)

where $\alpha^i$ and $\xi^i$ are scalars and $\gamma^i$ is a vector in $\mathbb{R}^{p-1}$ with components $\gamma^j_i$ for all $j \neq i$. Since the primal problem given in (42) has a convex objective and linear constraints (with finite optimal objective), strong duality holds and there exists at least one optimal solution for the dual problem in (44) (e.g., see [4]). Let $\hat{\rho}, \hat{\alpha}, \hat{\gamma}, \hat{\xi}$ be any dual optimal solution. The following implication directly follows from the optimality conditions of the primal-dual pair:

$$|\tilde{X}^T\hat{\rho} - (\hat{\gamma}^j + \hat{\gamma}^j_i)| < \lambda_2 \implies \theta^*_{ij} = 0$$  \hspace{1cm} (49)
Note that when $|\tilde{X}_{ij}^T\hat{\rho}| < \lambda_2$, we can w.l.o.g. assume that $\hat{\gamma}_j^i = \hat{\gamma}_i^j = 0$ (since if either of $\hat{\gamma}_j^i$ or $\hat{\gamma}_i^j$ is not zero, we can always set it to zero without affecting feasibility or the objective in Problem (44)). Therefore, when $|\tilde{X}_{ij}^T\hat{\rho}| < \lambda_2$, implication (49) can be equivalently written as:

$$|\tilde{X}_{ij}^T\hat{\rho}| < \lambda_2 \implies \theta_{ij}^* = 0.$$  \hspace{1cm} (50)

Define

$$h_{ij} = \max_{\rho, \xi} |\tilde{X}_{ij}^T\rho| \text{ s.t. } -\frac{1}{2}\|\rho\|^2_2 - \rho^T y - M \sum_i \xi^i \geq c, \quad \xi \geq 0. \hspace{1cm} (51)$$

By the definition of $c$ and from strong duality, we have $c \leq F(\beta^*, \theta^*) = -\frac{1}{2}\|\rho\|^2_2 - \rho^T y - M \sum_i \hat{\xi}^i$, which implies that $\hat{\rho}, \hat{\xi}$ is feasible for (51). Therefore, $h_{ij} \geq X_{ij}^T\hat{\rho}$ and consequently $h_{ij} < \lambda_2 \implies |\tilde{X}_{ij}^T\hat{\rho}| < \lambda_2 \implies \theta_{ij}^* = 0$. Note that $\{\rho \mid -\frac{1}{2}\|\rho\|^2_2 - \rho^T y - M \sum_i \xi^i \geq c, \quad \xi \geq 0\} = \{\rho \mid -\frac{1}{2}\|\rho\|^2_2 - \rho^T y \geq c\}$, which implies

$$h_{ij} = \max_{\rho, \xi} |\tilde{X}_{ij}^T\rho| \text{ s.t. } -\frac{1}{2}\|\rho\|^2_2 - \rho^T y \geq c \hspace{1cm} (52)$$

Solving the problem above (e.g., using the KKT conditions) leads to

$$h_{ij} = |\tilde{X}_{ij}^T y| + \|\tilde{X}_{ij}\|^2 \sqrt{\|y\|^2 - 2c}. \hspace{1cm} (53)$$

Finally, we derive a reasonable value for $c$ by constructing a dual feasible solution. Note that the solution $\rho = y\lambda_2/\|\tilde{X}^T y\|_{\infty}, \alpha = X^T \rho, \xi = 0$ is feasible for Problem (44) and its objective is equal to

$$\|y\|^2 \left( -\frac{\lambda_2}{\|\tilde{X}^T y\|_{\infty}} - \frac{1}{2} \frac{\lambda_2^2}{\|\tilde{X}^T y\|_{\infty}^2} \right).$$

Thus, setting $c$ equal to the expression above and plugging it into (53) we get:

$$h_{ij} = |\tilde{X}_{ij}^T y| + \|\tilde{X}_{ij}\|^2 \|y\| \left( 1 - \frac{\lambda_2}{\|\tilde{X}^T y\|_{\infty}} \right).$$  \hspace{1cm} (54)

Note on the choice of $\lambda_2$: Setting $\lambda_2 = \|\tilde{X}^T y\|_{\infty}$ will lead to $\theta_{ij}$’s all being zero (in the optimal solution). Thus, we always choose $\lambda_2 \leq \|\tilde{X}^T y\|_{\infty}$. 

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B  Results of Additional Experiments

Figure 4: Mean-squared Error (MSE) on the test data for synthetic data (Anti-hierarchical truth). XGBoost is limited to depth 2 trees.

Figure 5: Mean-squared Error (MSE) on the test data for synthetic data (Hierarchical truth). XGBoost is limited to depth 2 trees.
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