Fusing regression coefficients into homogenous groups can unveil those coefficients that share a common value within each group. Such groupwise homogeneity reduces the intrinsic dimension of the parameter space and unleashes sharper statistical accuracy. We propose and investigate a new combinatorial grouping approach called \(L_0\)-Fusion that is amenable to mixed integer optimization (MIO). On the statistical aspect, we identify a fundamental quantity called \textit{grouping sensitivity} that underpins the difficulty of recovering the true groups. We show that \(L_0\)-Fusion achieves grouping consistency under the weakest possible requirement of the grouping sensitivity: if this requirement is violated, then the minimax risk of group misspecification will fail to converge to zero. Moreover, we show that in the high-dimensional regime, one can apply \(L_0\)-Fusion coupled with a sure screening set of features without any essential loss of statistical efficiency, while reducing the computational cost substantially. On the algorithmic aspect, we provide a MIO formulation for \(L_0\)-Fusion along with a warm start strategy. Simulation and real data analysis demonstrate that \(L_0\)-Fusion exhibits superiority over its competitors in terms of grouping accuracy.

1. **Introduction.** Identifying homogeneous groups of regression coefficients has received increasing attention because the resulting regression model provides better scientific interpretations and enhance predictive performance in many applications. In some occasions, features or covariates naturally act in groups to influence outcomes, so knowing group structures of the features help scientists gain new knowledge about a physical system of interest. From a modeling perspective, aggregating covariates with similar effects along with the response reduces model complexity and improves interpretability, especially in the high-dimensional regime. There have been a flurry of works under this direction; see for example Bondell and Reich (2008); Shen and Huang (2010); Zhu, Shen and Pan (2013); Ke, Fan and Wu (2015); Jeon, Kwon and Choi (2017), among others. There is a vast literature in discovering homogeneous groups of observations or individuals in overly heterogeneous population. However, these existing methods cannot be applied to our problem that aims to group regression parameters. Identifying group structures of regression parameters is crucial to learn the underlying heterogeneous covariates’ effects, which is then leveraged to reach a more appropriate model for data analyses. A partial list of the literature includes Ke et al. (2016); Shen and He (2015); Ma and Huang (2017); Lian, Qiao and Zhang (2017), just name a few. The focus of this paper is on pursuing homogeneous groups of regression coefficients in which we do not have any prior knowledge about their true group structures.

Homogeneity fusion is carried out routinely in environmental health sciences in a manual and subjective manner to evaluate the effect of a given set of toxicants on certain health outcomes. Consider \(p\) toxicants, whose concentrations are denoted by \(X_1, \ldots, X_p\), respectively, \(q\) other covariates \(\{Z_k\}_{k=1}^q\) and a outcome variable \(Y\). Scientists typically consider a linear regression model \(Y \sim \sum_{j=1}^p \beta_j X_j + \sum_{k=1}^q \alpha_k Z_k\) to evaluate effect of a mixture \(A := \sum_{j=1}^p \beta_j X_j\) on outcome \(Y\). One common practice to reduce model complexity and facilitate scientific interpretation is aggregating the exposure of similar toxicants to yield a sum-mixture (e.g. \(\sum_{j} X_j\)). For example, SumDEHP is a sum of four phthalates, MECPP, MEOHP, MEHHP, and MEHP, which quantifies total DEHP exposure from products such as PVC plastics used in food processing/packaging materials as well as building materials and medical devices (Schettler, 2006; Kobrosly et al., 2012; Braun et al., 2012). See also

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**SUPERVISED HOMOGENEITY FUSION: A COMBINATORIAL APPROACH**

**BY WEN WANG, SHIHAO WU, ZIWEI ZHU, LING ZHOU, PETER X.-K. SONG**

Fusing regression coefficients into homogenous groups can unveil those coefficients that share a common value within each group. Such groupwise homogeneity reduces the intrinsic dimension of the parameter space and unleashes sharper statistical accuracy. We propose and investigate a new combinatorial grouping approach called \(L_0\)-Fusion that is amenable to mixed integer optimization (MIO). On the statistical aspect, we identify a fundamental quantity called \textit{grouping sensitivity} that underpins the difficulty of recovering the true groups. We show that \(L_0\)-Fusion achieves grouping consistency under the weakest possible requirement of the grouping sensitivity: if this requirement is violated, then the minimax risk of group misspecification will fail to converge to zero. Moreover, we show that in the high-dimensional regime, one can apply \(L_0\)-Fusion coupled with a sure screening set of features without any essential loss of statistical efficiency, while reducing the computational cost substantially. On the algorithmic aspect, we provide a MIO formulation for \(L_0\)-Fusion along with a warm start strategy. Simulation and real data analysis demonstrate that \(L_0\)-Fusion exhibits superiority over its competitors in terms of grouping accuracy.

1. **Introduction.** Identifying homogeneous groups of regression coefficients has received increasing attention because the resulting regression model provides better scientific interpretations and enhance predictive performance in many applications. In some occasions, features or covariates naturally act in groups to influence outcomes, so knowing group structures of the features help scientists gain new knowledge about a physical system of interest. From a modeling perspective, aggregating covariates with similar effects along with the response reduces model complexity and improves interpretability, especially in the high-dimensional regime. There have been a flurry of works under this direction; see for example Bondell and Reich (2008); Shen and Huang (2010); Zhu, Shen and Pan (2013); Ke, Fan and Wu (2015); Jeon, Kwon and Choi (2017), among others. There is a vast literature in discovering homogeneous groups of observations or individuals in overly heterogeneous population. However, these existing methods cannot be applied to our problem that aims to group regression parameters. Identifying group structures of regression parameters is crucial to learn the underlying heterogeneous covariates’ effects, which is then leveraged to reach a more appropriate model for data analyses. A partial list of the literature includes Ke et al. (2016); Shen and He (2015); Ma and Huang (2017); Lian, Qiao and Zhang (2017), just name a few. The focus of this paper is on pursuing homogeneous groups of regression coefficients in which we do not have any prior knowledge about their true group structures.

Homogeneity fusion is carried out routinely in environmental health sciences in a manual and subjective manner to evaluate the effect of a given set of toxicants on certain health outcomes. Consider \(p\) toxicants, whose concentrations are denoted by \(X_1, \ldots, X_p\), respectively, \(q\) other covariates \(\{Z_k\}_{k=1}^q\) and a outcome variable \(Y\). Scientists typically consider a linear regression model \(Y \sim \sum_{j=1}^p \beta_j X_j + \sum_{k=1}^q \alpha_k Z_k\) to evaluate effect of a mixture \(A := \sum_{j=1}^p \beta_j X_j\) on outcome \(Y\). One common practice to reduce model complexity and facilitate scientific interpretation is aggregating the exposure of similar toxicants to yield a sum-mixture (e.g. \(\sum_{j} X_j\)). For example, SumDEHP is a sum of four phthalates, MECPP, MEOHP, MEHHP, and MEHP, which quantifies total DEHP exposure from products such as PVC plastics used in food processing/packaging materials as well as building materials and medical devices (Schettler, 2006; Kobrosly et al., 2012; Braun et al., 2012). See also
To obtain this estimator, we formulate the corresponding optimization problem as a mixed group constraint (\(L \) are small (e.g. weak signals). We propose to pursue homogeneity and sparsity simultaneously through a combinatorial objective with respect to \(\beta \), where \(\|\cdot\|_0 \) is a tuning parameter that is associated with fusion strength, and \(J_\tau(z) = \min(z\tau^{-1},1) \) is a surrogate of the indicator function \(1_{z\neq 0}(z) \) with \(\tau > 0\) representing the approximation error of \(J_\tau(z) \) to the \(L_0\) penalty \(1_{z\neq 0}(z) \). Such penalty on the pairwise difference can lead to redundant comparisons and extra computational complexity. Note that there is no sparsity regularization in \(S_1(\beta) \). An extension, Zhu, Shen and Pan (2013) considered simultaneous grouping pursuit and feature selection by further penalizing individual coefficients, that is, minimizing \(S_2(B) = n^{-1} \sum_{i=1}^n (y_i - \sum_{j=1}^p x_{ij} \beta_j)^2 + \lambda_2 \sum_{j=1}^p \sum_{j' \neq j} \gamma_j |\beta_j - \beta_{j'}|) + \lambda_2 \sum_{j=1}^p J_\tau(|\beta_j|) \). Here \(E \) is the edge set of an undirected graph with \(p \) nodes representing \(\{X_j\}_{j=1}^p \). If \(X_i \) and \(X_j \) can be grouped, then there is an edge between nodes \(i \) and \(j \); otherwise, there is no edge. Available prior knowledge of \(E \) reduces computational burden and improves estimation efficiency. However, it is always challenging in practice to obtain a plausible estimate of \(E \), which makes the method less appealing. Ke, Fan and Wu (2015) proposed a different method named as clustering algorithm in regression via data-driven segmentation (CARDS). They use a preliminary estimate to determine “adjacent” coefficient pairs for fusion and only penalize distances between the two coefficients in each adjacent pairs by folded concave penalty function. Therefore, the CARDS estimator depends on the initial ordering of the coefficients, which could be unstable especially when the effect sizes are small (e.g. weak signals).

We propose to pursue homogeneity and sparsity simultaneously through a combinatorial approach called \(L_0\)-Fusion. Specifically, we estimate \(\beta^* \) by the least squares with an exact group constraint (\(\beta_j^* \) can only take \(K_0 \) distinct nonzero values) and an \(L_0\) sparsity constraint. To obtain this estimator, we formulate the corresponding optimization problem as a mixed

\begin{equation}
Y = \sum_{j=1}^p \beta_j^* X_j + \sum_{k=1}^q \alpha_k^* Z_k + \varepsilon, \quad \beta_j^* \in \{0, \gamma_{1}^*, \gamma_{2}^*, \ldots, \gamma_{K_0}^*\}, \quad \forall j \in [p],
\end{equation}

where \(\varepsilon \sim \mathcal{N}(0, \sigma^2)\), and where the coefficients \(\{\beta_j^*\}_{j=1}^p \) belong to a set including 0 and \(K_0 \) unknown different nonzero values \(\{\gamma_k^*\}_{k=1}^{K_0} \). Note that the group membership of each nonzero \(\beta_j \) is not observed in data collection. Write \(\alpha^* = (\alpha_1^*, \ldots, \alpha_q^*)^\top \in \mathbb{R}^q, \beta^* = (\beta_1^*, \ldots, \beta_p^*)^\top \in \mathbb{R}^p \) and \(\gamma^* = (\gamma_1^*, \ldots, \gamma_{K_0}^*)^\top \in \mathbb{R}^{K_0} \). Our main goal in this paper is to estimate \(\gamma^*, \beta^* \) and \(\alpha^* \) simultaneously based on an independent and identically distributed (i.i.d.) sample \(\{(x_i, z_i, y_i)\}_{i=1}^n \) of size \(n \). In the case of high dimension, \(\beta \) is often assumed sparse so that we perform feature selection and grouping simultaneously to ensure statistical consistency.

We now review and discuss some important works related to model (1.1). Shen and Huang (2010) considered model (1.1) without \(\{Z_k\}_{k\in[q]} \) and proposed to minimize the following objective with respect to \(\beta \): \(S_1(\beta) = n^{-1} \sum_{i=1}^n (y_i - \sum_{j=1}^p x_{ij} \beta_j)^2 + \lambda_1 \sum_{j<j'} J_\tau(|\beta_j - \beta_{j'}|) \), where \(\lambda_1 \) is a tuning parameter that is associated with fusion strength, and \(J_\tau(z) = \min(z\tau^{-1},1) \) is a surrogate of the indicator function \(1_{z\neq 0}(z) \) with \(\tau > 0\) representing the approximation error of \(J_\tau(z) \) to the \(L_0\) penalty \(1_{z\neq 0}(z) \). Such penalty on the pairwise difference can lead to redundant comparisons and extra computational complexity. Note that there is no sparsity regularization in \(S_1(\beta) \). As an extension, Zhu, Shen and Pan (2013) considered simultaneous grouping pursuit and feature selection by further penalizing individual coefficients, that is, minimizing \(S_2(B) = n^{-1} \sum_{i=1}^n (y_i - \sum_{j=1}^p x_{ij} \beta_j)^2 + \lambda_1 \sum_{j<j'} J_\tau(|\beta_j - \beta_{j'}|) + \lambda_2 \sum_{j=1}^p J_\tau(|\beta_j|) \). Here \(E \) is the edge set of an undirected graph with \(p \) nodes representing \(\{X_j\}_{j=1}^p \). If \(X_i \) and \(X_j \) can be grouped, then there is an edge between nodes \(i \) and \(j \); otherwise, there is no edge. Available prior knowledge of \(E \) reduces computational burden and improves estimation efficiency. However, it is always challenging in practice to obtain a plausible estimate of \(E \), which makes the method less appealing. Ke, Fan and Wu (2015) proposed a different method named as clustering algorithm in regression via data-driven segmentation (CARDS). They use a preliminary estimate to determine “adjacent” coefficient pairs for fusion and only penalize distances between the two coefficients in each adjacent pairs by folded concave penalty function. Therefore, the CARDS estimator depends on the initial ordering of the coefficients, which could be unstable especially when the effect sizes are small (e.g. weak signals).
integer optimization (MIO) problem. Bertsimas et al. (2016) demonstrated that MIO provides a computationally tractable approach to solve the classical best subset selection (BSS) problem of a practical scale: With the sample size in thousands and the dimension in hundreds, a MIO algorithm can achieve provable optimality in minutes. Such success of MIO and the similar combinatorial nature of the BSS problem inspire us to seek for a MIO formulation of the $L_0$-Fusion problem. Our main contributions are summarized as follows: (a) To the best of our knowledge, it is the first time that we formulate the group pursuing as a MIO problem; (b) we show that the estimator derived from the $L_0$-Fusion problem achieves grouping consistency once the loss function is reasonably sensitive to a certain grouping error; (c) we discover that the grouping sensitivity requirement in (b) turns out to be necessary (up to a universal constant) for any approach to achieve selection and grouping consistency; (d) we provide a warm start algorithm with convergence guarantee for the $L_0$-Fusion problem, in order to accelerate the MIO solver.

The rest of the article is organized as follows. Section 2 introduces the $L_0$-Fusion method and a “screen then group” strategy to tackle high dimension. It also presents all the statistical theory, including the selection and grouping consistency of the $L_0$-Fusion method and a necessary condition to achieve such consistency. Section 3 introduces our MIO formulation for the $L_0$-Fusion problem together with a warm up algorithm. Section 4 demonstrates significant superiority of the $L_0$-Fusion method over existing ones in terms of grouping accuracy in both low-dimensional and high-dimensional regimes. We also apply $L_0$-Fusion to a metabolomics dataset to aggregate concentration of similar lipids to predict the body mass index (BMI). The appendix includes all technical details, including the proofs of major theoretical results.

2. Statistical methodology and theory.

2.1. Notation. We use regular letters, bold regular letters and bold capital letters to denote scalars, vectors and matrices respectively. For any positive integer $n$, we denote $\{1, \ldots, n\}$ by $[n]$. For any two sets $A$ and $B$, let $A \setminus B := A \cap B^c$. For any vector $a$ and matrix $A$, we use $a^\top$ and $A^\top$ to denote the transpose of $a$ and $A$ respectively. Given $B = \{i_1, \ldots, i_{|B|}\} \subset [p]$, we use $X_B$ to denote the submatrix of $X$ with columns indexed in $B$ and use $\beta_B$ to denote $(\beta_{i_1}, \ldots, \beta_{i_{|B|}})^\top$. Given any $a,b \in \mathbb{R}$, we say $a \lesssim b$ if there exists a universal constant $C > 0$ such that $a \leq Cb$; we say $a \gtrsim b$ if there exists a universal constant $c > 0$ such that $a \geq cb$; we say $a \asymp b$ if $a \lesssim b$ and $a \gtrsim b$. For any event $A$, we use $I(A)$ to denote the indicator function associated with $A$, i.e., $I(A) = 1$ if $A$ occurs, and $I(A) = 0$ otherwise.

2.2. $L_0$-Fusion with feature screening. Suppose we have $n$ independent observations $(x_{i}, z_{i}, y_{i})_{i \in [n]}$ from model (1.1). Our paper revolves around the following combinatorial optimization problem to achieve feature selection and homogeneity fusion simultaneously:

$$\begin{align*}
\min_{\alpha \in \mathbb{R}^s, \beta \in \mathbb{R}^p, \gamma \in \mathbb{R}^K} & \sum_{i=1}^{n} (y_i - x_i^\top \beta - z_i^\top \alpha)^2, \\
\text{subject to:} & \quad \beta_j \in \{0, \gamma_1, \gamma_2, \ldots, \gamma_K\}, \forall j \in [p], \\
& \quad \|eta\|_0 := \sum_{j=1}^{p} I(\beta_j \neq 0) \leq s.
\end{align*}$$  

(2.1)

The first constraint requires the non-zero group number to be bounded by $K$, and the second constraint requires the sparsity of $\beta$ to be bounded by $s$. Given that the problem above restricts the $\ell_0$-norm of $\beta$ and also fuses the components of $\beta$, we refer to it as the $L_0$-Fusion...
Algorithm 1: CoSaMP($X, y, \hat{\beta}_0, \pi, l, \tau$)

**Input:** Design matrix $X$, response $y$, initial value $\hat{\beta}_0$, projection size $\pi$, expansion size $l$, convergence threshold $\tau > 0$

1: $t \leftarrow 0$
2: repeat
3: $G_t \leftarrow T_{abs}(\nabla L(\hat{\beta}_t), l)$
4: $S_t^\dagger \leftarrow \text{supp}(\hat{\beta}_t) \cup G_t$
5: $\hat{\beta}_t^\dagger \leftarrow (X_{S_t^\dagger}^T X_{S_t^\dagger})^{-1} X_{S_t^\dagger}^T y$
6: $S_t \leftarrow T_{abs}(\hat{\beta}_t^\dagger, \pi)$
7: $\hat{\beta}_{t+1} \leftarrow (X_{S_t} X_{S_t})^{-1} X_{S_t} y$
8: $t \leftarrow t + 1$
9: until $\|\hat{\beta}_t - \hat{\beta}_{t-1}\|_2 < \tau$
10: $\hat{\beta}_{cs} \leftarrow \hat{\beta}_t$

**Output:** $\hat{\beta}_{cs}$

Without the grouping constraint, (2.1) boils down the well-known best subset selection (BSS) problem (Garside, 1965; Hocking and Leslie, 1967; Beale, Kendall and Mann, 1967) with subset size $s$. Note that problem (2.1) is NP-hard because of the cardinality and grouping constraint. Despite of the computational challenge, Section 3.1 provides a MIO formulation of (2.1) that is amenable to modern integer optimization solvers such as GUROBI and MOSEK. In our numerical study, when the dimension $p \leq 100$, GUROBI can solve the $L_0$-Fusion problem within seconds.

However, under practical setups, $p$ is often in thousands or even millions. Directly solving the $L_0$-Fusion problem under such a scale is computationally burdensome or even prohibitive. To tackle this, we propose a “screen then group” strategy. In the screening stage, let $\tilde{S}$ denote a screening set generated by a preliminary feature screening procedure, the examples of which include, but are not limited to, penalized least squares methods (Tibshirani, 1996; Fan and Li, 2001; Zhang et al., 2010), sure independence screening (Fan and Lv, 2008) or sparsity constraint method (Needell and Tropp, 2009; Fan, Guo and Zhu, 2020). Suppose $\tilde{S}$ enjoys the sure screening property, i.e., the true support set $S^0 \subseteq \tilde{S}$ with high probability. Then in the grouping stage, we perform $L_0$-Fusion on the reduced design $X_{\tilde{S}}$ to generate groups of nonzero coefficients, so that we work with lower-dimensional version of problem (2.1).

We choose CoSaMP (Compressive Sampling Matching Pursuit), an iterative two-stage hard thresholding algorithm proposed by Needell and Tropp (2009), as our variable screener. Algorithm 1 presents its pseudocode. CoSaMP performs two rounds of hard thresholding in each iteration: it first expands the model by recruiting the largest coordinates of the gradient (lines 3-4) and then contracts the model by discarding the smallest components of the refitted signal on the expanded model (lines 5-7). Fan, Guo and Zhu (2020) showed that under a high-dimensional sparse regression setup, CoSaMP (referred to as IHT therein) can achieve sure screening properties within few iterations under highly correlated designs. In addition, Zhu and Wu (2021) showed numerically that CoSaMP yields much fewer false discoveries than LASSO, SCAD and MCP on early solution paths, particularly in the presence of high correlations among predictors. These supporting results signify CoSaMP as an efficient and reliable screener that can help substantially reduce the dimension while retaining the true signals. We emphasize that the low false discovery rate (FDR) here is crucial to controlling the dimension of the reduced design on which the $L_0$-Fusion procedure becomes computationally tractable.
2.3. Statistical theory. In this section, we prove that the global minimizers of problem (2.1) reconstruct the ideal “oracle estimator”, i.e., the estimator with prior knowledge of the true grouping, under a “degree-of-separation” condition. To understand how the proposed method performs under high dimensions, in the following we derive necessary and sufficient conditions to achieve grouping consistency as well as selection consistency. Define the parameter space \( \Theta(K, s) := \{ \theta = (\beta^*, \alpha^*)^\top \in \mathbb{R}^{p+q} \mid \gamma \in \mathbb{R}^K, \beta_j \in \{0, \gamma_1, \ldots, \gamma_K\}, \forall j \in [p], ||\beta||_0 \leq s \} \). Denote the index operator for the elements of \( \beta \) with value \( r \) by \( G(\beta; r) = \{ j \in [p] \mid \beta_j = r \} \) and the grouping operator by \( G(\beta) = \{ G(\beta; r) \mid r \neq 0, G(\beta; r) \neq \emptyset \} \). Let \( |G(\beta; r)| \) and \( |G(\beta)| \) be the cardinality of \( G(\beta; r) \) and \( G(\beta) \), respectively.

Throughout this section, we write the \( n \times p \) design matrix \( X = (X_1, \ldots, X_p) \) and the \( n \times q \) matrix \( Z = (Z_1, \ldots, Z_q) \), where \( X_j \) and \( Z_k \) are the \( j \)th and \( k \)th columns of \( X \) and \( Z \), respectively.

2.3.1. Sensitivity to grouping accuracy. We first define a distance \( d(\beta, \beta') \) between two groupings that correspond to \( \beta \) and \( \beta' \) respectively:

**Definition 2.1** (Distance between groupings). Let \( F(\beta, \beta') := \{ f \text{ is injective} : \mathcal{G}(\beta) \rightarrow \mathcal{G}(\beta') \} \). Then for any \( \beta, \beta' \) such that \( |G(\beta)| \leq |G(\beta')| \), define

\[
(2.2) \quad d(\beta, \beta') := \min_{f \in F(\beta, \beta')} \left\| \bigcup_{G_2 \in G(\beta)} \left\{ G_2 \setminus \bigcup_{G_1 \in G(\beta)} \{ G_1 \cap f(G_1) \} \right\} \right\|
\]

This distance is the minimum number of grouping labels that need to be changed to match \( \mathcal{G}(\beta) \) and \( \mathcal{G}(\beta') \). Specifically, \( \cup_{G_1 \in G(\beta)} \{ G_1 \cap f(G_1) \} \) collects all the variables that are consistently labeled by \( G(\beta) \) and \( G(\beta') \) based on a mapping \( f \). Therefore, \( \cup_{G_2 \in G(\beta)} \bigcup_{G_1 \in G(\beta)} \{ G_1 \cap f(G_1) \} \) means to capture all the variables with inconsistent group labels in \( \mathcal{G}(\beta) \) and \( \mathcal{G}(\beta') \) based on mapping \( f \). Figure 1 illustrates a specific setup with two possible grouping maps \( f^{(1)} \) and \( f^{(2)} \) in \( F(\beta, \beta') \). One can see that \( f^{(1)} \) gives three inconsistent group labels (three crosses) between \( \mathcal{G}(\beta) \) and \( \mathcal{G}(\beta') \), while \( f^{(2)} \) gives four. Therefore, \( f^{(1)} \) minimizes the objective in (2.2), implying that \( d(\beta, \beta') = 3 \).

Next, we define a sensitivity measure of mean squared error (MSE) with respect to grouping error, which is shown later to determine the difficulty of identifying the true grouping:

**Definition 2.2** (Grouping sensitivity).

\[
(2.3) \quad c_{\text{min}} \equiv c_{\text{min}}(\theta^*, X, Z) = \min_{\theta \in \Theta(\|G(\beta^*)\|, \|\beta^*\|_0)} \frac{\|X(\beta - \beta^*) + Z(\alpha - \alpha^*)\|^2_2}{n \max(d(\beta, \beta^*), 1)}.
\]

In words, \( c_{\text{min}} \) is the minimum increase of MSE due to a falsely grouped variable. A small \( c_{\text{min}} \) suggests that the MSE is insensitive to false grouping and thus makes it difficult to identify the true grouping.

2.3.2. Sufficient condition. Given a grouping status \( \mathcal{G}(\beta) \), define

\[
X_{\mathcal{G}(\beta)} := \left( \sum_{k \in \mathcal{G}(\beta; \gamma_1)} X_k, \ldots, \sum_{k \in \mathcal{G}(\beta; \gamma_1)} X_k \right),
\]

which is a groupwise collapsed matrix by summing up columns of \( X \) according to the groups in \( \mathcal{G}(\beta) \).
DEFINITION 2.3 (Oracle least squares estimator). Given the true coefficient \( \beta^* \), the oracle least squares estimator \( \hat{\theta}^{ol} = (\hat{\beta}^{olT}, \hat{\alpha}^{olT})^T \) is defined as
\[
\hat{\theta}^{ol} := \arg\min_{\theta: G(\beta) = \hat{G}(\beta^*)} \| Y - X\beta - Z\alpha \|_2^2.
\]
More specifically, in \( \hat{\beta}^{ol} = (\hat{\beta}_1, \ldots, \hat{\beta}_p)^T \), \( \hat{\beta}_j \) is \( \hat{\gamma}_k \) if \( j \in \hat{G}(\beta^*; \gamma_k) \), \( k = 1, \ldots, K_0 \), and \( \hat{\beta}_j = 0 \) if \( j \notin \hat{G}(\beta^*; 0) \), where
\[
(\hat{\gamma}^T, \hat{\alpha}^T) = (\hat{\gamma}_1, \ldots, \hat{\gamma}_{K_0}, \hat{\alpha}^T) = \arg\min_{(\gamma^T, \alpha^T) \in \mathbb{R}^{K_0 + q}} \| Y - X_{G(\beta^*)}\gamma - Z\alpha \|_2^2.
\]

For any estimator \( \hat{\theta} = (\hat{\beta}^T, \hat{\alpha}^T)^T \) of \( \theta^* \), define the 0-1 grouping risk \( \mathcal{L}_g(\hat{\theta}; \theta^*) := \mathbb{P}(G(\beta) \neq G(\beta^*)) \). Denote the solution to the \( L_0 \)-Fusion problem (2.1) by \( \hat{\theta}^g = (\hat{\beta}^g, \hat{\alpha}^g)^T \). Recall that \( K_0 = |G(\beta^*)| \) and further define \( s_0 = |\beta^*|_0 \). The next theorem says that \( \hat{\theta}^g \) consistently recovers \( \theta^{ol} \) when the grouping sensitivity \( c_{min} \geq \log(pK_0)/n \). Section 2.3.3 shows that this lower bound is necessary to achieve grouping consistency.

THEOREM 2.4. Suppose that \( K = K_0 \) and \( s = s_0 \) in (2.1). We have
\[
\mathbb{P}(\hat{\theta}^g \neq \theta^{ol}) \leq 6 \exp\left\{ -\frac{3n}{40\sigma^2} \left\{ c_{min} - \frac{\sigma^2}{n} \left( 27 \log(pK_0) + 12 \right) \right\} \right\},
\]
which implies that when \( c_{min} \geq \frac{\sigma^2}{n} \{ d_1 \log(pK_0) + 12 \} \) for some universal constant \( d_1 > 27 \), \( \hat{\theta}^g \) consistently reconstructs \( \theta^{ol} \), i.e., as \( n, p \to \infty \), \( \mathcal{L}_g(\hat{\theta}^g; \theta^*) \to 0 \).

Define the sure screening event as \( \mathcal{E} := \{ S^0 \subseteq \hat{S} \} \). Let \( \hat{\theta}^{sg} \) denote the solution under the “screen then group” strategy. The following corollary says that as long as \( \mathcal{E} \) enjoys sure screening with high probability, \( \hat{\theta}^{sg} \) also consistently recovers \( \theta^{ol} \). Many variable screening techniques provably yield such a sure screening set under reasonable assumptions on the signal and design, e.g., Sure Independence Screening (Fan and Lv, 2008), LASSO (Wainwright,
the RHS of the inequality above is well bounded from below, so that
\[ n \geq \frac{\sigma^2}{\sigma^2/n} \left( 27\log(pK_0) + 12 \right), \]
we have
\[ \mathbb{P}(\hat{\theta}^{\text{ols}} = \hat{\theta}^{\text{opt}}) \geq 1 - \exp \left[-\frac{3n}{40\sigma^2} \left( c_{\min} - \frac{\sigma^2}{n} \left( 27\log(pK_0) + 12 \right) \right) \right] - \mathbb{P}(\mathcal{E}^c). \]

2.3.3. Necessary condition. For \( \ell > 0 \), consider the following subspace of \( \Theta(K_0, s_0) \):
\[ \Theta_c(K_0, s_0, \ell) := \{ \theta : \theta \in \Theta(K_0, s_0), c_{\min}(\theta, X, Z) \geq \ell \}. \]
We now present a lower bound for the minimax 0-1 grouping risk over \( \Theta_c(K_0, s_0, \ell) \), which enables us to deduce the necessity of the lower bound of \( c_{\min} \) in Theorem 2.4 (up to a universal constant) in connection to a theoretical guarantee for the selection and grouping consistency simultaneously. For notational convenience, define the following subspace \( \Theta(K_0, s_0) \) of \( \Theta(K_0, s_0) \) with well separated signal strengths across groups and balanced group sizes:
\[ \Theta_c(K_0, s_0) := \{ \theta^* \in \Theta(K_0, s_0) : |\beta_j^* - \beta_{j'}^*| \geq 1, \forall \beta_j^* \neq \beta_{j'}, |\mathcal{G}(\beta^*, \gamma_k^*)| \leq 2 |\mathcal{G}(\beta^*, \gamma_{k'}^*)|, \forall k, k' \in |K_0| \}. \]

THEOREM 2.5. Define
\[ r(X, Z, K_0, s_0) := \max_{1 \leq j \leq p} n^{-1} \|X_j\|_2^2 \]
\[ \min_{\theta^*: \theta \in \Theta(K_0, s_0)} c_{\min}(\theta^*, X, Z). \]
For any \( K_0 \geq 1, p \geq s_0 \geq K_0 \) and \( \ell > 0 \), we have
\[ \inf_{\theta} \sup_{\theta^*: \theta \in \Theta_c(K_0, s_0, \ell)} \mathcal{L}_g(\hat{\theta}; \theta^*) \geq 1 - \frac{2nr(X, Z, K_0, s_0) \ell + \sigma^2 \log 2}{\sigma^2 \log \left( \frac{K_0+3}{4} p \right)}. \]
Consequently, if \( \inf_{\theta} \sup_{\theta^*: \theta \in \Theta_c(K_0, s_0, \ell)} \mathcal{L}_g(\hat{\theta}; \theta^*) \to 0 \), as \( n, p \to \infty \), one must have that
\[ \ell \geq \frac{\sigma^2 \left\{ \log \left( \frac{K_0+3}{4} p \right) - \log 2 \right\}}{2nr(X, Z, K_0, s_0)}. \]

Quantity \( r(X, Z, K_0, s_0) \) plays an important role in the lower bound above, which deserves some discussion. We conjecture that under an restricted eigenvalue (RE) assumption (Bickel et al., 2009; Van De Geer and B"uhlmann, 2009; Negahban et al., 2012) and an assumption of bounded marginal variance of the features, \( r(X, Z, K_0, s_0) \lesssim 1 \). Specifically, write \( \tilde{X} = (X, Z) \). Under the RE condition that \( n^{-1} |\tilde{X}v|_2^2 \geq \kappa |v|_2^2 \) for any \( v \in \mathbb{R}^{p+q} \) with \( |v|_0 \leq (2s_0 + q) \) and some \( \kappa > 0 \), we have that
\[ \min_{\theta^*: \theta \in \Theta(K_0, s_0)} c_{\min}(\theta^*, X, Z) \geq \min_{\theta^*: \theta \in \Theta(K_0, s_0)} \min_{\theta (1 \notin \mathcal{G}(\beta^*), |\beta|_0)} \min_{\mathcal{G}(\beta) \neq \mathcal{G}(\beta^*)} \frac{\kappa |\beta - \beta^*|_2^2}{\max(d(\beta, \beta^*), 1)}. \]

The following proposition considers a special case of two groups \( (K_0 = 2) \) and shows that the \( \text{RHS} \) of the inequality above is well bounded from below, so that \( r(X, Z, K_0, s_0) \lesssim 1 \) if \( n^{-1} \max_{j \in [p]} \|X_j\|_2^2 \lesssim 1 \).
PROPOSITION 2.1. Under the RE condition above, we have for any \( s_0 \geq 2 \) that

\[
\min_{\theta^* \in \tilde{\Theta}(2, s_0)} \frac{\min_{G(\beta) \neq G(\beta^*)} \|\beta - \beta^*\|_2^2}{\max\{d(\beta, \beta^*), 1\}} \gtrsim 1.
\]

We emphasize that the well-separated signals and balanced group sizes in the definition of \( \tilde{\Theta} \) are both essential to guarantee the conclusion of Proposition 2.1. Violating either of the two constraints in the definition of \( \tilde{\Theta} \) can let the double minimum above vanish asymptotically as \( s_0 \to \infty \).

3. Mixed integer optimization formulation. Given the strong statistical guarantee established for \( L_0 \)-Fusion in the previous section, we now switch our focus to the computational aspect of the problem. In this section, we leverage mixed integer optimization techniques to solve the combinatorial problem (2.1). Recently, Bertsimas et al. (2016) proposed a MIO approach to solve the best subset selection problem of a remarkably enhanced scale. This inspires us to formulate \( L_0 \)-Fusion as a MIO problem, for which we can resort to modern MIO solvers. In Section 3.1, we introduce the MIO formulation of \( L_0 \)-Fusion. Then we present a warm start algorithm in Section 3.2 to further accelerate the MIO solver.

3.1. MIO formulations for homogeneity fusion. Generally speaking, a MIO problem is formulated as follows:

\[
\min_{\alpha \in \mathbb{R}^m} \alpha^\top Q \alpha + \alpha^\top a \tag{3.1}
\]

subject to:

\[
A \alpha \leq b,
\]

\[
\alpha_j \in \{0, 1\}, \quad j \in I,
\]

\[
\alpha_j \geq 0, \quad j \notin I,
\]

where \( a \in \mathbb{R}^m, A \in \mathbb{R}^{h \times m}, b \in \mathbb{R}^h, \) and \( Q \in \mathbb{R}^{m \times m} \) is positive semi-definite. The symbol \( \leq \) represents element-wise inequalities. \( I \), an index subset of \([m]\), identifies the binary components of \( \alpha \). The mixture of discrete and continuous components of \( \alpha \) justifies the name of mixed integer programming. For more comprehensive background of MIO, we refer the readers to Bertsimas and Weismantel (2005) and Jünger and Reinelt (2013). Some popular MIO solvers include CPLEX, GLPK, MOSEK and GUROBI. Thanks to the branch-and-bound techniques (Cook et al., 1995), these solvers can provide both feasible solutions and lower bounds of the optimal objective value, from which we can learn how far a current solution is from the global optimum.

Now we introduce the MIO formulation for problem (2.1):

\[
\min_{\alpha \in \mathbb{R}^p, \beta \in \mathbb{R}^p, \gamma \in \mathbb{R}^K, \Omega \in \{0, 1\}^{p \times (K+1)}} \sum_{i=1}^n (y_i - x_i^\top \beta - z_i^\top \alpha)^2, \tag{3.2}
\]

subject to:

\[
\omega_{jk} \in \{0, 1\}, \quad \forall k \in \{0\} \cup [K], j \in [p]
\]

\[
\omega_{jk} (\beta_j - \gamma_k) = 0, \quad \forall k \in [K], j \in [p]
\]

\[
\omega_{j0} \beta_j = 0, \quad \forall j \in [p]
\]

\[
\gamma_k \leq \gamma_{k+1}, \quad \forall k \in [K-1]
\]

\[
\sum_{k=0}^{K} \omega_{jk} = 1, \quad \forall j \in [p]
\]
Consider the following generalized
\[
\sum_{j=1}^{p} \omega_j \theta_j \geq p - s.
\]

Here the number of groups \( K \) and the sparsity \( s \) are prespecified, which will be tuned by, for example, cross-validation. For any \( j \in [p] \) and \( k \in \{0\} \cup [K] \), we use \( \omega_{jk} \) to denote the \((j, k + 1)\) entry of \( \Omega \). For any \( j \in [p] \) and \( k \in [K] \), \( \omega_{jk} = 1 \) (\( \omega_{jk} = 0 \)) means that the \( j \)th covariate is (not) in the \( k \)-th group. To see why this is true, note that \( \omega_{jk}(\beta_j - \gamma_k) = 0 \) enforces \( \beta_j = \gamma_k \) when \( \omega_{jk} = 1 \). Similarly, \( \omega_{j0} = 1 \) implies that \( \beta_j = 0 \), given the constraint that \( \omega_{j0}\beta_j = 0 \). These types of constraints correspond to Specially Ordered Sets of type 1 (SOS-1) in Beale and Tomlin (1970) and can be replaced by linear constraints (Vielma and Nemhauser, 2011; Markowitz and Manne, 1957; Dantzig, 1960). The constraint \( \gamma_k < \gamma_{k+1} \) resolves the identifiability issue so that \( \{\gamma_k\}_{k \in [K]} \) can be uniquely determined. \( \sum_{k=1}^{K} \omega_{jk} = 1 \) implies that each covariate belongs to exactly one group. Finally, \( \sum_{j=1}^{p} \omega_{j0} \geq p - s \) ensures the size of the zero-valued group to be bigger than \( p - s \), thereby constraining the sparsity of \( \beta \) below \( s \). It is noteworthy that the solution of problem (3.2) can have fewer than \( K \) groups.

Problem (3.2) can be easily extended to accommodate prior knowledge regarding group structures. For instance, some covariates are known in advance to be in the same group, say \( \beta_{j \in \mathcal{J}} \) are equal for a set \( \mathcal{J} \subset [p] \). Then we can incorporate this information into (3.2) by adding the constraint that \( \omega_{jk} = \omega_{j,k}, \forall j_1, j_2 \in \mathcal{J}, j_1 \neq j_2, k \in \{0\} \cup [K] \). Another example is that we know no pair of covariates among \( \{X_{j}\}_{j \in \mathcal{J}} \) should belong to the same group. Then we can add the constraint that \( \sum_{j \in \mathcal{J}} \omega_{jk} \leq 1, k = \{0\} \cup [K] \).

### 3.2. Warm start algorithm.
This section introduces a discrete first-order algorithm to provide a warm start for the MIO problem (3.2). Our algorithm is inspired by Bertsimas et al. (2016), who proposed a similar algorithm to initialize a MIO solver to solve the BSS problem. Since this algorithm is not limited to the square loss objective in the \( L_0 \)-Fusion problem, we extend the original \( L_0 \)-Fusion problem to embrace a wider range of objective functions.

Suppose we are interested in a convex objective function \( g(\theta) \) satisfying that:

(i) \( g(\theta) \geq C_2 > -\infty \) for some universal constant \( C_2 \);
(ii) \( g(\theta) \) has Lipschitz continuous gradient, i.e., \( \|\nabla g(\theta) - \nabla g(\tilde{\theta})\|_2 \leq l\|\theta - \tilde{\theta}\|_2 \) for some positive \( l \) and any \( \theta, \tilde{\theta} \in \Theta(K, s) \), which is defined in the beginning of Section 2.3.

Consider the following generalized \( L_0 \)-Fusion problem:

\[
(3.3) \quad \min_{\theta \in \Theta(K, s)} g(\theta).
\]

We propose an algorithm to attain a feasible point close to the solution of problem (3.3), based on ideas from projected gradient descent methods (Nesterov, 2004, 2013). Note that this point can serve as a starting point for MIO solvers and the objective function value at this point is an upper bound of the global minimum. To do so, we construct a curve \( h_L(\theta, \theta') \) defined in the following proposition, which lies above \( g(\theta) \) and is tangent to \( g(\theta) \) at \( \theta' \):

**Proposition 3.1** (Nesterov (2004, 2013)). For a convex function \( g(\theta) \) satisfying (ii), and for any \( L \geq l \), we have:

\[
(3.4) \quad g(\theta) \leq h_L(\theta, \theta') := g(\theta') + (\theta - \theta')^\top \nabla g(\theta') + \frac{L}{2} \|\theta - \theta'\|_2^2
\]

for all \( \theta, \theta' \) with equality holding at \( \theta = \theta' \).
As illustrated in Figure 2, given a point $\theta_m$, we can always improve the current objective value $g(\theta_m)$ through the descending route:

\[
g(\theta_{m+1}) \leq h_L(\theta_{m+1}, \theta_m) \leq h_L(\theta_m, \theta_m) = g(\theta_m),
\]

where

\[
\theta_{m+1} \in \arg\min_{\theta \in \Theta(K,s)} h_L(\theta, \theta_m) = \arg\min_{\theta \in \Theta(K,s)} \left\| \theta - (\theta_m - \frac{1}{L} \nabla g(\theta_m)) \right\|^2_2.
\]

For convenience, for any constant vector $c = (c_1, \ldots, c_{p+q})^\top$, define

\[
\mathcal{H}_{K,s}(c) := \arg\min_{\theta \in \Theta(K,s)} \|\theta - c\|^2_2.
\]

Then $\theta_{m+1} \in \mathcal{H}_{K,s}(\theta_m - \frac{1}{L} \nabla g(\theta_m))$. By doing this improvement iteratively, we implement Algorithm 2 below that supplies our warm starts to solve problem (3.3).

**Algorithm 2: Warm Start**

**Input:** Loss function $g(\theta)$, number of groups $K$, sparsity constraint $s$, step size parameter $L$ and convergence tolerance $\varepsilon$.

1: Initialize with $\theta_1 \in \mathbb{R}^{p+q}$.
2: For $m \geq 1$, $\theta_{m+1} \in \mathcal{H}_{K,s}(\theta_m - \frac{1}{L} \nabla g(\theta_m))$.
3: Repeat Step 2 until $g(\theta_m) - g(\theta_{m+1}) \leq \varepsilon$.

**Output:** $\theta_{m+1}$.

Algorithm 2 is essentially a projected gradient descent algorithm: In each iteration, we perform a gradient descent step followed by projection onto $\mathcal{H}_{K,s}$. To obtain an element in $\mathcal{H}_{K,s}(c)$ for any $c \in \mathbb{R}^{p+q}$, we can exploit the subroutine Algorithm 3 in Appendix A.1, which is a generalization of the segment neighbourhood method (Auger and Lawrence, 1989) with sparsity constraint. To investigate the algorithmic convergence of Algorithm 2, we first define the first-order stationary points of problem (3.3) as follows.
DEFINITION 3.1 (First-order stationary point). We say a vector $\theta \in \Theta(K, s)$ is a first-order stationary point for problem (3.3) if $\theta' \in \mathcal{H}_{K,s}(\theta - \frac{1}{L}\nabla g(\theta))$ for some positive constant $L \geq 1$.

The following proposition establishes two important properties of the first-order stationary points that underpin the effectiveness and stability of our warm start Algorithm 2.

PROPOSITION 3.2. Suppose a positive constant $L > l$.

1. If $\theta$ is a solution to problem (3.3), then it is a first-order stationary point.
2. If $\theta$ is a first-order stationary point, then the set $\mathcal{H}_{K,s}(\theta - \frac{1}{L}\nabla g(\theta))$ has exactly one element $\theta$.

PROOF. 1. From (3.5) and that $\theta$ is a solution to problem (3.3), we know $\min_{\theta' \in \Theta(K, s)} h_L(\theta', \theta) = h_L(\theta, \theta)$. Then $\theta \in \mathcal{H}_{K,s}(\theta - \frac{1}{L}\nabla g(\theta))$.

2. Assume $\theta \in \mathcal{H}_{K,s}(\theta - \frac{1}{L}\nabla g(\theta))$ and $\theta \neq \theta$. Then $(\theta - \theta)^\top \nabla g(\theta) = \frac{L}{2}\|\theta - \theta\|_2^2 > 0$. Since $g$ is convex, we have $g(\theta) > g(\theta)$. This contradicts with (3.5).

Now we present the convergence property and convergence rate of Algorithm 2 through Proposition 3.3 and Theorem 3.2, respectively.

PROPOSITION 3.3. For problem (3.3) and some positive constant $L > l$, let $\theta_m, m \geq 1$ be the sequence generated by Algorithm 2. We have

1. $g(\theta_m) - g(\theta_{m+1}) \geq \frac{L - l}{2}\|\theta_m - \theta_{m+1}\|_2^2$;
2. $\|\theta_{m+1} - \theta_m\|_2 \rightarrow 0$ as $m \rightarrow \infty$.

PROOF. The first statement holds because

$$g(\theta_m) = h_L(\theta_m, \theta_m) \geq h_L(\theta_{m+1}, \theta_m)$$

$$= g(\theta_m) + (\theta_m - \theta_{m+1})^\top \nabla g(\theta_m) + \frac{L}{2}\|\theta_m - \theta_{m+1}\|_2^2 \quad \text{ (From (3.4))}$$

$$= g(\theta_m) + (\theta_m - \theta_{m+1})^\top \nabla g(\theta_m) + \frac{l}{2}\|\theta_m - \theta_{m+1}\|_2^2 + \frac{L - l}{2}\|\theta_m - \theta_{m+1}\|_2^2$$

$$\geq g(\theta_{m+1}) + \frac{L - l}{2}\|\theta_m - \theta_{m+1}\|_2^2. \quad \text{ (From Proposition 3.1)}$$

To prove the second statement, we note that from (3.5) and Condition (i), $\{g(\theta_m)\}|_{m=1}^{\infty}$ is decreasing and bounded from below, so it is convergent. Then $\lim_{m \rightarrow \infty} g(\theta_m) = 0$. From Proposition 3.3 Statement 1, we have $\lim_{m \rightarrow \infty} \|\theta_{m+1} - \theta_m\|_2^2 = 0$.

THEOREM 3.2. For the sequence $\{\theta_m\}|_{m=1}^{\infty}$ generated by Algorithm 2, if $L > l$, then there exists $c \in \mathbb{R}$, such that for any $M \in \mathbb{Z}^+$ we have

$$\min_{m=1, \ldots, M} \|\theta_{m+1} - \theta_m\|_2^2 \leq \frac{2(g(\theta_1) - c)}{M(L - l)},$$

where $g(\theta_m) \downarrow c$ as $m \rightarrow \infty$. 

PROOF. From (3.5) and Condition (i), we have the fact that \{g(\theta_m)\}_{m=1}^\infty is decreasing and bounded from below, so it is convergent to some \(c \in \mathbb{R}\). For this \(c\), the conclusion follows directly from Proposition 3.3 Statement 1.

Finally, we show that Algorithm 2 gives a feasible solution whose objective value is the same as some first-order stationary point under mild conditions:

**Proposition 3.4.** Consider problem (3.3) and some constant \(L > l\), let \(\theta_m, m \geq 1\) be the sequence generated by Algorithm 2. Suppose \(g\) satisfies the following conditions:

1. \(g\) has second-order derivative;
2. there exists \(l' > 0\) such that \(l'\|\theta - \hat{\theta}\|_2 \leq \|\nabla g(\theta) - \nabla g(\hat{\theta})\|_2\) for any \(\theta, \hat{\theta} \in \Theta(K, s)\) satisfying \(G(\hat{\beta}) = G(\hat{\beta});\)
3. \(\{\theta \in \Theta(K, s) | g(\theta) \leq C\}\) is bounded for any \(C \in \mathbb{R}\).

Then \(g(\theta_m)\) converges to \(g(\theta)\) where \(\theta\) is a first-order stationary point.

The detailed proof of Proposition 3.4 is given in Proposition A.5.1 and Remark A.5.1 in Appendix A.2.1.

**4. Numerical studies.** We conduct a variety of numerical experiments to assess the performance of \(L_0\)-Fusion. We use the normalized mutual information (NMI, Ana and Jain (2003)) to evaluate grouping accuracy. Specifically, given \(G_1 = \{G_1^{(1)}, G_1^{(2)}, \ldots\}\) and \(G_2 = \{G_2^{(1)}, G_2^{(2)}, \ldots\}\) as two sets of disjoint clusters of \([p]\), define the mutual information \(I(G_1; G_2)\) between \(G_1\) and \(G_2\) as

\[
I(G_1; G_2) := \sum_{i \in [G_1], j \in [G_2]} \frac{|G_1^{(i)} \cap G_2^{(j)}|}{p} \log \left( \frac{p|G_1^{(i)} \cap G_2^{(j)}|}{|G_1^{(i)}||G_2^{(j)}|} \right),
\]

and define the entropy of \(G_1\) as

\[
H(G_1) := I(G_1; G_1) = - \sum_{i \in [G_1]} \frac{|G_1^{(i)}|}{p} \log \left( \frac{|G_1^{(i)}|}{p} \right).
\]

Now we are ready to define the NMI between \(G_1\) and \(G_2\) as

\[
\text{NMI}(G_1, G_2) := \frac{I(G_1; G_2)}{\{H(G_1) + H(G_2)\}/2}.
\]

Note that if \(G_1\) and \(G_2\) share the same group structure, we have \(\text{NMI}(G_1, G_2) = 1\).

The rest of the section is organized as follows. Section 4.1 compares \(L_0\)-Fusion with its competitors in terms of grouping accuracy and investigates the effectiveness of the warm start Algorithm 2 under low-dimensional regimes. Section 4.2 implements the “screening then grouping” strategy discussed in Section 2.2 to perform homogeneity fusion under ultrahigh-dimensional sparse setups. Finally, Section 4.3 applies \(L_0\)-Fusion to group lipids in a study of metabolomic effects on body mass index (BMI).

**4.1. Low-dimensional regime.** We consider a collection of low-dimensional setups where the design vectors \(\{x_i\}_{i=1}^n\) are independent realizations from a \(p\)-dimensional multivariate normal distribution \(\mathcal{N}(0, \Sigma)\) with mean zero and covariance matrix \(\Sigma := (\Sigma_{ij})\).

We adopt the autoregressive design in the sense that \(\Sigma_{ij} = \rho^{|i-j|}\) with \(\rho \in (0, 0.5]\). In particular, \(\rho = 0\) gives the independent design. For each fixed \(X\), we generate the responses
\[ y = X\beta^* + \epsilon \text{ with } \epsilon \sim \mathcal{N}(0, I) \]. Throughout this section, we always set the group number \( K_0 = 4 \), while \( n, p \) and \( \beta^* \) are specified in the following subsections.

In Sections 4.1.1 and 4.1.2, we compare six methods when group sizes are equal and unequal respectively: \( L_0 \)-Fusion, ordinary least squares (OLS), fused LASSO (fLASSO, Tibshirani et al. (2005)), pairwise fusion (pairReg, Ma and Huang (2017)), feature grouping and selection over an undirected graph (FGSG, Zhu, Shen and Pan (2013)) and clustering algorithm in regression via data-driven segmentation (CARDS, Ke et al. (2016)). For \( L_0 \)-Fusion, CARDS and fLASSO, the tuning parameters are chosen via Bayesian Information Criterion (BIC). For OLS, FGSG and pairReg, we first tune the parameters (if any) in these methods via 10-fold cross-validation in terms of mean squared error (MSE). Note that these methods encourage coefficients within the same group to be close but not exactly the same. To derive grouping structures and gauge their accuracy, we perform \textit{k-means} clustering on the solutions of OLS, FGSG, pairReg with oracle cluster number \( K = 4 \). We use OLS+, FGSG+, pairReg+ to represent the corresponding post-clustering results. In Section 4.1.3, we present the NMI of the warm-start solution in Section 3.2 with varying \( n \) and \( p \), and illustrate how warm starts help the convergence of \( L_0 \)-Fusion, especially in the early stage. All the results are based on 200 independent Monte Carlo experiments.

4.1.1. Equal group sizes. We start with the case where all the coefficient groups have equal sizes. Specifically, we let \( p = 80 \) and have 4 coefficient groups of size 20, which take values \(-2r, -r, r, 2r\) respectively with \( r \in \{0.5, 0.8\} \). Figure 3 displays the boxplots of NMI for correlation coefficient \( \rho \in \{0, 0.5\} \) and signal strength \( r \in \{0.5, 0.8\} \). The results are based on \( n = 120 \) observations. We have the following observations:

(i) \( L_0 \)-Fusion exhibits significantly higher NMI than the other methods under all the cases, even though OLS+, pairReg+ and FGSG+ have oracle knowledge of the true number of groups.

(ii) Nearly all the methods yield higher grouping accuracy when \( r \) is larger (compare left red and right blue boxplots) or \( \rho \) is smaller (compare panels (a) and (b)).

4.1.2. Unequal group sizes. Now we consider groups of different sizes. Particular challenges can arise from identifying small groups whose collective explanation power is typically weak. To assess the capability of detecting small groups, we let \( p = 80 \) and divide the true predictors into 4 groups of sizes 1, 20, 20, 39, whose coefficient values are \(-4r, -r, r, 2r\) respectively. Figure 4 shows the boxplots of NMI for all the aforementioned approaches for \( \rho \in \{0, 0.5\} \) and \( r \in \{0.5, 0.8\} \). The results are based on \( n = 120 \) observations. We have the following observations:

(i) Similarly to Section 4.1.1, \( L_0 \)-Fusion outperforms the competing methods in terms of NMI uniformly under all the cases.

(ii) Similarly to Section 4.1.1, all the methods yield higher grouping accuracy when \( r \) is larger (compare red and blue boxplots) or \( \rho \) is smaller (compare panels (a) and (b)).

(iii) The performance gap between \( L_0 \)-Fusion and fLASSO is further enlarged here compared with the case of equal group sizes, which suggests the robustness of \( L_0 \)-Fusion with respect to group size heterogeneity.

4.1.3. Warm-start algorithm. We first assess the grouping accuracy of the solution of the discrete first-order algorithm introduced in Section 3.2 with initial value \( \theta_0 = 0 p+q \) in simulation. Figure 5 presents the NMI of this algorithm with oracle \( K \) as \( n \) and \( p \) vary. The plot shows its deteriorating performance as \( p \) grows or \( n \) decreases. However, it is clear that
Fig 3: Grouping accuracy with equal group sizes under different covariance designs and signal strengths. We set the correlation coefficient $\rho \in \{0, 0.5\}$ and signal strength $r \in \{0.5, 0.8\}$.

Next, we exploit the discrete first-order algorithm to provide a warm start for $L_0$-Fusion. The MIO solver in *Gurobi* (Gurobi Optimization, LLC, 2021) terminates when the gap between the lower and upper objective bounds is less than the Mixed-Integer Programming (MIP) Gap (a user-determined parameter between 0 and 1) times the absolute value of the incumbent objective value. More precisely, let $z_P$ be the incumbent primal objective value, which is an upper bound for the global minimum, and $z_D$ be the dual objective value, which is a lower bound for the global minimum. Then the MIP Gap is defined as $|z_P - z_D|/|z_P|$. Figure 6 tracks the MIP Gap and the NMI of $L_0$-Fusion against its running time on the University of Michigan High Performance Linux cluster. Each job uses 4 CPUs and 16 GB memory, which can be satisfied on most personal computers.

We have the following three observations from the plots above:

(i) The warm-start solution yields NMI = 0.6, which is plausible but far from optimal.
(ii) $L_0$-Fusion with a warm start yields significantly higher NMI than that with a cold start within the first 50 seconds.
(iii) Even when the MIP Gap is not exactly 0, $L_0$-Fusion can achieve near perfect group recovery. Therefore, one can still expect decent grouping results even if the algorithm has to halt before the MIP Gap vanishes.
4.2. **Ultra-high dimensional regime.** For ultra-high dimensional cases, we let \( p = 20,000, s_0 = 60, n = \left\lfloor 2s \log p \right\rfloor \) and \( K_0 = 4 \). All the entries of the design matrix \( \mathbf{X} \in \mathbb{R}^{n \times p} \) are independent standard Gaussian random variables. The true predictors are set as the first 60 predictors and divided into 4 groups of size 15 with coefficient values \(-2r, -r, r, 2r\) respectively.
spectively, where \( r \in \{0.15, 0.2, 0.25, 0.3\} \). All the results in this section are based on 100 independent Monte Carlo repetitions.

In the screening step, we first estimate the true sparsity \( s_0 \) by the size of the model from MCP (Zhang et al., 2010) that yields the lowest 10-fold cross validation (CV) MSE. Given that the following \( L_0 \)-Fusion algorithm can hardly handle hundreds of dimensions, we truncate our sparsity estimator below 100. Denote the resulting sparsity estimator by \( \hat{s} \). Then we use CoSaMP with projection size \( \pi = \hat{s} \) and expansion size \( l = \lceil \hat{s}/2 \rceil \) to generate a screening set \( \hat{S} \) of size \( \hat{s} \). To evaluate the quality of the screened set \( \hat{S} \), in Figure 7 we investigate the cardinality and true positive proportion (TPP) of \( \hat{S} \), the latter of which is defined as

\[
\text{TPP}(\hat{S}) := \frac{|\hat{S} \cap S^0|}{|S^0|},
\]

where \( S^0 \) denotes the true support set. We then perform grouping on the reduced design. The implementations for all the grouping methods are similar as those in Section 4.1. All the zero coefficients are considered as forming one group when we calculate the NMI. Figure 8 reports the NMI of \( L_0 \)-Fusion, CARDS, fLASSO, OLS+, pairReg+ and FGSG+. We have the following observations from the two figures:

(i) Figure 7 shows that as signal strength grows, CoSaMP yields higher TPP and smaller screening sizes, meaning that both accuracy and efficiency of CoSaMP improve.
(ii) Combining Figures 7 and 8, we observe that when \( r \in \{0.2, 0.25, 0.3\} \), CoSaMP achieves sure screening while the grouping can be far from the truth. This suggests that the grouping error is due to the grouping stage rather than the screening stage.
(iii) \( L_0 \)-Fusion still outperforms all the competing methods on the reduced designs.

4.3. **Real data analysis.** We further illustrate the proposed method by an empirical study of metabolomics data collected from \( n = 397 \) adolescents consisting of 197 boys and 200 girls aged 8 to 18 years during a critical period of growth and sexuality maturation. Early onset of obesity in the adolescent years has been found to be associated with an increased risk of many diseases (e.g., hypertension, diabetics, and cancer) during adulthood. Thus, it is of great scientific interest to detect key groups of lipids (largest metabolites among metabolomics) that predict body mass index (BMI), adjusted by age and sex (1 for boy and 0 for girl). We investigate a total of \( p = 234 \) lipids to determine the number of lipid groups, group memberships and associated average contribution of a group predictor to BMI. We fit the following
linear model with a group homogeneity pursuit on the outcome of BMI:

\[
(4.2) \quad \text{BMI} = \alpha_0 + \alpha_1 \text{age} + \alpha_2 \text{sex} + \sum_{j=1}^{234} \beta_j \text{lip}_j + \varepsilon, \quad \beta_j \in \{0, \gamma_1, \gamma_2, \ldots, \gamma_K\}, \quad \forall j \in [p],
\]

where the number of signal groups \((K)\) as well as the group of null lipids with \(\gamma_0 = 0\) is determined by 10-fold CV. Each group represents a subset of lipids with a shared nonzero effect size \(\gamma_k, k = 1, \ldots, K\). We normalize the design matrix to ensure mean 0 and variance 1 except intercept and sex. To calibrate the effect sizes with respect to different group sizes, for each group of lipids, we use their average measurement as the group’s overall measurement; therefore, the corresponding group-level effect size is \(\gamma_k\) multiplied by the group size.

Here we adopt the aforementioned “screen then group” strategy. Similarly to Section 4.2, we first estimate the true sparsity \(s\) by MCP with 10-fold CV and apply CoSaMP to identify...
promising individual lipids from the pool of 234 lipids. This screening step selects 18 potential lipids together with intercept, age and gender. In the second phase, we perform $L_0$-Fusion on these selected lipids. Through 10-fold cross-validation over $K = \{1, \ldots, 10\}$, we detect six groups with nonzero effect sizes. It is noteworthy that GUROBI solves the $L_0$-Fusion problem within few seconds. The results are summarized in Table 1. For group 1 consisting of 7 similar lipids, the group-level average lipid measurement has a 4.0 effect size on BMI.

We also conduct a confirmatory semi-simulation using the metabolomics design matrix of this real dataset. Assume that a variable of interest $y$ relates to the metabolomics as follows:

\begin{equation}
    y = \alpha_1 \text{age} + \alpha_2 \text{sex} + \sum_{j=1}^{234} \beta_j \text{lip}_j + \epsilon, \ \beta_j \in \{0, \gamma_1, \gamma_2, \ldots, \gamma_K\}, \ \forall j \in [p].
\end{equation}

We set $\alpha_1 = 0.5$, $\alpha_2 = 1$ and randomly assign the coefficients $\beta$ with a sparse (20 nonzero values) and grouped (4 groups of size 5) structure, where the true coefficients within each group are equal to $-2r, -r, r, 2r$ respectively with $r \in \{0.5, 1\}$. Then we generate $n = 397$ responses from the metabolomics design according to (4.3), where $\epsilon$’s are i.i.d. $\mathcal{N}(0, 1)$. We assess the prediction performance with/without group structure along with the grouping accuracy by randomly splitting the observations into a training set and a testing set at each repetition. We then implement both the screening procedure alone and the screening then grouping procedure on the training set and compare their prediction accuracy in terms of MSE on the testing set. Table 2 reports the testing MSE with standard error as well as the quantiles of NMI based on 100 independent Monte Carlo repetitions. It is clear from the table that leveraging the existing group structure by $L_0$-Fusion improves the prediction accuracy.

| Group (size) | Features                  | Group-level effect size |
|--------------|---------------------------|-------------------------|
| Intercept    |                           | 21.88                   |
| Boys versus girls |                   | -1.05                   |
| Age          |                           | 0.62                    |
| Group 1 (7)  | “cholesterol biosynthesis” | 4.00                    |
| Group 2 (6)  | “nutritional energy support and regulation” | -3.13                  |
| Group 3 (2)  | “energy transport”        | 4.44                    |
| Group 4 (1)  | “diet signaling”          | -2.00                   |
| Group 5 (1)  | “energy production”       | -1.28                   |
| Group 6 (1)  | “peptide hormones on food consumption” | 0.99                  |

**TABLE 1**

The analysis results of lipid groups and effect sizes among 18 promising metabolites from preliminary screening by CoSaMP.

5. Discussion. This paper studies a combinatorial approach called $L_0$-Fusion that enables simultaneous operation of clustering and estimation for regression coefficients in a linear model. This analytic task addresses a practical need for learning homogeneous groups of nonzero regression coefficients in a regression analysis to assess the relationship between outcomes and clustered signal features. We propose to formulate the $L_0$-Fusion problem as a mixed integer optimization (MIO) problem and then leverage modern MIO solvers to compute the corresponding estimators. When the dimension is too high for the MIO solver to handle, we invoke CoSaMP as a preliminary variable screening procedure to reduce dimension prior to the $L_0$-Fusion. As shown theoretically and numerically in Section 4.2, such a “screen then group” strategy dramatically broadens the applicability of the homogeneity fusion technique, which can scale $L_0$-Fusion up to the ambient dimension $p = 20,000$ with high accuracy of recovering the true group structure of regression coefficients. This level of methodological capacity allows to handle a large number of modern biomedical datasets.
| Signal Strength | Prediction Error (with grouping) | Prediction Error (without grouping) | NMI (quantiles) |
|-----------------|---------------------------------|------------------------------------|----------------|
|                 |                                 |                                    | Max: 1.00       |
|                 |                                 |                                    | 3rd Qu: 1.00    |
|                 |                                 |                                    | Median: 1.00    |
|                 |                                 |                                    | 1st Qu: 1.00    |
|                 |                                 |                                    | Min: 0.75       |
| $r = 1$         | **1.092(0.031)**                | 1.186(0.029)                       |                |
|                 |                                 |                                    |                |
| $r = 0.5$       | **1.120(0.023)**                | 1.223(0.001)                       | Max: 1.00       |
|                 |                                 |                                    | 3rd Qu: 1.00    |
|                 |                                 |                                    | Median: 0.91    |
|                 |                                 |                                    | 1st Qu: 0.85    |
|                 |                                 |                                    | Min: 0.58       |

**TABLE 2**

Results of grouping and prediction accuracy for the semi-simulation.

Thus, this two-stage approach as well as its variants provide efficient toolboxes to solve many homogeneity fusion problems on large-scale datasets.

Theoretically, we establish grouping consistency of the $L_0$-Fusion estimator, for which the sample size $n$ only needs to grow at the same rate as the sum of logarithms of the true sparsity and true group number, i.e., $\log(pK)$. This sample size requirement is also shown to be necessary for any procedure to achieve grouping consistency. These technical results are not only of theoretical interest, but also useful to guide practical work such as sample size determination in a study design.

An important future work concerns statistical inference after the operation of $L_0$-Fusion. A thorough investigation on the influence of selection errors on statistical inference, in both aspects of finite-sample and large-sample properties, is of great interest. This $L_0$-Fusion may be extended to other regression problems with the framework of generalized linear models where iterative procedures used in the parameter estimation rely on weighted least squares objective functions. Thus, this extension is technically manageable but may require substantial computational effort. Also, we would consider an extension of this method to the setting of estimating equations, which could cover a broad range of important statistical models, such as GEE regression, Cox regression and quantile regression.

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Appendices.

A.1. Segment neighborhood method. Algorithm 3 is a generalization of the segment neighbourhood method (Auger and Lawrence, 1989) with sparsity constraint.

Algorithm 3: Segment neighborhood method $\Omega(Ks^2 + p \log p + q)$

Input: $c \in \mathbb{R}^{q+p}$, the number of groups $K$ and the sparsity restriction $s$

Output: a member in $H_{K,s}(c)$

1: $\hat{\alpha} = (c_1, c_2, \ldots, c_q)$. 
2: Let $\delta$ be a bijection on $\{q+1, \ldots, q+p\}$ such that $c_{\delta(q+1)} \leq c_{\delta(q+2)} \leq \cdots \leq c_{\delta(q+p)}$.

3: set $x_{lk}, y_{lk}, x'_{lk}$ and $y'_{lk}$ to 0 for $l = 0, \ldots, p + 1$ and $k = 0, \ldots, K$.

4: For $l$ from 1 to $s$:
   
   5: For $k$ from 1 to $K$:
      
      6: $x_{lk} = \max_{1 \leq i \leq l} \{y_{i-1,k-1} + \frac{(\sum_{j=i}^{l} c_{\delta(j)})^2}{l-i+1}\}$.
      
      7: $y_{lk} = \max_{1 \leq i \leq l} \{y_{i-1,k-1} + \frac{(\sum_{j=i}^{l} c_{\delta(j)})^2}{l-i+1}\}$.

8: If $s < p$:
9:   
9: For $l$ from $p$ to $p - s + 1$:
10:   
10: For $k$ from 1 to $K$:
11:      
11: $x'_{lk} = \max_{1 \leq i \leq p} \{y'_{i,k} + 1 + \frac{(\sum_{j=i}^{l} c_{\delta(j)})^2}{l-i+1}\}$.
12:      
12: $y'_{lk} = \max_{1 \leq i \leq p} \{y_{i+1,k} + 1 + \frac{(\sum_{j=i}^{l} c_{\delta(j)})^2}{l-i+1}\}$.

13: 
14: $(k^*, l^*, m^*) = \arg \max_{0 \leq k \leq K} \max_{0 \leq l \leq s} \max_{0 \leq m \leq p} \sum_{s=p}^{m^*} x_{lk} + y_{lk}$.
15: 
15: For $l$ from $l^* + 1$ to $m^* - 1$:
16:      
16: $\hat{\beta}_{\delta(q+l)} = 0$.

17: 
17: Set $t = l^*$
18: 
18: For $k$ from $k^*$ to 1:
19:      
19: For $l$ from $t$ to $x_{tk}$:
20:         
20: $\hat{\beta}_{\delta(q+l)} = \frac{\sum_{s=t}^{l} c_{\delta(q+s)}}{l - x_{tk} + 1}$.
21:      
21: $t = x_{tk} - 1$.

22: 
22: Set $t = m^*$
23: 
23: For $k$ from $K - k^*$ to 1:
24:      
24: For $l$ from $t$ to $x'_{tk}$:
25:         
25: $\hat{\beta}_{\delta(q+l)} = \frac{\sum_{s=t}^{l} c_{\delta(q+s)}}{x'_{tk} - l + 1}$.
26:      
26: $t = x'_{tk} + 1$.

27: Return $(\hat{\alpha}^*, \hat{\beta}^\top)$.

A.2. Proofs of Propositions and Theorems.

A.2.1. Proof of Proposition 3.4.

PROPOSITION A.5.1. Consider problem (3.3) and some constant $L > 1$. Let $\{\theta_m\}_{m=1}^\infty$ be the sequence generated by Algorithm 2. Define

$$\rho_m = \begin{cases} 
\min_{\beta_{m,j} \neq \beta_{m,j'}} |\beta_{m,j} - \beta_{m,j'}|, & \text{if there are } K \text{ distinct non-zero values in } \beta_m, \\
0, & \text{otherwise};
\end{cases}$$

where $\theta_m = p_0 \sum_{j=1}^M |\beta_{m,j}|$ and $p_0$ is a constant.
3. When the following properties hold.
2. a) Since \( \theta \) (\( \{m \beta_m \}^\top P \)) is a convergent subsequence then \( \liminf_{m \to \infty} \tau_m \) is bounded and converges to a first-order stationary point.

3. When \( \liminf_{m \to \infty} \rho_m = 0 \) and \( \liminf_{m \to \infty} \tau_m > 0 \), we have
   a) \( G(\beta_m; 0) \) converges and \( \liminf_{m \to \infty} \max_{j \in [p]} |g(\theta_m, 0)| \frac{\partial g(\theta_m)}{\partial \beta_j} = 0 \).
   b) If there exists a convergent subsequence \( \{\theta_{f(m)}\}_{m=1}^\infty \) such that \( \lim_{m \to \infty} \tau_{f(m)} = 0 \), then \( \lim_{m \to \infty} g(\theta_m) = \min_{\theta \in \mathbb{R}^p} g(\theta) \).

Remark A.5.1. The convergent subsequence condition could be satisfied under some weak conditions such as \( \{\theta \in \Theta(K, s) | g(\theta) \leq C\} \) being bounded for any \( C \in \mathbb{R} \).

Proof. In the following proof, \( \beta_{m,j} \) denotes the \( j \)th element in \( \beta_m \) where \( \theta_m = (\beta^\top_m, \alpha^\top_m)^\top \). Likewise, \( c_{m,j} \) denotes the \( j \)th element in \( c_m := \theta_m - \frac{1}{2} \nabla g(\theta_m) \).

1. a) For large enough \( m \), if \( G(\beta_m) \neq G(\beta_{m+1}) \), then
   \[
   \|\beta_{m+1} - \beta_m\|_2 > \min(\liminf_{m \to \infty} \rho_m, \liminf_{m \to \infty} \tau_m) / \sqrt{2},
   \]
   in contradiction to Proposition 3.3 Statement 2.

   b) Due to Statement 1a, there exists \( M \) such that for any \( m \geq M \), \( G(\beta_m) \) are the same. Then for any \( m > M \), we have
   \[
   \|\theta_{m+2} - \theta_{m+1}\|_2 = \left\| \begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \theta_{m+1} - \theta_m \\ \frac{1}{L} \left( \nabla g(\theta_{m+1}) - \nabla g(\theta_m) \right) \end{bmatrix} \right\|_2
   \]
   \[
   = \left\| \begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix} \left( I - \frac{1}{L} \nabla^2 g(\theta') \right)(\theta_{m+1} - \theta_m) \right\|_2 \leq \sqrt{1 - \frac{l^2}{L^2}} \|\theta_{m+1} - \theta_m\|_2,
   \]
   where \( A_{p \times p} \) is an idempotent matrix \( \left( \frac{I_{\{\beta_{m,j}=\beta_{m,j}'\}}}{|G(\beta_m; \beta_{m,j}')|} \right)_{j,j' \in [p]} \). Since \( 0 < \tfrac{l}{L} \leq 1 \), \( \theta_m \) converges to a first order stationary point.

2. a) Since \( \theta_{m+1} - \theta_m \) converges, we have \( \lim_{m \to \infty} \left\| \frac{\partial g(\theta_m)}{\partial \alpha} \right\|_\infty = 0 \). There exists a subsequence \( \{\theta_{f(m)}\}_{m=1}^\infty \) such that \( \lim_{m \to \infty} \tau_{f(m)} = 0 \). Without loss of generality, we assume \( |G(\beta_{f(m)}, \tau_{f(m)})| = t > 0 \). Fixing \( m \), for any \( j \in [p] \) such that \( |G(\beta_{f(m)}, \tau_{f(m)})| = \tau' > 1 \), we create \( \tilde{\theta} \) whose grouping is the same as \( \theta_{f(m)} \) except that the 0-group and \( \tau_{f(m)} \)-group in \( \theta_{f(m)} \) are merged as the new 0-group and that \( \beta_{f(m),j} \) is singled out as a new group. Then
   \[
   0 \geq \frac{2}{L} \left\{ h_L(\theta_{f(m)}, \theta_{f(m) - 1}) - h_L(\tilde{\theta}, \theta_{f(m) - 1}) \right\}
   \]
   \[
   = \begin{cases} 
   -t \tau^2_{f(m)} + c^2_{f(m) - 1,j} & \text{if } \beta_{f(m),j} = 0 \text{ or } \tau_{f(m)}; \\
   -t \tau^2_{f(m)} + \tau'^2 - (\beta_{f(m),j} - c_{f(m) - 1,j})^2 & \text{otherwise.}
   \end{cases}
   \]
So for any \( j \in [p] \), we have \( \frac{1}{L} |\frac{\partial g(\theta_{f(m)-1})}{\partial \beta_j}| = |\beta_{f(m)-1,j} - c_{f(m)-1,j}| \leq |\beta_{f(m)-1,j} - \beta_{f(m),j}| + |\beta_{f(m),j} - c_{f(m)-1,j}| \leq \|\theta_{f(m)} - \theta_{f(m)-1}\|_2 + (\sqrt{s} + 1)\tau_f(m) \). Thus \( \lim_{m \to \infty} \left\| \frac{\partial g(\theta_{f(m)-1})}{\partial \beta_j} \right\| = 0 \).

b) Due to Statement 2a, we have \( \lim_{m \to \infty} \|\nabla g(\theta_{f(m)-1})\| = 0 \). Since \( \lim_{m \to \infty} \theta_{f(m)-1} = \theta' \), we have \( g(\theta') = \min_{\theta} g(\theta) \). Since \( g(\theta_m) \) converges, we have \( \lim_{m \to \infty} g(\theta_m) = \min_{\theta} g(\theta) \).

3. a) Due to the proof of Statement 1a, if \( \lim_{m \to \infty} \rho_m = 0 \), then \( \mathcal{G}(\beta_m; 0) \) converges. There exists sequences \( \{\theta_{f(m)}\}_{m=1}^\infty, \{j_m\}_{m=1}^\infty \) and \( \{j_m'\}_{m=1}^\infty \) such that for any \( m > 0 \) we have \( \beta_{f(m),j_m} \neq 0, \beta_{f(m),j_m'} \neq 0, |\beta_{f(m),j_m} - \beta_{f(m),j_m'}| = \rho_f(m) \) and \( \lim_{m \to \infty} \beta_{f(m),j_m} = \beta_{f(m),j_m'} = 0 \). Fixing \( m \), let \( t \) and \( t' \) denote \( \mathcal{G}(\beta_{f(m)}, \beta_{f(m),j_m}) \) and \( \mathcal{G}(\beta_{f(m)}, \beta_{f(m),j_m'}) \). For any \( j'' \in [p] \) such that \( \beta_{f(m),j''} \neq 0 \) and \( t'' := |\mathcal{G}(\beta_{f(m)}, \beta_{f(m),j''})| > 1 \), we create \( \tilde{\theta} \) whose grouping is the same as \( \theta_{f(m)} \) except that the \( \beta_{f(m),j_m} \)-group and \( \beta_{f(m),j_m'} \)-group in \( \theta_{f(m)} \) are merged as a new group and that \( \beta_{f(m),j''} \) is singled out as a new group. Then

\[
0 \geq \frac{2}{L} \left\langle h_L(\theta_{f(m)}; \theta_{f(m)-1}) - h_L(\tilde{\theta}; \theta_{f(m)-1}) \right\rangle
\]

where

\[
\left\langle (1 + \frac{1}{t})^{-1} (\beta_{f(m),j_m} - \beta_{f(m),j_m'})^2 + \frac{t + t'}{t + t'} - 1 (\beta_{f(m),j_m'} - \beta_{f(m),j_m})^2 \frac{t + t'}{t + t'} \right\rangle
\]

if \( \beta_{f(m),j_m'} = \beta_{f(m),j_m} \) or \( \beta_{f(m),j_m'} \); otherwise.

So for any \( j'' \in [p] \) such that \( \beta_{f(m),j''} \neq 0 \), we have \( \frac{1}{L} |\frac{\partial g(\theta_{f(m)-1})}{\partial \beta_{j''}}| = |\beta_{f(m)-1,j''} - c_{f(m)-1,j''}| \leq |\beta_{f(m)-1,j''} - \beta_{f(m),j''}| + |\beta_{f(m),j''} - c_{f(m)-1,j''}| \leq \|\theta_{f(m)} - \theta_{f(m)-1}\|_2 + (s + 1)\rho_f(m) \).

b) On top of the proof of Statement 3a, for fixed \( m \) and any \( j'_m, j''_m \in [p] \) such that \( \beta_{f(m),j'_m} = 0 \) and \( \beta_{f(m),j''_m} \neq 0 \), we create \( \tilde{\theta} \) whose grouping is the same with \( \theta_{f(m)} \) except that the \( \beta_{f(m),j_m} \)-group and \( \beta_{f(m),j_m'} \)-group in \( \theta_{f(m)} \) are merged as a new group and that \( \beta_{j'} \) is singled out as a new non-zero group and \( \beta_{j''} \) is put in 0-group. Let \( t'' \) denote \( \mathcal{G}(\beta_{f(m)}, \beta_{f(m),j''}) \). Then

\[
0 \geq \frac{2}{L} \left\langle h_L(\theta_{f(m)}; \theta_{f(m)-1}) - h_L(\tilde{\theta}; \theta_{f(m)-1}) \right\rangle
\]

where

\[
\left\langle (1 + \frac{1}{t})^{-1} (\beta_{f(m),j_m} - \beta_{f(m),j_m'})^2 + \frac{t + t'}{t + t'} - 1 (\beta_{f(m),j_m'} - \beta_{f(m),j_m})^2 \frac{t + t'}{t + t'} \right\rangle
\]

if \( \beta_{f(m),j_m'} = \beta_{f(m),j_m} \) or \( \beta_{f(m),j_m'} \); otherwise.

Thus \( |c_{f(m)-1,j''}| \leq |c_{f(m)-1,j''}| \).

Since \( \lim_{m \to \infty} \theta_{f(m)} = \theta' \), we have \( \lim_{m \to \infty} \theta_{f(m)-1} = \theta' \) and \( \lim_{m \to \infty} \nabla g(\theta_{f(m)-1}) = \nabla g(\theta') \). It is easy to check that \( \Theta(K, s) \) is a closed set, so \( \theta' \in \Theta(K, s) \). And \( \mathcal{G}(\theta'; 0) = \lim_{m \to \infty} \mathcal{G}(\beta_m; 0) \) because of Statement 3a. Therefore, we have

\[
|\beta_{j'_m} - \frac{1}{L} \frac{\partial g(\theta')}{\partial \beta_{j'_m}}| = \lim_{m \to \infty} |c_{f(m)-1,j''_m}| \leq \lim_{m \to \infty} |c_{f(m)-1,j''_m}| = |\beta_{j'_m} - \frac{1}{L} \frac{\partial g(\theta')}{\partial \beta_{j'_m}}|,
\]
for any \( j, j' \in [p] \) such that \( \beta_j' = 0 \) and \( \beta_j' \neq 0 \). Due to Statement 3a, we have \( \frac{\partial \theta_j}{\partial \beta_j'} = 0 \) for any \( j \in [p] \) such that \( \beta_j' = 0 \). So \( \theta' \in \mathcal{H}_{K,n}(\theta' - \frac{1}{2} \nabla g(\theta')) \).

\[ \tag{A.2} \]

\[ \tag{A.3} \]

\[ \tag{A.4} \]

\[ = \mathbb{P} \left( 2 \varepsilon^\top (I - P_{G(\beta)})(X, Z)\theta^* + \| (I - P_{G(\beta)})(X, Z)\theta^* \|_2^2 - \varepsilon^\top (P_{G(\beta)} - P_{G(\beta^*)})\varepsilon < 0 \right). \]

For any \( 0 < \delta < 1 \), we have:

Equation (A.1) \( \leq \mathbb{E} \left[ \exp \left\{ - \frac{2t_1 \varepsilon^\top (I - P_{G(\beta)})(X, Z)\theta^*}{\sigma^2} \right\} \right] \exp \left\{ - \frac{t_1 \delta \| (I - P_{G(\beta)})(X, Z)\theta^* \|_2^2}{\sigma^2} \right\} + \]

\[ \mathbb{E} \left[ \exp \left\{ \frac{t_2 \varepsilon^\top (P_{G(\beta)} - P_{G(\beta^*)})\varepsilon}{\sigma^2} \right\} \right] \exp \left\{ - \frac{t_2 (1 - \delta) \| (I - P_{G(\beta)})(X, Z)\theta^* \|_2^2}{\sigma^2} \right\}. \]

By moment generating function, when \( 2t_1^2 - t_1 \delta < 0 \), the term in Equation (A.2) equals to:

\[ \exp \left\{ \frac{2t_1^2 \| (I - P_{G(\beta)})(X, Z)\theta^* \|_2^2}{\sigma^2} \right\} \exp \left\{ - \frac{t_1 \delta \| (I - P_{G(\beta)})(X, Z)\theta^* \|_2^2}{\sigma^2} \right\}, \]

\[ \leq \exp \left\{ \frac{2t_1^2 - t_1 \delta}{\sigma^2} \right\} \frac{n d(\beta, \beta^*) c_{\min}}{2}. \]

By geometry interpretation of projection matrix, the term in Equation (A.3) is smaller than or equal to:

\[ \mathbb{E} \left[ \exp \left\{ \frac{t_2 \varepsilon^\top P_{G(\beta) \setminus G(\beta^*)}\varepsilon}{\sigma^2} \right\} \right] \exp \left\{ - \frac{t_2 (1 - \delta) \| (I - P_{G(\beta)})(X, Z)\theta^* \|_2^2}{\sigma^2} \right\}, \]

\[ = (1 - 2t_2)^{-|G(\beta) \setminus G(\beta^*)|/2} \exp \left\{ - \frac{t_2 (1 - \delta) \| (I - P_{G(\beta)})(X, Z)\theta^* \|_2^2}{\sigma^2} \right\}, \]

where \( P_{G(\beta) \setminus G(\beta^*)} \) indicates the projection matrix of the columns in \( X_{G(\beta)} \) but not in \( X_{G(\beta^*)} \), and \( |G(\beta) \setminus G(\beta^*)| \) is the number of those columns. By the fact that \( 2t_2 \geq - \log(1 - 2t_2)/2 \)
for any $0 < t_2 < 0.398$, we can restrict $t_2 \leq 0.398$. Then, the term in Equation (A.3) is less than or equal to:

$$\exp \left\{ 2t_2 |G(\beta) \backslash G(\beta^*)| \right\} \exp \left\{ -\frac{t_2(1-\delta)}{\sigma^2} \| (I - P_{G(\beta)})(X, Z)\theta^* \|_2^2 \right\}$$

$$\leq \exp \left\{ 2t_2 |G(\beta) \backslash G(\beta^*)| - \frac{t_2(1-\delta)}{\sigma^2} nd(\beta, \beta^*)c_{\text{min}} \right\}$$

Combining the two terms and set $t_1 = \frac{1}{5}$, $t_2 = \frac{3}{5}$, $\delta = \frac{4}{5}$, we have that Equation (A.1) is less than or equal to:

$$\exp \left\{ \frac{2t_1^2 - t_1 \delta}{\sigma^2} nd(\beta, \beta^*)c_{\text{min}} \right\} + \exp \left\{ 2t_2 |G(\beta) \backslash G(\beta^*)| - \frac{t_2(1-\delta)}{\sigma^2} nd(\beta, \beta^*)c_{\text{min}} \right\},$$

$$= 2 \exp \left\{ - \frac{3}{40} \frac{nd(\beta, \beta^*)c_{\text{min}}}{\sigma^2} + \frac{3}{4} |G(\beta) \backslash G(\beta^*)| \right\}.$$

Finally, we bound the probability that the $L_0$ estimator fails to specify the true grouping:

(A.4)

$$\mathbb{P}(\hat{\theta} \neq \hat{\theta}^{ol})$$

$$\leq \sum_{\omega \in \{G(\beta) \mid \theta \in \Theta(K_0, s_0), G(\beta) \neq G(\beta^*) \}} \mathbb{P} \left( \min_{G(\beta) = \omega} \mathbb{E} \left( Y - (X, Z)\theta \right) \right)$$

$$\leq \sum_{i=1}^{s_0} \sum_{j=0}^{i} \left( \begin{array}{c} s_0 \\ i \end{array} \right) K_0^i \left( \begin{array}{c} p - s_0 \\ j \end{array} \right) K_0^j 2 \exp \left\{ - \frac{3nic_{\text{min}}}{40\sigma^2} + \frac{3}{4} (2i + j) \right\},$$

$$\leq \sum_{i=1}^{s_0} \sum_{j=0}^{i} (K_0s_0)^i (K_0(p - s_0))^j 2 \exp \left\{ - \frac{3nic_{\text{min}}}{40\sigma^2} + \frac{3}{4} (2i + j) \right\},$$

$$= \sum_{i=1}^{s_0} 2 \exp \left\{ - \frac{3nic_{\text{min}}}{40\sigma^2} + \frac{3}{2} i + i \log(K_0s_0) \right\} \sum_{j=0}^{i} \exp \left[ j \left( \frac{3}{4} + \log(K_0(p - s_0)) \right) \right],$$

$$\leq \frac{2}{1 - e^{-3/4}} \sum_{i=1}^{s_0} \exp \left\{ - \frac{3nic_{\text{min}}}{40\sigma^2} + \frac{3}{2} i + i \log(K_0s_0) + \frac{3}{4} i + i \log(K_0(p - s_0)) \right\}.$$
Due to the fact that $\mathbb{P}(\hat{\theta} \neq \tilde{\theta}^{(0)}) \leq 1$ and that $\frac{2}{1 - e^{-3/4}} \frac{x}{1 - x} \leq 6x$ when $0 \leq \frac{2}{1 - e^{-3/4}} \frac{x}{1 - x} \leq 1$ and $0 < x < 1$, we have Equation (A.4) less than or equal to:

$$6 \exp \left[ - \frac{3n}{40\sigma^2} \left( c_{\min} - \frac{\sigma^2}{n} \left( 27 \log(pK_0) + 12 \right) \right) \right].$$

\[ \square \]

A.2.3. Proof of Corollary 2.1.

PROOF. Note that $\{\hat{\theta}^{\bar{k}} = \tilde{\theta}^{(0)}\} = \{\hat{\theta}^{\bar{k}} = \tilde{\theta}^{(0)}\} \cap \mathcal{E}$. Then

$$\mathbb{P}(\hat{\theta}^{\bar{k}} = \tilde{\theta}^{(0)}) = \mathbb{P}(\{\hat{\theta}^{\bar{k}} = \tilde{\theta}^{(0)}\} \cap \mathcal{E})$$

$$= 1 - \mathbb{P}(\{\hat{\theta}^{\bar{k}} \neq \tilde{\theta}^{(0)}\} \cup \mathcal{E}^c)$$

$$\geq 1 - \mathbb{P}(\{\hat{\theta}^{\bar{k}} \neq \tilde{\theta}^{(0)}\} - \mathbb{P}(\mathcal{E}^c).$$

The conclusion immediately follows by combining this with Theorem 2.4.

\[ \square \]

A.2.4. Proof of Theorem 2.5.

PROOF. Consider a measurable space $(\mathcal{X}, \mathcal{A})$ and a measurable function class $\Psi_t := \{\psi : \mathcal{X} \to [t]\}$. By Lemma 2.7 in Birgé (1983): for any sequence of $t \geq 2$ probability distributions $\mathbb{P}_1, \ldots, \mathbb{P}_t$ on the same measurable space $(\mathcal{X}, \mathcal{A})$, we have that

$$\inf_{\psi \in \Psi_t} \sup_{j = 1, \ldots, t} \mathbb{P}_j(\psi(x) = j) \geq 1 - \frac{t^{-2} \sum_{1 \leq j, k \leq t} \text{KL}(\mathbb{P}_j, \mathbb{P}_k) + \log 2}{\log(t - 1)},$$

where $\text{KL}(\mathbb{P}_j, \mathbb{P}_k)$ is the Kullback-Leibler information for distributions $\mathbb{P}_j$ versus $\mathbb{P}_k$.

For any $\gamma_{\min} > 0$, we can construct a collection of parameters of distinct groupings $\mathcal{S}_{\gamma_{\min}} := \{\beta^{(j)}\}_{j=0}^{K_0 - 1} \subseteq \Theta(K_0, s_0)$ satisfying that

i. each entry of $\beta^{(j)}$ belongs to $\mathcal{V} := \{-\lceil \frac{K_0}{2} \rceil \gamma_{\min}, \ldots, -\gamma_{\min} K_0, 0, \gamma_{\min} K_0, \ldots, \lceil \frac{K_0 + 1}{2} \rceil \gamma_{\min}\}$;

ii. for any $0 < j \leq \lceil \frac{K_0 + 3}{4} \rceil$, we have $\|\beta^{(j)} - \beta^{(0)}\|_0 \leq 2$;

iii. for any $0 < j \leq \lceil \frac{K_0 + 3}{4} \rceil$, we have $\|\beta^{(j)} - \beta^{(0)}\|_1 = \frac{1}{K_0} \gamma_{\min}$ or $\frac{2}{K_0} \gamma_{\min}$;

iv. for any $0 < j \leq \lceil \frac{K_0 + 3}{4} \rceil$, we have $\|\beta^{(j)} - \beta^{(0)}\|_\infty = \frac{1}{K_0} \gamma_{\min}$ or $\frac{2}{K_0} \gamma_{\min}$.

Below we give the detailed construction of $\mathcal{S}_{\gamma_{\min}} \subseteq \{\beta^{(0)}\} \cup \mathcal{S}_{\gamma_{\min}}^\dagger \cup \mathcal{S}_{\gamma_{\min}} \cup \{\beta^{(0)}(1), \beta^{(0)}(2)\}$ where $\beta^{(0)}(1)$ and $\beta^{(0)}(2)$ are two variants of $\beta^{(0)}$ defined blow.

1. Set $\beta^{(0)}$ as any parameter with components valued in $\mathcal{V}$ such that $|\mathcal{G}(\beta^{(0)}; 0)| = p - K_0 + 1, |\mathcal{G}(\beta^{(0)}; \gamma_{\min})| = 0$ and each of the rest $K_0 - 1$ groups has only one covariate, as shown in Figure 9a.

2. Consider multiset $\tilde{\mathcal{S}}_{\gamma_{\min}} := \{\tilde{\beta}^{(j,k)}\}_{j \in [p-K_0+1], k \leq \lceil \frac{K_0+1}{2} \rceil}$. Each $\tilde{\beta}^{(j,1)}$ is generated by modifying $\beta^{(0)}$ via moving the $j$th covariate of $0$-group in $\beta^{(0)}$, i.e., $\mathcal{G}(\beta^{(0)}; 0)$, to $\gamma_{\min} K_0$-group. Each $\tilde{\beta}^{(j,k)}$ with $k > 1$ is created by modifying $\tilde{\beta}^{(j,1)}$ through moving the covariate in $\gamma_{\min}$-group to $\gamma_{\min} K_0$-group. (see Figure 9b)

3. When $K_0 \geq 5$, consider multiset $\mathcal{S}_{\gamma_{\min}} := \{\beta^{(j,k)}\}_{j \in \lceil \frac{K_0+2}{4} \rceil - 2, k \in \lceil \frac{K_0+1}{4} \rceil + 1}$. Each $\beta^{(j,1)}$ is generated by modifying $\beta^{(0)}$ via moving the covariate in $\gamma_{\min}$-group to $\gamma_{\min} K_0$-group. Each $\beta^{(j,k)}$ with $k > 1$ is created by modifying $\beta^{(j,1)}$ through moving the covariate in $-\frac{k}{K_0} \gamma_{\min}$-group to $-\frac{k+1}{K_0} \gamma_{\min}$-group. (see Figure 9c)
Fig 9: Illustration of constructing $S_{\gamma_{\min}}$ in the proof of Theorem 2.5. A rectangle represents a group in $\beta$ corresponding to the coefficient value above the rectangle. Circles in a rectangle represent the covariates in the group, which are labeled by their indices. In each subgraph, rectangles and circles collectively specify an element in $S_{\gamma_{\min}}$. An arrow means to move a covariate to a different group to generate another $\beta$. (a) An example of $\beta^{(0)}$ in Step 1. (b) An example of Step 2. (c) An example of Step 3.

4. When $K_0 \geq 2$, consider multiset $\tilde{S}_{\gamma_{\min}} := \{\tilde{\beta}^{(j)}\}_{j \in \lfloor \frac{K_0}{2} \rfloor}$. Each $\tilde{\beta}^{(j)}$ is generated by modifying $\beta^{(0)}$ via moving the covariate in $-\frac{j}{K_0} \gamma_{\min}$-group to $-\frac{j-1}{K_0} \gamma_{\min}$-group. (see Figure 9d)

5. When $K_0 \geq 2$, construct $\beta^{(01)}$ by modifying $\beta^{(0)}$ by moving one covariate in 0-group to $-\frac{1}{K_0} \gamma_{\min}$-group. When $K_0 \geq 4$, construct $\beta^{(02)}$ by modifying $\beta^{(0)}$ by moving one covariate in 0-group to $-\frac{2}{K_0} \gamma_{\min}$-group. (see Figure 9e)

Note that the constructed $\beta$’s in Steps 1-5 are distinct and with cardinality at least $\lfloor \frac{K_0+3}{4} \rfloor p + 1$. 
Then for any $0 \leq j < j' \leq \lfloor \frac{K_0 + 3}{2} \rfloor p$, we have

$$\text{KL}\{N(X\hat{\beta}(j), \sigma^2 I_n), N(X\beta(j'), \sigma^2 I_n)\} = \frac{1}{2\sigma^2} \|X(\beta(j) - \beta(j'))\|^2 \leq \frac{2\max_{1 \leq j \leq p} \|X_j\|^2 \gamma^2_{\min}}{\sigma^2 K_0^2} = \frac{2n\gamma^2}{\sigma^2 K_0^2} \min_{\theta \in \Theta(K_0, s_0)} c_{\min}(\theta, X, Z) \leq \frac{2nr(\theta, X, K_0, s_0)}{\sigma^2} \min_{\theta \in \Theta(K_0, s_0)} c_{\min}(\theta, X, Z).$$

For any estimator $\hat{\beta}$ of $\beta^*$, we can define $\hat{\beta}^\dagger = \begin{cases} \hat{\beta}, & \text{when } \hat{\beta} \in S_{\gamma_{\min}}, \\ \text{uniform}(S_{\gamma_{\min}}), & \text{otherwise}. \end{cases}$

Then we can apply Lemma 2.7 in Birgé (1983) to probability distributions $\{N(X\beta, \sigma^2 I_n) | \beta \in S_{\gamma_{\min}}\}$. It follows that

$$\inf_{\beta} \sup_{\theta' \in \Theta_{L}(K_0, s_0, \text{min})} \min_{\beta' \in S_{\gamma_{\min}}} \mathbb{P}(G(\hat{\beta}) \neq G(\beta^*)) \geq \inf_{\beta} \sup_{\theta' \in \Theta_{L}(K_0, s_0, \text{min})} \min_{\beta' \in S_{\gamma_{\min}}} \mathbb{P}(G(\hat{\beta}^\dagger) \neq G(\beta^*)) \geq \inf_{\beta} \sup_{\theta' \in \Theta_{L}(K_0, s_0, \text{min})} \min_{\beta' \in S_{\gamma_{\min}}} \mathbb{P}(G(\hat{\beta}) \neq G(\beta^*)) \geq \inf_{\beta} \sup_{\theta' \in \Theta_{L}(K_0, s_0, \text{min})} \min_{\beta' \in S_{\gamma_{\min}}} \mathbb{P}(G(\hat{\beta}^\dagger) \neq G(\beta^*)) \geq \inf_{\beta} \sup_{\theta' \in \Theta_{L}(K_0, s_0, \text{min})} \min_{\beta' \in S_{\gamma_{\min}}} \mathbb{P}(G(\hat{\beta}) \neq G(\beta^*)).$$
\[
\begin{align*}
&= \inf_{\psi \in \Psi} \sup_{\beta:|\beta|_{\infty} \leq 0, p+1} \mathbb{P}(G(\beta) \neq G(\beta^*)) \\
&\geq 1 - \frac{2nr(X, Z, K_0, s_0) \min_{\beta, \beta \in S_{\min}} c_{\min}(\theta, X, Z) + \sigma^2 \log 2}{\sigma^2 \log (\lfloor \frac{K_0 + 3}{4} \rfloor p)}.
\end{align*}
\]

When \( \gamma_{\min} \) varies from 0 to \( \infty \), \( \min_{\beta, \beta \in S_{\min}} c_{\min}(\theta, X, Z) \) varies from 0 to \( \infty \). Then for any \( \ell > 0 \) we have

\[
\begin{align*}
&\inf_{\beta^*} \sup_{\theta^* \in \Theta_{s}(K_0, s_0, \ell)} \mathbb{P}(G(\hat{\beta}^*) \neq G(\beta^*)) \\
&\geq 1 - \frac{2nr(X, Z, s) \ell + \sigma^2 \log 2}{\sigma^2 \log (\lfloor \frac{K_0 + 3}{4} \rfloor p)}.
\end{align*}
\]

Then \( \inf_{\beta^*} \sup_{\theta^* \in \Theta_{s}(K_0, s_0, \ell)} \mathbb{P}(G(\hat{\beta}^*) \neq G(\beta^*)) \to 0 \), as \( n, p \to \infty \) implies

\[
l \geq \frac{\sigma^2 (\log (\lfloor \frac{K_0 + 3}{4} \rfloor p) - \log 2)}{2nr(X, Z, K_0, s_0)}.
\]

\[\square\

A.3. Proof of Proposition 2.1.

PROOF. Consider \( s_0 = p \) and \( K_0 = 2 \). We have \( G(\beta^*) = \{G_1^*, G_2^*\} \), where \( G_1^* = \{j: \beta_j^* = \gamma_1^*\} \) and \( G_2^* = \{j: \beta_j^* = \gamma_2^*\} \) with \( |\gamma_1^* - \gamma_2^*| \geq 1 \). Write \( k_1^* = |G_1^*| \) and \( k_2^* = |G_2^*| \). For any \( \beta \) such that \( G(\beta) = \{G_1, G_2\} \neq G(\beta^*) \), let \( k_1 = |G_1| \) and \( k_2 = |G_2| \). We now consider two possible grouping structures.

Case (i): Without loss of generality, \( G_1 \subset G_1^* \) and \( G_2 \subset G_2^* \). In this case, we have

\[
d(\beta, \beta^*) = |G_1^* \setminus G_1| = k_1^* - k_1,
\]

\[
\arg\min_{\beta \in \Theta_{s}(K_0, s_0, \ell)} \|\beta'_{G_1} - \beta_{G_1^*}\|^2 = \gamma_1^* 1_{|G_1^*|},
\]

\[
\arg\min_{\beta \in \Theta_{s}(K_0, s_0, \ell)} \|\beta'_{G_2} - \beta_{G_2^*}\|^2 = \frac{(k_1^* - k_1)(\gamma_1^* + k_2^* \gamma_2^*)}{k_2} 1_{|G_2^*|}.
\]

Note that \( k_1 + k_2 = s_0 \) and \( k_1^* + k_2^* = s_0 \). Accordingly,

\[
\begin{align*}
\min_{\beta \in \Theta_{s}(K_0, s_0, \ell)} \|\beta' - \beta^*\|^2
&= (k_1^* - k_1) \left( \gamma_1^* - \frac{(k_1^* - k_1) \gamma_1^* + k_2^* \gamma_2^*}{k_2} \right)^2 + k_2 \left( \gamma_2^* - \frac{(k_1^* - k_1) \gamma_1^* + k_2^* \gamma_2^*}{k_2} \right)^2 \\
&= \frac{(k_1^* - k_1)(s_0 - k_1)^2 (\gamma_1^* - \gamma_2^*)^2}{(s_0 - k_1)^2} + \frac{(s_0 - k_1^*)(k_1^* - k_1)^2 (\gamma_1^* - \gamma_2^*)^2}{(s_0 - k_1)^2} \\
&= \frac{(k_1^* - k_1)(s_0 - k_1^*)(\gamma_1^* - \gamma_2^*)^2}{s_0 - k_1}.
\end{align*}
\]

Since \( C_1 \leq k_1^*/k_2^* \leq C_h \) for some universal constants \( C_h > C_1 > 0 \), we always have that \( k_1^* = c_1^* s_0 \) and \( k_2^* = (1 - c_1^*) s_0 \) for some constant \( 0 < c_1^* < 1 \). Then

\[
\begin{align*}
\min_{\beta \in \Theta_{s}(K_0, s_0, \ell)} \|\beta' - \beta^*\|^2
\quad &d(\beta, \beta^*) \\
&= \frac{(s_0 - k_1^*)(\gamma_1^* - \gamma_2^*)^2}{s_0 - k_1} \geq \frac{(1 - c_1^*) s_0 (\gamma_1^* - \gamma_2^*)^2}{s_0} = (1 - c_1^*) (\gamma_1^* - \gamma_2^*)^2 \geq 1 - c_1^*.
\end{align*}
\]
Case (ii): $\mathcal{G}_1 \cap \mathcal{G}_1^* \neq \emptyset$ and $\mathcal{G}_2 \cap \mathcal{G}_2^* \neq \emptyset$. Let $d = |\mathcal{G}_1^* \setminus \mathcal{G}_1|$. Then
\[
d(\beta, \beta^*) = \min \{k_1 - k_1^* + 2d, s_0 - (k_1 - k_1^* + 2d)\}
\]
Also,
\[
\arg\min_{\beta' \in \mathcal{G}(\beta') = \mathcal{G}(\beta)} \|\beta'_{\mathcal{G}_1} - \beta_{\mathcal{G}_1}^*\|_2^2 = \frac{(k_1^* - d)\gamma_1^* + (k_1 - k_1^* + d)\gamma_2^*}{k_1} 1_{|\mathcal{G}_1|},
\]
\[
\arg\min_{\beta'_{\mathcal{G}_2} \in \mathcal{G}(\beta)} \|\beta'_{\mathcal{G}_2} - \beta_{\mathcal{G}_2}^*\|_2^2 = \frac{d\gamma_1^* + (k_2 - d)\gamma_2^*}{k_2} 1_{|\mathcal{G}_2|}.
\]
Accordingly we have
\[
\min_{\beta' \in \mathcal{G}(\beta')} \|\beta' - \beta^*\|_2^2 = \frac{(k_1^* - d)(k_1 - k_1^* + d)\gamma_2^*}{k_1} + \frac{d(k_2 - d)(\gamma_1^* - \gamma_2^*)^2}{k_2}.
\]
Similar to case (i), we have
\[
\min_{\beta' \in \mathcal{G}(\beta')} \frac{\|\beta' - \beta^*\|_2^2}{d(\beta, \beta^*)} = \frac{(k_1^* - d)(k_1 - k_1^* + d)/k_1 + d(k_2 - d)/k_2}{\min\{k_1 - k_1^* + 2d, s_0 - (k_1 - k_1^* + 2d)\}} (\gamma_1^* - \gamma_2^*)^2.
\]
The numerator term in (A.5) equals to
\[
k_1 \left(\frac{k_1^* - d}{k_1} \right) \left(1 - \frac{k_1^* - d}{k_1} \right) + k_2 \left(\frac{d}{k_2} \right) \left(1 - \frac{d}{k_2} \right).
\]
The denominator term in (A.5) is always upper bounded by $s_0/2$. Note that $k_1 - k_1^* + d > 0$ and $d < k_1^*$. We consider two situations with different orders of $d$.
(i) Under $d = o(s_0)$, we have
\[
k_1 \left(\frac{k_1^* - d}{k_1} \right) \left(1 - \frac{k_1^* - d}{k_1} \right) \approx c_1 s_0 \frac{k_1 - k_1^* + d}{k_1}.
\]
Now it is possible that $k_1 - k_1^* + d = c_1 s_0$ with some $c_1 \in (0, 1)$ or $k_1 - k_1^* + d = o(s_0)$. If $k_1 - k_1^* + d = c_1 s_0$ with some $c_1 \in (0, 1)$, we have (A.6) $\geq s_0$ and consequently (A.5) $\geq 1$.
If $k_1 - k_1^* + d = o(s_0)$, it holds that $\min\{k_1 - k_1^* + 2d, s_0 - (k_1 - k_1^* + 2d)\} = k_1 - k_1^* + 2d$ with sufficiently large $s_0$. We have
\[
(A.5) = \frac{(k_1^* - d)(k_1 - k_1^* + d)/k_1}{k_1 - k_1^* + 2d} \geq 1.
\]
(ii) Under $d \approx s_0$, by noticing that $d < k_2$, we have $k_2 \approx s_0$ and

$$k_2 \left(\frac{d}{k_2}\right) \left(1 - \frac{d}{k_2}\right) = d \frac{k_2 - d}{k_2} \approx k_2 - d.$$ 

If $k_2 - d \approx s_0$, then (A.6) $\geq s_0$ and (A.5) $\geq 1$. If $k_2 - d = o(s_0)$, we have $k_1 - k_1^* + d = c_2^* s_0 - o(s_0)$, thus the first term of the numerator in (A.5) is lower bounded by the order of $s_0$.

Combining all the cases concludes the proof. □

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