

# Optimality of Graphlet Screening in High Dimensional Variable Selection

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## Abstract

Consider a linear model  $Y = X\beta + \sigma z$ , where  $X$  has  $n$  rows and  $p$  columns and  $z \sim N(0, I_n)$ . We assume both  $p$  and  $n$  are large, including the case of  $p \gg n$ . The unknown signal vector  $\beta$  is assumed to be sparse in the sense that only a small fraction of its components is nonzero. The goal is to identify such nonzero coordinates (i.e., variable selection).

We are primarily interested in the regime where signals are both *rare and weak* so that successful variable selection is challenging but is still possible. We assume the Gram matrix  $G = X'X$  is sparse in the sense that each row has relatively few large entries (diagonals of  $G$  are normalized to 1). The sparsity of  $G$  naturally induces the sparsity of the so-called *Graph of Strong Dependence* (GOSD). The key insight is that there is an interesting interplay between the signal sparsity and graph sparsity: in a broad context, the signals decompose into many small-size components of GOSD that are disconnected to each other.

We propose *Graphlet Screening* for variable selection. This is a two-step Screen and Clean procedure, where in the first step, we screen subgraphs of GOSD with sequential  $\chi^2$ -tests, and in the second step, we clean with penalized MLE. The main methodological innovation is to use GOSD to guide both the screening and cleaning processes.

For any variable selection procedure  $\hat{\beta}$ , we measure its performance by the Hamming distance between the sign vectors of  $\hat{\beta}$  and  $\beta$ , and assess the optimality by the minimax Hamming distance. Compared with more stringent criteria such as exact support recovery or oracle property, which demand strong signals, the Hamming distance criterion is more appropriate for weak signals since it naturally allows a small fraction of errors.

We show that in a broad class of situations, Graphlet Screening achieves the optimal rate of convergence in terms of the Hamming distance. Unlike Graphlet Screening, well-known procedures such as the  $L^0/L^1$ -penalization methods do not utilize local graphic structure for variable selection, so they generally do not achieve the optimal rate of convergence, even in very simple settings and even if the tuning parameters are ideally set.

The the presented algorithm is implemented as R-CRAN package *ScreenClean* and in *matlab* (available at <http://www.stat.cmu.edu/~jiashun/Research/software/GS-matlab/>).

**Keywords:** asymptotic minimaxity, graph of least favorables (GOLF), graph of strong dependence (GOSD), graphlet screening (GS), Hamming distance, phase diagram, rare and weak signal model, screen and clean, sparsity

## 1. Introduction

Consider a linear regression model

$$Y = X\beta + \sigma z, \quad X = X_{n,p}, \quad z \sim N(0, I_n). \quad (1)$$

We write

$$X = [x_1, x_2, \dots, x_p], \quad \text{and} \quad X' = [X_1, X_2, \dots, X_n], \quad (2)$$

so that  $x_j$  is the  $j$ -th design vector and  $X_i$  is the  $i$ -th sample. Motivated by the recent interest in ‘Big Data’, we assume both  $p$  and  $n$  are large but  $p \geq n$  (though this should not be taken as a restriction). The vector  $\beta$  is unknown to us, but is presumably *sparse* in the sense that only a small proportion of its entries is nonzero. Calling a nonzero entry of  $\beta$  a signal, the main interest of this paper is to identify all signals (i.e., variable selection).

Variable selection is one of the most studied problem in statistics. However, there are important regimes where our understanding is very limited.

One of such regimes is the *rare and weak* regime, where the signals are both *rare* (or sparse) and *individually weak*. Rare and weak signals are frequently found in research areas such as Genome-wide Association Study (GWAS) or next generation sequencing. Unfortunately, despite urgent demand in applications, the literature of variable selection has been focused on the regime where the signals are rare but *individually strong*. This motivates a revisit to variable selection, focusing on the rare and weak regime.

For variable selection in this regime, we need new methods and new theoretical frameworks. In particular, we need a loss function that is appropriate for rare and weak signals to evaluate the optimality. In the literature, given a variable selection procedure  $\hat{\beta}$ , we usually use the probability of exact recovery  $P(\text{sgn}(\hat{\beta}) \neq \text{sgn}(\beta))$  as the measure of loss (Fan and Li, 2001);  $\text{sgn}(\hat{\beta})$  and  $\text{sgn}(\beta)$  are the sign vectors of  $\hat{\beta}$  and  $\beta$  respectively. In the rare and weak regime, the signals are so rare and weak that exact recovery is impossible, and the Hamming distance between  $\text{sgn}(\hat{\beta})$  and  $\text{sgn}(\beta)$  is a more appropriate measure of loss.

Our focus on the rare and weak regime and the Hamming distance loss provides new perspectives to variable selection, in methods and in theory.

Throughout this paper, we assume the diagonals of the Gram matrix

$$G = X'X \quad (3)$$

are normalized to 1 (and approximately 1 in the random design model), instead of  $n$  as often used in the literature. The difference between two normalizations is non-essential, but the signal vector  $\beta$  are different by a factor of  $n^{1/2}$ .

We also assume the Gram matrix  $G$  is ‘sparse’ (aka. graph sparsity) in the sense that each of its rows has relatively few large entries. Signal sparsity and graph sparsity can be simultaneously found in the following application areas.

- *Compressive sensing.* We are interested in a very high dimensional sparse vector  $\beta$ . The goal is to store or transmit  $n$  linear functionals of  $\beta$  and then reconstruct it. For  $1 \leq i \leq n$ , we choose a  $p$ -dimensional coefficient vector  $X_i$  and observe  $Y_i = X_i' \beta + \sigma z_i$  with an error  $\sigma z_i$ . The so-called Gaussian design is often considered (Donoho, 2006a,b; Bajwa et al., 2007), where  $X_i \stackrel{iid}{\sim} N(0, \Omega/n)$  and  $\Omega$  is sparse; the sparsity of  $\Omega$  induces the sparsity of  $G = X'X$ .
- *Genetic Regulatory Network (GRN).* For  $1 \leq i \leq n$ ,  $W_i = (W_i(1), \dots, W_i(p))'$  represents the expression level of  $p$  different genes of the  $i$ -th patient. Approximately,  $W_i \stackrel{iid}{\sim} N(\alpha, \Sigma)$ , where the contrast mean vector  $\alpha$  is sparse reflecting that only few genes are differentially expressed between a normal patient and a diseased one (Peng et al., 2009). Frequently, the concentration matrix  $\Omega = \Sigma^{-1}$  is believed to be sparse, and can be effectively estimated in some cases (e.g., Bickel and Levina, 2008 and Cai et al., 2010), or can be assumed as known in others, with the so-called “data about data” available (Li and Li, 2011). Let  $\hat{\Omega}$  be a positive-definite estimate of  $\Omega$ , the setting can be re-formulated as the linear model  $(\hat{\Omega})^{1/2} Y \approx \Omega^{1/2} Y \sim N(\Omega^{1/2} \beta, I_p)$ , where  $\beta = \sqrt{n} \alpha$  and the Gram matrix  $G \approx \Omega$ , and both are sparse.

Other examples can be found in Computer Security (Ji and Jin, 2011) and Factor Analysis (Fan et al., 2011).

The sparse Gram matrix  $G$  induces a sparse graph which we call the *Graph of Strong Dependence* (GOSD), denoted by  $\mathcal{G} = (V, E)$ , where  $V = \{1, 2, \dots, p\}$  and there is an edge between nodes  $i$  and  $j$  if and only the design vectors  $x_i$  and  $x_j$  are *strongly correlated*. Let

$$S = S(\beta) = \{1 \leq j \leq p : \beta_j \neq 0\}$$

be the support of  $\beta$  and  $\mathcal{G}_S$  be the subgraph of  $\mathcal{G}$  formed by all nodes in  $S$ . The key insight is that, there is an interesting interaction between signal sparsity and graph sparsity, which yields the subgraph  $\mathcal{G}_S$  decomposable:  $\mathcal{G}_S$  splits into many “graphlet”; each “graphlet” is a small-size component and different components are not connected (in  $\mathcal{G}_S$ ).

While we can always decompose  $\mathcal{G}_S$  in this way, our emphasis in this paper is that, in many cases, the maximum size of the graphlets is small; see Lemma 1 and related discussions.

The decomposability of  $\mathcal{G}_S$  motivates a new approach to variable selection, which we call *Graphlet Screening* (GS). GS is a Screen and Clean method (Wasserman and Roeder, 2009). In the screening stage, we use multivariate screening to identify candidates for all the graphlets. Let  $\hat{S}$  be all the nodes that survived the screening, and let  $\mathcal{G}_{\hat{S}}$  be the subgraph of GOSD formed by all nodes in  $\hat{S}$ . Although  $\hat{S}$  is expected to be somewhat larger than  $S$ , the subgraph  $\mathcal{G}_{\hat{S}}$  is still likely to resemble  $\mathcal{G}_S$  in structure in the sense that it, too, splits into many small-size disconnected components. We then clean each component separately to remove false positives.

The objective of the paper is two-fold.

- To propose a “fundamentally correct” solution in the rare and weak paradigm along with a computationally fast algorithm for the solution.
- To show that GS achieves the optimal rate of convergence in terms of the Hamming distance, and achieves the optimal phase diagram for variable selection.

Phase diagram can be viewed as an optimality criterion which is especially appropriate for rare and weak signals. See Donoho and Jin (2004) and Jin (2009) for example.

In the settings we consider, most popular approaches are *not* rate optimal; we explain this in Sections 1.1-1.3. In Section 1.4, we explain the basic idea of GS and why it works.

### 1.1 Non-optimality of the $L^0$ -penalization Method for Rare and Weak Signals

When  $\sigma = 0$ , Model (1) reduces to the “noiseless” model  $Y = X\beta$ . In this model, Donoho and Stark (1989) (see also Donoho and Huo, 2001) reveals a fundamental phenomenon on sparse representation. Fix  $(X, Y)$  and consider the equation  $Y = X\beta$ . Since  $p > n$ , the equation has infinitely many solutions. However, a *very sparse solution*, if exists, is *unique* under mild conditions on the design  $X$ , with all other solutions being much denser. In fact, if the sparsest solution  $\beta_0$  has  $k$  elements, then all other solutions of the equation  $Y = X\beta$  must have at least  $(\text{rank}(X) - k + 1)$  nonzero elements, and  $\text{rank}(X) = n$  when  $X$  is in a “general position”.

From a practical viewpoint, we frequently believe that this unique sparse solution is the truth (i.e., Occam’s razor). Therefore, the problem of variable selection can be solved by some *global methods* designed for finding the sparsest solution to the equation  $Y = X\beta$ .

Since the  $L^0$ -norm is (arguably) the most natural way to measure the sparsity of a vector, the above idea suggests that the  $L^0$ -penalization method is a “fundamentally correct” (but computationally intractable) method for variable selection, provided some mild conditions on the noise, signal and design matrix, e.g., noiseless, Signal-to-Noise Ratio (SNR) is high, or signals are sufficiently sparse (Donoho and Stark, 1989; Donoho and Huo, 2001).

Motivated by this, in the past two decades, a long list of computationally tractable algorithms have been proposed that approximate the solution of the  $L^0$ -penalization method, including the lasso, SCAD, MC+, and many more (Akaike, 1974; Candes and Tao, 2007; Efron et al., 2004; Fan and Li, 2001; Schwarz, 1978; Tibshirani, 1996; Zhang, 2010, 2011; Zhao and Yu, 2006; Zou, 2006).

With that being said, we must note that these methodologies were built upon a framework with four tightly woven core components: “signals are rare but strong”, “the truth is also the sparsest solution to  $Y = X\beta$ ”, “probability of exact recovery is an appropriate loss function”, and “ $L^0$ -penalization method is a fundamentally correct approach”. Unfortunately, when signals are rare and weak, such a framework is no longer suitable.

- When signals are “rare and weak”, the fundamental uniqueness property of the sparse solution in the noiseless case is no longer valid in the noisy case. Consider the model  $Y = X\beta + \sigma z$  and suppose that a sparse  $\beta_0$  is the true signal vector. There are many vectors  $\beta$  that are small perturbations of  $\beta_0$  such that the two models  $Y = X\beta + \sigma z$  and  $Y = X\beta_0 + \sigma z$  are indistinguishable (i.e., all tests are asymptotically powerless). In the “rare and strong” regime,  $\beta_0$  is the sparsest solution among all such “eligible” solutions of  $Y = X\beta + \sigma z$ . However, this claim no longer holds in the “rare and weak” regime and the principle of Occam’s razor may not be as relevant as before.
- The  $L^0$ -penalization method is originally designed for “rare and strong” signals where “exact recovery” is used to measure its performance (Donoho and Stark, 1989; Donoho and Huo, 2001; Donoho, 2006a). When we must consider “rare and weak” signals and

when we use the Hamming distance as the loss function, it is unclear whether the  $L^0$ -penalization method is still “fundamentally correct”.

In fact, in Section 2.8 (see also Ji and Jin, 2011), we show that the  $L^0$ -penalization method is not optimal in Hamming distance when signals are rare and weak, even with very simple designs (i.e., Gram matrix is tridiagonal or block-wise) and even when the tuning parameter is ideally set. Since the  $L^0$ -penalization method is used as the benchmark in the development of many other penalization methods, its sub-optimality is expected to imply the sub-optimality of other methods designed to match its performance (e.g., lasso, SCAD, MC+).

## 1.2 Limitation of Univariate Screening and UPS

Univariate Screening (also called marginal regression or Sure Screening in Fan and Lv, 2008; Genovese et al., 2012) is a well-known variable selection method. For  $1 \leq j \leq p$ , recall that  $x_j$  is the  $j$ -th column of  $X$ . Univariate Screening selects variables with large marginal correlations:  $|(x_j, Y)|$ , where  $(\cdot, \cdot)$  denotes the inner product. The method is computationally fast, but it can be seriously corrupted by the so-called phenomenon of “signal cancellation” (Wasserman and Roeder, 2009). In our model (1)-(3), the SNR associated with  $(x_j, Y)$  is

$$\frac{1}{\sigma} \sum_{\ell=1}^p (x_j, x_\ell) \beta_\ell = \frac{\beta_j}{\sigma} + \frac{1}{\sigma} \sum_{\ell \neq j} (x_j, x_\ell) \beta_\ell.$$

“Signal cancellation” happens if SNR is significantly smaller than  $\beta_j/\sigma$ . For this reason, the success of Univariate Screening needs relatively strong conditions (e.g., Faithfulness Condition Genovese et al., 2012), under which signal cancellation does not have a major effect.

In Ji and Jin (2011), Ji and Jin proposed *Univariate Penalized Screening (UPS)* as a refinement of Univariate Screening, where it was showed to be optimal in the rare and weak paradigm, for the following two scenarios. The first scenario is where the nonzero effects of variables are all positively correlated:  $(x_j \beta_j)'(x_k \beta_k) \geq 0$  for all  $\{j, k\}$ . This guarantees the faithfulness of the univariate association test. The second scenario is a Bernoulli model where the “signal cancellation” only has negligible effects over the Hamming distance of UPS.

With that being said, UPS attributes its success mostly to the cleaning stage; the screening stage of UPS uses nothing but Univariate Screening, so UPS does not adequately address the challenge of “signal cancellation”. For this reason, we should not expect UPS to be optimal in much more general settings.

## 1.3 Limitations of Brute-force Multivariate Screening

One may attempt to overcome “signal cancellation” by multivariate screening, with Brute-force Multivariate Screening (BMS) being the most straightforward version. Fix an integer  $1 \leq m_0 \ll p$ . BMS consists of a series of screening phases, indexed by  $m$ ,  $1 \leq m \leq m_0$ , that are increasingly more ambitious. In Phase- $m$  BMS, we test the significance of the association between  $Y$  and any set of  $m$  different design variables  $\{x_{j_1}, x_{j_2}, \dots, x_{j_m}\}$ ,  $j_1 < j_2 < \dots < j_m$ ,

and retain all such design variables if the test is significant. The problem of BMS is, it enrolls too many candidates for screening, which is both unnecessary and unwise.

- (*Screening inefficiency*). In Phase- $m$  of BMS, we test about  $\binom{p}{m}$  hypotheses involving different subsets of  $m$  design variables. The larger the number of hypotheses we consider, the higher the threshold we need to set for the tests, in order to control the false positives. When we enroll too many candidates for hypothesis testing, we need signals that are stronger than necessary in order for them to survive the screening.
- (*Computational challenge*). Testing  $\binom{p}{m}$  hypotheses is computationally infeasible when  $p$  is large, even when  $m$  is very small, e.g.,  $(p, m) = (10^4, 3)$ .

#### 1.4 Graphlet Screening: How It Is Different and How It Works

Graphlet Screening (GS) uses a similar screening strategy as BMS does, except for a major difference. When it comes to the test of significance between  $Y$  and design variables  $\{x_{j_1}, x_{j_2}, \dots, x_{j_m}\}$ ,  $j_1 < j_2 < \dots < j_m$ , GS only carries out such a test if  $\{j_1, j_2, \dots, j_m\}$  is a connected subgraph of the GOSD. Otherwise, the test is safely skipped!

Fixing an appropriate threshold  $\delta > 0$ , we let  $\Omega^{*,\delta}$  be the regularized Gram matrix:

$$\Omega^{*,\delta}(i, j) = G(i, j)1\{|G(i, j)| \geq \delta\}, \quad 1 \leq i, j \leq p. \quad (4)$$

The GOSD  $\mathcal{G} \equiv \mathcal{G}^{*,\delta} = (V, E)$  is the graph where  $V = \{1, 2, \dots, p\}$  and there is an edge between nodes  $i$  and  $j$  if and only if  $\Omega^{*,\delta}(i, j) \neq 0$ . See Section 2.6 for the choice of  $\delta$ .

**Remark.** GOSD and  $\mathcal{G}$  are generic terms which vary from case to case, depending on  $G$  and  $\delta$ . GOSD is very different from the Bayesian conditional independence graphs (Pearl, 2000).

Fixing  $m_0 \geq 1$  as in BMS, we define

$$\mathcal{A}(m_0) = \mathcal{A}(m_0; G, \delta) = \{\text{all connected subgraphs of } \mathcal{G}^{*,\delta} \text{ with size } \leq m_0\}.$$

GS is a Screen and Clean method, consisting of a graphical screening step (GS-step) and a graphical cleaning step (GC-step).

- *GS-step*. We test the significance of association between  $Y$  and  $\{x_{j_1}, x_{j_2}, \dots, x_{j_m}\}$  if and only if  $\{j_1, j_2, \dots, j_m\} \in \mathcal{A}(m_0)$  (i.e., graph guided multivariate screening). Once  $\{j_1, \dots, j_m\}$  is retained, it remains there until the end of the GS-step.
- *GC-step*. The set of surviving nodes decompose into many small-size components, which we fit separately using an efficient low-dimensional test for small graphs.

GS is similar to Wasserman and Roeder (2009) for both of them have a screening and a cleaning stage, but is more sophisticated. For clarification, note that Univariate Screening or BMS introduced earlier does not contain a cleaning stage and can be viewed as a counterpart of the GS-step.

We briefly explain why GS works. We discuss the GS-step and GC-step separately.

Consider the GS-step first. Compared with BMS, the GS-step recruits far fewer candidates for screening, so it is able to overcome the two major shortcomings of BMS aforementioned: high computational cost and low statistical efficiency. In fact, fix  $K \geq 1$  and

suppose  $\mathcal{G}^{*,\delta}$  is  $K$ -sparse (see Section 1.5 for the definition). By a well-known result in graph theory (Frieze and Molloy, 1999),

$$|\mathcal{A}(m_0)| \leq Cm_0p(eK)^{m_0}. \tag{5}$$

The right hand side is much smaller than the term  $\binom{p}{m_0}$  as we encounter in BMS.

At the same time, recall that  $S = S(\beta)$  is the support of  $\beta$ . Let  $\mathcal{G}_S \equiv \mathcal{G}_S^{*,\delta}$  be the subgraph of  $\mathcal{G}^{*,\delta}$  consisting all signal nodes. We can always split  $\mathcal{G}_S^{*,\delta}$  into ‘‘graphlets’’ (arranged lexicographically) as follows:

$$\mathcal{G}_S^{*,\delta} = \mathcal{G}_{S,1}^{*,\delta} \cup \mathcal{G}_{S,2}^{*,\delta} \dots \cup \mathcal{G}_{S,M}^{*,\delta}, \tag{6}$$

where each  $\mathcal{G}_{S,i}^{*,\delta}$  is a component (i.e., a maximal connected subgraph) of  $\mathcal{G}_S^{*,\delta}$ , and different  $\mathcal{G}_{S,i}^{*,\delta}$  are not connected in  $\mathcal{G}_S^{*,\delta}$ . Let

$$m_0^* = m_0^*(S(\beta), G, \delta) = \max_{1 \leq i \leq M} |\mathcal{G}_{S,i}^{*,\delta}|$$

be the maximum size of such graphlets. Note that  $M$  also depends on  $S(\beta)$ ,  $G$  and  $\delta$ .

In many cases,  $m_0^*$  is small. One such case is when we have a Bernoulli signal model.

**Lemma 1** *Fix  $K \geq 1$  and  $\epsilon > 0$ . If  $\mathcal{G}^{*,\delta}$  is  $K$ -sparse and  $\text{sgn}(|\beta_1|), \text{sgn}(|\beta_2|), \dots, \text{sgn}(|\beta_p|)$  are iid from Bernoulli( $\epsilon$ ), then except for a probability  $p(\epsilon K)^{m_0^*+1}$ ,  $m_0^*(S(\beta), G, \delta) \leq m_0$ .*

Lemma 1 is not tied to the Bernoulli model and holds more generally. For example, it holds when  $\{\text{sgn}(|\beta_i|)\}_{i=1}^p$  are generated according to certain Ising models (Ising, 1925).

We recognize that in order for the GS-step to be efficient both in screening and in computation, it is sufficient that

$$m_0 \geq m_0^*. \tag{7}$$

In fact, first, if (7) holds, then for each  $1 \leq \ell \leq M$ ,  $\mathcal{G}_{S,\ell}^{*,\delta} \in \mathcal{A}(m_0)$ . Therefore, at some point of the screening process of the GS-step, we must have considered a significance test between  $Y$  and the set of design variables  $\{x_j : j \in \mathcal{G}_{S,\ell}^{*,\delta}\}$ . Consequently, the GS-step is able to overcome the ‘‘signal cancellations’’ (the explanation is a little bit long, and we slightly defer it). Second, since  $m_0^*$  is small in many situations, we could choose a relatively small  $m_0$  such that (7) holds. When  $m_0$  is small, as long as  $K$  is small or moderately large, the GS-step is computationally feasible. In fact, the right hand side of (5) is only larger than  $p$  by a moderate factor. See Section 2.2 for more discussion on the computation complexity.

We now explain the first point above. The notations below are frequently used.

**Definition 2** *For  $X$  in Models (1)-(2) and any subset  $\mathcal{I} \subset \{1, 2, \dots, p\}$ , let  $P^{\mathcal{I}} = P^{\mathcal{I}}(X)$  be the projection from  $\mathbb{R}^n$  to the subspace spanned by  $\{x_j : j \in \mathcal{I}\}$ .*

**Definition 3** *For an  $n \times p$  matrix  $A$  and sets  $\mathcal{I} \subset \{1, \dots, n\}$  and  $\mathcal{J} \subset \{1, \dots, p\}$ ,  $A^{\mathcal{I},\mathcal{J}}$  is the  $|\mathcal{I}| \times |\mathcal{J}|$  sub-matrix formed by restricting the rows of  $A$  to  $\mathcal{I}$  and columns to  $\mathcal{J}$ .*

When  $p = 1$ ,  $A$  is a vector, and  $A^{\mathcal{I}}$  is the sub-vector of  $A$  formed by restricting the rows of  $A$  to  $\mathcal{I}$ . When  $\mathcal{I} = \{1, 2, \dots, n\}$  (or  $\mathcal{J} = \{1, 2, \dots, p\}$ ), we write  $A^{\mathcal{I}, \mathcal{J}}$  as  $A^{\otimes, \mathcal{J}}$  (or  $A^{\mathcal{I}, \otimes}$ ). Note that indices in  $\mathcal{I}$  or  $\mathcal{J}$  are not necessarily sorted ascendingly.

Recall that for each  $1 \leq \ell \leq M$ , at some point of the GS-step, we must have considered a significance test between  $Y$  and the set of design variables  $\{x_j : j \in \mathcal{G}_{S, \ell}^{*, \delta}\}$ . By (6), we rewrite Model (1) as

$$Y = \sum_{\ell=1}^M X^{\otimes, \mathcal{G}_{S, \ell}^{*, \delta}} \beta^{\mathcal{G}_{S, \ell}^{*, \delta}} + \sigma z, \quad z \sim N(0, I_n).$$

The key is the set of matrices  $\{X^{\otimes, \mathcal{G}_{S, \ell}^{*, \delta}} : 1 \leq \ell \leq M\}$  are nearly orthogonal (i.e., for any column  $\xi$  of  $X^{\otimes, \mathcal{G}_{S, k}^{*, \delta}}$  and any column  $\eta$  of  $X^{\otimes, \mathcal{G}_{S, \ell}^{*, \delta}}$ ,  $|(\xi, \eta)|$  is small when  $k \neq \ell$ ).

When we test the significance between  $Y$  and  $\{x_j, j \in \mathcal{G}_{S, \ell}^{*, \delta}\}$ , we are testing the null hypothesis  $\beta^{\mathcal{G}_{S, \ell}^{*, \delta}} = 0$  against the alternative  $\beta^{\mathcal{G}_{S, \ell}^{*, \delta}} \neq 0$ . By the near orthogonality aforementioned, approximately,  $(X^{\otimes, \mathcal{G}_{S, \ell}^{*, \delta}})'Y$  is a sufficient statistic for  $\beta^{\mathcal{G}_{S, \ell}^{*, \delta}}$ , and the optimal test is based on the  $\chi^2$ -test statistic  $\|P^{\mathcal{G}_{S, \ell}^{*, \delta}}Y\|^2$ .

The near orthogonality also implies that significant ‘‘signal cancellation’’ only happens among signals within the same graphlet. When we screen each graphlet *as a whole* using the  $\chi^2$ -statistic above, ‘‘signal cancellation’’ between different graphlets only has negligible effects. In this way, GS-step is able to retain all nodes in  $\mathcal{G}_{S, \ell}^{*, \delta}$  in a nearly optimal way, and so overcome the challenge of ‘‘signal cancellation’’. This explains the first point.

Note that the GS-step consists of a sequence of sub-steps, each sub-step is associated with an element of  $\mathcal{A}(m_0)$ . When we screen  $\mathcal{G}_{S, \ell}^{*, \delta}$  as a whole, it is possible some of the nodes have already been retained in the previous sub-steps. In this case, we implement the  $\chi^2$ -test slightly differently, but the insight is similar. See Section 2.1 for details.

We now discuss the GC-step. Let  $\hat{S}$  be all the surviving nodes of the GS-step, and let  $\mathcal{G}_{\hat{S}}^{*, \delta}$  be the subgraph of  $\mathcal{G}^{*, \delta}$  formed by confining all nodes to  $\hat{S}$ . Similarly, we have (a) the decomposition  $\mathcal{G}_{\hat{S}}^{*, \delta} = \mathcal{G}_{\hat{S}, 1}^{*, \delta} \cup \mathcal{G}_{\hat{S}, 2}^{*, \delta} \dots \cup \mathcal{G}_{\hat{S}, \hat{M}}^{*, \delta}$ , (b) the near orthogonality between the  $\hat{M}$  different matrices, each is formed by  $\{x_j : j \in \mathcal{G}_{\hat{S}, \ell}^{*, \delta}\}$ . Moreover, a carefully tuned screening stage of the GS ensures that most of the components  $\mathcal{G}_{\hat{S}, \ell}^{*, \delta}$  are only small perturbations of their counterparts in the decomposition of  $\mathcal{G}_S^{*, \delta} = \mathcal{G}_{S, 1}^{*, \delta} \cup \mathcal{G}_{S, 2}^{*, \delta} \dots \cup \mathcal{G}_{S, M}^{*, \delta}$  as in (6), and the maximum size of  $\mathcal{G}_{\hat{S}, \ell}^{*, \delta}$  is not too much larger than  $m_0^* = m_0^*(S(\beta), G, \delta)$ . Together, these allow us to clean  $\mathcal{G}_{\hat{S}, \ell}^{*, \delta}$  separately, without much loss of efficiency. Since the maximum size of  $\mathcal{G}_{\hat{S}, \ell}^{*, \delta}$  is small, the computational complexity in the cleaning stage is moderate.

### 1.5 Content

The remaining part of the paper is organized as follows. In Section 2, we show that GS achieves the minimax Hamming distance in the Asymptotic Rare and Weak (ARW) model, and use the phase diagram to visualize the optimality of GS, and to illustrate the advantage of GS over the  $L^0/L^1$ -penalization methods. In Section 3, we explain that GS attributes

its optimality to the so-called *Sure Screening* property and the *Separable After Screening* property, and use these two properties to prove our main result, Theorem 8. Section 4 contains numeric results, Section 5 discusses more connections to existing literature and possible extensions of GS, and Section 6 contains technical proofs.

Below are some notations we use in this paper.  $L_p$  denotes a generic multi- $\log(p)$  term that may vary from occurrence to occurrence; see Definition 5. For a vector  $\beta \in R^p$ ,  $\|\beta\|_q$  denotes the  $L^q$ -norm, and when  $q = 2$ , we drop  $q$  for simplicity. For two vectors  $\alpha$  and  $\beta$  in  $R^p$ ,  $\alpha \circ \beta \in R^p$  denotes the vector in  $R^p$  that satisfies  $(\alpha \circ \beta)_i = \alpha_i \beta_i$ ,  $1 \leq i \leq p$ ; “ $\circ$ ” is known as the Hadamard product.

For an  $n \times p$  matrix  $A$ ,  $\|A\|_\infty$  denotes the matrix  $L^\infty$ -norm, and  $\|A\|$  denotes the spectral norm (Horn and Johnson, 1990). Recall that for two sets  $\mathcal{I}$  and  $\mathcal{J}$  such that  $\mathcal{I} \subset \{1, 2, \dots, n\}$  and  $\mathcal{J} \subset \{1, 2, \dots, p\}$ ,  $A^{\mathcal{I}, \mathcal{J}}$  denotes the submatrix of  $A$  formed by restricting the rows and columns of  $A$  to  $\mathcal{I}$  and  $\mathcal{J}$ , respectively. Note that the indices in  $\mathcal{I}$  and  $\mathcal{J}$  are not necessarily sorted in the ascending order. In the special case where  $\mathcal{I} = \{1, 2, \dots, n\}$  (or  $\mathcal{J} = \{1, 2, \dots, p\}$ ), we write  $A^{\mathcal{I}, \mathcal{J}}$  as  $A^{\otimes, \mathcal{J}}$  (or  $A^{\mathcal{I}, \otimes}$ ). In the special case where  $n = p$  and  $A$  is positive definite,  $\lambda_k^*(A)$  denotes the minimum eigenvalue of all the size  $k$  principal submatrices of  $A$ ,  $1 \leq k \leq p$ . For  $X$  in (1),  $P^{\mathcal{I}}$  denotes the projection to the column space of  $X^{\otimes, \mathcal{I}}$ .

Recall that in Model (1),  $Y = X\beta + \sigma z$ . Fixing a threshold  $\delta > 0$ . Let  $G = X'X$  be the Gram matrix, and let  $\Omega^{*, \delta}$  be the regularized Gram matrix defined by  $\Omega^{*, \delta}(i, j) = G(i, j)1\{|G(i, j)| \geq \delta\}$ ,  $1 \leq i, j \leq p$ . Let  $\mathcal{G}^{*, \delta}$  be the graph where each index in  $\{1, 2, \dots, p\}$  is a node, and there is an edge between node  $i$  and node  $j$  if and only if  $\Omega^{*, \delta}(i, j) \neq 0$ . We let  $S(\beta)$  be the support of  $\beta$ , and denote  $\mathcal{G}_S^{*, \delta}$  by the subgraph of  $\mathcal{G}^{*, \delta}$  formed by all nodes in  $S(\beta)$ . We call  $\mathcal{G}^{*, \delta}$  the Graph of Strong Dependence (GOSD) and sometimes write it by  $\mathcal{G}$  for short. The GOSD and  $\mathcal{G}$  are generic notations which depend on  $(G, \delta)$  and may vary from occurrence to occurrence. We also denote  $\mathcal{G}^\diamond$  by the Graph of Least Favorable (GOLF). GOLF only involves the study of the information lower bound. For an integer  $K \geq 1$ , a graph  $\mathcal{G}$ , and one of its subgraph  $\mathcal{I}_0$ , we write  $\mathcal{I}_0 \triangleleft \mathcal{G}$  if and only if  $\mathcal{I}_0$  is a component of  $\mathcal{G}$  (i.e., a maximal connected subgraph of  $\mathcal{G}$ ), and we call  $\mathcal{G}$   $K$ -sparse if its maximum degree is no greater than  $K$ .

## 2. Main Results

In Section 2.1, we formally introduce GS. In Section 2.2, we discuss the computational complexity of GS. In Sections 2.3-2.6, we show that GS achieves the optimal rate of convergence in the Asymptotic Rare and Weak model. In Sections 2.7-2.8, we introduce the notion of phase diagram and use it to compare GS with the  $L^0/L^1$ -penalization methods. We conclude the section with a summary in Section 2.9.

### 2.1 Graphlet Screening: The Procedure

GS consists of a GS-step and a GC-step. We describe two steps separately. Consider the GS-step first. Fix  $m_0 \geq 1$  and  $\delta > 0$ , recall that  $\mathcal{G}^{*, \delta}$  denotes the GOSD and  $\mathcal{A}(m_0)$  consists of all connected subgraphs of  $\mathcal{G}^{*, \delta}$  with size  $\leq m_0$ .

- *Initial sub-step.* Let  $\mathcal{U}_p^* = \emptyset$ . List all elements in  $\mathcal{A}(m_0)$  in the ascending order of the number of nodes it contains, with ties broken lexicographically. Since a node is thought of as connected to itself, the first  $p$  connected subgraphs on the list are simply the nodes  $1, 2, \dots, p$ . We screen all connected subgraphs in the order they are listed.
- *Updating sub-step.* Let  $\mathcal{I}_0$  be the connected subgraph under consideration, and let  $\mathcal{U}_p^*$  be the current set of retained indices. We update  $\mathcal{U}_p^*$  with a  $\chi^2$  test as follows. Let  $\hat{F} = \mathcal{I}_0 \cap \mathcal{U}_p^*$  and  $\hat{D} = \mathcal{I}_0 \setminus \mathcal{U}_p^*$ , so that  $\hat{F}$  is the set of nodes in  $\mathcal{I}_0$  that have already been accepted, and  $\hat{D}$  is the set of nodes in  $\mathcal{I}_0$  that is currently under investigation. Note that no action is needed if  $\hat{D} = \emptyset$ . For a threshold  $t(\hat{D}, \hat{F}) > 0$  to be determined, we update  $\mathcal{U}_p^*$  by adding all nodes in  $\hat{D}$  to it if

$$T(Y, \hat{D}, \hat{F}) = \|P^{\mathcal{I}_0} Y\|^2 - \|P^{\hat{F}} Y\|^2 > t(\hat{D}, \hat{F}), \quad (8)$$

and we keep  $\mathcal{U}_p^*$  the same otherwise (by default,  $\|P^{\hat{F}} Y\| = 0$  if  $\hat{F} = \emptyset$ ). We continue this process until we finish screening all connected subgraphs on the list. The final set of retained indices is denoted by  $\mathcal{U}_p^*$ .

See Table 1 for a recap of the procedure. In the *GS*-step, once a node is kept in any sub-stage of the screening process, it remains there until the end of the *GS*-step (however, it may be killed in the *GC*-step). This has a similar flavor to that of the Forward regression.

In principle, the procedure depends on how the connected subgraphs of the same size are initially ordered, and different ordering could give different numeric results. However, such differences are usually negligibly small. Alternatively, one could revise the procedure so that it does not depend on the ordering. For example, in the updating sub-step, we could choose to update  $\mathcal{U}_p^*$  only when we finish screening all connected sub-graphs of size  $k$ ,  $1 \leq k \leq m_0$ . While the theoretic results below continue to hold if we revise GS in this way, we must note that from a numeric perspective, the revision would not produce a very different result. For reasons of space, we skip discussions along this line.

The GS-step uses a set of tuning parameters:

$$\mathcal{Q} \equiv \{t(\hat{D}, \hat{F}) : (\hat{D}, \hat{F}) \text{ are as defined in (8)}\}.$$

A convenient way to set these parameters is to let  $t(\hat{D}, \hat{F}) = 2\sigma^2 q \log p$  for a fixed  $q > 0$  and all  $(\hat{D}, \hat{F})$ . More sophisticated choices are given in Section 2.6.

The *GS*-step has two important properties: *Sure Screening* and *Separable After Screening (SAS)*. With tuning parameters  $\mathcal{Q}$  properly set, the Sure Screening property says that  $\mathcal{U}_p^*$  retains all but a negligible fraction of the signals. The SAS property says that as a subgraph of  $\mathcal{G}^{*,\delta}$ ,  $\mathcal{U}_p^*$  decomposes into many disconnected components, each has a size  $\leq \ell_0$  for a fixed small integer  $\ell_0$ . Together, these two properties enable us to reduce the original large-scale regression problem to many small-size regression problems that can be solved parallelly in the *GC*-step. See Section 3 for elaboration on these ideas.

We now discuss the *GC*-step. For any  $1 \leq j \leq p$ , we have either  $j \notin \mathcal{U}_p^*$ , or that there is a unique connected subgraph  $\mathcal{I}_0$  such that  $j \in \mathcal{I}_0 \triangleleft \mathcal{U}_p^*$ . In the first case, we estimate  $\beta_j$  as 0. In the second case, for two tuning parameters  $u^{gs} > 0$  and  $v^{gs} > 0$ , we estimate the whole set of variables  $\beta^{\mathcal{I}_0}$  by minimizing the functional

$$\|P^{\mathcal{I}_0} (Y - X^{\otimes, \mathcal{I}_0} \xi)\|^2 + (u^{gs})^2 \|\xi\|_0 \quad (9)$$

<i>GS</i> -step:	List $\mathcal{G}^{*,\delta}$ -connected submodels $\mathcal{I}_{0,k}$ with $ \mathcal{I}_{0,1}  \leq  \mathcal{I}_{0,2}  \leq \dots \leq m_0$ Initialization: $\mathcal{U}_p^* = \emptyset$ and $k = 1$ Test $H_0 : \mathcal{I}_{0,k} \cap \mathcal{U}_p^*$ against $H_1 : \mathcal{I}_{0,k}$ with $\chi^2$ test (8) Update: $\mathcal{U}_p^* \leftarrow \mathcal{U}_p^* \cup \mathcal{I}_{0,k}$ if $H_0$ rejected, $k \leftarrow k + 1$
<i>GC</i> -step:	As a subgraph of $\mathcal{G}^{*,\delta}$ , $\mathcal{U}_p^*$ decomposes into many components $\bar{\mathcal{I}}_0$ Use the $L^0$ -penalized test (9) to select a subset $\hat{\mathcal{I}}_0$ of each $\bar{\mathcal{I}}_0$ Return the union of $\hat{\mathcal{I}}_0$ as the selected model

Table 1: Graphlet Screening Algorithm.

over all  $|\mathcal{I}_0| \times 1$  vectors  $\xi$ , each nonzero coordinate of which  $\geq v^{gs}$  in magnitude. The resultant estimator is the final estimate of GS, and we use  $\hat{\beta}^{gs} = \hat{\beta}^{gs}(Y; \delta, \mathcal{Q}, u^{gs}, v^{gs}, X, p, n)$  to denote it. See Section 1.5 for notations used in this paragraph.

Sometimes for linear models with random designs, the Gram matrix  $G$  is very noisy, and GS is more effective if we use it iteratively for a few times ( $\leq 5$ ). This can be implemented in a similar way as that in Ji and Jin (2011, Section 3). Here, the main purpose of iteration is to denoise  $G$ , not for variable selection. See Ji and Jin (2011, Section 3) and Section 4 for more discussion.

## 2.2 Computational Complexity

If we exclude the overhead of obtaining  $\mathcal{G}^{*,\delta}$ , then the computation cost of GS contains two parts, that of the GS-step and that of the GC-step. In each part, the computation cost hinges on the sparsity of  $\mathcal{G}^{*,\delta}$ . In Section 2.3, we show that with a properly chosen  $\delta$ , for a wide class of design matrices,  $\mathcal{G}^{*,\delta}$  is  $K$ -sparse for some  $K = K_p \leq C \log^\alpha(p)$  as  $p \rightarrow \infty$ , where  $\alpha > 0$  is a constant. As a result (Frieze and Molloy, 1999),

$$|\mathcal{A}(m_0)| \leq pm_0(eK_p)^{m_0} \leq Cm_0p \log^{m_0\alpha}(p). \tag{10}$$

We now discuss two parts separately.

In the GS-step, the computation cost comes from that of listing all elements in  $\mathcal{A}(m_0)$ , and that of screening all connected-subgraphs in  $\mathcal{A}(m_0)$ . Fix  $1 \leq k \leq m_0$ . By (10) and the fact that every size  $k$  ( $k > 1$ ) connected subgraph at least contains one size  $k - 1$  connected subgraph, greedy algorithm can be used to list all sub-graphs with size  $k$  with computational complexity  $\leq Cp(K_pk)^k \leq Cp \log^{k\alpha}(p)$ , and screening all connected subgraphs of size  $k$  has computational complexity  $\leq Cnp \log^{k\alpha}(p)$ . Therefore, the computational complexity of the GS-step  $\leq Cnp(\log(p))^{(m_0+1)\alpha}$ .

The computation cost of the GC-step contains the part of breaking  $\mathcal{U}_p^*$  into disconnected components, and that of cleaning each component by minimizing (9). As a well-known application of the breadth-first search (Hopcroft and Tarjan, 1973), the first part  $\leq |\mathcal{U}_p^*|(K_p + 1)$ . For the second part, by the SAS property of the GS-step (i.e., Lemma 16), for a broad class of design matrices, with the tuning parameters chosen properly, there is a *fixed* integer  $\ell_0$  such that with overwhelming probability,  $|\mathcal{I}_0| \leq \ell_0$  for any  $\mathcal{I}_0 \triangleleft \mathcal{U}_p^*$ . As a result, the

total computational cost of the  $GC$ -step is no greater than  $C(2^{\ell_0} \log^\alpha(p))|\mathcal{U}_p^*|n$ , which is moderate.

The computational complexity of GS is only moderately larger than that of Univariate Screening or UPS (Ji and Jin, 2011). UPS uses univariate thresholding for screening which has a computational complexity of  $O(np)$ , and GS implements multivariate screening for all connected subgraphs in  $\mathcal{A}(m_0)$ , which has a computational complexity  $\leq Cnp(\log(p))^{(m_0+1)\alpha}$ . The latter is only larger by a multi-log( $p$ ) term.

### 2.3 Asymptotic Rare and Weak Model and Random Design Model

To analyze GS, we consider the regression model  $Y = X\beta + \sigma z$  as in (1), and use an Asymptotic Rare and Weak (ARW) model for  $\beta$  and a random design model for  $X$ .

We introduce the ARW first. Fix parameters  $\epsilon \in (0, 1)$ ,  $\tau > 0$ , and  $a \geq 1$ . Let  $b = (b_1, \dots, b_p)'$  be the  $p \times 1$  random vector where

$$b_i \stackrel{iid}{\sim} \text{Bernoulli}(\epsilon). \tag{11}$$

We model the signal vector  $\beta$  in Model (1) by

$$\beta = b \circ \mu, \tag{12}$$

where “ $\circ$ ” denotes the Hadamard product (see Section 1.5) and  $\mu \in \Theta_p^*(\tau, a)$ , with

$$\Theta_p^*(\tau, a) = \{\mu \in \Theta_p(\tau), \|\mu\|_\infty \leq a\tau\}, \quad \Theta_p(\tau) = \{\mu \in \mathbb{R}^p : |\mu_i| \geq \tau, 1 \leq i \leq p\}. \tag{13}$$

In this model,  $\epsilon$  calibrates the sparsity level and  $\tau$  calibrates the minimum signal strength. We are primarily interested in the case where  $\epsilon$  is small and  $\tau$  is smaller than the required signal strength for the exact recovery of the support of  $\beta$ , so the signals are both rare and weak. The constraint of  $\|\mu\|_\infty \leq a\tau_p$  is mainly for technical reasons (only needed for Lemma 16); see Section 2.6 for more discussions.

We let  $p$  be the driving asymptotic parameter, and tie  $(\epsilon, \tau)$  to  $p$  through some fixed parameters. In detail, fixing  $0 < \vartheta < 1$ , we model

$$\epsilon = \epsilon_p = p^{-\vartheta}. \tag{14}$$

For any fixed  $\vartheta$ , the signals become increasingly sparser as  $p \rightarrow \infty$ . Also, as  $\vartheta$  ranges, the sparsity level ranges from very dense to very sparse, and covers all interesting cases.

It turns out that the most interesting range for  $\tau$  is  $\tau = \tau_p = O(\sqrt{\log(p)})$ . In fact, when  $\tau_p \ll \sigma\sqrt{\log(p)}$ , the signals are simply too rare and weak so that successful variable selection is impossible. On the other hand, exact support recovery requires  $\tau \gtrsim \sigma\sqrt{2\log p}$  for orthogonal designs and possibly even larger  $\tau$  for correlated designs. In light of this, we fix  $r > 0$  and calibrate  $\tau$  by

$$\tau = \tau_p = \sigma\sqrt{2r\log(p)}. \tag{15}$$

Next, consider the random design model. The use of random design model is mainly for simplicity in presentation. The main results in the paper can be translated to fixed design models with a careful modification of the notations; see Corollary 7 and Section 5.

For any positive definite matrix  $A$ , let  $\lambda(A)$  be the smallest eigenvalue, and let

$$\lambda_k^*(\Omega) = \min\{\lambda(A) : A \text{ is a } k \times k \text{ principle submatrix of } \Omega\}. \quad (16)$$

For  $m_0$  as in the GS-step, let  $g = g(m_0, \vartheta, r)$  be the smallest integer such that

$$g \geq \max\{m_0, (\vartheta + r)^2 / (2\vartheta r)\}. \quad (17)$$

Fixing a constant  $c_0 > 0$ , introduce

$$\mathcal{M}_p(c_0, g) = \{\Omega : p \times p \text{ correlation matrix, } \lambda_g^*(\Omega) \geq c_0\}. \quad (18)$$

Recall  $X_i$  is the  $i$ -th row of  $X$ ; see (2). In the random design model, we fix an  $\Omega \in \mathcal{M}(c_0, g)$  ( $\Omega$  is unknown to us), and assume

$$X_i \stackrel{iid}{\sim} N(0, \frac{1}{n}), \quad 1 \leq i \leq n. \quad (19)$$

In the literature, this is called the Gaussian design, which can be found in Compressive Sensing (Bajwa et al., 2007), Computer Security (Dinur and Nissim, 2003), and other application areas.

At the same time, fixing  $\kappa \in (0, 1)$ , we model the sample size  $n$  by

$$n = n_p = p^\kappa. \quad (20)$$

As  $p \rightarrow \infty$ ,  $n_p$  becomes increasingly large but is still much smaller than  $p$ . We assume

$$\kappa > (1 - \vartheta), \quad (21)$$

so that  $n_p \gg p\epsilon_p$ . Note  $p\epsilon_p$  is approximately the total number of signals. Condition (21) is almost necessary for successful variable selection (Donoho, 2006a,b).

**Definition 4** We call model (11)-(15) for  $\beta$  the *Asymptotic Rare Weak model* ARW( $\vartheta, r, a, \mu$ ), and call model (19)-(21) for  $X$  the *Random Design model* RD( $\vartheta, \kappa, \Omega$ ).

## 2.4 Minimax Hamming Distance

In many works on variables selection, one assesses the optimality by the ‘oracle property’, where the probability of non-exact recovery  $P(\text{sgn}(\hat{\beta}) \neq \text{sgn}(\beta))$  is the loss function. When signals are rare and weak,  $P(\text{sgn}(\hat{\beta}) \neq \text{sgn}(\beta)) \approx 1$  and ‘exact recovery’ is usually impossible. A more appropriate loss function is the Hamming distance between  $\text{sgn}(\hat{\beta})$  and  $\text{sgn}(\beta)$ .

For any fixed  $\beta$  and any variable selection procedure  $\hat{\beta}$ , we measure the performance by the Hamming distance:

$$h_p(\hat{\beta}, \beta | X) = E \left[ \sum_{j=1}^p 1\{\text{sgn}(\hat{\beta}_j) \neq \text{sgn}(\beta_j)\} | X \right].$$

In the Asymptotic Rare Weak model,  $\beta = b \circ \mu$ , and  $(\epsilon_p, \tau_p)$  depend on  $p$  through  $(\vartheta, r)$ , so the overall Hamming distance for  $\hat{\beta}$  is

$$H_p(\hat{\beta}; \epsilon_p, n_p, \mu, \Omega) = E_{\epsilon_p} E_{\Omega} [h_p(\hat{\beta}, \beta | X)] \equiv E_{\epsilon_p} E_{\Omega} [h_p(\hat{\beta}, b \circ \mu | X)],$$

where  $E_{\epsilon_p}$  is the expectation with respect to the law of  $b$ , and  $E_{\Omega}$  is the expectation with respect to the law of  $X$ ; see (11) and (19). Finally, the minimax Hamming distance is

$$\text{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) = \inf_{\hat{\beta}} \sup_{\mu \in \Theta_p^*(\tau_p, a)} \{H_p(\hat{\beta}; \epsilon_p, n_p, \mu, \Omega)\}.$$

The Hamming distance is no smaller than the sum of the expected number of signal components that are misclassified as noise and the expected number of noise components that are misclassified as signal.

### 2.5 Lower Bound for the Minimax Hamming Distance, and GOLF

We first construct lower bounds for “local risk” at different  $j$ ,  $1 \leq j \leq p$ , and then aggregate them to construct a lower bound for the global risk. One challenge we face is the least favorable configurations for different  $j$  overlap with each other. We resolve this by exploiting the sparsity of a new graph to be introduced: Graph of Least Favorable (GOLF).

To recap, the model we consider is Model (1), where

$$\beta \text{ is modeled by } \text{ARW}(\vartheta, r, a, \mu), \quad \text{and} \quad X \text{ is modeled by } \text{RD}(\vartheta, \kappa, \Omega).$$

Fix  $1 \leq j \leq p$ . The “local risk” at an index  $j$  is the risk of estimating the set of variables  $\{\beta_k : d(k, j) \leq g\}$ , where  $g$  is defined in (17) and  $d(j, k)$  denotes the geodesic distance between  $j$  and  $k$  in the graph  $\mathcal{G}^{*, \delta}$ . The goal is to construct two subsets  $V_0$  and  $V_1$  and two realizations of  $\beta$ ,  $\beta^{(0)}$  and  $\beta^{(1)}$  such that  $j \in V_0 \cup V_1$  and

$$\text{If } k \notin V_0 \cup V_1, \beta_k^{(0)} = \beta_k^{(1)}; \text{ otherwise, } \beta_k^{(i)} \neq 0 \text{ if and only if } k \in V_i, i = 0, 1,$$

where in the special case of  $V_0 = V_1$ , we require  $\text{sgn}(\beta^{(0)}) \neq \text{sgn}(\beta^{(1)})$ . In the literature, it is known that how well we can estimate  $\{\beta_k : d(k, j) \leq g\}$  depends on how well we can separate two hypotheses (where  $\beta^{(0)}$  and  $\beta^{(1)}$  are assumed as known):

$$H_0^{(j)} : Y = X\beta^{(0)} + \sigma z \quad \text{vs.} \quad H_1^{(j)} : Y = X\beta^{(1)} + \sigma z, \quad z \sim N(0, I_n). \quad (22)$$

The least favorable configuration for the local risk at index  $j$  is the quadruple  $(V_0, V_1, \beta^{(0)}, \beta^{(1)})$  for which two hypotheses are the most difficult to separate.

For any  $V \subset \{1, 2, \dots, p\}$ , let  $I_V$  be the indicator vector of  $V$  such that for any  $1 \leq k \leq p$ , the  $k$ -th coordinate of  $I_V$  is 1 if  $k \in V$  and is 0 otherwise. Define

$$B_V = \{I_V \circ \mu : \mu \in \Theta_p^*(\tau_p, a)\},$$

where we recall “ $\circ$ ” denotes the Hadamard product (see Section 1.5). Denote for short  $\theta^{(i)} = I_{V_0 \cup V_1} \circ \beta^{(i)}$ , and so  $\beta^{(1)} - \beta^{(0)} = \theta^{(1)} - \theta^{(0)}$  and  $\theta^{(i)} \in B_{V_i}$ ,  $i = 0, 1$ . Introduce

$$\alpha(\theta^{(0)}, \theta^{(1)}) = \alpha(\theta^{(0)}, \theta^{(1)}; V_0, V_1, \Omega, a) = \tau_p^{-2}(\theta^{(0)} - \theta^{(1)})' \Omega (\theta^{(0)} - \theta^{(1)}).$$

For the testing problem in (22), the optimal test is to reject  $H_0^{(j)}$  if and only if  $(\theta^{(1)} - \theta^{(0)})' X'(Y - X\beta^{(0)}) \geq t\sigma\tau_p \sqrt{\alpha(\theta^{(0)}, \theta^{(1)})}$  for some threshold  $t > 0$  to be determined. In the ARW and RD models,  $P(\beta_k \neq 0, \forall k \in V_i) \sim \epsilon_p^{|V_i|}$ ,  $i = 0, 1$ , and  $(\theta^{(0)} - \theta^{(1)})' G(\theta^{(0)} - \theta^{(1)}) \approx$

$(\theta^{(0)} - \theta^{(1)})' \Omega (\theta^{(0)} - \theta^{(1)})$ , since the support of  $\theta^{(0)} - \theta^{(1)}$  is contained in a small-size set  $V_0 \cup V_1$ . Therefore the sum of Type I and Type II error of any test associated with (22) is no smaller than (up to some negligible differences)

$$\epsilon_p^{|V_0|} \bar{\Phi}(t) + \epsilon_p^{|V_1|} \Phi(t - (\tau_p/\sigma)[\alpha(\theta^{(0)}, \theta^{(1)})]^{1/2}), \quad (23)$$

where  $\bar{\Phi} = 1 - \Phi$  is the survival function of  $N(0, 1)$ .

For a lower bound for the ‘‘local risk’’ at  $j$ , we first optimize the quantity in (23) over all  $\theta^{(0)} \in B_{V_0}$  and  $\theta^{(1)} \in B_{V_1}$ , and then optimize over all  $(V_0, V_1)$  subject to  $j \in V_0 \cup V_1$ . To this end, define  $\alpha^*(V_0, V_1) = \alpha^*(V_0, V_1; a, \Omega)$ ,  $\eta(V_0, V_1) = \eta(V_0, V_1; \vartheta, r, a, \Omega)$ , and  $\rho_j^* = \rho_j^*(\vartheta, r, a, \Omega)$  by

$$\alpha^*(V_0, V_1) = \min\{\alpha(\theta^{(0)}, \theta^{(1)}; V_0, V_1, \Omega, a) : \theta^{(i)} \in B_{V_i}, i = 0, 1, \text{sgn}(\theta^{(0)}) \neq \text{sgn}(\theta^{(1)})\}, \quad (24)$$

$$\eta(V_0, V_1) = \max\{|V_0|, |V_1|\} \vartheta + \frac{1}{4} \left[ \left( \sqrt{\alpha^*(V_0, V_1)r} - \frac{(|V_1| - |V_0|) \vartheta}{\sqrt{\alpha^*(V_0, V_1)r}} \right)_+ \right]^2,$$

and

$$\rho_j^*(\vartheta, r, a, \Omega) = \min_{\{(V_0, V_1): j \in V_1 \cup V_0\}} \eta(V_0, V_1).$$

The following shorthand notation is frequently used in this paper, which stands for a generic multi- $\log(p)$  term that may vary from one occurrence to another.

**Definition 5**  $L_p > 0$  denotes a multi- $\log(p)$  term such that when  $p \rightarrow \infty$ , for any  $\delta > 0$ ,  $L_p p^\delta \rightarrow \infty$  and  $L_p p^{-\delta} \rightarrow 0$ .

By (23) and Mills’ ratio (Wasserman and Roeder, 2009), a lower bound for the ‘‘local risk’’ at  $j$  is

$$\begin{aligned} & \sup_{\{(V_0, V_1): j \in V_0 \cup V_1\}} \left\{ \inf_t [\epsilon_p^{|V_0|} \bar{\Phi}(t) + \epsilon_p^{|V_1|} \Phi(t - (\tau_p/\sigma)[\alpha^*(V_0, V_1)]^{1/2})] \right\} \\ &= \sup_{\{(V_0, V_1): j \in V_0 \cup V_1\}} \left\{ L_p \exp(-\eta(V_0, V_1) \cdot \log(p)) \right\} = L_p \exp(-\rho_j^*(\vartheta, r, a, \Omega) \log(p)). \end{aligned}$$

We now aggregate such lower bounds for ‘‘local risk’’ for a global lower bound. Since the ‘‘least favorable’’ configurations of  $(V_0, V_1)$  for different  $j$  may overlap with each other, we need to consider a graph as follows. Revisit the optimization problem in (24) and let

$$(V_{0j}^*, V_{1j}^*) = \operatorname{argmin}_{\{(V_0, V_1): j \in V_1 \cup V_0\}} \eta(V_0, V_1; \vartheta, r, a, \Omega). \quad (25)$$

When there is a tie, pick the pair that appears first lexicographically. Therefore, for any  $1 \leq j \leq p$ ,  $V_{0j}^* \cup V_{1j}^*$  is uniquely defined. In Lemma 22 of the appendix, we show that  $|V_{0j}^* \cup V_{1j}^*| \leq (\vartheta + r)^2 / (2\vartheta r)$  for all  $1 \leq j \leq p$ .

We now define a new graph, Graph of Least Favorable (GOLF),  $\mathcal{G}^\circ = (V, E)$ , where  $V = \{1, 2, \dots, p\}$  and there is an edge between  $j$  and  $k$  if and only if  $(V_{0j}^* \cup V_{1j}^*)$  and  $(V_{0k}^* \cup V_{1k}^*)$  have non-empty intersections. Denote the maximum degree of GOLF by  $d_p(\mathcal{G}^\circ)$ .

**Theorem 6** Fix  $(\vartheta, \kappa) \in (0, 1)^2$ ,  $r > 0$ , and  $a \geq 1$  such that  $\kappa > (1 - \vartheta)$ , and let  $\mathcal{M}_p(c_0, g)$  be as in (18). Consider Model (1) where  $\beta$  is modeled by ARW $(\vartheta, r, a, \mu)$  and  $X$  is modeled by RD $(\vartheta, \kappa, \Omega)$  and  $\Omega \in \mathcal{M}_p(c_0, g)$  for sufficiently large  $p$ . Then as  $p \rightarrow \infty$ ,  $\text{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) \geq L_p [d_p(\mathcal{G}^\circ)]^{-1} \sum_{j=1}^p p^{-\rho_j^*(\vartheta, r, a, \Omega)}$ .

A similar claim holds for deterministic design models; the proof is similar so we omit it.

**Corollary 7** For deterministic design models, the parallel lower bound holds for the minimax Hamming distance with  $\Omega$  replaced by  $G$  in the calculation of  $\rho_j^*(\vartheta, r, a, \Omega)$  and  $d_p(\mathcal{G}^\circ)$ .

**Remark.** The lower bounds contain a factor of  $[d_p(\mathcal{G}^\circ)]^{-1}$ . In many cases including that considered in our main theorem (Theorem 8), this factor is a multi-log( $p$ ) term so it does not have a major effect. In some other cases, the factor  $[d_p(\mathcal{G}^\circ)]^{-1}$  could be much smaller, say, when the GOSD has one or a few hubs, the degrees of which grow algebraically fast as  $p$  grows. In these cases, the associated GOLF may (or may not) have large-degree hubs. As a result, the lower bounds we derive could be very conservative, and can be substantially improved if we treat the hubs, neighboring nodes of the hubs, and other nodes separately. For the sake of space, we leave such discussion to future work.

**Remark.** A similar lower bound holds if the condition  $\mu \in \Theta_p^*(\tau_p, a)$  of ARW is replaced by  $\mu \in \Theta_p(\tau_p)$ . In (24), suppose we replace  $\Theta_p^*(\tau_p, a)$  by  $\Theta_p(\tau_p)$ , and the minimum is achieved at  $(\theta^{(0)}, \theta^{(1)}) = (\theta_*^{(0)}(V_0, V_1; \Omega), \theta_*^{(1)}(V_0, V_1; \Omega))$ . Let  $g = g(m_0, \vartheta, r)$  be as in (17) and define

$$a_g^*(\Omega) = \max_{\{(V_0, V_1): |V_0 \cup V_1| \leq g\}} \{ \|\theta_*^{(0)}(V_0, V_1; \Omega)\|_\infty, \|\theta_*^{(1)}(V_0, V_1; \Omega)\|_\infty \}.$$

By elementary calculus, it is seen that for  $\Omega \in \mathcal{M}_p(c_0, g)$ , there is a constant  $C = C(c_0, g)$  such that  $a_g^*(\Omega) \leq C$ . If additionally we assume

$$a > a_g^*(\Omega), \tag{26}$$

then  $\alpha^*(V_0, V_1) = \alpha^*(V_0, V_1; \Omega, a)$ ,  $\eta(V_0, V_1; \Omega, a, \vartheta, r)$ , and  $\rho_j^*(\vartheta, r, a, \Omega)$  do not depend on  $a$ . Especially, we can derive an alternative formula for  $\rho_j^*(\vartheta, r, a, \Omega)$ ; see Lemma 18 for details.

When (26) holds,  $\Theta_p^*(\tau_p, a)$  is broad enough in the sense that the least favorable configurations  $(V_0, V_1, \beta^{(0)}, \beta^{(1)})$  for all  $j$  satisfy  $\|\beta^{(i)}\|_\infty \leq a\tau_p$ ,  $i = 0, 1$ . Consequently, neither the minimax rate nor GS needs to adapt to  $a$ . In Section 2.6, we assume (26) holds; (26) is a mild condition for it only involves small-size sub-matrices of  $\Omega$ .

### 2.6 Upper Bound and Optimality of Graphlet Screening

Fix constants  $\gamma \in (0, 1)$  and  $A > 0$ . Let  $\mathcal{M}_p(c_0, g)$  be as in (18). In this section, we further restrict  $\Omega$  to the following set:

$$\mathcal{M}_p^*(\gamma, c_0, g, A) = \left\{ \Omega \in \mathcal{M}_p(c_0, g) : \sum_{j=1}^p |\Omega(i, j)|^\gamma \leq A, 1 \leq i \leq p \right\}.$$

Note that any  $\Omega \in \mathcal{M}_p^*(\gamma, c_0, g, A)$  is sparse in the sense that each row of  $\Omega$  has relatively few large coordinates. The sparsity of  $\Omega$  implies the sparsity of the Gram matrix  $G$ , since small-size sub-matrices of  $G$  approximately equal to their counterparts of  $\Omega$ .

In GS, when we regularize GOSD as in (4), we set the threshold  $\delta$  by

$$\delta = \delta_p = 1/\log(p). \tag{27}$$

Such a choice for threshold is mainly for convenience, and can be replaced by any term that tends to 0 logarithmically fast as  $p \rightarrow \infty$ .

For any subsets  $D$  and  $F$  of  $\{1, 2, \dots, p\}$ , define  $\omega(D, F; \Omega) = \omega(D, F; \vartheta, r, a, \Omega, p)$  by

$$\omega(D, F; \Omega) = \min_{\xi \in \mathbb{R}^{|D|}, \min_{i \in D} |\xi_i| \geq 1} \left\{ \xi' (\Omega^{D,D} - \Omega^{D,F} (\Omega^{F,F})^{-1} \Omega^{F,D}) \xi \right\}, \tag{28}$$

Write  $\omega = \omega(\hat{D}, \hat{F}; \Omega)$  for short. We choose the tuning parameters in the GS-step in a way such that

$$t(\hat{D}, \hat{F}) = 2\sigma^2 q(\hat{D}, \hat{F}) \log p, \tag{29}$$

where  $q = q(\hat{D}, \hat{F}) > 0$  satisfies

$$\begin{cases} \sqrt{q_0} \leq \sqrt{q} \leq \sqrt{\omega r} - \sqrt{\frac{(\vartheta + \omega r)^2}{4\omega r} - \frac{|\hat{D}|+1}{2}\vartheta}, & |\hat{D}| \text{ is odd \& } \omega r/\vartheta > |\hat{D}| + (|\hat{D}|^2 - 1)^{1/2}, \\ \sqrt{q_0} \leq \sqrt{q} \leq \sqrt{\omega r} - \sqrt{\frac{1}{4}\omega r - \frac{1}{2}|\hat{D}|\vartheta}, & |\hat{D}| \text{ is even \& } \omega r/\vartheta \geq 2|\hat{D}|, \\ q \text{ is a constant such that } q \geq q_0, & \text{otherwise.} \end{cases} \tag{30}$$

We set the GC-step tuning parameters by

$$u^{gs} = \sigma\sqrt{2\vartheta \log p}, \quad v^{gs} = \tau_p = \sigma\sqrt{2r \log p}. \tag{31}$$

The main theorem of this paper is the following theorem.

**Theorem 8** Fix  $m_0 \geq 1$ ,  $(\vartheta, \gamma, \kappa) \in (0, 1)^3$ ,  $r > 0$ ,  $c_0 > 0$ ,  $g > 0$ ,  $a > 1$ ,  $A > 0$  such that  $\kappa > 1 - \vartheta$  and (17) is satisfied. Consider Model (1) where  $\beta$  is modeled by ARW( $\vartheta, r, a, \mu$ ),  $X$  is modeled by RD( $\vartheta, \kappa, \Omega$ ), and where  $\Omega \in \mathcal{M}_p^*(\gamma, c_0, g, A)$  and  $a > a_g^*(\Omega)$  for sufficiently large  $p$ . Let  $\hat{\beta}^{gs} = \hat{\beta}^{gs}(Y; \delta, \mathcal{Q}, u^{gs}, v^{gs}, X, p, n)$  be the Graphlet Screening procedure defined as in Section 2.1, where the tuning parameters  $(\delta, \mathcal{Q}, u^{gs}, v^{gs})$  are set as in (27)-(31). Then as  $p \rightarrow \infty$ ,  $\sup_{\mu \in \Theta_p^*(\tau_p, a)} H_p(\hat{\beta}^{gs}; \epsilon_p, n_p, \mu, \Omega) \leq L_p \left[ p^{1-(m_0+1)\vartheta} + \sum_{j=1}^p p^{-\rho_j^*(\vartheta, r, a, \Omega)} \right] + o(1)$ .

Note that  $\rho_j^* = \rho_j^*(\vartheta, r, a, \Omega)$  does not depend on  $a$ . Also, note that in the most interesting range,  $\sum_{j=1}^p p^{-\rho_j^*} \gg 1$ . So if we choose  $m_0$  properly large, e.g.,  $(m_0 + 1)\vartheta > 1$ , then  $\sup_{\mu \in \Theta_p^*(\tau_p, a)} H_p(\hat{\beta}^{gs}; \epsilon_p, n_p, \mu, \Omega) \leq L_p \sum_{j=1}^p p^{-\rho_j^*(\vartheta, r, a, \Omega)}$ . Together with Theorem 6, this says that GS achieves the optimal rate of convergence, adaptively to all  $\Omega$  in  $\mathcal{M}_p^*(\gamma, c_0, g, A)$  and  $\beta \in \Theta_p^*(\tau_p, a)$ . We call this property *optimal adaptivity*. Note that since the diagonals of  $\Omega$  are scaled to 1 approximately,  $\kappa \equiv \log(n_p)/\log(p)$  does not have a major influence over the convergence rate, as long as (21) holds.

**Remark.** Theorem 8 addresses the case where (26) holds so  $a > a_g^*(\Omega)$ . We now briefly discuss the case where  $a < a_g^*(\Omega)$ . In this case, the set  $\Theta_p^*(\tau_p, a)$  becomes sufficiently narrow and  $a$  starts to have some influence over the optimal rate of convergence, at least for some choices of  $(\vartheta, r)$ . To reflect the role of  $a$ , we modify GS as follows: (a) in the GC-step (9), limit  $\xi$  to the class where either  $\xi_i = 0$  or  $\tau_p \leq |\xi_i| \leq a\tau_p$ , and (b) in the

GS-step, replacing the  $\chi^2$ -screening by the likelihood based screening procedure; that is, when we screen  $\mathcal{I}_0 = \hat{D} \cup \hat{F}$ , we accept nodes in  $\hat{D}$  only when  $h(\hat{F}) > h(\mathcal{I}_0)$ , where for any subset  $D \subset \{1, 2, \dots, p\}$ ,  $h(D) = \min\{\frac{1}{2}\|P^D(Y - X^{\otimes, D}\xi)\|^2 + \vartheta\sigma^2 \log(p)|D|\}$ , where the minimum is computed over all  $|D| \times 1$  vectors  $\xi$  whose nonzero elements all have magnitudes in  $[\tau_p, a\tau_p]$ . From a practical point of view, this modified procedure depends more on the underlying parameters and is harder to implement than is GS. However, this is the price we need to pay when  $a$  is small. Since we are primarily interested in the case of relatively larger  $a$  where  $a > a_g^*(\Omega)$  holds, we skip further discussion along this line.

**2.7 Phase Diagram and Examples Where  $\rho_j^*(\vartheta, r, a, \Omega)$  Have Simple Forms**

In general, the exponents  $\rho_j^*(\vartheta, r, a, \Omega)$  may depend on  $\Omega$  in a complicated way. Still, from time to time, one may want to find a simple expression for  $\rho_j^*(\vartheta, r, a, \Omega)$ . It turns out that in a wide class of situations, simple forms for  $\rho_j^*(\vartheta, r, a, \Omega)$  are possible. The surprise is that, in many examples,  $\rho_j^*(\vartheta, r, a, \Omega)$  depends more on the trade-off between the parameters  $\vartheta$  and  $r$  (calibrating the signal sparsity and signal strength, respectively), rather than on the large coordinates of  $\Omega$ .

We begin with the following theorem, which is proved in Ji and Jin (2011, Theorem 1.1).

**Theorem 9** *Fix  $(\vartheta, \kappa) \in (0, 1)$ ,  $r > 0$ , and  $a > 1$  such that  $\kappa > (1 - \vartheta)$ . Consider Model (1) where  $\beta$  is modeled by ARW( $\vartheta, r, a, \mu$ ) and  $X$  is modeled by RD( $\vartheta, \kappa, \Omega$ ). Then as  $p \rightarrow \infty$ ,*

$$\frac{\text{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega)}{p^{1-\vartheta}} \gtrsim \begin{cases} 1, & 0 < r < \vartheta, \\ L_p p^{-(r-\vartheta)^2/(4r)}, & r > \vartheta. \end{cases}$$

Note that  $p^{1-\vartheta}$  is approximately the number of signals. Therefore, when  $r < \vartheta$ , the number of selection errors can not get substantially smaller than the number of signals. This is the most difficult case where no variable selection method can be successful.

In this section, we focus on the case  $r > \vartheta$ , so that successful variable selection is possible. In this case, Theorem 9 says that a *universal* lower bound for the Hamming distance is  $L_p p^{1-(\vartheta+r)^2/(4r)}$ . An interesting question is, to what extent, this lower bound is tight.

Recall that  $\lambda_k^*(\Omega)$  denotes the minimum of smallest eigenvalues across all  $k \times k$  principle submatrices of  $\Omega$ , as defined in (16). The following corollaries are proved in Section 6.

**Corollary 10** *Suppose the conditions of Theorem 8 hold, and that additionally,  $1 < r/\vartheta < 3 + 2\sqrt{2} \approx 5.828$ , and  $|\Omega(i, j)| \leq 4\sqrt{2} - 5 \approx 0.6569$  for all  $1 \leq i, j \leq p$ ,  $i \neq j$ . Then as  $p \rightarrow \infty$ ,  $\text{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) = L_p p^{1-(\vartheta+r)^2/(4r)}$ .*

**Corollary 11** *Suppose the conditions of Theorem 8 hold. Also, suppose that  $1 < r/\vartheta < 5 + 2\sqrt{6} \approx 9.898$ , and that  $\lambda_3^*(\Omega) \geq 2(5 - 2\sqrt{6}) \approx 0.2021$ ,  $\lambda_4^*(\Omega) \geq 5 - 2\sqrt{6} \approx 0.1011$ , and  $|\Omega(i, j)| \leq 8\sqrt{6} - 19 \approx 0.5959$  for all  $1 \leq i, j \leq p$ ,  $i \neq j$ . Then as  $p \rightarrow \infty$ ,  $\text{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) = L_p p^{1-(\vartheta+r)^2/(4r)}$ .*

In these corollaries, the conditions on  $\Omega$  are rather relaxed. Somewhat surprisingly, the off-diagonals of  $\Omega$  do not necessarily have a major influence on the optimal rate of convergence, as one might have expected.

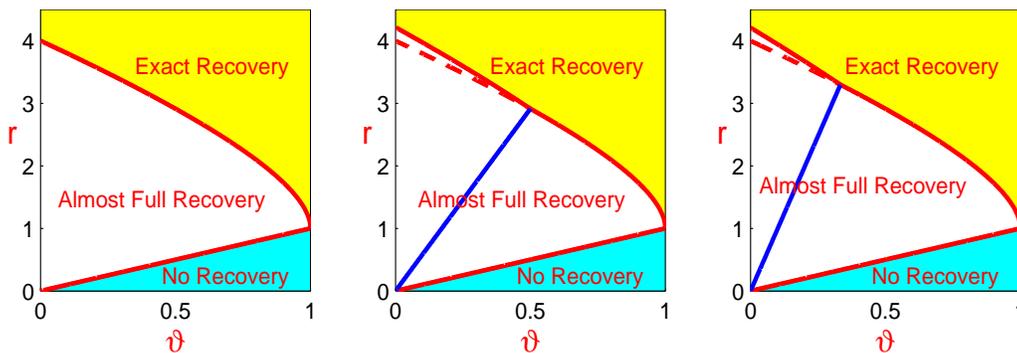


Figure 1: Phase diagram for  $\Omega = I_p$  (left), for  $\Omega$  satisfying conditions of Corollary 10 (middle), and for  $\Omega$  satisfying conditions of Corollary 11 (right). Red line:  $r = \vartheta$ . Solid red curve:  $r = \rho(\vartheta, \Omega)$ . In each of the last two panels, the blue line intersects with the red curve at  $(\vartheta, r) = (1/2, [3 + 2\sqrt{2}]/2)$  (middle) and  $(\vartheta, r) = (1/3, [5 + 2\sqrt{6}]/3)$  (right), which splits the red solid curve into two parts; the part to the left is illustrative for it depends on  $\Omega$  in a complicated way; the part to the right, together with the dashed red curve, represent  $r = (1 + \sqrt{1 - \vartheta})^2$  (in the left panel, this is illustrated by the red curve).

Note also that by Theorem 8, under the condition of either Corollaries 10 or Corollary 11, GS achieves the optimal rate in that

$$\sup_{\mu \in \Theta_p^*(\tau_p, a)} H_p(\hat{\beta}^{gs}; \epsilon_p, n_p, \mu, \Omega) \leq L_p p^{1 - (\vartheta + r)^2 / (4r)}. \tag{32}$$

Together, Theorem 9, Corollaries 10-11, and (32) have an interesting implication on the so-called *phase diagram*. Call the two-dimensional *parameter space*  $\{(\vartheta, r) : 0 < \vartheta < 1, r > 0\}$  the phase space. There are two curves  $r = \vartheta$  and  $r = \rho(\vartheta, \Omega)$  (the latter can be thought of as the solution of  $\sum_{j=1}^p p^{-\rho_j^*(\vartheta, r, a, \Omega)} = 1$ ; recall that  $\rho_j^*(\vartheta, r, a, \Omega)$  does not depend on  $a$ ) that partition the whole phase space into three different regions:

- *Region of No Recovery.*  $\{(\vartheta, r) : 0 < r < \vartheta, 0 < \vartheta < 1\}$ . In this region, as  $p \rightarrow \infty$ , for any  $\Omega$  and any procedures, the minimax Hamming error equals approximately to the total expected number of signals. This is the most difficult region, in which no procedure can be successful in the minimax sense.
- *Region of Almost Full Recovery.*  $\{(\vartheta, r) : \vartheta < r < \rho(\vartheta, \Omega)\}$ . In this region, as  $p \rightarrow \infty$ , the minimax Hamming distance satisfies  $1 \ll \text{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) \ll p^{1 - \vartheta}$ , and it is possible to recover most of the signals, but it is impossible to recover all of them.
- *Region of Exact Recovery.* In this region, as  $p \rightarrow \infty$ , the minimax Hamming distance  $\text{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) = o(1)$ , and it is possible to exactly recover all signals with overwhelming probability.

In general, the function  $\rho(\vartheta, \Omega)$  depends on  $\Omega$  in a complicated way. However, by Theorem 9 and Corollaries 10-11, we have the following conclusions. First, for all  $\Omega$  and  $a > 1$ ,  $\rho(\vartheta, \Omega) \geq (1 + \sqrt{1 - \vartheta})^2$  for all  $0 < \vartheta < 1$ . Second, in the simplest case where  $\Omega = I_p$ ,  $\text{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) = L_p p^{1 - (\vartheta+r)^2/(4r)}$ , and  $\rho(\vartheta, \Omega) = (1 + \sqrt{1 - \vartheta})^2$  for all  $0 < \vartheta < 1$ . Third, under the conditions of Corollary 10,  $\rho(\vartheta, \Omega) = (1 + \sqrt{1 - \vartheta})^2$  if  $1/2 < \vartheta < 1$ . Last, under the conditions of Corollary 11,  $\rho(\vartheta, \Omega) = (1 + \sqrt{1 - \vartheta})^2$  if  $1/3 < \vartheta < 1$ . The phase diagram for the last three cases are illustrated in Figure 1. The blue lines are  $r/\vartheta = 3 + 2\sqrt{2}$  (middle) and  $r/\vartheta = 5 + 2\sqrt{6}$  (right).

Corollaries 10-11 can be extended to more general situations, where  $r/\vartheta$  may get arbitrary large, but consequently, we need stronger conditions on  $\Omega$ . Towards this end, we note that for any  $(\vartheta, r)$  such that  $r > \vartheta$ , we can find a unique integer  $N = N(\vartheta, r)$  such that  $2N - 1 \leq (\vartheta/r + r/\vartheta)/2 < 2N + 1$ . Suppose that for any  $2 \leq k \leq 2N - 1$ ,

$$\lambda_k^*(\Omega) \geq \max_{\{(k+1)/2 \leq j \leq \min\{k, N\}\}} \left\{ \frac{(r/\vartheta + \vartheta/r)/2 - 2j + 2 + \sqrt{[(r/\vartheta + \vartheta/r)/2 - 2j + 2]^2 - 1}}{(2k - 2j + 1)(r/\vartheta)} \right\}, \tag{33}$$

and that for any  $2 \leq k \leq 2N$ ,

$$\lambda_k^*(\Omega) \geq \max_{\{k/2 \leq j \leq \min\{k-1, N\}\}} \left\{ \frac{(r/\vartheta + \vartheta/r)/2 + 1 - 2j}{(k - j)(r/\vartheta)} \right\}. \tag{34}$$

Then we have the following corollary.

**Corollary 12** *Suppose the conditions in Theorem 8 and that in (33)-(34) hold. Then as  $p \rightarrow \infty$ ,  $\text{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) = L_p p^{1 - (\vartheta+r)^2/(4r)}$ .*

The right hand sides of (33)-(34) decrease with  $(r/\vartheta)$ . For a constant  $s_0 > 1$ , (33)-(34) hold for all  $1 < r/\vartheta \leq s_0$  as long as they hold for  $r/\vartheta = s_0$ . Hence Corollary 12 implies a similar partition of the phase diagram as do Corollaries 10-11.

**Remark.** Phase diagram can be viewed as a new criterion for assessing the optimality, which is especially appropriate for rare and weak signals. The phase diagram is a partition of the phase space  $\{(\vartheta, r) : 0 < \vartheta < 1, r > 0\}$  into different regions where statistical inferences are distinctly different. In general, a phase diagram has the following four regions:

- An “exact recovery” region corresponding to the “rare and strong” regime in which high probability of completely correct variable selection is feasible.
- An “almost full recovery” region as a part of the “rare and weak” regime in which completely correct variable selection is not achievable with high probability but variable selection is still feasible in the sense that with high probability, the number of incorrectly selected variables is a small fraction of the total number of signals.
- A “detectable” region in which variable selection is infeasible but the detection of the existence of a signal (somewhere) is feasible (e.g., by the Higher Criticism method).
- An “undetectable” region where signals are so rare and weak that nothing can be sensibly done.

In the sparse signal detection (Donoho and Jin, 2004) and classification (Jin, 2009) problems, the main interest is to find the detectable region, so that the exact recovery and almost full recovery regions were lumped into a single “estimable” region (e.g., Donoho and Jin, 2004, Figure 1). For variable selection, the main interest is to find the boundaries of the almost full discovery region so that the detectable and non-detectable regions are lumped into a single “no recovery” region as in Ji and Jin (2011) and Figure 1 of this paper.

Variable selection in the “almost full recovery” region is a new and challenging problem. It was studied in Ji and Jin (2011) when the effect of signal cancellation is negligible, but the hardest part of the problem was unsolved in Ji and Jin (2011). This paper (the second in this area) deals with the important issue of signal cancellation, in hopes of gaining a much deeper insight on variable selection in much broader context.

## 2.8 Non-optimality of Subset Selection and the Lasso

Subset selection (also called the  $L^0$ -penalization method) is a well-known method for variable selection, which selects variables by minimizing the following functional:

$$\frac{1}{2}\|Y - X\beta\|^2 + \frac{1}{2}(\lambda_{ss})^2\|\beta\|_0, \quad (35)$$

where  $\|\beta\|_q$  denotes the  $L^q$ -norm,  $q \geq 0$ , and  $\lambda_{ss} > 0$  is a tuning parameter. The AIC, BIC, and RIC are methods of this type (Akaike, 1974; Schwarz, 1978; Foster and George, 1994). Subset selection is believed to have good “theoretic property”, but the main drawback of this method is that it is computationally NP hard. To overcome the computational challenge, many *relaxation* methods are proposed, including but are not limited to the lasso (Chen et al., 1998; Tibshirani, 1996), SCAD (Fan and Li, 2001), MC+ (Zhang, 2010), and Dantzig selector (Candes and Tao, 2007). Take the lasso for example. The method selects variables by minimizing

$$\frac{1}{2}\|Y - X\beta\|^2 + \lambda_{lasso}\|\beta\|_1, \quad (36)$$

where the  $L^0$ -penalization is replaced by the  $L^1$ -penalization, so the functional is convex and the optimization problem is solvable in polynomial time under proper conditions.

Somewhat surprisingly, subset selection is generally *rate non-optimal* in terms of selection errors. This sub-optimality of subset selection is due to its lack of flexibility in adapting to the “local” graphic structure of the design variables. Similarly, other global relaxation methods are sub-optimal as well, as the subset selection is the “idol” these methods try to mimic. To save space, we only discuss subset selection and the lasso, but a similar conclusion can be drawn for SCAD, MC+, and Dantzig selector.

For mathematical simplicity, we illustrate the point with an idealized regression model where the Gram matrix  $G = X'X$  is diagonal block-wise and has  $2 \times 2$  blocks

$$G(i, j) = 1\{i = j\} + h_0 \cdot 1\{|j - i| = 1, \max(i, j) \text{ is even}\}, \quad |h_0| < 1, \quad 1 \leq i, j \leq p. \quad (37)$$

Using an idealized model is mostly for technical convenience, but the non-optimality of subset selection or the lasso holds much more broadly than what is considered here. On the other hand, using a simple model is sufficient here: if a procedure is non-optimal in an idealized case, we can not expect it to be optimal in a more general context.

At the same time, we continue to model  $\beta$  with the Asymptotic Rare and Weak model  $ARW(\vartheta, r, a, \mu)$ , but where we relax the assumption of  $\mu \in \Theta_p^*(\tau_p, a)$  to that of  $\mu \in \Theta_p(\tau_p)$  so that the strength of each signal  $\geq \tau_p$  (but there is no upper bound on the strength). Consider a variable selection procedure  $\hat{\beta}^\star$ , where  $\star = gs, ss, lasso$ , representing GS, subset selection, and the lasso and the tuning parameters for each method are ideally set. Note that for the worst-case risk considered below, the ideal tuning parameters depend on  $(\vartheta, r, p, h_0)$  but do not depend on  $\mu$ . Since the index groups  $\{2j - 1, 2j\}$  are exchangeable in (37) and the ARW models, the Hamming error of  $\beta^\star$  in its worst case scenario has the form of  $\sup_{\{\mu \in \Theta_p(\tau_p)\}} H_p(\hat{\beta}^\star; \epsilon_p, \mu, G) = L_p p^{1-\rho_\star(\vartheta, r, h_0)}$ .

We now study  $\rho_\star(\vartheta, r, h_0)$ . Towards this end, we first introduce  $\rho_{lasso}^{(3)}(\vartheta, r, h_0) = \{(2|h_0|)^{-1}[(1 - h_0^2)\sqrt{r} - \sqrt{(1 - h_0^2)(1 - |h_0|^2)r - 4|h_0|(1 - |h_0|)\vartheta}]\}^2$  and  $\rho_{lasso}^{(4)}(\vartheta, r, h_0) = \vartheta + \frac{(1-|h_0|)^3(1+|h_0|)}{16h_0^2} [(1 + |h_0|)\sqrt{r} - \sqrt{(1 - |h_0|^2)r - 4|h_0|\vartheta/(1 - h_0^2)}]^2$ . We then let

$$\rho_{ss}^{(1)}(\vartheta, r, h_0) = \begin{cases} 2\vartheta, & r/\vartheta \leq 2/(1 - h_0^2) \\ [2\vartheta + (1 - h_0^2)r]^2/[4(1 - h_0^2)r], & r/\vartheta > 2/(1 - h_0^2) \end{cases},$$

$$\rho_{ss}^{(2)}(\vartheta, r, h_0) = \begin{cases} 2\vartheta, & r/\vartheta \leq 2/(1 - |h_0|) \\ 2[\sqrt{2(1 - |h_0|)r} - \sqrt{(1 - |h_0|)r - \vartheta}]^2, & r/\vartheta > 2/(1 - |h_0|) \end{cases},$$

$$\rho_{lasso}^{(1)}(\vartheta, r, h_0) = \begin{cases} 2\vartheta, & r/\vartheta \leq 2/(1 - |h_0|)^2 \\ \rho_{lasso}^{(3)}(\vartheta, r, h_0), & r/\vartheta > 2/(1 - |h_0|)^2 \end{cases},$$

and

$$\rho_{lasso}^{(2)}(\vartheta, r, h_0) = \begin{cases} 2\vartheta, & r/\vartheta \leq (1 + |h_0|)/(1 - |h_0|)^3 \\ \rho_{lasso}^{(4)}(\vartheta, r, h_0), & r/\vartheta > (1 + |h_0|)/(1 - |h_0|)^3 \end{cases}.$$

The following theorem is proved in Section 6.

**Theorem 13** Fix  $\vartheta \in (0, 1)$  and  $r > 0$  such that  $r > \vartheta$ . Consider Model (1) where  $\beta$  is modeled by  $ARW(\vartheta, r, a, \mu)$  and  $X$  satisfies (37). For GS, we set the tuning parameters  $(\delta, m_0) = (0, 2)$ , and set  $(\mathcal{Q}, u^{gs}, v^{gs})$  as in (29)-(31). For subset selection as in (35) and the lasso as in (36), we set their tuning parameters ideally given that  $(\vartheta, r)$  are known. Then as  $p \rightarrow \infty$ ,

$$\rho_{gs}(\vartheta, r, h_0) = \min\left\{\frac{(\vartheta + r)^2}{4r}, \vartheta + \frac{(1 - |h_0|)}{2}r, 2\vartheta + \frac{\{[(1 - h_0^2)r - \vartheta]_+\}^2}{4(1 - h_0^2)r}\right\}, \quad (38)$$

$$\rho_{ss}(\vartheta, r, h_0) = \min\left\{\frac{(\vartheta + r)^2}{4r}, \vartheta + \frac{(1 - |h_0|)}{2}r, \rho_{ss}^{(1)}(\vartheta, r, h_0), \rho_{ss}^{(2)}(\vartheta, r, h_0)\right\}, \quad (39)$$

and

$$\rho_{lasso}(\vartheta, r, h_0) = \min\left\{\frac{(\vartheta + r)^2}{4r}, \vartheta + \frac{(1 - |h_0|)r}{2(1 + \sqrt{1 - h_0^2})}, \rho_{lasso}^{(1)}(\vartheta, r, h_0), \rho_{lasso}^{(2)}(\vartheta, r, h_0)\right\}. \quad (40)$$

It can be shown that  $\rho_{gs}(\vartheta, r, h_0) \geq \rho_{ss}(\vartheta, r, h_0) \geq \rho_{lasso}(\vartheta, r, h_0)$ , where depending on the choices of  $(\vartheta, r, h_0)$ , we may have equality or strict inequality (note that a larger exponent means a better error rate). This fits well with our expectation, where as far as the convergence rate is concerned, GS is optimal for all  $(\vartheta, r, h_0)$ , so it outperforms the subset selection, which in turn outperforms the lasso. Table 2 summarizes the exponents for some representative  $(\vartheta, r, h_0)$ . It is seen that differences between these exponents become increasingly prominent when  $h_0$  increase and  $\vartheta$  decrease.

$\vartheta/r/h_0$	.1/11/.8	.3/9/.8	.5/4/.8	.1/4/.4	.3/4/.4	.5/4/.4	.1/3/.2	.3/3/.2
$\star = gs$	1.1406	1.2000	0.9000	0.9907	1.1556	1.2656	0.8008	0.9075
$\star = ss$	0.8409	0.9047	0.9000	0.9093	1.1003	1.2655	0.8007	0.9075
$\star = lasso$	0.2000	0.6000	0.7500	0.4342	0.7121	1.0218	0.6021	0.8919

Table 2: The exponents  $\rho_{\star}(\vartheta, r, h_0)$  in Theorem 13, where  $\star = gs, ss, lasso$ .

As in Section 2.7, each of these methods has a phase diagram plotted in Figure 2, where the phase space partitions into three regions: *Region of Exact Recovery*, *Region of Almost Full Recovery*, and *Region of No Recovery*. Interestingly, the separating boundary for the last two regions are the same for three methods, which is the line  $r = \vartheta$ . The boundary that separates the first two regions, however, vary significantly for different methods. For any  $h_0 \in (-1, 1)$  and  $\star = gs, ss, lasso$ , the equation for this boundary can be obtained by setting  $\rho_{\star}(\vartheta, r, h_0) = 1$  (the calculations are elementary so we omit them). Note that the lower the boundary is, the better the method is, and that the boundary corresponding to the lasso is discontinuous at  $\vartheta = 1/2$ . In the non-optimal region of either subset selection or the lasso, the Hamming errors of the procedure are much smaller than  $p\epsilon_p$ , so the procedure gives “almost full recovery”; however, the rate of Hamming errors is slower than that of the optimal procedure, so subset selection or the lasso is non-optimal in such regions.

Subset selection and the lasso are rate non-optimal for they are so-called *one-step* or *non-adaptive* methods (Ji and Jin, 2011), which use only one tuning parameter, and which do not adapt to the local graphic structure. The non-optimality can be best illustrated with the diagonal block-wise model presented here, where each block is a  $2 \times 2$  matrix. Correspondingly, we can partition the vector  $\beta$  into many size 2 blocks, each of which is of the following three types (i) those have no signal, (ii) those have exactly one signal, and (iii) those have two signals. Take the subset selection for example. To best separate (i) from (ii), we need to set the tuning parameter ideally. But such a tuning parameter may not be the “best” for separating (i) from (iii). This explains the non-optimality of subset selection.

Seemingly, more complicated penalization methods that use multiple tuning parameters may have better performance than the subset selection and the lasso. However, it remains open how to design such extensions to achieve the optimal rate for general cases. To save space, we leave the study along this line to the future.

## 2.9 Summary

We propose GS as a new approach to variable selection. The key methodological innovation is to use the GOSD to guide the multivariate screening. While a brute-force  $m$ -variate

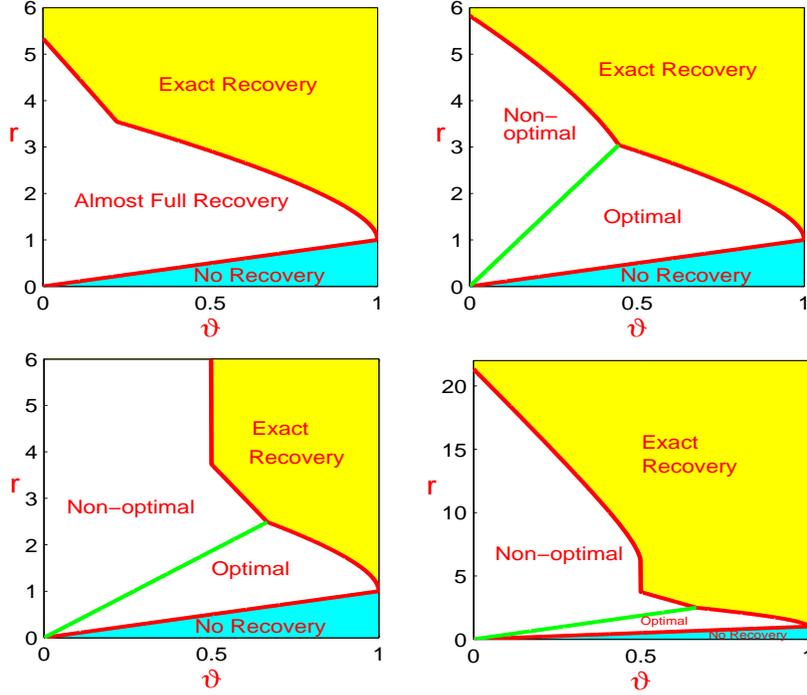


Figure 2: Phase diagrams for GS (top left), subset selection (top right), and the lasso (bottom; zoom-in on the left and zoom-out on the right), where  $h_0 = 0.5$ .

screening has a computation cost of  $O(p^m + np)$ , GS only has a computation cost of  $L_p np$  (excluding the overhead of obtaining the GOSD), by utilizing graph sparsity. Note that when the design matrix  $G$  is approximately banded, say, all its large entries are confined to a diagonal band with bandwidth  $\leq K$ , the overhead of GS can be reduced to  $O(npK)$ . One such example is in Genome-Wide Association Study (GWAS), where  $G$  is the empirical Linkage Disequilibrium (LD) matrix, and  $K$  can be as small as a few tens. We remark that the lasso has a computational complexity of  $O(npk)$ , where  $k$ , dominated by the number steps requiring re-evaluation of the correlation between design vectors and updated residuals, could be smaller than the  $L_p$  term for GS (Wang et al., 2013).

We use *asymptotic minimaxity of the Hamming distance* as the criterion for assessing optimality. Compared with existing literature on variable selection where we use the *oracle property* or *probability of exact support recovery* to assess optimality, our approach is mathematically more demanding, yet scientifically more relevant in the rare/weak paradigm.

We have proved that GS achieves the optimal rate of convergence of Hamming errors, especially when signals are rare and weak, provided that the Gram matrix is sparse. Subset selection and the lasso are not rate optimal, even with very simple Gram matrix  $G$  and

even when the tuning parameters are ideally set. The sub-optimality of these methods is due to that they do not take advantage of the ‘local’ graphical structure as GS does.

GS has three key tuning parameters:  $q$  for the threshold level  $t(\hat{D}, \hat{F}) = 2\sigma^2 q \log p$  in the *GS*-step, and  $(u^{gs}, v^{gs}) = (\sigma\sqrt{2\vartheta \log p}, \sigma\sqrt{2r \log p})$  in the *GC*-step. While the choice of  $q$  is reasonably flexible and a sufficiently small fixed  $q > 0$  is usually adequate, the choice of  $u^{gs}$  and  $v^{gs}$  are more directly tied to the signal sparsity and signal strength. Adaptive choice of these tuning parameters is a challenging direction of further research. One of our ideas to be developed in this direction is a subsampling scheme similar to the Stability Selection (Meinshausen and Bühlmann, 2010). On the other hand, as shown in our numeric results in Section 4, the performance of GS is relatively insensitive to mis-specification of  $(\epsilon_p, \tau_p)$ ; see details therein.

### 3. Properties of Graphlet Screening, Proof of Theorem 8

GS attributes the success to two important properties: the Sure Screening property and the *Separable After Screening* (SAS) property.

The Sure Screening property means that in the  $m_0$ -stage  $\chi^2$  screening, by picking an appropriate threshold, the set  $\mathcal{U}_p^*$  (which is the set of retained indices after the GS-step) contains all but a small fraction of true signals. Asymptotically, this fraction is comparably smaller than the minimax Hamming errors, and so negligible. The SAS property means that except for a negligible probability, as a subgraph of the GOSD,  $\mathcal{U}_p^*$  decomposes into many disconnected components of the GOSD, where the size of each component does not exceed a fixed integer. These two properties ensure that the original regression problem reduces to many small-size regression problems, and thus pave the way for the *GC*-step.

Below, we explain these ideas in detail, and conclude the section by the proof of Theorem 8. Since the only place we need the knowledge of  $\sigma$  is in setting the tuning parameters, so without loss of generality, we assume  $\sigma = 1$  throughout this section.

First, we discuss the *GS*-step. For short, write  $\hat{\beta} = \hat{\beta}^{gs}(Y; \delta, \mathcal{Q}, u^{gs}, v^{gs}, X, p, n)$  throughout this section. We first discuss the computation cost of the *GS*-step. As in Theorem 8, we take the threshold  $\delta$  in  $\mathcal{G}^{*,\delta}$  to be  $\delta = \delta_p = 1/\log(p)$ . The proof of the following lemma is similar to that of Ji and Jin (2011, Lemma 2.2), so we omit it.

**Lemma 14** *Suppose the conditions of Theorem 8 hold, where we recall  $\delta = 1/\log(p)$ , and  $\Omega^{*,\delta}$  is defined as in (4). As  $p \rightarrow \infty$ , with probability  $1 - o(1/p^2)$ ,  $\|\Omega - \Omega^{*,\delta}\|_\infty \leq C(\log(p))^{-(1-\gamma)}$ , and  $\mathcal{G}^{*,\delta}$  is  $K$ -sparse, where  $K \leq C(\log(p))^{1/\gamma}$ .*

Combining Lemma 14 and Frieze and Molloy (1999), it follows that with probability  $1 - o(1/p^2)$ ,  $\mathcal{G}^{*,\delta}$  has at most  $p(Ce(\log(p))^{1/\gamma})^{m_0}$  connected subgraphs of size  $\leq m_0$ . Note that the second factor is at most logarithmically large, so the computation cost in the *GS*-step is at most  $L_p p$  flops.

Consider the performance of the *GS*-step. The goal of this step is two-fold: on one hand, it tries to retain as many signals as possible during the screening; on the other hand, it tries to minimize the computation cost of the *GC*-step by controlling the maximum size of all components of  $\mathcal{U}_p^*$ . The key in the *GS*-step is to set the collection of thresholds  $\mathcal{Q}$ . The tradeoff is that, setting the thresholds too high may miss too many signals during the screening, and setting the threshold too low may increase the maximum size of the

components in  $\mathcal{U}_p^*$ , and so increase the computational burden of the  $GC$ -step. The following lemma characterizes the Sure Screening property of GS, and is proved in Section 6.

**Lemma 15** (*Sure Screening*). *Suppose the settings and conditions are as in Theorem 8. In the  $m_0$ -stage  $\chi^2$  screening of the  $GS$ -step, if we set the thresholds  $t(\hat{D}, \hat{F})$  as in (29), then as  $p \rightarrow \infty$ , for any  $\Omega \in \mathcal{M}_p^*(\gamma, c_0, g, A)$ ,  $\sum_{j=1}^p P(\beta_j \neq 0, j \notin \mathcal{U}_p^*) \leq L_p [p^{1-(m_0+1)\vartheta} + \sum_{j=1}^p p^{-\rho_j^*(\vartheta, r, a, \Omega)}] + o(1)$ .*

Next, we formally state the SAS property. Viewing it as a subgraph of  $\mathcal{G}^{*,\delta}$ ,  $\mathcal{U}_p^*$  decomposes into many disconnected components  $\mathcal{I}^{(k)}$ ,  $1 \leq k \leq N$ , where  $N$  is an integer that may depend on the data.

**Lemma 16** (*SAS*). *Suppose the settings and conditions are as in Theorem 8. In the  $m_0$ -stage  $\chi^2$  screening in the  $GS$ -step, suppose we set the thresholds  $t(\hat{D}, \hat{F})$  as in (29) such that  $q(\hat{D}, \hat{F}) \geq q_0$  for some constant  $q_0 = q_0(\vartheta, r) > 0$ . As  $p \rightarrow \infty$ , under the conditions of Theorem 8, for any  $\Omega \in \mathcal{M}_p^*(\gamma, c_0, g, A)$ , there is a constant  $\ell_0 = \ell_0(\vartheta, r, \kappa, \gamma, A, c_0, g) > 0$  such that with probability at least  $1 - o(1/p)$ ,  $|\mathcal{I}^{(k)}| \leq \ell_0$ ,  $1 \leq k \leq N$ .*

We remark that a more convenient way of picking  $q$  is to let

$$\begin{cases} q_0 \leq q \leq \left(\frac{\omega r + \vartheta}{2\omega r}\right)^2 \omega r, & |\hat{D}| \text{ is odd \& } \omega r / \vartheta > |\hat{D}| + (|\hat{D}|^2 - 1)^{1/2}, \\ q_0 \leq q \leq \frac{1}{4}\omega r, & |\hat{D}| \text{ is even \& } \omega r / \vartheta \geq 2|\hat{D}|, \end{cases}$$

and let  $q$  be any other number otherwise, with which both lemmas continue to hold with this choice of  $q$ . Here, for short,  $\omega = \omega(\hat{D}, \hat{F}; \Omega)$ . Note that numerically this choice is comparably more conservative.

Together, the above two lemmas say that the  $GS$ -step makes only negligible false non-discoveries, and decomposes  $\mathcal{U}_p^*$  into many disconnected components, each has a size not exceeding a fixed integer. As a result, the computation cost of the following  $GC$ -step is moderate, at least in theory.

We now discuss the  $GC$ -step. The key to understanding the  $GC$ -step is that the original regression problem reduces to many disconnected small-size regression problems. To see the point, define  $\tilde{Y} = X'Y$  and recall that  $G = X'X$ . Let  $\mathcal{I}_0 \triangleleft \mathcal{U}_p^*$  be a component, we limit our attention to  $\mathcal{I}_0$  by considering the following regression problem:

$$\tilde{Y}^{\mathcal{I}_0} = G^{\mathcal{I}_0, \otimes} \beta + (X'z)^{\mathcal{I}_0}, \quad (41)$$

where  $(X'z)^{\mathcal{I}_0} \sim N(0, G^{\mathcal{I}_0, \mathcal{I}_0}) \approx N(0, \Omega^{\mathcal{I}_0, \mathcal{I}_0})$ , and  $G^{\mathcal{I}_0, \otimes}$  is a  $|\mathcal{I}_0| \times p$  matrix according to our notation. What is non-obvious here is that, the regression problem still involves the whole vector  $\beta$ , and is still high-dimensional. To see the point, letting  $V = \{1, 2, \dots, p\} \setminus \mathcal{U}_p^*$ , we write  $G^{\mathcal{I}_0, \otimes} \beta = G^{\mathcal{I}_0, \mathcal{I}_0} \beta^{\mathcal{I}_0} + I + II$ , where  $I = \sum_{\mathcal{J}_0: \mathcal{J}_0 \triangleleft \mathcal{U}_p^*, \mathcal{J}_0 \neq \mathcal{I}_0} G^{\mathcal{I}_0, \mathcal{J}_0} \beta^{\mathcal{J}_0}$  and  $II = G^{\mathcal{I}_0, V} \beta^V$ . First, by Sure Screening property,  $\beta^V$  contains only a negligible number of signals, so we can think  $II$  as negligible. Second, for any  $\mathcal{J}_0 \neq \mathcal{I}_0$  and  $\mathcal{J}_0 \triangleleft \mathcal{U}_p^*$ , by the SAS property,  $\mathcal{I}_0$  and  $\mathcal{J}_0$  are disconnected and so the matrix  $G^{\mathcal{I}_0, \mathcal{J}_0}$  is a small size matrix whose coordinates are uniformly small. This heuristic is made precise in the proof of Theorem 8. It is now seen that the regression problem in (41) is indeed low-dimensional:

$$\tilde{Y}^{\mathcal{I}_0} \approx G^{\mathcal{I}_0, \mathcal{I}_0} \beta^{\mathcal{I}_0} + (X'z)^{\mathcal{I}_0} \approx N(\Omega^{\mathcal{I}_0, \mathcal{I}_0} \beta^{\mathcal{I}_0}, \Omega^{\mathcal{I}_0, \mathcal{I}_0}), \quad (42)$$

The above argument is made precise in Lemma 17, see details therein. Finally, approximately, the *GC*-step is to minimize  $\frac{1}{2}(\tilde{Y}^{\mathcal{I}_0} - \Omega^{\mathcal{I}_0, \mathcal{I}_0} \xi)'(\Omega^{\mathcal{I}_0, \mathcal{I}_0})^{-1}(\tilde{Y}^{\mathcal{I}_0} - \Omega^{\mathcal{I}_0, \mathcal{I}_0} \xi) + \frac{1}{2}(u^{gs})^2 \|\xi\|_0$ , where each coordinate of  $\xi$  is either 0 or  $\geq v^{gs}$  in magnitude. Comparing this with (42), the procedure is nothing but the penalized MLE of a low dimensional normal model, and the main result follows by exercising basic statistical inferences.

We remark that in the *GC*-step, removing the constraints on the coordinates of  $\xi$  will not give the optimal rate of convergence. This is one of the reasons why the classical subset selection procedure is rate non-optimal. Another reason why the subset selection is non-optimal is that, the procedure has only one tuning parameter, but GS has the flexibility of using different tuning parameters in the *GS*-step and the *GC*-step. See Section 2.8 for more discussion.

We are now ready for the proof of Theorem 8.

### 3.1 Proof of Theorem 8

For notational simplicity, we write  $\rho_j^* = \rho_j^*(\vartheta, r, a, \Omega)$ . By Lemma 15,

$$\sum_{j=1}^p P(\beta_j \neq 0, j \notin \mathcal{U}_p^*) \leq L_p [p^{1-(m_0+1)\vartheta} + \sum_{j=1}^p p^{-\rho_j^*}] + o(1).$$

So to show the claim, it is sufficient to show

$$\sum_{j=1}^p P(j \in \mathcal{U}_p^*, \text{sgn}(\beta_j) \neq \text{sgn}(\hat{\beta}_j)) \leq L_p [\sum_{j=1}^p p^{-\rho_j^*} + p^{1-(m_0+1)\vartheta}] + o(1). \tag{43}$$

Towards this end, let  $S(\beta)$  be the support of  $\beta$ ,  $\Omega^{*,\delta}$  be as in (4), and  $\mathcal{G}^{*,\delta}$  be the GOSD. Let  $\mathcal{U}_p^*$  be the set of retained indices after the GS-step. Note that when  $\text{sgn}(\hat{\beta}_j) \neq 0$ , there is a unique component  $\mathcal{I}_0$  such that  $j \in \mathcal{I}_0 \triangleleft \mathcal{U}_p^*$ . For any connected subgraph  $\mathcal{I}_0$  of  $\mathcal{G}^{*,\delta}$ , let  $B(\mathcal{I}_0) = \{k: k \notin \mathcal{I}_0, \Omega^{*,\delta}(k, \ell) \neq 0 \text{ for some } \ell \in \mathcal{I}_0, 1 \leq k \leq p\}$ . Note that when  $\mathcal{I}_0$  is a component of  $\mathcal{U}_p^*$ , we must have  $B(\mathcal{I}_0) \cap \mathcal{U}_p^* = \emptyset$  as for any node in  $B(\mathcal{I}_0)$ , there is at least one edge between it and some nodes in the component  $\mathcal{I}_0$ . As a result,

$$P(j \in \mathcal{I}_0 \triangleleft \mathcal{U}_p^*, B(\mathcal{I}_0) \cap S(\beta) \neq \emptyset) \leq \sum_{\mathcal{I}_0: j \in \mathcal{I}_0} \sum_{k \in B(\mathcal{I}_0)} P(k \notin \mathcal{U}_p^*, \beta_k \neq 0), \tag{44}$$

where the first summation is over all connected subgraphs that contains node  $j$ . By Lemma 16, with probability at least  $1 - o(1/p)$ ,  $\mathcal{G}^{*,\delta}$  is  $K$ -sparse with  $K = C(\log(p))^{1/\gamma}$ , and there is a finite integer  $\ell_0$  such that  $|\mathcal{I}_0| \leq \ell_0$ . As a result, there are at most finite  $\mathcal{I}_0$  such that the event  $\{j \in \mathcal{I}_0 \triangleleft \mathcal{U}_p^*\}$  is non-empty, and for each of such  $\mathcal{I}_0$ ,  $B(\mathcal{I}_0)$  contains at most  $L_p$  nodes. Using (44) and Lemma 15, a direct result is

$$\sum_{j=1}^p P(j \in \mathcal{I}_0 \triangleleft \mathcal{U}_p^*, B(\mathcal{I}_0) \cap S(\beta) \neq \emptyset) \leq L_p [\sum_{j=1}^p p^{-\rho_j^*} + p^{1-(m_0+1)\vartheta}] + o(1). \tag{45}$$

Comparing (45) with (43), to show the claim, it is sufficient to show that

$$\sum_{j=1}^p P(\text{sgn}(\beta_j) \neq \text{sgn}(\hat{\beta}_j), j \in \mathcal{I}_0 \triangleleft \mathcal{U}_p^*, B(\mathcal{I}_0) \cap S(\beta) = \emptyset) \leq L_p [\sum_{j=1}^p p^{-\rho_j^*} + p^{1-(m_0+1)\vartheta}] + o(1). \tag{46}$$

Fix  $1 \leq j \leq p$  and a connected subgraph  $\mathcal{I}_0$  such that  $j \in \mathcal{I}_0$ . For short, let  $S$  be the support of  $\beta^{\mathcal{I}_0}$  and  $\hat{S}$  be the support of  $\hat{\beta}^{\mathcal{I}_0}$ . The event  $\{\text{sgn}(\beta_j) \neq \text{sgn}(\hat{\beta}_j), j \in \mathcal{I}_0 \triangleleft \mathcal{U}_p^*\}$  is identical to the event of  $\{\text{sgn}(\beta_j) \neq \text{sgn}(\hat{\beta}_j), j \in S \cup \hat{S}\}$ . Moreover, Since  $\mathcal{I}_0$  has a finite size, both  $S$  and  $\hat{S}$  have finite possibilities. So to show (46), it is sufficient to show that for any fixed  $1 \leq j \leq p$ , connected subgraph  $\mathcal{I}_0$ , and subsets  $S_0, S_1 \subset \mathcal{I}_0$  such that  $j \in S_0 \cup S_1$ ,

$$P(\text{sgn}(\beta_j) \neq \text{sgn}(\hat{\beta}_j), S = S_0, \hat{S} = S_1, j \in \mathcal{I}_0 \triangleleft \mathcal{U}_p^*, B(\mathcal{I}_0) \cap S(\beta) = \emptyset) \leq L_p [p^{-\rho_j^*} + p^{-(m_0+1)\vartheta}]. \quad (47)$$

We now show (47). The following lemma is proved in Ji and Jin (2011, A.4).

**Lemma 17** *Suppose the conditions of Theorem 8 hold. Over the event  $\{j \in \mathcal{I}_0 \triangleleft \mathcal{U}_p^*\} \cap \{B(\mathcal{I}_0) \cap S(\beta) = \emptyset\}$ ,  $\|(\Omega\beta)^{\mathcal{I}_0} - \Omega^{\mathcal{I}_0, \mathcal{I}_0} \beta^{\mathcal{I}_0}\|_\infty \leq C\tau_p(\log(p))^{-(1-\gamma)}$ .*

Write for short  $\hat{M} = G^{\mathcal{I}_0, \mathcal{I}_0}$  and  $M = \Omega^{\mathcal{I}_0, \mathcal{I}_0}$ . By definitions,  $\hat{\beta}^{\mathcal{I}_0}$  is the minimizer of the following functional  $Q(\xi) \equiv \frac{1}{2}(\tilde{Y}^{\mathcal{I}_0} - \hat{M}\xi)' \hat{M}^{-1}(\tilde{Y}^{\mathcal{I}_0} - \hat{M}\xi) + \frac{1}{2}(u^{gs})^2 \|\xi\|_0$ , where  $\xi$  is an  $|\mathcal{I}_0| \times 1$  vector whose coordinates are either 0 or  $\geq v^{gs}$  in magnitude,  $u^{gs} = \sqrt{2\vartheta \log(p)}$ , and  $v^{gs} = \sqrt{2r \log(p)}$ . In particular,  $Q(\beta^{\mathcal{I}_0}) \geq Q(\hat{\beta}^{\mathcal{I}_0})$ , or equivalently

$$(\hat{\beta}^{\mathcal{I}_0} - \beta^{\mathcal{I}_0})'(\tilde{Y}^{\mathcal{I}_0} - \hat{M}\beta^{\mathcal{I}_0}) \geq \frac{1}{2}(\hat{\beta}^{\mathcal{I}_0} - \beta^{\mathcal{I}_0})' \hat{M}(\hat{\beta}^{\mathcal{I}_0} - \beta^{\mathcal{I}_0}) + (|S_1| - |S_0|)\vartheta \log(p). \quad (48)$$

Now, write for short  $\delta = \tau_p^{-2}(\hat{\beta}^{\mathcal{I}_0} - \beta^{\mathcal{I}_0})' M(\hat{\beta}^{\mathcal{I}_0} - \beta^{\mathcal{I}_0})$ . First, by Schwartz inequality,  $[(\hat{\beta}^{\mathcal{I}_0} - \beta^{\mathcal{I}_0})'(\tilde{Y}^{\mathcal{I}_0} - \hat{M}\beta^{\mathcal{I}_0})]^2 \leq \delta \tau_p^2 (\tilde{Y}^{\mathcal{I}_0} - \hat{M}\beta^{\mathcal{I}_0})' M^{-1}(\tilde{Y}^{\mathcal{I}_0} - \hat{M}\beta^{\mathcal{I}_0})$ . Second, by Lemma 17,  $\tilde{Y}^{\mathcal{I}_0} = w + M\beta^{\mathcal{I}_0} + rem$ , where  $w \sim N(0, M)$  and with probability  $1 - o(1/p)$ ,  $|rem| \leq C(\log(p))^{-(1-\gamma)}\tau_p$ . Last, with probability at least  $(1 - o(1/p))$ ,  $\|\hat{M} - M\|_\infty \leq C\sqrt{\log(p)}p^{-[\kappa-(1-\vartheta)]/2}$ . Inserting these into (48) gives that with probability at least  $(1 - o(1/p))$ ,  $w'M^{-1}w \geq \frac{1}{4} \left[ (\sqrt{\delta r} + \frac{(|S_1| - |S_0|)\vartheta}{\sqrt{\delta r}})_+ \right]^2 (2 \log(p)) + O((\log(p))^\gamma)$ . Since  $\gamma < 1$ ,  $O((\log(p))^\gamma)$  is negligible. We note that  $w'M^{-1}w \sim \chi_{|\mathcal{I}_0|}^2(0)$ . Inserting this back to (47), the left hand side  $\leq \epsilon_p^{|S_0|} P(\chi_{|\mathcal{I}_0|}^2(0) \geq [(\sqrt{\delta r} + (|S_1| - |S_0|)\vartheta/\sqrt{\delta r})_+]^2 (\log(p)/2)) + o(1/p)$ . Assume  $\text{sgn}(\beta_j) \neq \text{sgn}(\hat{\beta}_j)$ , and fix all parameters except  $\delta$ ,  $S_0$  and  $S_1$ . By arguments similar to the proof of Lemma 18, the above quantity cannot achieve its maximum in the cases where  $S_0 = S_1$ . Hence we only need to consider the cases where  $S_0 \neq S_1$ . We also only need to consider the cases where  $\max(|S_0|, |S_1|) \leq m_0$ , since the sum of the probabilities of other cases is controlled by  $p^{1-(m_0+1)\vartheta}$ . The claim follows by the definitions of  $\rho_j^*$ .  $\blacksquare$

#### 4. Simulations

We conduct a small-scale simulation study to investigate the numerical performance of Graphlet Screening and compare it with the lasso and the UPS. The subset selection is not included for comparison since it is computationally NP hard. We consider the experiments for both random design and fixed design, where as before, the parameters  $(\epsilon_p, \tau_p)$  are tied to  $(\vartheta, r)$  by  $\epsilon_p = p^{-\vartheta}$  and  $\tau_p = \sqrt{2r \log(p)}$  (we assume  $\sigma = 1$  for simplicity in this section).

In random design settings where  $p$  is not very large, we follow the spirit of the refined UPS in Ji and Jin (2011) and propose the iterative Graphlet Screening algorithm where we

iterate Graphlet Screening for a few times ( $\leq 5$ ). The main purpose for the iteration is to denoise the Gram matrix; see Ji and Jin (2011, Section 3) for more discussion.

Even with the refinement as in Ji and Jin (2011, Section 3), UPS behaves poorly for most examples presented below. Over close investigations, we find out that this is due to the threshold choice in the initial  $U$ -step is too low, and increasing the threshold largely increases the performance. Note that the purpose of this step is to denoise the Gram matrix (Ji and Jin, 2011, Section 3), not for signal retainment, and so a larger threshold helps.

In this section, we use this improved version of refined UPS, but for simplicity, we still call it the refined UPS. With that being said, recall that UPS is unable to resolve the problem of signal cancellation, so it usually performs poorer than GS, especially when the effect of signal cancellation is strong. For this reason, part of the comparison is between GS and the lasso only.

The experiments with random design contain the following steps.

1. Fix  $(p, \vartheta, r, \mu, \Omega)$  such that  $\mu \in \Theta_p(\tau_p)$ . Generate a vector  $b = (b_1, b_2, \dots, b_p)'$  such that  $b_i \stackrel{iid}{\sim} \text{Bernoulli}(\epsilon_p)$ , and set  $\beta = b \circ \mu$ .
2. Fix  $\kappa$  and let  $n = n_p = p^\kappa$ . Generate an  $n \times p$  matrix with *iid* rows from  $N(0, (1/n)\Omega)$ .
3. Generate  $Y \sim N(X\beta, I_n)$ , and apply the iterative Graphlet Screening, the refined UPS and the lasso.
4. Repeat 1-3 independently, and record the average Hamming distances or the Hamming ratio, the ratio of the Hamming distance and the number of the signals.

The steps for fixed design experiments are similar, except for that  $n_p = p$ ,  $X = \Omega^{1/2}$  and we apply GS and UPS directly.

GS uses tuning parameters  $(m_0, \mathcal{Q}, u^{gs}, v^{gs})$ . We set  $m_0 = 3$  for our experiments, which is usually large enough due to signal sparsity. The choice of  $\mathcal{Q}$  is not critical, as long as the corresponding parameter  $q$  satisfies (30), and we use the maximal  $\mathcal{Q}$  satisfying (30) in most experiments. Numerical studies below (e.g., Experiment 5a) support this point. In principle, the optimal choices of  $(u^{gs}, v^{gs})$  depend on the unknown parameters  $(\epsilon_p, \tau_p)$ , and how to estimate them in general settings is a lasting open problem (even for linear models with orthogonal designs). Fortunately, our studies (e.g., Experiment 5b-5d) show that mis-specifying parameters  $(\epsilon_p, \tau_p)$  by a reasonable amount does not significantly affect the performance of the procedure. For this reason, in most experiments below, assuming  $(\epsilon_p, \tau_p)$  are known, we set  $(u^{gs}, v^{gs})$  as  $(\sqrt{2 \log(1/\epsilon_p)}, \tau_p)$ . For the iterative Graphlet Screening, we use the same tuning parameters in each iteration.

For the UPS and the refined UPS, we use the tuning parameters  $(u^{ups}, v^{ups}) = (u^{gs}, v^{gs})$ . For both the iterative Graphlet Screening and the refined UPS, we use the following as the initial estimate:  $\hat{\beta}_i = \text{sgn}(\tilde{Y}_i) \cdot 1\{|\tilde{Y}_i| \geq \tau_p\}$ ,  $1 \leq i \leq p$ , where  $\tilde{Y} = X'Y$ . The main purpose of initial estimate is to denoise the Gram matrix, not for screening. We use *glmnet* package (Friedman et al., 2010) to perform lasso. To be fair in comparison, we apply the lasso with all tuning parameters, and we report the Hamming error associated with the “best” tuning parameter.

The simulations contain 6 different experiments which we now describe separately.

*Experiment 1.* The goal of this experiment is two-fold. First, we compare GS with UPS and the lasso in the fixed design setting. Second, we investigate the minimum signal strength levels  $\tau_p$  required by these three methods to yield exact recovery, respectively.

Fixing  $p = 0.5 \times 10^4$ , we let  $\epsilon_p = p^{-\vartheta}$  for  $\vartheta \in \{0.25, 0.4, 0.55\}$ , and  $\tau_p \in \{6, 7, 8, 9, 10\}$ . We use a fixed design model where  $\Omega$  is a symmetric diagonal block-wise matrix, where each block is a  $2 \times 2$  matrix, with 1 on the diagonals, and  $\pm 0.7$  on the off-diagonals (the signs alternate across different blocks). Recall the  $\beta = b \circ \mu$ . For each pair of  $(\epsilon_p, \tau_p)$ , we generate  $b$  as  $p$  iid samples from  $Bernoulli(\epsilon_p)$ , and we let  $\mu$  be the vector where the signs of  $\mu_i = \pm 1$  with equal probabilities, and  $|\mu_i| \stackrel{iid}{\sim} 0.8\nu_{\tau_p} + 0.2h$ , where  $\nu_{\tau_p}$  is the point mass at  $\tau_p$  and  $h(x)$  is the density of  $\tau_p(1 + V/6)$  with  $V \sim \chi_1^2$ . The average Hamming errors across 40 repetitions are tabulated in Table 3. For all  $(\vartheta, \tau_p)$  in this experiment, GS behaves more satisfactorily than the UPS, which in turn behaves more satisfactorily than the lasso.

Suppose we say a method yields ‘exact recovery’ if the average Hamming error  $\leq 3$ . Then, when  $\vartheta = 0.25$ , the minimum  $\tau_p$  for GS to yield exact recovery is  $\tau_p \approx 8$ , but that for UPS and the lasso are much larger ( $\geq 10$ ). For larger  $\vartheta$ , the differences are less prominent, but the pattern is similar.

The comparison between GS and UPS is particularly interesting. Due to the block structure of  $\Omega$ , as  $\vartheta$  decreases, the signals become increasingly less sparse, and the effects of signal cancellation become increasingly stronger. As a result, the advantage of GS over the UPS becomes increasingly more prominent.

	$\tau_p$	6	7	8	9	10
$\vartheta = 0.25$	Graphic Screening	24.7750	8.6750	2.8250	0.5250	0.1250
	UPS	48.5500	34.6250	36.3500	30.8750	33.4000
	lasso	66.4750	47.7000	43.5250	35.2500	35.0500
$\vartheta = 0.40$	Graphic Screening	6.9500	2.1500	0.4000	0.0750	0.0500
	UPS	7.7500	4.0000	2.2000	2.7750	2.4250
	lasso	12.8750	6.8000	4.3250	3.7500	2.6750
$\vartheta = 0.55$	Graphic Screening	1.8750	0.8000	0.3250	0.2250	0.1250
	UPS	1.8750	0.8000	0.3250	0.2250	0.1250
	lasso	2.5000	1.1000	0.7750	0.2750	0.1250

Table 3: Comparison of average Hamming errors (Experiment 1).

*Experiment 2.* In this experiment, we compare GS, UPS and the lasso in the random design setting, and investigate the effect of signal cancellation on their performances. We fix  $(p, \kappa, \vartheta, r) = (0.5 \times 10^4, 0.975, 0.35, 3)$ , and assume  $\Omega$  is blockwise diagonal. We generate  $\mu$  as in Experiment 1, but to better illustrate the difference between UPS and GS in the presence of signal cancellation, we generate the vector  $b$  differently and allow it to depend on  $\Omega$ . The experiment contains 2 parts, 2a and 2b.

In Experiment 2a,  $\Omega$  is the block-wise matrix where each block is 2 by 2 matrix with 1 on the diagonals and  $\pm 0.5$  on the off diagonals (the signs alternate on adjacent blocks). According to the blocks in  $\Omega$ , the set of indices  $\{1, 2, \dots, p\}$  are also partitioned into blocks accordingly. For any fixed  $\vartheta$  and  $\eta \in \{0, 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.1, 0.2\}$ , we ran-

domly choose  $(1 - 2p^{-\vartheta})$  fraction of the blocks (of indices) where  $b$  is 0 at both indices,  $2(1 - \eta)p^{-\vartheta}$  fraction of the blocks where  $b$  is 0 at one index and 1 at the other (two indices are equally likely to be 0),  $2\eta p^{-\vartheta}$  fraction of the blocks where  $b$  is 1 on both indices.

Experiment 2b has similar settings, where the difference is that (a) we choose  $\Omega$  to be a diagonal block matrix where each block is a 4 by 4 matrix (say, denoted by  $A$ ) satisfying  $A(i, j) = 1\{i = j\} + 0.4 \cdot 1\{|i - j| = 1\} \cdot \text{sgn}(6 - i - j) + 0.05\{|i - j| \geq 2\} \cdot \text{sgn}(5.5 - i - j)$ ,  $1 \leq i, j \leq 4$ , and (b)  $(1 - 4p^{-\vartheta})$  is the fraction of blocks where  $b$  is nonzero in  $k = 0$  indices,  $4(1 - \eta)p^{-\vartheta}$  is that for  $k = 1$ , and  $4\eta p^{-\vartheta}$  is that for  $k \in \{2, 3, 4\}$  in total. In a block where  $\beta$  is nonzero at  $k$  indices, all configurations with  $k = 1$  are equally likely, and all those with  $k \in \{2, 3, 4\}$  are equally likely.

The average Hamming ratio results across 40 runs for two Experiment 2a and 2b are reported in Figure 3, where UPS and GS consistently outperform the lasso. Additionally, when  $\eta$  is small, the effect of signal cancellation is negligible, so UPS and GS have similar performances. However, when  $\eta$  increases, the effects of signal cancellation grows, and the advantage of GS over UPS becomes increasingly more prominent.

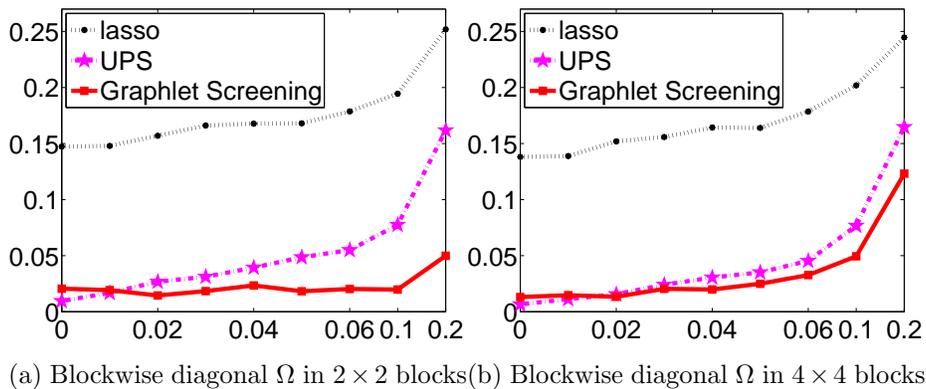


Figure 3: Hamming ratio results in Experiment 2

Through Experiment 1-2, the comparison of UPS and GS is more or less understood. For this reason, we do not include UPS for study in Experiment 3-5, but we include UPS for study in Experiment 6 where we investigate robustness of all three methods.

*Experiment 3.* In this experiment, we investigate how different choices of signal vector  $\beta$  affect the comparisons of GS and the lasso. We use a random design model, and  $\Omega$  is a symmetric tri-diagonal correlation matrix where the vector on each sub-diagonal consists of blocks of  $(.4, .4, -.4)'$ . Fix  $(p, \kappa) = (0.5 \times 10^4, 0.975)$  (note  $n = p^\kappa \approx 4,000$ ). We let  $\epsilon_p = p^{-\vartheta}$  with  $\vartheta \in \{0.35, 0.5\}$  and let  $\tau_p \in \{6, 8, 10\}$ . For each combination of  $(\epsilon_p, \tau_p)$ , we consider two choices of  $\mu$ . For the first choice, we let  $\mu$  be the vector where all coordinates equal to  $\tau_p$  (note  $\beta$  is still sparse). For the second one, we let  $\mu$  be as in Experiment 1. The average Hamming ratios for both procedures across 40 repetitions are tabulated in Table 4.

*Experiment 4.* In this experiment, we generate  $\beta$  the same way as in Experiment 1, and investigate how different choices of design matrices affect the performance of the two methods. Setting  $(p, \vartheta, \kappa) = (0.5 \times 10^4, 0.35, 0.975)$  and  $\tau_p \in \{6, 7, 8, 9, 10, 11, 12\}$ , we use

$\tau_p$		6		8		10	
Signal Strength		Equal	Unequal	Equal	Unequal	Equal	Unequal
$\vartheta = 0.35$	Graphic Screening	0.0810	0.0825	0.0018	0.0034	0	0.0003
	lasso	0.2424	0.2535	0.1445	0.1556	0.0941	0.1109
$\vartheta = 0.5$	Graphic Screening	0.0315	0.0297	0.0007	0.0007	0	0
	lasso	0.1107	0.1130	0.0320	0.0254	0.0064	0.0115

Table 4: Hamming ratio results of Experiment 3, where “Equal” and “Unequal” stand for the first and the second choices of  $\mu$ , respectively.

Gaussian random design model for the study. The experiment contains 3 sub-experiments 4a-4c.

In Experiment 4a, we set  $\Omega$  as the symmetric diagonal block-wise matrix, where each block is a  $2 \times 2$  matrix, with 1 on the diagonals, and  $\pm 0.5$  on the off-diagonals (the signs alternate across different blocks). The average Hamming ratios of 40 repetitions are reported in Figure 4.

In Experiment 4b, we set  $\Omega$  as a symmetric penta-diagonal correlation matrix, where the main diagonal are ones, the first sub-diagonal consists of blocks of  $(.4, .4, -.4)'$ , and the second sub-diagonal consists of blocks of  $(.05, -.05)'$ . The average Hamming ratios across 40 repetitions are reported in Figure 4.

In Experiment 4c, we generate  $\Omega$  as follows. First, we generate  $\Omega$  using the function *sprandsym*( $p, K/p$ ) in *matlab*. We then set the diagonals of  $\Omega$  to be zero, and remove some of entries so that  $\Omega$  is  $K$ -sparse for a pre-specified  $K$ . We then normalize each non-zero entry by the sum of the absolute values in that row or that column, whichever is larger, and multiply each entry by a pre-specified positive constant  $A$ . Last, we set the diagonal elements to be 1. We choose  $K = 3$  and  $A = 0.7$ , draw 5 different  $\Omega$  with this method, and for each of them, we draw  $(X, \beta, z)$  10 times independently. The average Hamming ratios are reported in Figure 4. The results suggest that GS is consistently better than the lasso.

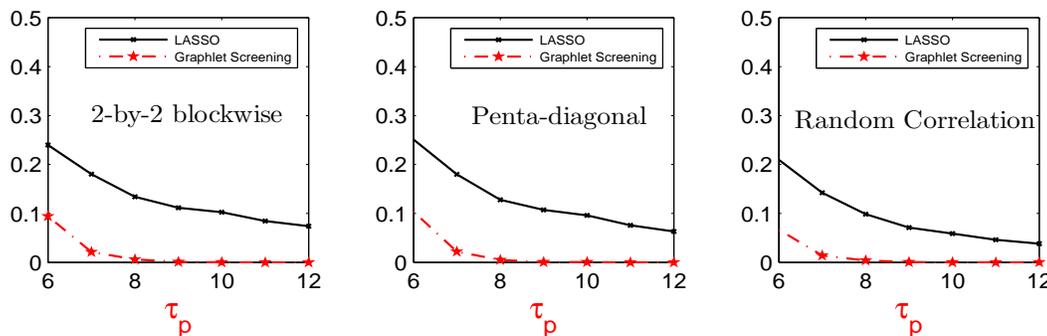


Figure 4:  $x$ -axis:  $\tau_p$ .  $y$ -axis: Hamming ratios. Left to right: Experiment 4a, 4b, and 4c.

*Experiment 5.* In this experiment, we investigate how sensitive GS is with respect to the tuning parameters. The experiment contains 4 sub-experiments, 5a-5d. In Experiment 5a, we investigate how sensitive the procedure is with respect to the tuning parameter  $q$  in  $\mathcal{Q}$  where we assume  $(\epsilon_p, \tau_p)$  are known; recall that the main results hold as long as  $q$  fall into the range given in (30). In Experiment 5b-5d, we mis-specify  $(\epsilon_p, \tau_p)$  by a reasonably small amount, and investigate how the mis-specification affect the performance of the procedure. For the whole experiment, we choose  $\beta$  the same as in Experiment 1, and  $\Omega$  the same as in Experiment 4b. We use a fixed design model in Experiment 5a-5c, and a random design model in Experiment 5d. For each sub-experiment, the results are based on 40 independent repetitions. We now describe the sub-experiments with details.

In Experiment 5a, we choose  $\vartheta \in \{0.35, 0.6\}$  and  $r \in \{1.5, 3\}$ . In GS, let  $q_{max} = q_{max}(\hat{D}, \hat{F})$  be the maximum value of  $q$  satisfying (30). For each combination of  $(\vartheta, r)$  and  $(\hat{D}, \hat{F})$ , we choose  $q(\hat{D}, \hat{F}) = q_{max}(\hat{D}, \hat{F}) \times \{0.7, 0.8, 0.9, 1, 1.1, 1.2\}$  for our experiment. The results are tabulated in Table 5, which suggest that different choices of  $q$  have little influence over the variable selection errors. We must note that the larger we set  $q(\hat{D}, \hat{F})$ , the faster the algorithm runs.

$q(\hat{F}, \hat{D})/q_{max}(\hat{F}, \hat{D})$	0.7	0.8	0.9	1	1.1	1.2
$(\vartheta, r) = (0.35, 1.5)$	0.0782	0.0707	0.0661	0.0675	0.0684	0.0702
$(\vartheta, r) = (0.35, 3)$	0.0066	0.0049	0.0036	0.0034	0.0033	0.0032
$(\vartheta, r) = (0.6, 1.5)$	0.1417	0.1417	0.1417	0.1417	0.1417	0.1417
$(\vartheta, r) = (0.6, 3)$	0.0089	0.0089	0.0089	0.0089	0.0089	0.0089

Table 5: Hamming ratio results in Experiment 5a.

In Experiment 5b, we use the same settings as in Experiment 5a, but we assume  $\vartheta$  (and so  $\epsilon_p$ ) is unknown (the parameter  $r$  is assumed as known, however), and let  $\vartheta^*$  is the misspecified value of  $\vartheta$ . We take  $\vartheta^* \in \vartheta \times \{0.85, 0.925, 1, 1.075, 1.15, 1.225\}$  for the experiment.

In Experiment 5c, we use the same settings as in Experiment 5b, but we assume  $r$  (and so  $\tau_p$ ) is unknown (the parameter  $\vartheta$  is assumed as known, however), and let  $r^*$  is the misspecified value of  $r$ . We take  $r^* = r \times \{0.8, 0.9, 1, 1.1, 1.2, 1.3\}$  for the experiment.

In Experiment 5b-5c, we run GS with tuning parameters set as in Experiment 1, except  $\vartheta$  or  $r$  are replaced by the misspecified counterparts  $\vartheta^*$  and  $r^*$ , respectively. The results are reported in Table 6, which suggest that the mis-specifications have little effect as long as  $r^*/r$  and  $\vartheta^*/\vartheta$  are reasonably close to 1.

In Experiment 5d, we re-examine the mis-specification issue in the random design setting. We use the same settings as in Experiment 5b and Experiment 5c, except for (a) while we use the same  $\Omega$  as in Experiment 5b, the design matrix  $X$  are generated according to the random design model as in Experiment 4b, and (b) we only investigate for the case of  $r = 2$  and  $\vartheta \in \{0.35, 0.6\}$ . The results are summarized in Table 7, which is consistent with the results in 5b-5c.

*Experiment 6.* In this experiment, we investigate the robustness of all three methods for the mis-specification of the linear model (1). We use the random design setting as in Experiment 4b, except that we fix  $(\vartheta, r) = (0.35, 3)$ . The experiment contains 3 sub-

$\vartheta^*/\vartheta$	0.85	0.925	1	1.075	1.15	1.225
$(\vartheta, r) = (0.35, 1.5)$	0.0799	0.0753	0.0711	0.0710	0.0715	0.0746
$(\vartheta, r) = (0.35, 3)$	0.0026	0.0023	0.0029	0.0030	0.0031	0.0028
$(\vartheta, r) = (0.6, 1.5)$	0.1468	0.1313	0.1272	0.1280	0.1247	0.1296
$(\vartheta, r) = (0.6, 3)$	0.0122	0.0122	0.0139	0.0139	0.0130	0.0147
$r^*/r$	0.8	0.9	1	1.1	1.2	1.3
$(\vartheta, r) = (0.35, 1.5)$	0.0843	0.0731	0.0683	0.0645	0.0656	0.0687
$(\vartheta, r) = (0.35, 3)$	0.0062	0.0039	0.0029	0.0030	0.0041	0.0054
$(\vartheta, r) = (0.6, 1.5)$	0.1542	0.1365	0.1277	0.1237	0.1229	0.1261
$(\vartheta, r) = (0.6, 3)$	0.0102	0.0076	0.0085	0.0059	0.0051	0.0076

Table 6: Hamming ratio results in Experiment 5b (top) and in Experiment 5c (bottom).

$\vartheta^*/\vartheta$	0.85	0.925	1	1.075	1.15	1.225
$(\vartheta, r) = (0.35, 2)$	0.1730	0.1367	0.1145	0.1118	0.0880	0.0983
$(\vartheta, r) = (0.6, 2)$	0.0583	0.0591	0.0477	0.0487	0.0446	0.0431
$r^*/r$	0.8	0.9	1	1.1	1.2	1.3
$(\vartheta, r) = (0.35, 2)$	0.1881	0.1192	0.1275	0.1211	0.1474	0.1920
$(\vartheta, r) = (0.6, 2)$	0.0813	0.0515	0.0536	0.0397	0.0442	0.0510

Table 7: Hamming ratio results in Experiment 5d.

experiments, 6a-6c, where we consider three scenarios where the linear model (1) is in question: the presence of non-Gaussianity, the presence of missing predictors, and the presence of non-linearity, correspondingly.

In Experiment 6a, we assume the noise vector  $z$  in Model (1) is non-Gaussian, where the coordinates are iid samples from a  $t$ -distribution with the same degree of freedom (df) (we assume that  $z$  is normalized so each coordinate has unit variance), where the df range in  $\{3, 4, 5, 6, 7, 8, 9, 10, 30, 50\}$ . Figure 5a shows how the Hamming ratios (based on 40 independent repetitions) change when the  $df$  decreases. The results suggest that all three methods are reasonably robust against non-Gaussianity, but GS continues to have the best performance.

In Experiment 6b, we assume that the true model is  $Y = X\beta + z$  where  $(X, \beta, z)$  are generated as in 4b, but the model that is accessible to us is a misspecified model where the some of the true predictors are missing. Fix  $\eta \in (0, 1)$ , and let  $S(\beta)$  be the support of  $\beta$ . For each  $i \in S(\beta)$ , we flip a coin that lands on head with probability  $\eta$ , and we retain  $i$  if and only if the coin lands on tail. Let  $S^* \subset S(\beta)$  be the set of retained indices, and let  $R = S^* \cup S^c$ . The misspecified model we consider is then  $Y = X^{\otimes, R}\beta^R + z$ .

For the experiment, we let  $\eta$  range in  $0.02 \times \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$ . The average Hamming ratios (based on 40 independent repetitions) are reported in Figure 5b. The results suggest that all three results are reasonably robust to missing predictors, with the lasso being the most robust. However, as long as the proportion of true predictors that are missing is reasonably small (say,  $\eta \leq .1$ ), GS continues to outperform UPS and the lasso.

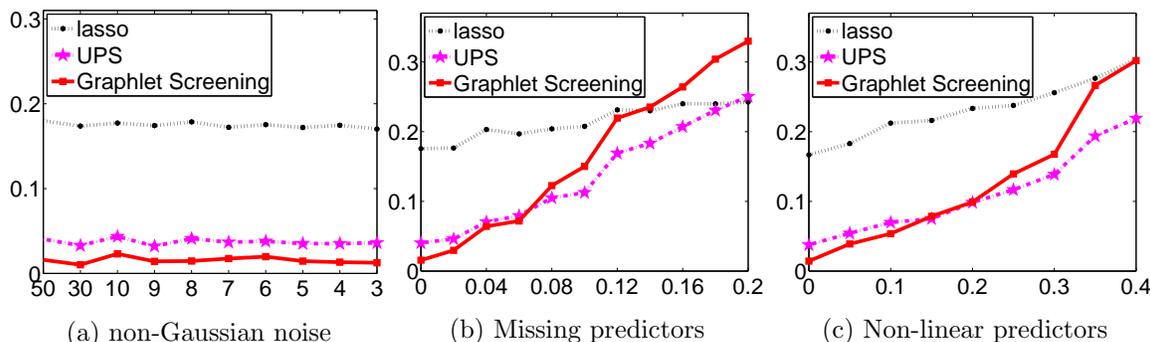


Figure 5: Hamming ratio results in Experiment 6

In Experiment 6c, for  $i = 1, \dots, n$ , the true model is an additive model in the form of  $Y_i = \sum_{j=1}^p f_j(X_{ij})\beta_j + z_i$ , but what is accessible to us is the linear model  $Y_i = \sum_{j=1}^p X_{ij}\beta_j + z_i$  (and thus misspecified; the true model is non-linear). For experiment, we let  $(X, \beta, z)$  be generated as in 4b, and  $S(\beta)$  be the support of  $\beta$ . Fixing  $\eta \in (0, 1)$ , for each  $i \in S(\beta)$ , we flip a coin that lands on head with probability  $\eta$ , and let  $S_{nl} \subset S(\beta)$  be all indices of the heads. We then randomly split  $S_{nl}$  into two sets  $S_1$  and  $S_2$  evenly. For  $j = 1, \dots, p$ , we define  $f_j(x) = [\text{sgn}(x)x^2 \cdot \mathbf{1}\{j \in S_1\} + (e^{\sqrt{n}x} - a_j) \cdot \mathbf{1}\{j \in S_2\} + x \cdot \mathbf{1}\{j \in S_{nl}^c\}]/c_j$ , where  $a_j$  and  $c_j$  are constants such that  $\{f_j(X(i, j))\}_{i=1}^n$  has mean 0 and variance  $1/n$ .

For the experiment, we let  $\eta$  range in  $.05 \times \{0, 1, 2, 3, 4, 5, 6, 7, 8\}$ . The average Hamming ratios (based on 40 independent repetitions) are reported in Figure 5c. The results suggest that all three methods are reasonably robust to the presence of nonlinearity, and GS continues to outperform UPS and the lasso when the degree of nonlinearity is moderate (say,  $\eta < .2$ ).

## 5. Connection to Existing Literature and Possible Extensions

Our idea of utilizing graph sparsity is related to the graphical lasso (Meinshausen and Bühlmann, 2006; Friedman et al., 2008), which also attempts to exploit graph structure. However, the setting we consider here is different from that in Meinshausen and Bühlmann (2006); Friedman et al. (2008), and our emphasis on precise optimality and calibration is also very different. Our method allows nearly optimal detection of very rare and weak effects, because they are based on careful analysis that has revealed a number of subtle high-dimensional effects (e.g., phase transitions) that we properly exploit. Existing methodologies are not able to exploit or capture these phenomena, and can be shown to fail at the levels of rare and weak effects where we are successful.

The paper is closely related to the recent work by Fan and Lv (2008), Ji and Jin (2011) and Genovese et al. (2012). Both Ji and Jin (2011) and this paper use a similar rare and weak signal framework and a similar random design model. However, they are different in important ways, since the technical device developed in Ji and Jin (2011) can not be extended to the current study. For example, the lower bound derived in this paper is different and sharper than that in Ji and Jin (2011). Also, the procedure in Ji and Jin (2011) relies on marginal regression for screening. The limitation of marginal regression

is that it neglects the graph structure of GOSD for the regularized Gram matrix (1.5), so that it is incapable of picking variables that have *weak marginal* correlation but *significant joint* correlation to  $Y$ . Correct selection of such hidden significant variables, termed as the challenge of *signal cancellation* (Wasserman and Roeder, 2009), is the difficulty at the heart of the variable selection problem. One of the main innovation of GS is that it uses the graph structure to guide the screening, so that it is able to successfully overcome the challenge of signal cancellation.

Additionally, two papers have very different objectives, and consequently the underlying analysis are very different. The main results of each of these two papers can not be deduced from the other. For example, to assess optimality, Ji and Jin (2011) uses the criterion of the partition of the phase diagram, while the current paper uses the minimax Hamming distance. Given the complexity of the high dimensional variable selection, one type of optimality does not imply the other, and vice versa. Also, the main result in Ji and Jin (2011) focuses on conditions under which the optimal rate of convergence is  $L_p p^{1-(\vartheta+r)^2/(4r)}$  for the *whole* phase space. While this overlaps with our Corollaries 10 and 11, we must note that Ji and Jin (2011) deals with the much more difficult cases where  $r/\vartheta$  can get arbitrary large; and to ensure the success in that case, they assume very strong conditions on the design matrix and the range of the signal strength. On the other hand, the main focus of the current paper is on optimal variable selection under conditions (of the Gram matrix  $G$  as well as the signal vector  $\beta$ ) that are as general as possible.

While the study in this paper has been focused on the Random Design model  $\text{RD}(\vartheta, \kappa, \Omega)$ , extensions to deterministic design models are straightforward (in fact, in Corollary 7, we have already stated some results on deterministic design models), and the omission of discussion on the latter is largely for technical simplicity and the sake of space. In fact, for models with deterministic designs, since the likelihood ratio test in the derivation of the lower bound matches the penalized MLE in the cleaning step of GS, the optimality of GS follows from the *Sure Screening and Separable After Screening* properties of GS. The proof of these properties, and therefore the optimality of GS, follows the same line as those for random design as long as  $\max_j |\sum_i \beta_i G(i, j) I\{\Omega^{*,\delta}(i, j) = 0\}|/\tau_p$  is small. This last condition on  $G$  holds when  $p^{1-\vartheta}\|G - \Omega\|_\infty = o(1)$  with a certain  $\Omega \in \mathcal{M}_p^*(\gamma, c_0, g, A)$ . Alternatively, this condition holds when  $p^{1-\vartheta}\|G - \Omega\|_\infty^2 \log p = o(1)$  with  $\Omega \in \mathcal{M}_p^*(\gamma, c_0, g, A)$ , provided that  $\text{sgn}(\beta_j)$  are iid symmetric random variables as in Candes and Plan (2009).

In this paper, we assume the signal vector  $\beta$  is independent of the design matrix  $X$ , and that  $\beta$  is modeled by a Bernoulli model through  $\beta = b \circ \mu$ . Both assumptions can be relaxed. In fact, in order for GS to work, what we really need is some *decomposability* condition similar to that in Lemma 1, where except for negligible probabilities, the maximum size of the graphlets  $m_0^* = m_0^*(S(\beta), G, \delta)$  is small. In many situations, we can show that  $m_0^*$  does not exceed a fixed integer. One of such examples is as follows. Suppose for any fixed integer  $m \geq 1$  and size- $m$  subset  $S$  of  $\{1, 2, \dots, p\}$ , there are constants  $C > 0$  and  $d > 0$  such that the conditional probability  $P(\beta_j \neq 0, \forall j \in S | X) \leq Cp^{-dm}$ . In fact, when such a condition holds, the claim follows since  $\mathcal{G}^{*,\delta}$  has no more than  $C(eK)^m$  size- $m$  connected subgraphs if it is  $K$ -sparse. See the proof of Lemma 1 for details. Note that when  $\epsilon_p = p^{-\vartheta}$  as in the ARW, then the condition holds for the Bernoulli model in Lemma 1, with  $d = \vartheta$ . Note also that the Bernoulli model can be replaced by some Ising models.

Another interesting direction of future research is the extension of GS to more general models such as logistic regression. The extension of the lower bound in Theorem 6 is relatively simple since the degree of GOLF can be bounded using the true  $\beta$ . This indicates the optimality of GS in logistic and other generalized linear models as long as proper generalized likelihood ratio or Bayes tests are used in both the *GS*- and *GC*-steps.

## 6. Proofs

In this section, we provide all technical proofs. We assume  $\sigma = 1$  for simplicity.

### 6.1 Proof of Lemma 1

When  $\mathcal{G}_S^{*,\delta}$  contains a connected subgraph of size  $\geq m_0 + 1$ , it must contain a connected subgraph with size  $m_0 + 1$ . By Frieze and Molloy (1999), there are  $\leq p(eK)^{m_0+1}$  connected subgraph of size  $m_0 + 1$ . Therefore, the probability that  $\mathcal{G}_S^{*,\delta}$  has a connected subgraph of size  $(m_0 + 1) \leq p(eK)^{m_0+1} \epsilon_p^{m_0+1}$ . Combining these gives the claim.  $\blacksquare$

### 6.2 Proof of Theorem 6

Write for short  $\rho_j^* = \rho_j^*(\vartheta, r, a, \Omega)$ . Without loss of generality, assume  $\rho_1^* \leq \rho_2^* \leq \dots \leq \rho_p^*$ . We construct indices  $i_1 < i_2 < \dots < i_m$  as follows. (a) start with  $B = \{1, 2, \dots, p\}$  and let  $i_1 = 1$ , (b) updating  $B$  by removing  $i_1$  and all nodes  $j$  that are neighbors of  $i_1$  in GOLF, let  $i_2$  be the smallest index, (c) defining  $i_3, i_4, \dots, i_m$  by repeating (b), and terminates the process when no indices is left in  $B$ . Since each time we remove at most  $d_p(\mathcal{G}^\circ)$  nodes, it follows that

$$\sum_{j=1}^p p^{-\rho_j^*} \leq d_p(\mathcal{G}^\circ) \sum_{k=1}^m p^{-\rho_{i_k}^*}. \quad (49)$$

For each  $1 \leq j \leq p$ , as before, let  $(V_{0j}^*, V_{1j}^*)$  be the least favorable configuration, and let  $(\theta_{*j}^{(0)}, \theta_{*j}^{(1)}) = \operatorname{argmin}_{\{\theta^{(0)} \in B_{V_{0j}^*}, \theta^{(1)} \in B_{V_{1j}^*}, \operatorname{sgn}(\theta^{(0)}) \neq \operatorname{sgn}(\theta^{(1)})\}} \alpha(\theta^{(0)}, \theta^{(1)}; \Omega)$ . By our notations, it is seen that

$$\rho_j^* = \eta(V_{0j}^*, V_{1j}^*; \Omega), \quad \alpha^*(V_{0j}^*, V_{1j}^*; \Omega) = \alpha(\theta_{*j}^{(0)}, \theta_{*j}^{(1)}; \Omega). \quad (50)$$

In case  $(\theta_{*j}^{(0)}, \theta_{*j}^{(1)})$  is not unique, pick one arbitrarily. We construct a  $p \times 1$  vector  $\mu^*$  as follows. Fix  $j \in \{i_1, \dots, i_m\}$ . For all indices in  $V_{0j}^*$ , set the constraint of  $\mu^*$  on these indices to be  $\theta_{*j}^{(0)}$ . For any index  $i \notin \cup_{k=1}^m V_{0i_k}^*$ , set  $\mu_i^* = \tau_p$ . Since

$$\operatorname{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) \geq \inf_{\hat{\beta}} H_p(\hat{\beta}; \epsilon_p, n_p, \mu^*, \Omega) = \inf_{\hat{\beta}} \sum_{i=1}^p P(\operatorname{sgn}(\hat{\beta}_i) \neq \operatorname{sgn}(\beta_i)), \quad (51)$$

it follows that

$$\operatorname{Hamm}_p^*(\vartheta, \kappa, r, a, \Omega) \geq \sum_{k=1}^m \sum_{j \in V_{0i_k}^* \cup V_{1i_k}^*} P(\operatorname{sgn}(\hat{\beta}_j) \neq \operatorname{sgn}(\beta_j)), \quad (52)$$

where  $\beta = b \circ \mu^*$  in (51)-(52). Combining (49) and (52), to show the claim, we only need to show that for any  $1 \leq k \leq m$  and any procedure  $\hat{\beta}$ ,

$$\sum_{j \in V_{0i_k} \cup V_{1i_k}} P(\text{sgn}(\hat{\beta}_j) \neq \text{sgn}(\beta_j)) \geq L_p p^{-\rho_{i_k}^*}. \tag{53}$$

Towards this end, we write for short  $V_0 = V_{0i_k}$ ,  $V_1 = V_{1i_k}$ ,  $V = V_0 \cup V_1$ ,  $\theta^{(0)} = \theta_{*i_k}^{(0)}$ , and  $\theta^{(1)} = \theta_{*i_k}^{(1)}$ . Note that by Lemma 22,

$$|V| \leq (\vartheta + r)^2 / (2\vartheta r).$$

Consider a test setting where under the null  $H_0$ ,  $\beta = \beta^{(0)} = b \circ \mu^*$  and  $I_V \circ \beta^{(0)} = I_V \circ \theta^{(0)}$ , and under the alternative  $H_1$ ,  $\beta = \beta^{(1)}$  which is constructed by keeping all coordinates of  $\beta^{(0)}$  unchanged, except those coordinates in  $V$  are perturbed in a way so that  $I_V \circ \beta^{(1)} = I_V \circ \theta^{(1)}$ . In this construction, both  $\beta^{(0)}$  and  $\beta^{(1)}$  are assumed as known, but we don't know which of  $H_0$  and  $H_1$  is true. In the literature, it is known that  $\inf_{\hat{\beta}} \sum_{j \in V} P(\text{sgn}(\hat{\beta}_j) \neq \text{sgn}(\beta_j))$  is not smaller than the minimum sum of Type I and Type II errors associated with this testing problem.

Note that by our construction and (50), the right hand side is  $\alpha^*(V_0, V_1; \Omega)$ . At the same time, it is seen the optimal test statistic is  $Z \equiv (\theta^{(1)} - \theta^{(0)})' X'(Y - X\beta^{(0)})$ . It is seen that up to some negligible terms,  $Z \sim N(0, \alpha^*(V_0, V_1; \Omega)\tau_p^2)$  under  $H_0$ , and  $Z \sim N(\alpha^*(V_0, V_1; \Omega)\tau_p^2, \alpha^*(V_0, V_1; \Omega)\tau_p^2)$  under  $H_1$ . The optimal test is to reject  $H_0$  when  $Z \geq t[\alpha^*(V_0, V_1; \Omega)]^{1/2}\tau_p$  for some threshold  $t$ , and the minimum sum of Type I and Type II error is

$$\inf_t \{ \epsilon_p^{|V_0|} \bar{\Phi}(t) + \epsilon_p^{|V_1|} \Phi(t - [\alpha^*(V_0, V_1; \Omega)]^{1/2}\tau_p) \}.$$

Here, we have used  $P(H_0) \sim \epsilon_p^{|V_0|}$  and  $P(H_1) \sim \epsilon_p^{|V_1|}$ , as a result of the Binomial structure in  $\beta$ . It follows that  $\sum_{j \in V} P(\text{sgn}(\hat{\beta}_j) \neq \text{sgn}(\beta_j)) \gtrsim \inf_t \{ \epsilon_p^{|V_0|} \bar{\Phi}(t) + \epsilon_p^{|V_1|} \Phi(t - [\alpha^*(V_0, V_1; \Omega)]^{1/2}\tau_p) \}$ . Using Mills' ratio and definitions, the right hand side  $\geq L_p p^{-\eta(V_0, V_1; \Omega)}$ , and (53) follows by recalling (50). ■

### 6.3 Proof of Corollaries 10, 11, and 12

When  $a > a_g^*(\Omega)$ ,  $\rho_j^*(\vartheta, r, a, \Omega)$  does not depend on  $a$ , and have an alternative expression as follows. For any subsets  $D$  and  $F$  of  $\{1, 2, \dots, p\}$ , let  $\omega(D, F; \Omega)$  be as in (28). Introduce  $\rho(D, F; \Omega) = \rho(D, F; \vartheta, r, a, \Omega, p)$  by

$$\rho(D, F; \Omega) = \frac{(|D| + 2|F|)\vartheta}{2} + \begin{cases} \frac{1}{4}\omega(D, F; \Omega)r, & |D| \text{ is even,} \\ \frac{\vartheta}{2} + \frac{1}{4}[(\sqrt{\omega(D, F; \Omega)}r - \frac{\vartheta}{\sqrt{\omega(D, F; \Omega)r}})_+]^2, & |D| \text{ is odd.} \end{cases} \tag{54}$$

The following lemma is proved in Section 6.3.4.

**Lemma 18** Fix  $m_0 \geq 1$ ,  $(\vartheta, \kappa) \in (0, 1)^2$ ,  $r > 0$ ,  $c_0 > 0$ , and  $g > 0$  such that  $\kappa > (1 - \vartheta)$ . Suppose the conditions of Theorem 6 hold, and that for sufficiently large  $p$ , (26) is satisfied. Then as  $p \rightarrow \infty$ ,  $\rho_j^*(\vartheta, r, a, \Omega)$  does not depend on  $a$ , and satisfies  $\rho_j^*(\vartheta, r, a, \Omega) = \min_{\{D, F\}: j \in D \cup F, D \cap F = \emptyset, D \neq \emptyset, |D \cup F| \leq g} \rho(D, F; \Omega)$ .

We now show Corollaries 10-12. Write for short  $\omega = \rho(D, F; \Omega)$ ,  $T = r/\vartheta$ , and  $\lambda_k^* = \lambda_k^*(\Omega)$ . The following inequality is frequently used below, the proof of which is elementary so we omit it:

$$\omega \geq \lambda_k^*|D|, \quad \text{where } k = |D| + |F|. \tag{55}$$

To show these corollaries, it is sufficient to show for all subsets  $D$  and  $F$  of  $\{1, 2, \dots, p\}$ ,

$$\rho(D, F; \Omega) \geq (\vartheta + r)^2/(4r), \quad |D| \geq 1, \tag{56}$$

where  $\rho(D, F; \Omega)$  is as in (54). By basic algebra, (56) is equivalent to

$$\begin{cases} (\omega T + 1/(\omega T) - 2)1\{\omega T \geq 1\} \geq (T + 1/T - 2(|D| + 2|F|)), & |D| \text{ is odd,} \\ \omega \geq \frac{2}{T}[(T + 1/T)/2 + 1 - (|D| + 2|F|)], & |D| \text{ is even.} \end{cases} \tag{57}$$

Note that when  $(|D|, |F|) = (1, 0)$ , this claim holds trivially, so it is sufficient to consider the case where

$$|D| + |F| \geq 2. \tag{58}$$

We now show that (57) holds under the conditions of each of corollaries.

### 6.3.1 PROOF OF COROLLARY 10

In this corollary,  $1 < (T + 1/T)/2 \leq 3$ , and if either (a)  $|D| + 2|F| \geq 3$  and  $|D|$  is odd or (b)  $|D| + 2|F| \geq 4$  and  $|D|$  is even, the right hand side of (57)  $\leq 0$ , so the claim holds trivially. Therefore, all we need to show is the case where  $(|D|, |F|) = (2, 0)$ . In this case, since each off-diagonal coordinate  $\leq 4\sqrt{2} - 5 \equiv \rho_0$ , it follows from definitions and basic algebra that  $\omega \geq 2(1 - \rho_0) = 4(3 - 2\sqrt{2})$ , and (57) follows by noting that  $\frac{2}{T}[(T + 1/T)/2 + 1 - (|D| + 2|F|)] = (1 - 1/T)^2 \leq 4(3 - 2\sqrt{2})$ . ■

### 6.3.2 PROOF OF COROLLARY 11

In this corollary,  $1 < (T + 1/T)/2 \leq 5$ . First, we consider the case where  $|D|$  is odd. By similar argument, (57) holds trivially when  $|D| + 2|F| \geq 5$ , so all we need to consider is the case  $(|D|, |F|) = (1, 1)$  and the case  $(|D|, |F|) = (3, 0)$ . In both cases,  $|D| + 2|F| = 3$ . By (55), when  $\omega T < 1$ , there must be  $T < 1/\min(\lambda_2^*, 3\lambda_3^*)$ . By the conditions of this corollary, it follows  $T < (5 + 2\sqrt{6})/4 < 3 + 2\sqrt{2}$ . When  $1 < T < 3 + 2\sqrt{2}$ , there is  $T + 1/T - 6 < 0$ , and thus (57) holds for  $\omega T < 1$ . When  $\omega T \geq 1$ , (57) holds if and only if  $\omega T + \frac{1}{\omega T} - 2 \geq T + 1/T - 6$ . By basic algebra, this holds if

$$\omega \geq \frac{1}{4}[(1 - 1/T) + \sqrt{(1 - 1/T)^2 - 4/T}]^2. \tag{59}$$

Note that the right hand side of (59) is a monotone in  $T$  and has a maximum of  $(3 + 2\sqrt{2})(5 - 2\sqrt{6})$  at  $T = (5 + 2\sqrt{6})$ . Now, on one other hand, when  $(|D|, |F|) = (1, 0)$ , by (55) and conditions of the corollary,  $\omega \geq 3\lambda_3^* > (3 + 2\sqrt{2})(5 - 2\sqrt{6})$ . On the other hand, when  $(|D|, |F|) = (1, 1)$ , by basic algebra and that each off-diagonal coordinate of  $\Omega \leq \sqrt{1 + (\sqrt{6} - \sqrt{2})/(1 + \sqrt{3/2})} \equiv \rho_1$  in magnitude,  $\omega \geq 1 - \rho_1^2 = (3 + 2\sqrt{2})(5 - 2\sqrt{6})$ . Combining these gives (57).

We now consider the case where  $|D|$  is even. By similar argument, (57) holds when  $|D| + 2|F| \geq 6$ , so all we need is to show is that (57) holds for the following three cases:  $(|D|, |F|) = (4, 0), (2, 1), (2, 0)$ . Equivalently, this is to show that  $\omega \geq \frac{2}{T}[(T + 1/T)/2 - 3]$  in the first two cases and that  $\omega \geq \frac{2}{T}[(T + 1/T)/2 - 1]$  in the last case. Similarly, by the monotonicity of the right hand side of these inequalities, all we need to show is  $\omega \geq 4(5 - 2\sqrt{6})$  in the first two cases, and  $\omega \geq 8(5 - 2\sqrt{6})$  in the last case. Now, on one hand, using (55),  $\omega \geq 4\lambda_4^*$  in the first case, and  $\omega \geq 2\lambda_3^*$  in the second case, so by the conditions of the corollary,  $\omega \geq 4(5 - 2\sqrt{6})$  in the first two cases. On the other hand, in the last case, since all off-diagonal coordinates of  $\Omega \leq 8\sqrt{6} - 19 \equiv \rho_0$  in magnitude, and  $\omega \geq 2(1 - \rho_0) = 8(5 - 2\sqrt{6})$ . Combining these gives (57).  $\blacksquare$

### 6.3.3 PROOF OF COROLLARY 12

Let  $N$  be the unique integer such that  $2N - 1 \leq (T + 1/T)/2 < 2N + 1$ . First, we consider the case where  $|D|$  is odd. Note that when  $|D| + 2|F| \geq 2N + 1$ , the right hand side of (57)  $\leq 0$ , so all we need to consider is the case  $|D| + 2|F| \leq 2N - 1$ . Write for short  $k = k(D, F) = |D| + |F|$  and  $j = j(D, F) = (|D| + 2|F| + 1)/2$ . By (58), definitions, and that  $|D| + 2|F| \leq 2N - 1$ , it is seen that  $2 \leq k \leq 2N - 1$  and  $(k + 1)/2 \leq j \leq \min\{k, N\}$ .

By the condition of the corollary,  $\lambda_k^* \geq \frac{(T+1/T)/2-2j+2+\sqrt{[(T+1/T)/2-2j+2]^2-1}}{T(2k-2j+1)}$ . Note that  $|D| = 2k - 2j + 1$ . Combining these with (55) gives  $\omega T \geq (2k - 2j + 1)\lambda_k^* T \geq (T + 1/T)/2 - 2j + 2 + \sqrt{[(T + 1/T)/2 - 2j + 2]^2 - 1} \geq 1$ . and (57) follows by basic algebra.

We now consider the case where  $|D|$  is even. Similarly, the right hand side of (57) is negative when  $|D| + 2|F| \geq 2(N + 1)$ , so we only need to consider the case where  $|D| + 2|F| \leq 2N$ . Similarly, write for short  $k = k(D, F) = |D| + |F|$  and  $j = (|D| + 2|F|)/2$ . It is seen that  $2 \leq k \leq 2N$  and  $k/2 \leq j \leq \min\{k - 1, N\}$ . By the conditions of the corollary,  $\lambda_k^* \geq \frac{(T+1/T)/2+1-2j}{T(k-j)}$ . Note that  $|D| = k - j$ . It follows from (55) that  $\omega \geq 2(k - j)\lambda_k^* \geq \frac{2}{T}[(T + 1/T)/2 + 1 - 2j]$ , and (57) follows.  $\blacksquare$

### 6.3.4 PROOF OF LEMMA 18

Let sets  $V_0$  and  $V_1$  and vectors  $\theta^{(0)}$  and  $\theta^{(1)}$  be as in Section 2.5, and let  $V = V_0 \cup V_1$ . By definition,  $\rho_j^*(\vartheta, r, a, \Omega)$  can be written as the minimum of  $I$  and  $II$ , where  $I = \min_{\{(V_0, V_1): j \in V_1 \cup V_0, V_0 \neq V_1\}} \eta(V_0, V_1; \Omega)$  and  $II = \min_{\{V_0: j \in V_0 \cup V_1, V_0 = V_1\}} \eta(V_0, V_1; \Omega)$ . So to show the claim, it is sufficient to show

$$I = \min_{\{(D, F): j \in D \cup F, D \cap F = \emptyset, D \neq \emptyset, |D \cup F| \leq g\}} \rho(D, F; \Omega), \quad II \geq I. \quad (60)$$

Consider the first claim in (60). Write for short  $F = F(V_0, V_1) = V_0 \cap V_1$  and  $D = D(V_0, V_1) = V \setminus F$ . By the definitions,  $D \neq \emptyset$ . The key is to show that when  $|V_0 \cup V_1| \leq g$ ,

$$\alpha^*(V_0, V_1; \Omega) = \omega(D, F; \Omega). \quad (61)$$

Towards this end, note that by definitions,  $\alpha^*(V_0, V_1; \Omega) = \alpha(\theta_*^{(0)}, \theta_*^{(1)})$ , where  $(\theta_*^{(0)}, \theta_*^{(1)}) = \operatorname{argmin}_{\{\theta^{(0)} \in B_{V_0}, \theta^{(1)} \in B_{V_1}\}} \alpha(\theta^{(0)}, \theta^{(1)})$ . By  $a > a_g^*(\Omega)$  and the way  $a_g^*(\Omega)$  is defined,  $(\theta_*^{(0)}, \theta_*^{(1)})$  remains as the solution of the optimization problem if we relax the conditions  $\theta^{(i)} \in B_{V_i}$  to

that of  $\theta^{(i)} = I_{V_i} \circ \mu^{(i)}$ , where  $\mu^{(i)} \in \Theta_p(\tau_p)$  (so that upper bounds on the signal strengths are removed),  $i = 0, 1$ . As a result,

$$\alpha^*(V_0, V_1; \Omega) = \min_{\{\theta^{(i)} \in I_{V_i} \circ \mu^{(i)}, \mu^{(i)} \in \Theta_p(\tau_p), i=0,1\}} \alpha(\theta^{(0)}, \theta^{(1)}). \quad (62)$$

We now study (62). For short, write  $\xi = \tau_p^{-1}(\theta^{(1)} - \theta^{(0)})^V$ ,  $\Omega_{VV} = \Omega^{V,V}$ ,  $\xi_D = \tau_p^{-1}(\theta^{(1)} - \theta^{(0)})^D$ , and similarly for  $\Omega_{DD}$ ,  $\Omega_{DF}$ ,  $\Omega_{FD}$ ,  $\Omega_{FF}$ , and  $\xi_F$ . Without loss of generality, assume the indices in  $D$  come first in  $V$ . It follows

$$\Omega_{VV} = \begin{pmatrix} \Omega_{DD} & \Omega_{DF} \\ \Omega_{FD} & \Omega_{FF} \end{pmatrix},$$

and

$$\alpha(\theta^{(0)}, \theta^{(1)}) = \xi' \Omega_{VV} \xi = \xi'_D \Omega_{DD} \xi_D + 2\xi'_D \Omega_{DF} \xi_F + \xi'_F \Omega_{FF} \xi_F. \quad (63)$$

By definitions, it is seen that there is no constraint on the coordinates of  $\xi_F$ , so to optimize the quadratic form in (61), we need to choose  $\xi$  is a way such that  $\xi_F = -\Omega_{FF}^{-1} \Omega_{FD} \xi_D$ , and that  $\xi_D$  minimizes  $\xi'_D (\Omega_{DD} - \Omega_{DF} \Omega_{FF}^{-1} \Omega_{FD}) \xi_D$ , where every coordinate of  $\xi_D \geq 1$  in magnitude. Combining these with (62) gives (61).

At the same time, we rewrite

$$I = \min_{\{(D,F): j \in D \cup F, D \neq \emptyset, D \cap F = \emptyset\}} \left\{ \min_{\{(V_0, V_1): V_0 \cup V_1 = D \cup F, V_0 \cap V_1 = F\}} \eta(V_0, V_1; \Omega) \right\}. \quad (64)$$

By similar arguments as in the proof of Lemma 22, the subsets  $(V_0, V_1)$  that achieve the minimum of  $\eta(V_0, V_1; \Omega)$  must satisfy  $|V_0 \cup V_1| \leq g$ . Using (61), for any fixed  $D$  and  $F$  such that  $|D \cup F| \leq g$ ,  $D \neq \emptyset$  and  $D \cap F = \emptyset$ , the term in the big bracket on the right hand side is  $\min_{\{(V_0, V_1): V_0 \cup V_1 = D \cup F, V_0 \cap V_1 = F\}} \left\{ \frac{(2|F| + |D|)\vartheta}{2} + \frac{||V_1| - |V_0||\vartheta}{2} + \frac{1}{4} [(\sqrt{\omega(D, F; \Omega)r} - \frac{||V_1| - |V_0||\vartheta}{\sqrt{\omega(D, F; \Omega)r}})_+]^2 \right\}$ . It is worth noting that for fixed  $D$  and  $F$ , the above quantity is monotone increasing with  $||V_1| - |V_0||$ . When  $|D|$  is even, the minimum is achieved at  $(V_0, V_1)$  with  $|V_0| = |V_1|$ , and when  $|D|$  is odd, the minimum is achieved at  $(V_0, V_1)$  with  $||V_1| - |V_0|| = 1$ , and in both cases, the minimum is  $\rho(D, F; \Omega)$ . Inserting this to (64), it is seen that

$$I = \min_{\{(D,F): j \in D \cup F, D \cap F = \emptyset, D \neq \emptyset, |D \cup F| \leq g\}} \rho(D, F; \Omega),$$

which is the first claim in (60).

Consider the second claim of (60). In this case, by definitions,  $V_0 = V_1$  but  $\text{sgn}(\theta^{(0)}) \neq \text{sgn}(\theta^{(1)})$ . Redefine  $D$  as the subset of  $V_0$  where the signs of the coordinates of  $\theta^{(0)}$  do not equal to those of  $\theta^{(1)}$ , and let  $F = V \setminus D$ . By definitions, it is seen that  $\alpha^*(V_0, V_0; \Omega) = 4\alpha^*(F, V_0; \Omega)$ , where we note  $D \neq \emptyset$  and  $F \neq V_0$ . By the definition of  $\eta(V_0, V_1; \Omega)$ , it follows that  $\eta(V_0, V_0; \Omega) \geq \eta(F, V_0; \Omega)$ , and the claim follows.  $\blacksquare$

#### 6.4 Proof of Lemma 15

Write for short  $\rho_j^* = \rho_j^*(\vartheta, a, r, \Omega)$ . To show the claim, it is sufficient to show that for any fixed  $1 \leq j \leq p$ ,

$$P(j \notin \mathcal{U}_p^*, \beta_j \neq 0) \leq L_p [p^{-\rho_j^*} + p^{-(m_0+1)\vartheta} + o(1/p)]. \quad (65)$$

Using Lemma 14 and Ji and Jin (2011, Lemma 3.1), there is an event  $A_p$  that depends on  $(X, \beta)$  such that  $P(A_p^c) \leq o(1/p)$  and that over the event,  $\Omega^{*,\delta}$  is  $K$ -sparse with  $K = C(\log(p))^{1/\gamma}$ ,  $\|\Omega^{*,\delta} - \Omega\|_\infty \leq (\log(p))^{-(1-\gamma)}$ ,  $\|(X'X - \Omega)\beta\|_\infty \leq C\|\Omega\|\sqrt{2\log(p)}p^{-[(\kappa-(1-\vartheta)]/2}$ , and for all subset  $B$  with size  $\leq m_0$ ,  $\|G^{B,B} - \Omega^{B,B}\|_\infty \leq L_p p^{-\kappa/2}$ . Recall that  $\mathcal{G}^{*,\delta}$  is the GOSD and  $\mathcal{G}_S^{*,\delta}$  is the subgraph of the GOSD formed by the nodes in the support of  $\beta$ ,  $S(\beta) = \{1 \leq j \leq p : \beta_j \neq 0\}$ . When  $\beta_j \neq 0$ , there is a unique component  $\mathcal{I}_0$  such that  $j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*,\delta}$  ( $A \triangleleft B$  means that  $A$  is component or maximal connected subgraph of  $B$ ). Let  $B_p$  be the event  $|\mathcal{I}_0| \leq m_0$ . By Frieze Frieze and Molloy (1999), it is seen that  $P(B_p^c \cap A_p) \leq L_p p^{-(m_0+1)\vartheta}$ . So to show (65), it is sufficient to show that

$$P(j \notin \mathcal{U}_p^*, j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*,\delta}, A_p \cap B_p) \leq L_p p^{-\rho_j^*}. \quad (66)$$

Now, in the screening procedure, when we screen  $\mathcal{I}_0$ , we have  $\mathcal{I}_0 = \hat{D} \cup \hat{F}$  as in (8). Since the event  $\{j \notin \mathcal{U}_p^*, j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*,\delta}\}$  is contained in the event  $\{T(Y, \hat{D}, \hat{F}) < t(\hat{D}, \hat{F})\}$ ,  $P(j \notin \mathcal{U}_p^*, j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*,\delta}, A_p \cap B_p) \leq P(T(Y, \hat{D}, \hat{F}) \leq t(\hat{D}, \hat{F}), j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*,\delta}, A_p \cap B_p)$ , where the right hand side does not exceed

$$\sum_{(\mathcal{I}_0, D, F): j \in \mathcal{I}_0 \text{ \& } \mathcal{I}_0 = D \cup F \text{ is a partition}} P(T(Y, D, F) \leq t(D, F), j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*,\delta}, A_p \cap B_p);$$

note that  $(\mathcal{I}_0, D, F)$  do not depend on  $z$  (but may still depend on  $(X, \beta)$ ). First, note that over the event  $A_p$ , there are at most  $(eK)^{m_0+1}$   $\mathcal{I}_0$  such that  $j \in \mathcal{I}_0$  and  $|\mathcal{I}_0| \leq m_0$ . Second, note that for each  $\mathcal{I}_0$ , there are only finite ways to partition it to  $D$  and  $F$ . Last, note that for any fixed  $j$  and  $\mathcal{I}_0$ ,  $P(j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*,\delta}) \leq \epsilon_p^{|\mathcal{I}_0|}$ . Combining these observations, to show (66), it is sufficient to show that for any such triplet  $(\mathcal{I}_0, D, F)$ ,

$$\epsilon_p^{|\mathcal{I}_0|} P(T(Y, D, F) \leq t(D, F) | \{j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*,\delta}\} \cap A_p \cap B_p) \leq L_p p^{-\rho_j^*}. \quad (67)$$

We now show (67). Since  $\lambda_{m_0}^*(\Omega) \geq C > 0$ , it follows from the definition of  $A_p$  and basic algebra that for any realization of  $(X, \beta)$  in  $A_p \cap B_p$ ,

$$\|(G^{\mathcal{I}_0, \mathcal{I}_0})^{-1}\|_\infty \leq C. \quad (68)$$

Recall that  $\tilde{Y} = X'Y$  and denote for short  $y = (G^{\mathcal{I}_0, \mathcal{I}_0})^{-1}\tilde{Y}^{\mathcal{I}_0}$ . It is seen that

$$y = \beta^{\mathcal{I}_0} + w + rem, \quad w \sim N(0, (G^{\mathcal{I}_0, \mathcal{I}_0})^{-1}), \quad rem \equiv (G^{\mathcal{I}_0, \mathcal{I}_0})^{-1} G^{\mathcal{I}_0, \mathcal{I}_0^c} \beta^{\mathcal{I}_0^c}. \quad (69)$$

Since  $\mathcal{I}_0$  is a component of  $\mathcal{G}_S^{*,\delta}$ ,  $(\Omega^{*,\delta})_{\mathcal{I}_0, \mathcal{I}_0^c} \beta^{\mathcal{I}_0^c} = 0$ . Therefore, we can write  $rem = (G^{\mathcal{I}_0, \mathcal{I}_0})^{-1}(I + II)$ , where  $I = (G^{\mathcal{I}_0, \mathcal{I}_0^c} - \Omega^{\mathcal{I}_0, \mathcal{I}_0^c})\beta^{\mathcal{I}_0^c}$  and  $II = [\Omega^{\mathcal{I}_0, \mathcal{I}_0^c} - (\Omega^{*,\delta})_{\mathcal{I}_0, \mathcal{I}_0^c}]\beta^{\mathcal{I}_0^c}$ . By the definition of  $A_p$ ,  $\|I\|_\infty \leq C\sqrt{2\log(p)}p^{-[\kappa-(1-\vartheta)]/2}$ , and  $\|II\|_\infty \leq \|\Omega - \Omega^{*,\delta}\|_\infty \|\beta^{\mathcal{I}_0^c}\|_\infty \leq C\tau_p(\log(p))^{-(1-\gamma)}$ . Combining these with (68) gives  $\|rem\|_\infty \leq C\tau_p(\log(p))^{-(1-\gamma)}$ .

At the same time, let  $y_1, w_1$ , and  $rem^1$  be the restriction of  $y, w$ , and  $rem$  to indices in  $D$ , correspondingly, and let  $H = [G^{D,D} - G^{D,F}(G^{F,F})^{-1}G^{F,D}]$ . By (69) and direct calculations,  $T(Y, D, F) = y_1' H y_1$ ,  $y_1 \sim N(\beta^D + rem^1, H^{-1})$ , and so  $T(Y, D, F)$  is distributed as  $\chi_{|D|}^2(\delta)$ , where the non-central parameter is  $(\beta^D + rem^1)' H (\beta^D + rem^1) = \delta + O((\log(p))^\gamma)$  and  $\delta \equiv (\beta^D)' H \beta^D$ . Since  $\lambda_{m_0}^*(\Omega) \geq C$ ,  $\delta \geq C\tau_p^2$  and is the dominating term. It follows that

$$P(T(Y, D, F) \leq t(D, F) | \{j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*,\delta}\} \cap A_p \cap B_p) \lesssim P(\chi_{|D|}^2(\delta) \leq t(D, F)). \quad (70)$$

Now, first, by definitions,  $\delta \geq 2\omega(D, F; \Omega)r \log(p)$ , so by basic knowledge on non-central  $\chi^2$ ,

$$P(\chi_{|D|}^2(\delta) \leq t(D, F)) \leq P(\chi_{|D|}^2(2\omega(D, F; \Omega)r \log(p)) \leq t(D, F)). \quad (71)$$

Second, recalling  $t(D, F) = 2q \log(p)$ , we have

$$P(\chi_{|D|}^2(2\omega(D, F; \Omega)r \log(p)) \leq t(D, F)) \leq L_p p^{-[(\sqrt{\omega(D, F; \Omega)r} - \sqrt{q})_+]^2}. \quad (72)$$

Inserting (71)-(72) into (70) and recalling  $\epsilon_p = p^{-\vartheta}$ ,

$$\epsilon_p^{|\mathcal{I}_0|} P(T(Y, D, F) \leq t(D, F) | \{j \in \mathcal{I}_0 \triangleleft \mathcal{G}_S^{*, \delta}\} \cap A_p \cap B_p) \leq L_p p^{-(|\mathcal{I}_0| \vartheta + [(\sqrt{\omega(D, F; \Omega)r} - \sqrt{q})_+]^2)}. \quad (73)$$

By the choice of  $q$  and direct calculations,

$$|\mathcal{I}_0| \vartheta + [(\sqrt{\omega(D, F; \Omega)r} - \sqrt{q})_+]^2 \geq \rho(D, F; \Omega) \geq \rho_j^*, \quad (74)$$

where  $\rho(D, F; \Omega)$  as in (54). Combining (73)-(74) gives (67).  $\blacksquare$

## 6.5 Proof of Lemma 16

In the screening stage, suppose we pick the threshold  $t(\hat{D}, \hat{F}) = 2q \log(p)$  in a way such that there is a constant  $q_0(\vartheta, r, \kappa) > 0$  such that  $q = q(\hat{D}, \hat{F}) \geq q_0(\vartheta, r, \kappa) > 0$ . Recall that  $\mathcal{G}^{*, \delta}$  denotes the GOSD. Let  $\mathcal{U}_p^*$  be the set of retained indices. Viewing it as a subgraph of  $\mathcal{G}^{*, \delta}$ ,  $\mathcal{U}_p^*$  decomposes into many components  $\mathcal{U}_p^* = \mathcal{I}^{(1)} \cup \mathcal{I}^{(2)} \dots \cup \mathcal{I}^{(N)}$ . Recall that  $\tilde{Y} = X'Y$ . The following lemma is proved below.

**Lemma 19** *Suppose the settings and conditions are as in Lemma 16. There exists a constant  $c_1 = c_1(\vartheta, r, \kappa, \gamma, A) > 0$  such that with probability at least  $1 - o(1/p)$ , for any component  $\mathcal{I}_0 \triangleleft \mathcal{U}_p^*$ ,  $\|\tilde{Y}^{\mathcal{I}_0}\|^2 \geq 2c_1 |\mathcal{I}_0| \log(p)$ .*

The remaining part of the proof is similar to that of Ji and Jin (2011, Lemma 2.3) so we omit it. We note that however Lemma 19 is new and needs a much harder proof.  $\blacksquare$

### 6.5.1 PROOF OF LEMMA 19

First, we need some notations. Let  $\mathcal{I}_0$  be a component of  $\mathcal{U}_p^*$ , and let  $\mathcal{I}_0^{(i)}$ ,  $1 \leq i \leq N_0$ , be all connected subgraphs with size  $\leq m_0$ , listed in the order as in the GS-step, where  $N_0$  is an integer that may depend on  $(X, Y)$ . For each  $1 \leq i \leq N_0$ , let  $\mathcal{I}_0^{(i)} = \hat{D}^{(i)} \cup \hat{F}^{(i)}$  be the *exactly the same* partition when we screen  $\mathcal{I}_0^{(i)}$  in the  $m_0$ -stage  $\chi^2$ -screening of the GS-step. In our list, we only keep  $\mathcal{I}_0^{(i)}$  such that  $\hat{D}^{(i)} \cap \mathcal{I}_0 \neq \emptyset$ . Since  $\mathcal{I}_0$  is a component of  $\mathcal{U}_p^*$  and  $\mathcal{I}_0^{(i)}$  is a connected subgraph, it follows from the way that the  $\chi^2$ -screening is designed and the definition of  $\hat{D}^{(i)}$  that

$$\mathcal{I}_0^{(i)} \subset \mathcal{I}_0, \quad \text{and} \quad \hat{D}^{(i)} = \mathcal{I}_0^{(i)} \setminus (\cup_{j=1}^{i-1} \mathcal{I}_0^{(j)}), \quad 1 \leq i \leq N_0,$$

and

$$\mathcal{I}_0 = \hat{D}^{(1)} \cup \hat{D}^{(2)} \dots \cup \hat{D}^{(N_0)} \text{ is a partition,} \quad (75)$$

where  $\hat{F}^{(1)}$  is empty.

Now, for each  $1 \leq i \leq N_0$ , recall that as long as  $G^{\mathcal{I}_0^{(i)}, \mathcal{I}_0^{(i)}}$  is non-singular, the  $\chi^2$ -test score in GS is  $T(Y, \hat{D}^{(i)}, \hat{F}^{(i)}) = T(Y, \hat{D}^{(i)}, \hat{F}^{(i)}; \mathcal{I}_0^{(i)}, X, p, n) = (\tilde{Y}^{\mathcal{I}_0^{(i)}})'(G^{\mathcal{I}_0^{(i)}, \mathcal{I}_0^{(i)}})^{-1}\tilde{Y}^{\mathcal{I}_0^{(i)}} - (\tilde{Y}^{\hat{F}^{(i)}})'(G^{\hat{F}^{(i)}, \hat{F}^{(i)}})^{-1}\tilde{Y}^{\hat{F}^{(i)}}$ . By basic algebra and direct calculations, it can be verified that  $T(Y, \hat{D}^{(i)}, \hat{F}^{(i)}) = \|W_i\|^2$ , where  $W_i = W(\tilde{Y}, \hat{D}^{(i)}, \hat{F}^{(i)}; \mathcal{I}_0^{(i)}, X, p, n)$  is defined as  $W_i = V_i^{-1/2}y_i$ , and for short,  $V_i = G^{\hat{D}^{(i)}, \hat{D}^{(i)}} - G^{\hat{D}^{(i)}, \hat{F}^{(i)}}(G^{\hat{F}^{(i)}, \hat{F}^{(i)}})^{-1}G^{\hat{F}^{(i)}, \hat{D}^{(i)}}$ ,  $y_i = \tilde{Y}^{\hat{D}^{(i)}} - G^{\hat{D}^{(i)}, \hat{F}^{(i)}}(G^{\hat{F}^{(i)}, \hat{F}^{(i)}})^{-1}\tilde{Y}^{\hat{F}^{(i)}}$ . At the same time, for a constant  $\delta > 0$  to be determined, define  $\tilde{\Omega}$  by  $\tilde{\Omega}(i, j) = G(i, j) \cdot 1\{|G(i, j)| \geq \delta\}$ . The definition of  $\tilde{\Omega}$  is the same as that of  $\Omega^{*, \delta}$ , except for that the threshold  $\delta$  would be selected differently. We introduce a counterpart of  $W_i$  which we call  $W_i^*$ ,

$$W_i^* = V_i^{-1/2}y_i^*. \tag{76}$$

where  $y_i^* = \tilde{Y}^{\hat{D}^{(i)}} - \tilde{\Omega}^{\hat{D}^{(i)}, \hat{F}^{(i)}}(\tilde{\Omega}^{\hat{F}^{(i)}, \hat{F}^{(i)}})^{-1}\tilde{Y}^{\hat{F}^{(i)}}$ . Let  $W^* = ((W_1^*)', (W_2^*)', \dots, (W_{N_0}^*)')'$ , and define  $|\mathcal{I}_0| \times |\mathcal{I}_0|$  matrices  $H_1$  and  $H_2$  as follows:  $H_1$  is a diagonal block-wise matrix where the  $i$ -th block is  $V_i^{-1/2}$ , and  $H_2 = \tilde{H}_2^{\mathcal{I}_0, \mathcal{I}_0}$ , where  $\tilde{H}_2$  is a  $p \times p$  matrix such that for every component  $\mathcal{I}_0$  of  $\mathcal{U}_p^*$ , and  $\hat{D}^{(i)}$  and  $\hat{F}^{(i)}$  defined on each component,  $\tilde{H}_2^{\hat{D}^{(i)}, \hat{F}^{(i)}} = -(\tilde{\Omega})^{\hat{D}^{(i)}, \hat{F}^{(i)}}[(\tilde{\Omega})^{\hat{F}^{(i)}, \hat{F}^{(i)}}]^{-1}$ ,  $\tilde{H}_2^{\hat{D}^{(i)}, \hat{D}^{(i)}} = I_{|\hat{D}^{(i)}|}$ , and that the coordinates of  $\tilde{H}_2$  are zero elsewhere. Here  $I_k$  stands for  $k \times k$  identity matrix. From the definitions, it is seen that

$$W^* = H_1 H_2 \tilde{Y}^{\mathcal{I}_0}. \tag{77}$$

Compared with  $W_i$ ,  $W_i^*$  is relatively easier to study, for it induces column-sparsity of  $H_2$ . In fact, using (Ji and Jin, 2011, Lemma 2.2, 3.1), there is an event  $A_p$  that depends on  $(X, \beta)$  such that  $P(A_p^c) \leq o(1/p^2)$  and that over the event, for all subset  $B$  with size  $\leq m_0$ ,

$$\|G^{B, B} - \Omega^{B, B}\|_\infty \leq L_p p^{-\kappa/2}.$$

The following lemma is proved below.

**Lemma 20** *Fix  $\delta > 0$  and suppose the conditions in Lemma 19 hold. Over the event  $A_p$ , there is a constant  $C > 0$  such that each row and column of  $\tilde{H}_2$  has no more than  $C$  nonzero coordinates.*

We are now ready to show Lemma 19. To begin with, note that since we accept  $\hat{D}^{(i)}$  when we graphlet-screen  $\mathcal{I}_0^{(i)}$  and  $|\hat{D}^{(i)}| \leq m_0$ ,

$$\|W_i\|^2 \geq 2(q_0/m_0)|\hat{D}^{(i)}|\log(p). \tag{78}$$

At the same time, by basic algebra,  $\|W_i - W_i^*\| \leq \|V_i^{-1/2}\| \|y_i - y_i^*\|$ , and  $\|y_i - y_i^*\| \leq \|G^{\hat{D}^{(i)}, \hat{F}^{(i)}}(G^{\hat{F}^{(i)}, \hat{F}^{(i)}})^{-1} - (\tilde{\Omega})^{\hat{D}^{(i)}, \hat{F}^{(i)}}((\tilde{\Omega})^{\hat{F}^{(i)}, \hat{F}^{(i)}})^{-1}\|_\infty \cdot \|\tilde{Y}^{\hat{F}^{(i)}}\|$ . First, since  $\lambda_{m_0}^*(\Omega) \geq C$ , it is seen that over the event  $A_p$ ,  $\|V_i^{-1/2}\| \leq C$ . Second, by similar reasons, it is not hard to see that except for probability  $o(p^{-2})$ ,  $\|G^{\hat{D}^{(i)}, \hat{F}^{(i)}}(G^{\hat{F}^{(i)}, \hat{F}^{(i)}})^{-1} - (\tilde{\Omega})^{\hat{D}^{(i)}, \hat{F}^{(i)}}((\tilde{\Omega})^{\hat{F}^{(i)}, \hat{F}^{(i)}})^{-1}\|_\infty \leq C\delta^{1-\gamma}$ , and  $\|\tilde{Y}^{\hat{F}^{(i)}}\| \leq C\sqrt{\log(p)} \leq C\tau_p$ . Combining these gives

$$\|W_i - W_i^*\| \leq C\delta^{1-\gamma}\tau_p.$$

Inserting this to (78), if we choose  $\delta$  to be a sufficiently small constant,  $\|W_i^*\|^2 \geq \frac{1}{2}\|W_i\|^2 \geq (q_0/m_0)|\hat{D}^{(i)}|\log(p)$ .

At the same time, by definitions, it follows from  $\|V_i^{-1/2}\| \leq C$  that  $\|H_1\| \leq C$ . Also, since over the event  $A_p$ , each coordinate of  $H_2$  is bounded from above by a constant in magnitude, it follows from Lemma 20 that  $\|H_2\| \leq C$ . Combining this with (75)-(77), it follows from basic algebra that except for probability  $o(p^{-2})$ ,  $(q_0/m_0)|\mathcal{I}_0|\log(p) \leq \|W^*\|^2 \leq \|H_1 H_2 \tilde{Y}^{\mathcal{I}_0}\|^2 \leq C\|\tilde{Y}^{\mathcal{I}_0}\|^2$ , and the claim follows since  $m_0$  is a fixed integer.  $\blacksquare$

### 6.5.2 PROOF OF LEMMA 20

By definitions, it is equivalent to show that over the event  $A_p$ , each row and column of  $\tilde{H}_2$  has finite nonzero coordinates. It is seen that each row of  $\tilde{H}_2$  has  $\leq m_0$  nonzeros, so all we need to show is that each column of  $\tilde{H}_2$  has finite nonzeros.

Towards this end, we introduce a new graph  $\tilde{\mathcal{G}} = (V, E)$ , where  $V = \{1, 2, \dots, p\}$  and nodes  $i$  and  $j$  are connected if and only if  $|\tilde{\Omega}(i, j)| \neq 0$ . This definition is the same as GOSD, except that  $\Omega^{*,\delta}$  is substituted by  $\tilde{\Omega}$ . It is seen that over the event  $A_p$ , for any  $\Omega \in \mathcal{M}_p^*(\gamma, c_0, g, A)$ ,  $\tilde{\mathcal{G}}$  is  $K$ -sparse with  $K \leq C\delta^{-1/\gamma}$ . The key for the proof is to show that for any  $k \neq \ell$  such that  $\tilde{H}_2(k, \ell) \neq 0$ , there is a path with length  $\leq (m_0 - 1)$  in  $\tilde{\mathcal{G}}$  that connects  $k$  and  $\ell$ .

To see the point, we note that when  $\tilde{H}_2(k, \ell) \neq 0$ , there must be an  $i$  such that  $k \in \hat{D}^{(i)}$  and  $\ell \in \hat{F}^{(i)}$ . We claim that there is a path in  $\mathcal{I}_0^{(i)}$  (which is regarded as a subgraph of  $\tilde{\mathcal{G}}$ ) that connects  $k$  and  $\ell$ . In fact, if  $k$  and  $\ell$  are not connected in  $\mathcal{I}_0^{(i)}$ , we can partition  $\mathcal{I}_0^{(i)}$  into two separate sets of nodes such that one contains  $k$  and the other contains  $\ell$ , and two sets are disconnected. In effect, both the matrix  $\tilde{\Omega}^{\hat{D}^{(i)}, \hat{D}^{(i)}}$  and  $\tilde{\Omega}^{\hat{D}^{(i)}, \hat{F}^{(i)}}$  can be visualized as two by two blockwise matrix, with off-diagonal blocks being 0. As a result, it is seen that  $\tilde{H}_2(k, \ell) = 0$ . This contradiction shows that whenever  $\tilde{H}_2(k, \ell) \neq 0$ ,  $k$  and  $\ell$  are connected by a path in  $\mathcal{I}_0^{(i)}$ . Since  $|\mathcal{I}_0^{(i)}| \leq m_0$ , there is a path  $\leq m_0 - 1$  in  $\tilde{\mathcal{G}}$  that connects  $k$  and  $\ell$  where  $k \neq \ell$ .

Finally, since  $\tilde{\mathcal{G}}$  is  $K$ -sparse with  $K = C\delta^{-1/\gamma}$ , for any fixed  $\ell$ , there are at most finite  $k$  connecting to  $\ell$  by a path with length  $\leq (m_0 - 1)$ . The claim follows.  $\blacksquare$

## 6.6 Proof of Theorem 13

Since  $\sigma$  is known, for simplicity, we assume  $\sigma = 1$ . First, consider (38). By Theorem 8 and (54),  $\rho_{gs} = \min_{\{(D,F): D \cap F = \emptyset, D \neq \emptyset, D \cup F \subset \{1,2\}\}} \rho(D, F; \Omega)$ , where we have used that  $G$  is a diagonal block-wise matrix, each block is the same  $2 \times 2$  matrix. To calculate  $\rho(D, F; \Omega)$ , we consider three cases (a)  $(|D|, |F|) = (2, 0)$ , (b)  $(|D|, |F|) = (1, 0)$ , (c)  $(|D|, |F|) = (1, 1)$ . By definitions and direct calculations, it is seen that  $\rho(D, F; \Omega) = \vartheta + [(1 - |h_0|)r]/2$  in case (a),  $\rho(D, F; \Omega) = (\vartheta + r)^2/(4r)$  in case (b), and  $\rho(D, F; \Omega) = 2\vartheta + [(\sqrt{(1 - h_0^2)}r - \vartheta/\sqrt{(1 - h_0^2)}r)_+]^2/4$  in case (c). Combining these gives the claim.

Next, consider (39). Similarly, by the block-wise structure of  $G$ , we can restrict our attention to the first two coordinates of  $\beta$ , and apply the subset selection to the size 2 subproblem where the Gram matrix is the  $2 \times 2$  matrix with 1 on the diagonals and  $h_0$  on the off-diagonals. Fix  $q > 0$ , and let the tuning parameter  $\lambda_{ss} = \sqrt{2q_{ss} \log(p)}$ . Define  $f_{ss}^{(1)}(q) = \vartheta + [(\sqrt{r} - \sqrt{q})_+]^2$ ,  $f_{ss}^{(2)}(q) = 2\vartheta + [(\sqrt{r(1 - h_0^2)} - \sqrt{q})_+]^2$ , and  $f_{ss}^{(3)}(q) = 2\vartheta +$

$2[(\sqrt{r(1-|h_0|)} - \sqrt{q})_+]^2$ , where  $x_+ = \max\{x, 0\}$ . The following lemma is proved below, where the key is to use Ji and Jin (2011, Lemma 4.3).

**Lemma 21** *Fix  $q > 0$  and suppose the conditions in Theorem 13 hold. Apply the subset selection to the aforementioned size 2 subproblem with  $\lambda_{ss} = \sqrt{2q \log(p)}$ . As  $p \rightarrow \infty$ , the worst-case Hamming error rate is  $L_p p^{-f_{ss}(q)}$ , where  $f_{ss}(q) = f_{ss}(q, \vartheta, r, h_0) = \min\{\vartheta + (1 - |h_0|)r/2, q, f_{ss}^{(1)}(q), f_{ss}^{(2)}(q), f_{ss}^{(3)}(q)\}$ .*

By direct calculations,  $\rho_{ss}(\vartheta, r, h_0) = \max_{\{q>0\}} f_{ss}(q, r, h_0)$  and the claim follows.

Last, consider (40). The proof is very similar to that of the subset selection, except for that we need to use Ji and Jin (2011, Lemma 4.1), instead of Ji and Jin (2011, Lemma 4.3). For this reason, we omit the proof.  $\blacksquare$

### 6.6.1 PROOF OF LEMMA 21

By the symmetry in (35)-(36) when  $G$  is given by (37), we only need to consider the case where  $h_0 \in [0, 1)$  and  $\beta_1 \geq 0$ . Introduce events,  $A_0 = \{\beta_1 = \beta_2 = 0\}$ ,  $A_1 = \{\beta_1 \geq \tau_p, \beta_2 = 0\}$ ,  $A_{21} = \{\beta_1 \geq \tau_p, \beta_2 \geq \tau_p\}$ ,  $A_{22} = \{\beta_1 \geq \tau_p, \beta_2 \leq -\tau_p\}$ ,  $B_0 = \{\hat{\beta}_1 = \hat{\beta}_2 = 0\}$ ,  $B_1 = \{\hat{\beta}_1 > 0, \hat{\beta}_2 = 0\}$ ,  $B_{21} = \{\hat{\beta}_1 > 0, \hat{\beta}_2 > 0\}$  and  $B_{22} = \{\hat{\beta}_1 > 0, \hat{\beta}_2 < 0\}$ . It is seen that the Hamming error

$$= L_p(I + II + III), \quad (79)$$

where  $I = P(A_0 \cap B_0^c)$ ,  $II = P(A_1 \cap B_1^c)$  and  $III = P(A_{21} \cap B_{21}^c) + P(A_{22} \cap B_{22}^c)$ .

Let  $H$  be the  $2 \times 2$  matrix with ones on the diagonals and  $h_0$  on the off-diagonals,  $\alpha = (\beta_1, \beta_2)'$ , and  $w = (\tilde{Y}_1, \tilde{Y}_2)$ , where we recall  $\tilde{Y} = X'Y$ . It is seen that  $w \sim N(H\alpha, H)$ . Write for short  $\lambda = \sqrt{2q \log(p)}$ . Define regions on the plane of  $(\tilde{Y}_1, \tilde{Y}_2)$ ,  $D_0 = \{\max(|\tilde{Y}_1|, |\tilde{Y}_2|) > \lambda \text{ or } \tilde{Y}_1^2 + \tilde{Y}_2^2 - 2h_0\tilde{Y}_1\tilde{Y}_2 > 2\lambda^2(1-h_0^2)\}$ ,  $D_1 = \{|\tilde{Y}_1| < \lambda, \tilde{Y}_1 < \tilde{Y}_2 \text{ or } |\tilde{Y}_2 - h_0\tilde{Y}_1| > \lambda\sqrt{1-h_0^2}\}$ ,  $D_{21} = \{\tilde{Y}_2 - h_0\tilde{Y}_1 < \lambda\sqrt{1-h_0^2} \text{ or } \tilde{Y}_1 - h_0\tilde{Y}_2 < \lambda\sqrt{1-h_0^2}\}$  and  $D_{22} = \{\tilde{Y}_2 - h_0\tilde{Y}_1 > -\lambda\sqrt{1-h_0^2} \text{ or } \tilde{Y}_1 - h_0\tilde{Y}_2 > \lambda\sqrt{1-h_0^2} \text{ or } \tilde{Y}_1^2 + \tilde{Y}_2^2 - 2h_0\tilde{Y}_1\tilde{Y}_2 < 2\lambda^2(1-h_0^2)\}$ . Using (Ji and Jin, 2011, Lemma 4.3), we have  $B_0^c = \{(\tilde{Y}_1, \tilde{Y}_2)' \in D_0\}$ ,  $B_1^c = \{(\tilde{Y}_1, \tilde{Y}_2)' \in D_1\}$ ,  $B_{21}^c = \{(\tilde{Y}_1, \tilde{Y}_2)' \in D_{21}\}$ , and  $B_{22}^c = \{(\tilde{Y}_1, \tilde{Y}_2)' \in D_{22}\}$ . By direct calculation and Mills' ratio, it follows that for all  $\mu \in \Theta_p(\tau_p)$ ,

$$I = L_p \cdot (P(N(0, 1) > \lambda) + P(\chi_2^2 > 2\lambda^2)) = L_p \cdot p^{-q}, \quad (80)$$

$$II \leq L_p \cdot P(N((\tau_p, h_0\tau_p)', H) \in D_1) = L_p \cdot p^{-\vartheta - \min[(\sqrt{r}-\sqrt{q})^2, (1-h_0)r/2, q]}, \quad (81)$$

and when  $\beta_1 = \tau_p$  and  $\beta_2 = 0$ , the equality holds in (81). At the same time, note that over the event  $A_{21}$ , the worst case scenario, is where  $\beta_1 = \beta_2 = \tau_p$ . In such a case,  $(\tilde{Y}_1, \tilde{Y}_2)' \sim N(((1+h_0)\tau_p, (1+h_0)\tau_p)', H)$ . Combining this with Mills' ratio, it follows that for all  $\mu \in \Theta_p(\tau_p)$ ,

$$P(A_{21} \cap B_{21}^c) = P((\tilde{Y}_1, \tilde{Y}_2)' \in D_{21}) \leq L_p \cdot p^{-2\vartheta - (\sqrt{r(1-h_0^2)} - \sqrt{q})_+^2}, \quad (82)$$

and the equality holds when  $\beta_1 = \beta_2 = \tau_p$ . Similarly, note that over the event  $A_{22}$ , in the worst case scenario,  $\beta_1 = -\beta_2 = \tau_p$ . In such a case,  $(\tilde{Y}_1, \tilde{Y}_2)' \sim N(((1-h_0)\tau_p, -(1-h_0)\tau_p)', H)$ . Combining this with Mills' ratio, it follows that for all  $\mu \in \Theta_p(\tau_p)$ ,

$$P(A_{22} \cap B_{22}^c) = P((\tilde{Y}_1, \tilde{Y}_2)' \in D_{22}) \leq L_p \cdot p^{-2\vartheta - \min[(\sqrt{r(1-h_0^2)} - \sqrt{q})_+]^2, 2\{[\sqrt{r(1-h_0)} - \sqrt{q}]_+\}^2]}, \quad (83)$$

and the equality holds when  $\beta_1 = -\beta_2 = \tau_p$ . Inserting (80)-(83) into (79) gives the claim.  $\blacksquare$

### 6.7 Lemma 22 and the Proof

**Lemma 22** *Let  $(V_{0j}^*, V_{1j}^*)$  be defined as in (25). If the conditions of Theorem 6 hold, then  $\max\{|V_{0j}^* \cup V_{1j}^*|\} \leq (\vartheta + r)^2/(2\vartheta r)$ .*

**Proof.** Let  $V_0 = \emptyset$  and  $V_1 = \{j\}$ . It is seen that  $\alpha^*(V_0, V_1; \Omega) = 1$ , and  $\eta(V_0, V_1; \Omega) \leq (\vartheta + r)^2/(4r)$ . Using this and the definitions of  $V_{0j}^*$  and  $V_{1j}^*$ ,  $\max\{|V_{0j}^*|, |V_{1j}^*|\}\vartheta \leq (\vartheta + r)^2/(4r)$  and the claim follows.  $\blacksquare$

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