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Penalized Interaction Estimation for Ultrahigh Dimensional Quadratic Regression

Cheng Wang, Binyan Jiang and Liping Zhu

Shanghai Jiao Tong University, Hong Kong Polytechnic University, Renmin University of China

Abstract: Quadratic regression goes beyond the linear model by simultaneously including main effects and interactions between the covariates. The problem of interaction estimation in high dimensional quadratic regression has received extensive attention in the past decade. In this article we introduce a novel method which allows us to estimate the main effects and interactions separately. Unlike existing methods for ultrahigh dimensional quadratic regressions, our proposal does not require the widely used heredity assumption. In addition, our proposed estimates have explicit formulas and obey the invariance principle at the population level. We estimate the interactions of matrix form under penalized convex loss function. The resulting estimates are shown to be consistent even when the covariate dimension is an exponential order of the sample size. We develop an efficient ADMM algorithm to implement the penalized estimation. This ADMM algorithm fully explores the cheap computational cost of matrix multiplication and is much more efficient than existing penalized methods such as the all-pairs LASSO. We demonstrate the promising performance of our proposal through

extensive numerical studies.

Key words and phrases: High dimension, interaction estimation, quadratic regression, support recovery.

1. INTRODUCTION

In many scientific discoveries, a fundamental problem is to understand how the features under investigation interact with each other. Interaction estimation has been shown to be very attractive in both parameter estimation and model prediction (Bien et al., 2013; Hao et al., 2018), especially for data sets with complicated structures. Efron et al. (2004) pointed out that for Boston housing data, prediction accuracy can be significantly improved if interactions are included in addition to all main effects. In general, ignoring interactions by considering main effects alone may lead to an inaccurate or even a biased estimation, resulting in poor prediction of an outcome of interest, whereas considering interactions as well as main effects can improve model interpretability and prediction substantially, thus achieve a better understanding of how the outcome depends on the predictive features (Fan et al., 2015). While it is important to identify interactions which may reveal real relationship between the outcome and the predictive features, the number of parameters scales squarely with that of the predictive features,

making parameter estimation and model prediction very challenging for problems with large or even moderate dimensionality.

1.1 Interaction Estimation, Feature Selection and Screening

Estimating interactions is a challenging problem because the number of pairwise interactions increases quadratically with the number of the covariates. In the past decade, there has been a surge of interest in interaction estimation in quadratic regression. Roughly speaking, existing procedures for interaction estimation can be classified into three categories. In the first category of low or moderate dimensional setting, standard techniques such as ordinary least squares can be readily used to estimate all the pairwise interactions as well as the main effects. This simple one-stage strategy, however, becomes impractical or even infeasible for moderate or high dimensional problems, owing to rapid increase in dimensionality incurred by interactions. In the second category of moderate or high dimensional setting where feature selection becomes imperative, several one-stage regularization methods are proposed and some require either the strong or the weak heredity assumption. See, for example, Yuan et al. (2009), Choi et al. (2010), Bien et al. (2013), Lim and Hastie (2015), and Haris et al. (2016). These regularization methods are computationally feasible and the theoret-

ical properties of the resulting estimates are well understood for moderate or high dimensional problems. However, in the third category of ultrahigh dimension problems, these regularization methods are no longer feasible because their implementation requires storing and manipulating large scale design matrix and solving complex constrained optimization problems. The memory and computational cost is usually extremely expensive and prohibitive. Very recently, several two-stage approaches are proposed for both ultrahigh dimensional regression and classification problems, including Hao and Zhang (2014), Fan et al. (2015), Hao et al. (2018) and Kong et al. (2017). Two-stage approaches estimate main effects and interactions at two separate stages, so their computational complexity is dramatically reduced. However, these two-stage approaches hinge heavily on either the strong or weak heredity assumption. These methods are computationally scalable but may break down when the heredity assumption is violated.

1.2 Heredity Assumption and Invariance Principle

As an extra layer of flexibility to linear models, quadratic regressions include both main effects and pairwise interactions between the covariates. Denote Y the outcome variable and $\mathbf{x} = (X_1, \ldots, X_p)^{\mathrm{T}} \in \mathbb{R}^p$ the covariate vector. For notational clarity, we define $\mathbf{u} \stackrel{\text{def}}{=} \mathrm{E}(\mathbf{x}) \in \mathbb{R}^p$. In general, quadratic

regression has the form of

$$\mathrm{E}(Y \mid \mathbf{x}) = \alpha + (\mathbf{x} - \mathbf{u})^{\mathrm{T}}\boldsymbol{\beta} + (\mathbf{x} - \mathbf{u})^{\mathrm{T}}\boldsymbol{\Omega}(\mathbf{x} - \mathbf{u}), \tag{1.1}$$

where $\alpha \in \mathbb{R}^1$, $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)^{\mathrm{T}} \in \mathbb{R}^p$ and $\boldsymbol{\Omega} = (\boldsymbol{\Omega}_{k,l})_{p\times p} \in \mathbb{R}^{p\times p}$ are all unknown parameters. To ensure model identifiability, we further assume that $\boldsymbol{\Omega}$ is symmetric, that is, $\boldsymbol{\Omega}^{\mathrm{T}} = \boldsymbol{\Omega}$, or equivalently, $\boldsymbol{\Omega}_{k,l} = \boldsymbol{\Omega}_{l,k}$, $1 \leq k, l \leq p$. Our goal is to estimate $\boldsymbol{\beta}$ and $\boldsymbol{\Omega}$ which characterize respectively main effects and interactions. The intercept α is also useful for prediction.

In the literature, heredity structures (Nelder, 1977; Hamada and Wu, 1992) have been widely imposed to avoid quadratic computational cost of searching over all pairs of interactions. The heredity structures assume that the support of $\boldsymbol{\Omega}$ could be inferred from the support of $\boldsymbol{\beta}$. The strong heredity assumption requires that an interaction between two covariates be included in the model only if both main effects are important, while the weak one relaxes such a constraint to the presence of at least one main effect being important. In symbols, the strong and weak heredity structures are defined, respectively, as follows:

$$\begin{aligned} \text{strong heredity:} \quad & \boldsymbol{\Omega}_{k,l} \neq 0 \Rightarrow \beta_k^2 > 0 \text{ and } \beta_l^2 > 0, \\ \text{weak heredity:} \quad & \boldsymbol{\Omega}_{k,l} \neq 0 \Rightarrow \beta_k^2 + \beta_l^2 > 0. \end{aligned}$$

With the heredity assumptions, one can first seek a small number of im-

portant main effects and then only consider interactions involving these discovered main effects. It is however quite possible that main effects corresponding to important interactions are hard to detect. An example is $Y = (1 + X_1)(1 + X_2) + \varepsilon$, where X_1 and X_2 are drawn independently from $\mathcal{N}(-1, 1)$ and ε is standard normal. In this example, $\text{cov}(X_1, Y) = \text{cov}(X_2, Y) = 0$. The main effects X_1 and X_2 are thus unlikely detectable through a working linear model $Y = \alpha_0 + \alpha_1 X_1 + \alpha_2 X_2 + \epsilon$, indicating that the heredity assumptions do not facilitate to find interactions by searching for main effects first. From a practical perspective, Ritchie et al. (2001) provided a real data example to demonstrate the existence of pure interaction models in practice. Cordell (2009) also raised serious concerns that many existing methods that depend on the heredity assumption may miss pure interactions in the absence of main effects.

An ideal quantification of importance of the main effects and interactions should satisfy the invariance principle with respect to location-scale transformation of the covariates. It is natural and a common strategy to quantify the importance of main effects and interactions through the supports of $\boldsymbol{\beta}$ and $\boldsymbol{\Omega}$ in model (1.1). In conventional linear model where only main effects are present and interactions are absent (i.e., $\boldsymbol{\Omega} = \mathbf{0}_{p\times p}$ in model (1.1)), the invariance principle is satisfied. In contrast, in quadratic regres-

sion (1.1) with a general $\boldsymbol{\Omega}$ the invariance principle is very likely violated. To demonstrate this issue, we can recast model (1.1) as

$$\mathrm{E}(Y \mid \mathbf{x}) = (\alpha - \mathbf{u}^{\mathrm{T}}\boldsymbol{\beta} + \mathbf{u}^{\mathrm{T}}\boldsymbol{\Omega}\mathbf{u}) + \mathbf{x}^{\mathrm{T}}(\boldsymbol{\beta} - 2\boldsymbol{\Omega}\mathbf{u}) + \mathbf{x}^{\mathrm{T}}\boldsymbol{\Omega}\mathbf{x}. \tag{1.2}$$

In this model, the importance of main effects and interactions is naturally characterized through the support of $(\boldsymbol{\beta} - 2\boldsymbol{\Omega}\mathbf{u})$ and $\boldsymbol{\Omega}$, respectively, indicating that the interactions are invariant whereas the main effects are sensitive to location transformation. The heredity condition and the invariance principle were also discussed in details by Hao and Zhang (2017). In ultra-high dimensional quadratic regression, using one-stage approaches which simultaneously estimate main effects and interactions under the heredity assumption, or using two-stage approaches which search for main effects prior to searching for interactions, in model (1.1) and model (1.2), may lead to quite different conclusions. It is thus desirable to estimate interactions directly without knowing the main effects in advance. Direct interaction estimation without heredity constraints is, however, to the best of our knowledge, much more challenging and still unsolved in the literature. A careful anonymous referee pointed out that, if both $\boldsymbol{\beta}$ and $\boldsymbol{\Omega}$ in model (1.1) were treated as random rather than fixed, then the strong heredity condition would be satisfied almost surely. In this case, however, the main effects would be too weak to be used to search for interactions.

1.3 Our Contributions

In this article we consider interaction estimation in ultrahigh dimensional quadratic regressions without heredity assumption. We make at least the following two important contributions to the literature.

1. We obtain a general and explicit expression for quadratic regression with as minimal assumptions as possible. Surprisingly, it turns out that such an explicit solution only relies on certain moment conditions on the ultrahigh dimensional covariates, which is satisfied by the widely used normality assumption. Explicit forms can be derived for both the main effects and the interactions, from which it can be seen that the quadratic regression could be implemented as two independent tasks relating to the main effects and interactions separately. Under weaker moment assumptions, our approach is still valid in detecting the direction of the true interactions. Our proposal is different from existing one-step or two-step procedures in that we do not require the heredity assumption and our proposal give explicit forms for both the main effects and the interactions. Estimating the main effects through a separate working linear model ensures that the resulting estimate satisfies the desirable invariance principle. We show that our approach to detecting interactions is robust to the estima-

tion of main effects. Even when the main effects are not estimated precisely, we are still able to detect the interactions accurately.

2. We show that the interaction inference is equivalent to a particular matrix estimation at the population level. We estimate the interactions of matrix form under penalized convex loss function, which yields a sparse solution. We establish the consistency of our proposed estimates when the covariate dimension p grows, approximately, in an exponential order of the sample size n, to be precise, $p = o\left\{\exp(ns_p^{-2})\right\}$, where s_p stands for the size of the underlying true model. Compared with the conventional penalized least squares approach, the penalization of matrix form is appealing in both memory storage and computation cost. An efficient algorithm is developed to implement our procedure. This algorithm fully explores the cheap computational cost for matrix multiplication and is even much more efficient than existing penalized methods. For example, the algorithm can handle the case with $p = 10000$ covariates. The developed R package "PIE" is available at `https://github.com/cescwang85/PIE`. More details can be found in the package and the simulation part.

This paper is organized as follows. We begin with a quadratic regression model in Section 2 and derive closed forms for both the main effects

and the interactions. We propose a direct penalized estimation for high dimensional sparse quadratic model. To implement our proposal an efficient ADMM algorithm is provided. We also study the theoretical properties of our proposed estimates. We illustrate the performance of our proposal through simulations in Section 3 and an application to a real world problem in Section 4. We give some brief comments in Section 5. All technical details and additional simulations are deferred to the Supplementary Materials.

The following notations will be used repetitively in subsequent exposition. For a real $p \times q$ matrix $\mathbf{A}_{p\times q} = (\mathbf{A}_{k,l})_{p\times q}$, let $\lambda_{\max}(\mathbf{A})$ and $\lambda_{\min}(\mathbf{A})$ stand for its maximum and the minimum singular values, respectively. Let $\|\mathbf{A}\|_F \stackrel{\text{def}}{=} \{\text{tr}(\mathbf{A}^{\text{T}}\mathbf{A})\}^{1/2}$ be the Frobenius norm, $\|\mathbf{A}\|$ be the spectral norm, and $\text{tr}(\cdot)$ be the trace operator of $\mathbf{A}$. We further define

$$\|\mathbf{A}\|_\infty \stackrel{\text{def}}{=} \max_{1\le k\le p, 1\le l\le q} |\mathbf{A}_{k,l}|, \|\mathbf{A}\|_1 \stackrel{\text{def}}{=} \sum_{k=1}^{p}\sum_{l=1}^{q} |\mathbf{A}_{k,l}|, \text{ and } \|\mathbf{A}\|_L \stackrel{\text{def}}{=} \max_{1\le k\le p} \sum_{l=1}^{q} |\mathbf{A}_{k,l}|.$$

2. THE ESTIMATION PROCEDURE

2.1 The Rationale

In this section we discuss how to estimate $\boldsymbol{\beta}$ and $\boldsymbol{\Omega}$, which characterize the main effects and interactions in model (1.1), respectively. Note that $\boldsymbol{\beta} = E\{\partial E(Y \mid \mathbf{x})/(\partial \mathbf{x})\}$ and $\boldsymbol{\Omega} = E\{\partial^2 E(Y \mid \mathbf{x})/(\partial \mathbf{x}\partial \mathbf{x}^{\text{T}})\}/2$. Therefore, estimating $\boldsymbol{\beta}$ and $\boldsymbol{\Omega}$ amounts to estimating $E\{\partial E(Y \mid \mathbf{x})/(\partial \mathbf{x})\}$ and

$E\{\partial^2 E(Y \mid \mathbf{x})/(\partial\mathbf{x}\partial\mathbf{x}^{\mathrm{T}})\}$, respectively, which is however not straightforward, especially when $\mathbf{x}$ is ultrahigh dimensional. To illustrate the rationale of our proposal, we assume for now that $\mathbf{x}$ follows $\mathcal{N}(\mathbf{u}, \boldsymbol{\Sigma})$. It follows immediately from Stein's Lemma (Stein, 1981; Li, 1992) that

$$E\{\partial E(Y \mid \mathbf{x})/(\partial\mathbf{x})\} = \boldsymbol{\Sigma}^{-1}\mathrm{cov}(\mathbf{x}, Y) \text{ and}$$

$$E\{\partial^2 E(Y \mid \mathbf{x})/(\partial\mathbf{x}\partial\mathbf{x}^{\mathrm{T}})\} = \boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}_y\boldsymbol{\Sigma}^{-1},$$

where $\boldsymbol{\Lambda}_y \stackrel{\text{def}}{=} E\Big[\{Y - E(Y)\}(\mathbf{x}-\mathbf{u})(\mathbf{x}-\mathbf{u})^{\mathrm{T}}\Big]$. Define $r \stackrel{\text{def}}{=} Y - E(Y) - (\mathbf{x}-\mathbf{u})^{\mathrm{T}}\boldsymbol{\beta}$, which is the residual obtained by regressing Y on $\mathbf{x}$ linearly. The Hessians of $E(Y \mid \mathbf{x})$ and $E(r \mid \mathbf{x})$ are equal. Accordingly, we have

$$E\left\{\partial^2 E(Y \mid \mathbf{x})/(\partial\mathbf{x}\partial\mathbf{x}^{\mathrm{T}})\right\} = E\left\{\partial^2 E(r \mid \mathbf{x})/(\partial\mathbf{x}\partial\mathbf{x}^{\mathrm{T}})\right\}.$$

By Stein's Lemma, we can obtain that

$$E\left\{\partial^2 E(r \mid \mathbf{x})/(\partial\mathbf{x})(\partial\mathbf{x}^{\mathrm{T}})\right\} = \boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}_r\boldsymbol{\Sigma}^{-1},$$

where $\boldsymbol{\Lambda}_r \stackrel{\text{def}}{=} E\{r(\mathbf{x}-\mathbf{u})(\mathbf{x}-\mathbf{u})^{\mathrm{T}}\}$. This indicates that, if $\mathbf{x}$ is normal, we have explicit forms for $\boldsymbol{\beta}$ and $\boldsymbol{\Omega}$. Specifically,

$$\boldsymbol{\beta} = \boldsymbol{\Sigma}^{-1}\mathrm{cov}(\mathbf{x}, Y), \text{ and } \boldsymbol{\Omega} = \boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2,$$

where $\boldsymbol{\Lambda}$ stands for either $\boldsymbol{\Lambda}_y$ or $\boldsymbol{\Lambda}_r$.

We remark here that the normality assumption is widely used in the literature of interaction estimation. See, for example, Hao and Zhang (2014),

Simon and Tibshirani (2015), Bien et al. (2015) and Hao et al. (2018). In the present context we show that the normality assumption can be relaxed.

Proposition 1. Suppose that $\mathbf{x}$ is drawn from the factor model $\mathbf{x} = \mathbf{\Gamma}_0\mathbf{z} + \mathbf{u}$, where $\mathbf{\Gamma}_0$ satisfies $\mathbf{\Gamma}_0\mathbf{\Gamma}_0^{\mathrm{T}} = \mathbf{\Sigma} > 0$ and $\mathbf{z} \stackrel{\text{def}}{=} (Z_1, \ldots, Z_q)^{\mathrm{T}}$ where $Z_1, \cdots, Z_q$ are independent and identically distributed (i.i.d.) with $\mathrm{E}(Z_k) = 0$, $\mathrm{E}(Z_k^2) = 1$, $\mathrm{E}(Z_k^3) = 0$, $\mathrm{E}(Z_k^4) = \Delta$. We further assume either (C1): $\Delta = 3$ or (C2): $\mathrm{diag}(\mathbf{\Gamma}_0^{\mathrm{T}}\mathbf{\Omega}\mathbf{\Gamma}_0) = \mathbf{0}$. Then the parameters α, $\boldsymbol{\beta}$ and $\mathbf{\Omega}$ in model (1.1) have the following explicit forms:

$$\alpha = E(Y) - \mathrm{tr}(\mathbf{\Sigma}^{-1}\mathbf{\Lambda})/2,\ \boldsymbol{\beta} = \mathbf{\Sigma}^{-1}\mathrm{cov}(\mathbf{x}, Y) \text{ and } \mathbf{\Omega} = \mathbf{\Sigma}^{-1}\mathbf{\Lambda}\mathbf{\Sigma}^{-1}/2. \quad (2.3)$$

The factor model was widely assumed in random matrix theory (Bai and Saranadasa, 1996) and high dimensional inference (Chen et al., 2010), where higher order moment assumptions of $\mathbf{x}$ are often required. The moment conditions on $\mathbf{z}$ play an important role to derive an explicit form for $\mathbf{\Omega}$. Condition (C1) is satisfied if $\mathbf{x}$ is normal. When $\mathbf{\Gamma}_0 = \mathbf{I}_{p\times p}$, condition (C2) requires the absence of quadratic terms of the form X_k^2 in model (1.1), i.e.,

$$\mathrm{E}(Y \mid \mathbf{x}) = \alpha + \mathbf{x}^{\mathrm{T}}\boldsymbol{\beta} + \sum_{i\neq j} \mathbf{\Omega}_{i,j}X_iX_j,$$

where $X_1, \cdots, X_p$ are independent and identically distributed.

We provide two explicit forms for estimating $\mathbf{\Omega}$, one is based on the response Y and the other is based on the residual r. The difference between

$\mathbf{\Lambda}_y$ and $\mathbf{\Lambda}_r$ is that we remove the main effects in $\mathbf{\Lambda}_r$, or equivalently, the linear trend in model (1.1), before we estimate the interactions $\mathbf{\Omega}$. It is natural to expect that the residual-based $\mathbf{\Lambda}_r$ is superior to the response-based $\mathbf{\Lambda}_y$ in that the sample estimate of $\mathbf{\Lambda}_r$ has smaller variabilities than that of $\mathbf{\Lambda}_y$ (Cheng and Zhu, 2017). In effect, we can replace $\boldsymbol{\beta}$ with an arbitrary $\widetilde{\boldsymbol{\beta}} \in \mathbb{R}^p$, which yields that $\widetilde{r} \stackrel{\text{def}}{=} Y - E(Y) - (\mathbf{x}-\mathbf{u})^{\mathrm{T}}\widetilde{\boldsymbol{\beta}}$. Similarly, we can define $\mathbf{\Lambda}_{\widetilde{r}} \stackrel{\text{def}}{=} E\{\widetilde{r}(\mathbf{x}-\mathbf{u})(\mathbf{x}-\mathbf{u})^{\mathrm{T}}\}$. Under the normality assumption, $\mathbf{x}$ is symmetric about $\mathbf{u}$ and hence $\mathbf{\Lambda}_r = \mathbf{\Lambda}_{\widetilde{r}}$. This ensures that, to estimate $\mathbf{\Omega}$ accurately, our proposal does not hinge on the sparsity of main effects because we do not require $\boldsymbol{\beta}$ to be estimated consistently. Even if the main effects are not sufficiently sparse or are not estimated very accurately, we can either directly use the response-based method $\mathbf{\Sigma}^{-1}\mathbf{\Lambda}_y\mathbf{\Sigma}^{-1}$, or the residual-based method $\mathbf{\Sigma}^{-1}\mathbf{\Lambda}_{\widetilde{r}}\mathbf{\Sigma}^{-1}$ which utilizes a lousy residual $\widetilde{r} = Y - E(Y) - (\mathbf{x}-\mathbf{u})^{\mathrm{T}}\widetilde{\boldsymbol{\beta}}$ and $\widetilde{\boldsymbol{\beta}}$ can be a lousy estimate of $\boldsymbol{\beta}$. In effect $\mathbf{\Lambda}_y$ equals $\mathbf{\Lambda}_{\widetilde{r}}$ by setting $\widetilde{\boldsymbol{\beta}} = \mathbf{0}_{p\times 1}$ in $\widetilde{r}$. This makes our proposal quite different from existing procedures which assume the heredity conditions and require to estimate the main effects accurately in order to recover the interactions. By contrast, our proposal does not require to estimate the main effects precisely. We will illustrate this phenomenon through simulations in Section 3.

2.2 Interaction Estimation

We show that both $\boldsymbol{\beta}$ and $\boldsymbol{\Omega}$ have explicit forms under moment conditions in Section 2.1. In particular, $\boldsymbol{\beta} = \boldsymbol{\Sigma}^{-1}\text{cov}(\mathbf{x}, Y)$ and $\boldsymbol{\Omega} = \boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2$ for $\boldsymbol{\Lambda}$ being $\boldsymbol{\Lambda}_y$ or $\boldsymbol{\Lambda}_r$. In this section, we discuss how to estimate $\boldsymbol{\Sigma}^{-1}\text{cov}(\mathbf{x}, Y)$ and $\boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}$ at the sample level. Estimating $\boldsymbol{\Sigma}^{-1}\text{cov}(\mathbf{x}, Y)$ is straightforward by noting that it is a solution to the minimization problem

$$\arg\min_{\mathbf{b}} \text{E}\{Y - \text{E}(Y) - (\mathbf{x} - \mathbf{u})^{\text{T}}\mathbf{b}\}^2.$$

Therefore, we can simply estimate $\boldsymbol{\Sigma}^{-1}\text{cov}(\mathbf{x}, Y)$ with the penalized least squares by regressing $\{Y - \text{E}(Y)\}$ on the ultrahigh dimensional covariates $(\mathbf{x} - \mathbf{u})$ linearly. We do not provide details about how to estimate $\boldsymbol{\Sigma}^{-1}\text{cov}(\mathbf{x}, Y)$ because the penalized least squares estimation has already been well documented (Tibshirani, 1996; Fan and Li, 2001). Throughout our numerical studies we use the LASSO (Tibshirani, 1996) to estimate $\boldsymbol{\beta}$. The resulting solution is denoted by $\widehat{\boldsymbol{\beta}}$.

In what follows we concentrate on how to estimate $\boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2$, where $\boldsymbol{\Lambda}$ can be $\boldsymbol{\Lambda}_y$ or $\boldsymbol{\Lambda}_r$. For an arbitrary matrix $\mathbf{B} = (\mathbf{B}_{k,l})_{p\times p}$, we have

$$\begin{aligned}
\boldsymbol{\Omega} &= \arg\min_{\mathbf{B}} \Big[\text{tr}(\mathbf{B} - \boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2)^{\text{T}}(\mathbf{B} - \boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2)\Big] \\
&= \arg\min_{\mathbf{B}} \Big[\text{tr}(\mathbf{B} - \boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2)^{\text{T}}\boldsymbol{\Sigma}(\mathbf{B} - \boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2)\boldsymbol{\Sigma}\Big],
\end{aligned}$$

and

$$\begin{aligned}&\mathrm{tr}(\mathbf{B}-\boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2)^{\mathrm{T}}\boldsymbol{\Sigma}(\mathbf{B}-\boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2)\boldsymbol{\Sigma}\\&=\mathrm{tr}(\mathbf{B}^{\mathrm{T}}\boldsymbol{\Sigma}\mathbf{B}\boldsymbol{\Sigma})-\mathrm{tr}(\mathbf{B}\boldsymbol{\Lambda})+\mathrm{tr}(\boldsymbol{\Sigma}^{-2}\boldsymbol{\Lambda}^{2})/4.\end{aligned}$$

Ignoring the constant, we notice that, the term $\mathrm{tr}(\mathbf{B}^{\mathrm{T}}\boldsymbol{\Sigma}\mathbf{B}\boldsymbol{\Sigma})-\mathrm{tr}(\mathbf{B}\boldsymbol{\Lambda})$ quantifies the distance between $\mathbf{B}$ and $\boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2$. Therefore, to seek a $p\times p$ matrix $\mathbf{B}$ which can approximate $\boldsymbol{\Sigma}^{-1}\boldsymbol{\Lambda}\boldsymbol{\Sigma}^{-1}/2$ very well, it suffices to consider the following minimization problem

$$\arg\min_{\mathbf{B}}\Big[\mathrm{tr}(\mathbf{B}^{\mathrm{T}}\boldsymbol{\Sigma}\mathbf{B}\boldsymbol{\Sigma})-\mathrm{tr}(\mathbf{B}\boldsymbol{\Lambda})\Big], \tag{2.4}$$

as long as we have faithful estimates of $\boldsymbol{\Sigma}$ and $\boldsymbol{\Lambda}$. The above loss function of matrix form is convex which guarantees that local minimum must be a global minimum.

To construct faithful estimates for $\boldsymbol{\Sigma}$ and $\boldsymbol{\Lambda}$, we suppose $\{(\mathbf{x}_i,Y_i),i=1,\ldots,n\}$ is a random sample of $(\mathbf{x},Y)$. Denote

$$\begin{aligned}&\overline{\mathbf{x}}\overset{\text{def}}{=}n^{-1}\sum_{i=1}^{n}\mathbf{x}_i,\ \overline{Y}\overset{\text{def}}{=}n^{-1}\sum_{i=1}^{n}Y_i,\ \widehat{\boldsymbol{\Sigma}}\overset{\text{def}}{=}n^{-1}\sum_{i=1}^{n}(\mathbf{x}_i-\overline{\mathbf{x}})(\mathbf{x}_i-\overline{\mathbf{x}})^{\mathrm{T}},\\&\widehat{\boldsymbol{\Lambda}}_y\overset{\text{def}}{=}n^{-1}\sum_{i=1}^{n}(Y_i-\overline{Y})(\mathbf{x}_i-\overline{\mathbf{x}})(\mathbf{x}_i-\overline{\mathbf{x}})^{\mathrm{T}},\ \text{and}\\&\widehat{\boldsymbol{\Lambda}}_r\overset{\text{def}}{=}n^{-1}\sum_{i=1}^{n}\widehat{r}_i(\mathbf{x}_i-\overline{\mathbf{x}})(\mathbf{x}_i-\overline{\mathbf{x}})^{\mathrm{T}},\end{aligned}$$

where $\widehat{r}_i\overset{\text{def}}{=}Y_i-\overline{Y}-(\mathbf{x}_i-\overline{\mathbf{x}})^{\mathrm{T}}\widehat{\boldsymbol{\beta}}$. We propose the following penalized

interaction estimation (PIE) to estimate $\mathbf{\Omega}$, for $\widehat{\mathbf{\Lambda}}$ being $\widehat{\mathbf{\Lambda}}_y$ or $\widehat{\mathbf{\Lambda}}_r$:

$$\text{PIE:} \quad \widehat{\mathbf{\Omega}} = \underset{\mathbf{B}\in\mathbb{R}^{p\times p}}{\arg\min}\, \mathrm{tr}(\mathbf{B}^{\mathrm{T}}\widehat{\mathbf{\Sigma}}\mathbf{B}\widehat{\mathbf{\Sigma}}) - \mathrm{tr}(\mathbf{B}\widehat{\mathbf{\Lambda}}) + \lambda_n\|\mathbf{B}\|_1, \tag{2.5}$$

where λ_n is a tuning parameter and $\|\mathbf{B}\|_1 = \sum_{k=1}^{p}\sum_{l=1}^{p}|\mathbf{B}_{k,l}|$. To ease subsequent illustration, we further define the following two notations:

$$\text{PIE}_y: \quad \widehat{\mathbf{\Omega}}_y = \underset{\mathbf{B}\in\mathbb{R}^{p\times p}}{\arg\min}\, \mathrm{tr}(\mathbf{B}^{\mathrm{T}}\widehat{\mathbf{\Sigma}}\mathbf{B}\widehat{\mathbf{\Sigma}}) - \mathrm{tr}(\mathbf{B}\widehat{\mathbf{\Lambda}}_y) + \lambda_{1n}\|\mathbf{B}\|_1, \tag{2.6}$$

$$\text{PIE}_r: \quad \widehat{\mathbf{\Omega}}_r = \underset{\mathbf{B}\in\mathbb{R}^{p\times p}}{\arg\min}\, \mathrm{tr}(\mathbf{B}^{\mathrm{T}}\widehat{\mathbf{\Sigma}}\mathbf{B}\widehat{\mathbf{\Sigma}}) - \mathrm{tr}(\mathbf{B}\widehat{\mathbf{\Lambda}}_r) + \lambda_{2n}\|\mathbf{B}\|_1. \tag{2.7}$$

2.3 Implementation

In this section we develop an efficient algorithm to solve (2.5) which includes (2.6) and (2.7) as special cases. We rewrite the optimization problem as

$$\min_{\mathbf{B}\in\mathbb{R}^{p\times p}} \mathrm{tr}(\mathbf{B}^{\mathrm{T}}\widehat{\mathbf{\Sigma}}\mathbf{B}\widehat{\mathbf{\Sigma}}) - \mathrm{tr}(\mathbf{B}\widehat{\mathbf{\Lambda}}) + \lambda_n\|\mathbf{\Psi}\|_1, \text{ such that } \mathbf{\Psi} = \mathbf{B}, \tag{2.8}$$

which motivates us to form the augmented Lagrangian as

$$\begin{aligned} L(\mathbf{B}, \mathbf{\Psi}, \mathbf{L}) &= \mathrm{tr}(\mathbf{B}^{\mathrm{T}}\widehat{\mathbf{\Sigma}}\mathbf{B}\widehat{\mathbf{\Sigma}}) - \mathrm{tr}(\mathbf{B}\widehat{\mathbf{\Lambda}}) + \lambda_n\|\mathbf{\Psi}\|_1 \\ &\quad + \mathrm{tr}\left\{\mathbf{L}(\mathbf{B}-\mathbf{\Psi})\right\} + (\rho/2)\|\mathbf{B}-\mathbf{\Psi}\|_F^2, \end{aligned} \tag{2.9}$$

where $\rho > 0$ is a step size parameter. By standard Alternating Direction Method of Multipliers (Boyd et al., 2011, ADMM), the augmented

Lagrangian (2.9) can be solved by successively updating $(\mathbf{B}, \mathbf{\Psi}, \mathbf{L})$:

$$\text{The } \mathbf{B} \text{ step:} \quad \mathbf{B}^{k+1} = \underset{\mathbf{B}\in\mathbb{R}^{p\times p}}{\arg\min}\, L(\mathbf{B}, \mathbf{\Psi}^k, \mathbf{L}^k), \tag{2.10}$$

$$\text{The } \mathbf{\Psi} \text{ step:} \quad \mathbf{\Psi}^{k+1} = \underset{\mathbf{\Psi}\in\mathbb{R}^{p\times p}}{\arg\min}\, L(\mathbf{B}^{k+1}, \mathbf{\Psi}, \mathbf{L}^k), \tag{2.11}$$

$$\text{The } \mathbf{L} \text{ step:} \quad \mathbf{L}^{k+1} = \mathbf{L}^k + \rho(\mathbf{B}^{k+1} - \mathbf{\Psi}^{k+1}). \tag{2.12}$$

Define the elementwise soft thresholding operator $\text{soft}(\mathbf{A}, \lambda) \overset{\text{def}}{=} \{\max(\mathbf{A}_{k,l} - \lambda, 0)\}_{p\times p}$. For the $\mathbf{\Psi}$ step, given $\mathbf{B}^{k+1}$, $\mathbf{L}^k$, ρ and λ_n, the solution is

$$\mathbf{\Psi}^{k+1} \overset{\text{def}}{=} \text{soft}(\mathbf{B}^{k+1} + \rho^{-1}\mathbf{L}^k, \lambda_n/\rho).$$

The $\mathbf{B}$ step amounts to solving the equation

$$2\widehat{\mathbf{\Sigma}}\mathbf{B}^{k+1}\widehat{\mathbf{\Sigma}} + \rho\mathbf{B}^{k+1} = \mathbf{\Lambda}^k, \tag{2.13}$$

where $\mathbf{\Lambda}^k \overset{\text{def}}{=} \widehat{\mathbf{\Lambda}} - \mathbf{L}^k + \rho\mathbf{\Psi}^k$. We make the singular value decomposition to obtain $\widehat{\mathbf{\Sigma}} = \mathbf{U}\mathbf{D}_0\mathbf{U}^{\mathrm{T}}$, where $\mathbf{U} \in \mathbb{R}^{p\times m}$, $m = \min(n, p)$ and $\mathbf{D}_0 \overset{\text{def}}{=} \text{diag}(d_1, \cdots, d_m)$ is a diagonal matrix. Define $\mathbf{D} \overset{\text{def}}{=} (\mathbf{D}_{k,l})_{p\times p}$, where $\mathbf{D}_{k,l} \overset{\text{def}}{=} 2d_kd_l/(2d_kd_l + \rho)$. Given $\mathbf{\Psi}^k$, $\mathbf{L}^k$ and ρ, the solution to (2.13) is given by

$$\mathbf{B}^{k+1} = \rho^{-1}\mathbf{\Lambda}^k - \rho^{-1}\mathbf{U}\{\mathbf{D} \circ (\mathbf{U}^{\mathrm{T}}\mathbf{\Lambda}^k\mathbf{U})\}\mathbf{U}^{\mathrm{T}}.$$

where $\circ$ denotes the Hadamard product.

Details of the algorithm is summarized in Algorithm 1. This algorithm yields a symmetric estimate of $\mathbf{\Omega}$, which is denoted by $\widehat{\mathbf{\Omega}}$. The computational complexity of each iteration is no more than $\text{O}\{\min(n, p)p^2\}$ and the

memory requirement is no more than $O(p^2)$ since we only need to store a few $p \times p$ or $p \times \min(n, p)$ matrices in computer memory.

As a first-order method for convex problems, convergence analysis of the ADMM algorithm under various conditions has been well documented in the recent optimization literature. See, for example, Nishihara et al. (2015), Hong and Luo (2017) and Chen et al. (2017). The following lemma states the convergence of our proposed ADMM algorithm.

Lemma 1. Given $\widehat{\mathbf{\Sigma}}$ and $\widehat{\mathbf{\Lambda}}$. Suppose that the ADMM algorithm (2.10)-(2.12) generates a sequence of solutions $\{(\mathbf{B}^k, \mathbf{\Psi}^k, \mathbf{L}^k), k = 1, \ldots\}$. Then $\{(\mathbf{B}^k, \mathbf{\Psi}^k), k = 1, \ldots\}$ converges linearly to the minimizer of (2.8), and $\|\mathbf{B}^k - \mathbf{\Psi}^k\|_F$ converges linearly to zero, as $k \to \infty$.

It remains to choose an appropriate tuning parameter for PIE_y or PIE_r. Motivated by Efron et al. (2004), we use PIE to seek for a sparse model but not to estimate the coefficients. For a given λ_n, we fit least squares estimation on the support of $\widehat{\mathbf{\Omega}}$ estimated by PIE_y or PIE_r, which yields the residual sum of squares. We choose λ_n which minimizes the Bayesian information criterion (BIC). Our limited experience indicates that this procedure is very fast and effective.

Algorithm 1 ADMM algorithm for solving (2.5)

Initialization:

1: Input $\{(\mathbf{x}_i, Y_i), i = 1, \cdots, n\}$, the tuning parameter λ_n and ρ;

2: Calculate $\widehat{\mathbf{\Lambda}}$ and the singular value decomposition of the centered design matrix $(\mathbf{x}_1 - \overline{\mathbf{x}}, \cdots, \mathbf{x}_n - \overline{\mathbf{x}})_{p\times n}$ to get $\widehat{\mathbf{\Sigma}} = \mathbf{U}\mathbf{D}_0\mathbf{U}^{\mathrm{T}}$ where $\mathbf{U} \in \mathbb{R}^{p\times m}$, $\mathbf{D}_0 = \mathrm{diag}\{d_1, \ldots, d_m\}$ and $m = \min(n, p)$;

3: Define $\mathbf{D} \stackrel{\mathrm{def}}{=} (\mathbf{D}_{k,l})_{m\times m}$ where $\mathbf{D}_{k,l} = 2d_k d_l/(2d_k d_l + \rho)$;

4: Start from $k = 0$, $\mathbf{L}^0 = \mathbf{0}_{p\times p}, \mathbf{B}^0 = \mathbf{0}_{p\times p}$.

Iteration:

5: Define $\mathbf{\Lambda}^k \stackrel{\mathrm{def}}{=} \widehat{\mathbf{\Lambda}} - \mathbf{L}^k + \rho\mathbf{B}^k$. Update $\mathbf{B}^{k+1} = \rho^{-1}\mathbf{\Lambda}^k - \rho^{-1}\mathbf{U}\{\mathbf{D} \circ (\mathbf{U}^{\mathrm{T}}\mathbf{\Lambda}^k\mathbf{U})\}\mathbf{U}^{\mathrm{T}}$;

6: Update $\mathbf{\Psi}^{k+1} \stackrel{\mathrm{def}}{=} \mathrm{soft}(\mathbf{B}^{k+1} + \rho^{-1}\mathbf{L}^k, \lambda_n/\rho)$;

7: Update $\mathbf{L}^{k+1} \stackrel{\mathrm{def}}{=} \mathbf{L}^k + \rho(\mathbf{B}^{k+1} - \mathbf{\Psi}^{k+1})$;

8: Update $k = k + 1$;

9: Repeat step 5 through step 8 until convergence.

Output: $\widehat{\mathbf{\Omega}} = \mathbf{B}^{k+1}$.

2.4 Asymptotic Properties

For notational clarity, we denote the support of $\mathbf{\Omega} = (\mathbf{\Omega}_{k,l})_{p\times p}$ by $\mathcal{S} \stackrel{\text{def}}{=} \{(k,l) : \mathbf{\Omega}_{k,l} \neq 0\}$, the complement of $\mathcal{S}$ by $\mathcal{S}^c$, and the cardinality of $\mathcal{S}$ by $s_p \stackrel{\text{def}}{=} \|\mathbf{\Omega}\|_0$. Similarly, we denote by $\widehat{\mathcal{S}}_y$ and $\widehat{\mathcal{S}}_r$ the respective support of $\widehat{\mathbf{\Omega}}_y$ and $\widehat{\mathbf{\Omega}}_r$, and $\widehat{\mathcal{S}}_y^c$ and $\widehat{\mathcal{S}}_r^c$ the respective complement of $\widehat{\mathcal{S}}_y$ and $\widehat{\mathcal{S}}_r$. We further define $\mathbf{\Gamma} \stackrel{\text{def}}{=} \mathbf{\Sigma} \otimes \mathbf{\Sigma}$, $M \stackrel{\text{def}}{=} \|\mathbf{\Gamma}_{\mathcal{S},\mathcal{S}}^{-1}\|_L$ and $\kappa \stackrel{\text{def}}{=} 1 - \|\mathbf{\Gamma}_{\mathcal{S}^c,\mathcal{S}}\mathbf{\Gamma}_{\mathcal{S},\mathcal{S}}^{-1}\|_L$, where $\mathbf{\Gamma}_{\mathcal{S},\mathcal{S}}$ is a submatrix of $\mathbf{\Gamma}$ with rows and columns indexed by $\mathcal{S}$, and $\mathbf{\Gamma}_{\mathcal{S}^c,\mathcal{S}}$ is a submatrix of $\mathbf{\Gamma}$ with rows and columns indexed respectively by $\mathcal{S}^c$ and $\mathcal{S}$. Denote $c_0, C_0, c_1, C_1, \ldots$, a sequence of generic constants which may take different values at various places. We assume the following regularity conditions to study the asymptotic properties of $\widehat{\mathbf{\Omega}}_y$ and $\widehat{\mathbf{\Omega}}_r$.

(A1): Assume $c_0^{-1} \leq \lambda_{\min}(\mathbf{\Sigma}) \leq \lambda_{\max}(\mathbf{\Sigma}) \leq c_0$, where $\lambda_{\min}(\mathbf{\Sigma})$ and $\lambda_{\max}(\mathbf{\Sigma})$ are the respective smallest and largest eigenvalues of $\mathbf{\Sigma}$.

(A2): Assume X_ks are sub-Gaussian, i.e., $\mathrm{E}\{\exp(c_0|\mathbf{e}^{\mathrm{T}}\mathbf{x}|^2)\} \leq C_0 < \infty$ for any unit-length vector $\mathbf{e}$.

(A3) Assume $\mathrm{E}\{\exp(c_1|Y|^\alpha)\} \leq C_1 < \infty$ for some $0 < \alpha \leq 2$.

(A4) Assume the irrepresentability condition holds, i.e., $\kappa > 0$.

(A5) Assume $\mathbf{x}$ is symmetric about $\mathbf{u}$.

Conditions (A1) and (A2) are widely assumed in literature. Condition (A3) is assumed to control the tail behavior of Y through concentration inequalities. Condition (A4) is analog, but not identical, to the irrepresentability condition used for establishing model selection consistency in LASSO. In our context, the irrepresentability condition is imposed on $\mathbf{\Gamma} \stackrel{\text{def}}{=} \mathbf{\Sigma} \otimes \mathbf{\Sigma}$ because the interaction effects are concerned. This condition is also used to study the model consistency of the graphical LASSO (Ravikumar et al., 2011; Zhang and Zou, 2014; Liu and Luo, 2015). By contrast, if the linear effects are of primary interest, the irrepresentability condition is imposed on $\mathbf{\Sigma}$. See, for example, Zhao and Yu (2006) and Zou (2006). Condition (A5) is assumed to ensure the consistency of residual-based approaches.

Theorem 1. Let $\lambda_{1n} \stackrel{\text{def}}{=} c_1\{n^{-\alpha/(\alpha+1)}\log(p)\}^{1/2}$ for sufficiently large c_1 and assume $s_p\{n^{-1}\log(p)\}^{1/2} \to 0$. Under the conditions (A1)-(A4),

(i) if we further assume $\min_{(k,l)\in\mathcal{S}} |\mathbf{\Omega}_{k,l}| > c_2 M\lambda_{1n}$ for sufficiently large c_2, then $\text{pr}\big(\widehat{\mathcal{S}}_y = \mathcal{S}\big) = 1 - O(p^{-1})$.

(ii) $\text{pr}\big(\|\widehat{\mathbf{\Omega}}_y - \mathbf{\Omega}\|_\infty \le c_3\lambda_{1n}M\big) = 1 - O(p^{-1})$, for sufficiently large c_3.

(iii) $\text{pr}\big(\|\widehat{\mathbf{\Omega}}_y - \mathbf{\Omega}\|_F \le c_4 s_p^{1/2}\lambda_{1n}M\big) = 1 - O(p^{-1})$, for sufficiently large c_4.

Theorem 1 shows that, as long as the signal strength of the interactions is not too small, our proposal can identify the support correctly with a very

high probability. In other words, $\widehat{\boldsymbol{\Omega}}_y$ is asymptotically selection consistent. Theorem 1 also shows that $\widehat{\boldsymbol{\Omega}}_y$ is a consistent estimate of $\boldsymbol{\Omega}$ under both the infinity norm and the Frobenius norm.

Theorem 2. Let $\lambda_{2n} \stackrel{\text{def}}{=} c_5\{n^{-\alpha/(\alpha+1)}\log(p)\}^{1/2} + c_5\|\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}\|_1\{\log(p)/n\}^{1/2}$ for sufficiently large c_5 and assume that $s_p\{n^{-1}\log(p)\}^{1/2} \to 0$. Under the conditions (A1)-(A5), we have

(i) If we further assume $\min_{(k,l)\in\mathcal{S}} |\boldsymbol{\Omega}_{k,l}| > c_6 M\lambda_{2n}$ for sufficiently large c_6, then $\text{pr}\big(\widehat{\mathcal{S}}_r = \mathcal{S}\big) = 1 - O(p^{-1})$.

(ii) $\text{pr}\big(\|\widehat{\boldsymbol{\Omega}}_r - \boldsymbol{\Omega}\|_\infty \le c_7\lambda_{2n}M\big) = 1 - O(p^{-1})$, for sufficiently large c_7.

(iii) $\text{pr}\big(\|\widehat{\boldsymbol{\Omega}}_r - \boldsymbol{\Omega}\|_F \le c_8 s_p^{1/2}\lambda_{2n}M\big) = 1 - O(p^{-1})$, for sufficiently large c_8.

Theorem 2 shows that $\widehat{\boldsymbol{\Omega}}_r$, as well as $\widehat{\boldsymbol{\Omega}}_y$, possesses both the selection and estimation consistency asymptotically. Moreover, the convergence rate of $\widehat{\boldsymbol{\Omega}}_r$ depends on $\widehat{\boldsymbol{\beta}}$. If $\|\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}\|_1 = o\{n^{1/(2\alpha+2)}\}$, the convergence rate term involving $\widehat{\boldsymbol{\beta}}$ will be absorbed in the first term of Theorem 2. In other words, unless the estimation error of $\widehat{\boldsymbol{\beta}}$ diverges faster than $n^{1/(2\alpha+2)}$, $\widehat{\boldsymbol{\Omega}}_r$ and $\widehat{\boldsymbol{\Omega}}_y$ would share the same convergence rate.

3. SIMULATIONS

In this section we conduct simulations to evaluate the performance of our proposal and to compare it with the RAMP method (Hao et al., 2018) and the all-pairs-LASSO (Bien et al., 2013) which fits a LASSO model on all p main effects and $p(p+1)/2$ interactions. Hao et al. (2018) claimed that RAMP outperforms other methods such as iFOR(Hao and Zhang, 2014) and hierNet (Bien et al., 2013) under heredity assumptions. Therefore, we do not include iFOR and hierNet into our comparison. In what follows, we refer to the RAMP method under the strong heredity condition as "RAMPs" and the RAMP method under the weak heredity condition as "RAMPw". We also include the oracle estimate as a benchmark which assumes the main effects and the support of interactions are known in advance. The oracle estimate simply fits the least squares estimation on the support of interactions using the truly important main effects. We denote it as "Oracle". The RAMP method and all-pairs-LASSO are implemented by the R packages "RAMP" and "glmnet" (Friedman et al., 2010).

To ease illustration, we denote the estimate of $\mathbf{\Omega}$ by $\widehat{\mathbf{\Omega}}$ obtained with different approaches. We evaluate the accuracy of the estimation through five criteria: the support recovery rate, denoted by "rate", the Frobenius loss, denoted by "loss", the number of interactions that are estimated as

nonzero, denoted by "size" and the exact support recovery rate, denoted by "exact". To be specific, the criteria are defined as follows,

$$\begin{aligned}
\text{rate} &\stackrel{\text{def}}{=} B^{-1}\sum_{b=1}^{B}\sum_{l\le k} I(\widehat{\mathbf{\Omega}}_{k,l}^{(b)} \neq 0, \mathbf{\Omega}_{k,l} \neq 0)\Big/\sum_{l\le k} I(\mathbf{\Omega}_{k,l} \neq 0) \times 100\%, \\
\text{loss} &\stackrel{\text{def}}{=} B^{-1}\sum_{b=1}^{B} \|\widehat{\mathbf{\Omega}}^{(b)} - \mathbf{\Omega}\|_F, \text{ size} \stackrel{\text{def}}{=} B^{-1}\sum_{b=1}^{B}\sum_{l\le k} I(\widehat{\mathbf{\Omega}}_{k,l}^{(b)} \neq 0), \text{ and} \\
\text{exact} &\stackrel{\text{def}}{=} B^{-1}\sum_{b=1}^{B} I\big(\widehat{\mathcal{S}}^{(b)} = \mathcal{S}\big),
\end{aligned}$$

where $\mathcal{S}$ and $\widehat{\mathcal{S}}$ are the supports of $\mathbf{\Omega}$ and $\widehat{\mathbf{\Omega}}$, respectively, the superscript $^{(b)}$ stands for the b-th replication, the subscript $_{k,l}$ stands for the (k,l)-th entry of the associated matrix, $I(E)$ is an indicator function which equals 1 if the random event E is true and 0 otherwise. The closer the "rate" is to one, the "loss" to zero, the "size" to the number of truly important interactions, and the "exact" to one, the better performance a proposal has.

We consider the following four models.

$$Y = X_1 + X_6 + X_{10} + 2X_1X_6 + X_6^2 + 2X_6X_{10} + \varepsilon, \tag{3.14}$$

$$Y = X_6 + 2X_1X_6 + X_6^2 + 2X_6X_{10} + \varepsilon, \tag{3.15}$$

$$Y = X_1 + X_2 + 2X_1X_6 + X_6^2 + 2X_6X_{10} + \varepsilon, \tag{3.16}$$

$$Y = 2X_1X_6 + X_6^2 + 2X_6X_{10} + \varepsilon. \tag{3.17}$$

The strong heredity condition holds in (3.14) and the weak heredity condition holds in (3.15), respectively. Neither the strong nor the weak heredity

condition holds in (3.16) or (3.17). In particular, (3.17) is a pure interaction model. We replicate each scenario for $B = 100$ times to evaluate the performance of different proposals.

3.1 Estimation Accuracy

We draw $\mathbf{x}$ independently from $\mathcal{N}(\mathbf{0}_{p\times 1}, \mathbf{\Sigma})$, where $\mathbf{\Sigma} = (0.5^{|k-l|})_{p\times p}$, and generate an independent error ε from $\mathcal{N}(0, 1)$. We set the sample size $n = 200$ and the dimension $p = 100$ or 200.

Simulation results for models (3.15) and (3.17) are charted in Table 1 of the present main context, and those for models (3.14) and (3.16) are summarized in Table 1 of the Supplement. We observe that our proposal has a stable performance across almost all scenarios. It is not very surprising to see that, the RAMP method with strong heredity condition, denoted by RAMPs, completely fails in models (3.15)-(3.17) where the strong heredity condition is violated; in addition, the RAMP method with weak heredity condition, denoted by RAMPw, fails in models (3.16)-(3.17) where the weak heredity condition is violated. The RAMP method has a satisfactory performance when the required heredity condition is satisfied. In particular, the RAMPs performs quite well in model (3.14). For models (3.15)-(3.17), the oracle estimate has the smallest Frobenius loss, followed by our pro-

posals. Comparing with the all-pairs-LASSO, our proposal has a better performance in terms of Frobenious loss and model size. For the pure interaction model (3.17) where no main effects are present, fitting linear regression to obtain residuals very likely introduces some redundant bias. It is thus not surprising to see that our proposed response-based procedure (PIEy) slightly outperforms our residual-based procedure (PIEr).

3.2 Estimation of Main Effects

In this section we evaluate how the estimation of main effects affects the estimation of interactions. Both our proposed residual-based penalized interaction estimation and the RAMP method are relevant to estimating the main effects. To fixed the signal-to-noise ratio for all settings, we simply draw the covariates $\mathbf{x} = (X_1, \ldots, X_p)^{\mathrm{T}}$ from $\mathcal{N}(\mathbf{0}, \mathbf{I}_{p\times p})$ and consider the following quadratic model

$$\begin{aligned} Y = \;& d^{-1/2}\left(X_1 + X_6 + X_{10} + X_{k_1} + \cdots + X_{k_{d-3}}\right) \\ & + 2X_1X_6 + X_6^2 + 2X_6X_{10} + \varepsilon. \end{aligned}$$

The number of main effects is increased from $d = 3$ to 48. We always include X_1, X_6 and X_{10} to ensure that the strong heredity condition holds true. We also randomly choose $X_{k_1}, \ldots, X_{k_{d-3}}$ from $X_{11}, \ldots, X_p$. Figure 1 reports the support recovery rate of $\widehat{\mathbf{\Omega}}$ and the Frobenius loss of $\|\widehat{\mathbf{\Omega}} - \mathbf{\Omega}\|_F$.

Table 1: The averages (and standard deviations) of the support recovery rate ("rate"), the Frobenius loss ("loss"), the model size ("size") and the exact support recovery rate ("exact") for models (3.15) and (3.17). Simulation results for models (3.14) and (3.16) are given in the Supplement.

p		PIEy	PIEr	RAMPs	RAMPw	all-pairs-LASSO	Oracle
model (3.15) where the weak heredity condition is satisfied							
100	rate	98.67(6.56)	99.33(4.69)	40.67(26.20)	91.33(27.88)	100.00(0.00)	100.00(0.00)
	size	4.19(3.03)	3.73(2.11)	1.67(1.51)	3.91(3.39)	7.38(6.40)	3.00(0.00)
	loss	0.24(0.20)	0.18(0.16)	1.81(0.55)	0.30(0.68)	0.41(0.11)	0.09(0.05)
	exact	0.57(0.50)	0.70(0.46)	0.06(0.24)	0.75(0.43)	0.16(0.37)	1.00(0.00)
200	rate	99.00(5.71)	99.00(5.71)	29.67(23.16)	77.67(41.32)	100.00(0.00)	100.00(0.00)
	size	3.99(2.44)	3.42(1.08)	1.12(1.22)	4.09(4.34)	6.08(4.59)	3.00(0.00)
	loss	0.23(0.21)	0.19(0.19)	1.98(0.40)	0.62(0.97)	0.45(0.11)	0.09(0.04)
	exact	0.65(0.48)	0.73(0.45)	0.03(0.17)	0.68(0.47)	0.29(0.46)	1.00(0.00)
model (3.17) is a pure interaction model where the heredity conditions are violated							
100	rate	99.67(3.33)	100.00(0.00)	11.67(24.33)	31.67(44.79)	100.00(0.00)	100.00(0.00)
	size	4.18(4.24)	4.24(4.22)	0.71(1.58)	3.00(4.92)	5.57(3.86)	3.00(0.00)
	loss	0.13(0.12)	0.13(0.09)	2.11(0.41)	1.64(1.01)	0.42(0.11)	0.09(0.04)
	exact	0.72(0.45)	0.72(0.45)	0.03(0.17)	0.23(0.42)	0.27(0.45)	1.00(0.00)
200	rate	100.00(0.00)	100.00(0.00)	9.67(20.26)	24.33(41.26)	100.00(0.00)	100.00(0.00)
	size	3.45(1.00)	3.49(0.99)	0.51(1.21)	2.95(5.49)	5.46(5.27)	3.00(0.00)
	loss	0.11(0.06)	0.12(0.07)	2.15(0.21)	1.78(0.91)	0.44(0.11)	0.09(0.04)
	exact	0.72(0.45)	0.69(0.46)	0.00(0.00)	0.18(0.39)	0.45(0.50)	1.00(0.00)

It can be clearly seen that, as the number of main effects increases from $d = 3$ to 48, both RAMPs and RAMPw deteriorate gradually in terms of both criteria, indicating that the RAMP method requires to estimate the main effects accurately. For all-pairs-LASSO, the support recovery rate appears very stable while the Frobenius loss becomes worse when d increases. By contrast, our proposal is very robust to the number of main effects. When the number of main effects increases, PIEy is slightly better than PIEr in terms of Frobenius loss. Theses findings confirm our theoretical results in Theorem 2 since $\widehat{\boldsymbol{\beta}}$ becomes worse when d increases.

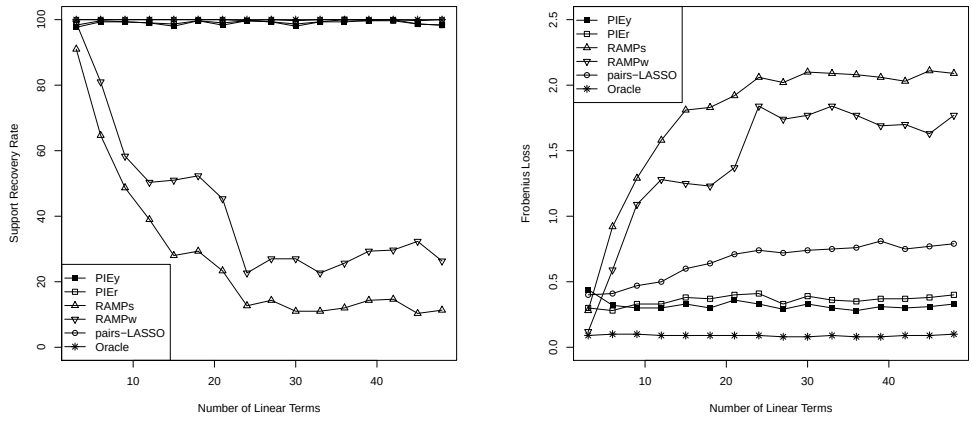


Figure 1: *The vertical axis is the support recovery rate (left) and Frobenius loss (right) of* $\widehat{\boldsymbol{\Omega}}$*, and the horizontal axis is the number of main effects.*

4. AN APPLICATION

In this section, we apply our proposal to the red wine dataset which is publicly available at `https://archive.ics.uci.edu/ml/datasets/Wine+Quality`. The data consist of 11 measurements of several chemical constituents, including determination of density, alcohol or pH values for 1599 red wine samples from the northwest region of Portugal. The response variable is the median of the scores evaluated by human experts and each score ranges from 0 (very bad) to 10 (very excellent). The same dataset was once analyzed by Cortez et al. (2009). In their analysis, interactions are found to be very helpful for prediction. The sampel size $n = 1599$ and the covariate dimension $p = 11$. Following Radchenko and James (2010), we standardize all the variables and conduct two experiments:

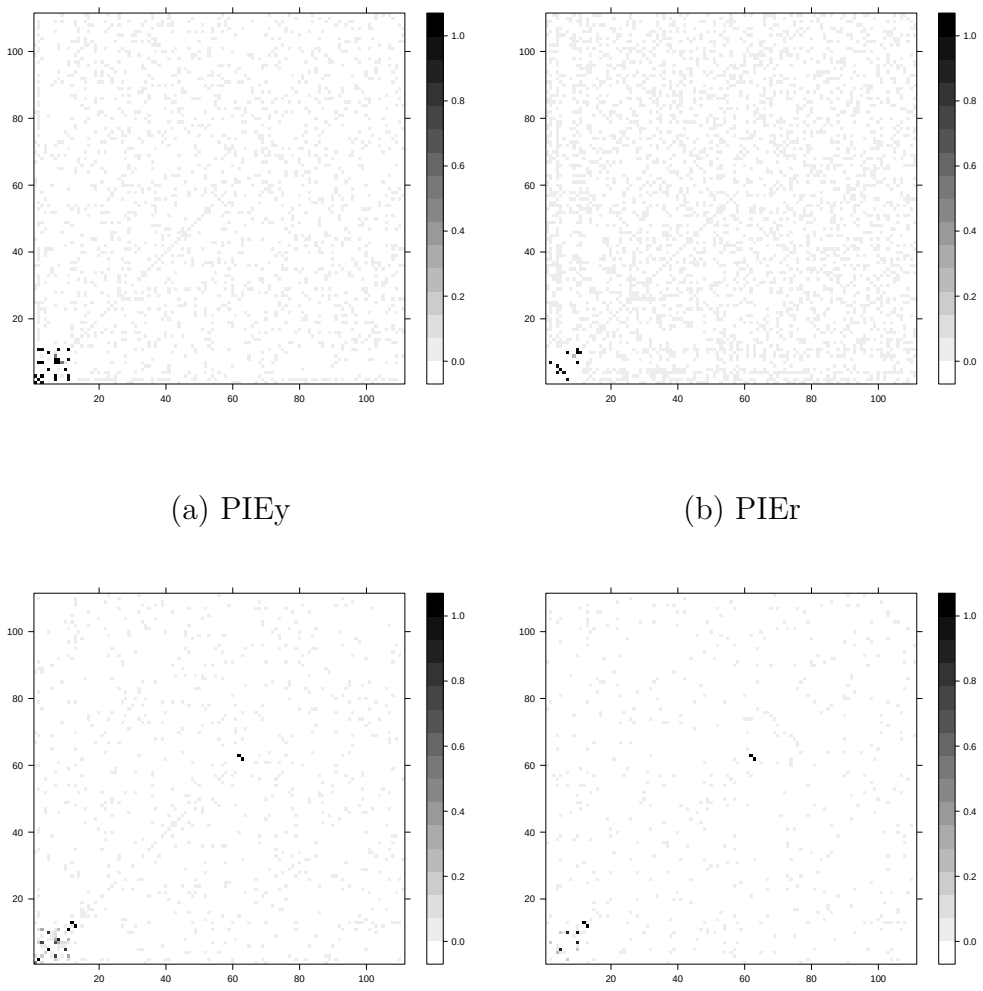
- **Experiment 1.** In addition to the original 11 covariates $X_1, \ldots, X_{11}$, we add 100 noise variables $X_{12}, \ldots, X_{111}$, among which the first 50 are generated from the standard normal distribution and the rest are generated from the uniform distribution on the interval $[-\sqrt{3}, \sqrt{3}]$.

- **Experiment 2.** We generate the covariates in the same way as in Experiment 1 and modify the response variable Y by adding two more interactions: $Y + 0.5X_{12}X_{13} + 0.5X_{61}X_{62}$. In this experiment, both

the strong and the weak heredity conditions are violated.

In both experiments the covariate dimension is updated to $p = 111$, leading to $111 \times 100/2 = 6,105$ possible interactions. We randomly select 400 observations as the sample and the procedure is repeated 100 times. The heat map of the frequencies of the identified interactions are summarized in Figure 2. It can be clearly seen that, in Experiment 1, the selected interactions mainly occur among the first 11 covariates collected in the original dataset while the interactions related to the remaining 100 noisy covariates are rarely detected. This indicates that both PIEy and PIEr are able to exclude irrelevant interactions. In Experiment 2, both methods are able to exclude irrelevant interactions with high probability. In addition, the interactions $X_{12}X_{13}$ and $X_{61}X_{62}$ are successfully identified throughout.

We further compare our proposed PIEy and PIEr with the all-pairs-LASSO in terms of prediction. We randomly split the observes into two halves. We use the first half as a training sample and the second as a test sample. We fit quadratic regressions using the training sample and perform prediction using the test sample. To implement the PIEy and PIEr, we follow Example 1 and generate 100 additional noise covariates. To implement the all-pairs-LASSO, we use the original 11 covariates only. We record the averages of the squared prediction errors for each random



(a) PIEy (b) PIEr

(c) PIEy (d) PIEr

Figure 2: *Heat maps of frequency of the interactions identified out of 100 replications using PIEy and PIEr. Upper panel: Experiment 1. Lower panel: Experiment 2.*

split. Table 2 summarizes the mean and standard deviation of the squared prediction errors and the model sizes based on 100 replications. Compared to the all-pairs-LASSO which includes around seven interactions, both PIEy and PIEr include less than four interactions and yield more parsimonious models. In terms of the prediction performance, both PIEy and PIEr are comparable with the all-pairs-LASSO method.

Table 2: The prediction performance on the red wine dataset. Both the PIEy and the PIEr are fitted with 100 additional noise covariates, while the all-pairs-LASSO are fitted with only 11 original covariates.

	PIEy	PIEr	all-pairs-LASSO
prediction error	0.706(0.035)	0.702(0.034)	0.671(0.032)
model size	3.600(1.980)	3.640(1.580)	7.020(1.880)

5. DISCUSSION

In this paper we propose a penalized estimation to detect interactions without requiring heredity conditions. We develop an efficient ADMM algorithm to implement our estimation. We demonstrate the effectiveness of our proposal through numerical studies. We remark here that, if the strong or

the weak heredity condition is satisfied, some existing methods, such as the RAMP method, may work pretty well as long as the main effects are sufficiently strong. However, if the main effects are too weak to be detectable, existing methods which require the heredity assumptions may have a deteriorating performance. Our proposal is very robust to the violation of the heredity assumptions, in that the estimation of interaction is separable from the estimation of the main effect. Even with a lousy estimate of the main effects, we are still able to estimate the interactions consistently. When we have little prior information about whether the heredity condition holds true or not in an application, we advocate using our proposal in that it does not require this assumption. If the heredity condition is known to be satisfied, we can also incorporate it into our proposal through a two-stage procedure. In the first stage, we use the penalized least squares to identify the main effects; In the second stage, we implement our procedure using only the main effects that are selected in the first stage. This allows us to handle ultrahigh dimensional problems efficiently. Moreover, it would also be interesting to combine our proposal with screening procedures such as the SIRI (Jiang and Liu, 2014), to further improve the estimation efficiency of our proposal.

Supplementary Materials

The supplementary materials contain the technical proofs and additional simulation results.

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School of Mathematical Sciences, MOE-LSC, Shanghai Jiao Tong University, Shanghai 200240, China.

E-mail: chengwang@sjtu.edu.cn

Department of Applied Mathematics, Hong Kong Polytechnic University, Hong Kong.

E-mail: by.jiang@polyu.edu.hk

Institute of Statistics and Big Data and Center for Applied Statistics, Renmin University of China, Beijing 100872, China.

E-mail: zhu.liping@ruc.edu.cn