Rare and Weak effects in Large-Scale Inference: methods and phase diagrams

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Abstract

Often when we deal with ‘Big Data’, the true effects we are interested in are Rare and Weak (RW). Researchers measure a large number of features, hoping to find perhaps only a small fraction of them to be relevant to the research in question; the effect sizes of the relevant features are individually small so the true effects are not strong enough to stand out for themselves.

Higher Criticism (HC) and Graphlet Screening (GS) are two classes of methods that are specifically designed for the Rare/Weak settings. HC was introduced to determine whether there are any relevant effects in all the measured features. More recently, HC was applied to classification, where it provides a method for selecting useful predictive features for trained classification rules. GS was introduced as a graph-guided multivariate screening procedure, and was used for variable selection.

We develop a theoretic framework where we use an Asymptotic Rare and Weak (ARW) model simultaneously controlling the size and prevalence of useful/significant features among the useless/null bulk. At the heart of the ARW model is the so-called phase diagram, which is a way to visualize clearly the class of ARW settings where the relevant effects are so rare or weak that desired goals (signal detection, variable selection, etc.) are simply impossible to achieve. We show that HC and GS have important advantages over better known procedures and achieve the optimal phase diagrams in a variety of ARW settings.

HC and GS are flexible ideas that adapt easily to many interesting situations. We review the basics of these ideas and some of the recent extensions, discuss their connections to existing literature, and suggest some new applications of these ideas.

Key words. Classification, control of FDR, feature ranking, feature selection, Graphlet Screening, Hamming distance, Higher Criticism, Large-Scale Inference, Rare and Weak effects, phase diagram, sparse precision matrix, sparse signal detection, variable selection.


1 Introduction

We are often said to be entering the era of ‘Big Data’. High-throughput devices measure thousands or even millions of different features per single subject on a daily basis. Such an activity is the driving force of many areas of science and technology, including a new branch of statistical practice which Efron [31] calls Large-Scale Inference (LSI).

In many high-throughput data sets, the relevant effects are Rare and Weak (RW). The researchers expect that only a small fraction of these measured features are relevant for the research in question, and the effect sizes of the relevant features are individually small. The researchers do not know in advance which features are relevant and which are not, so
they choose to measure all features within a certain range systematically and automatically, hoping to identify a small fraction of relevant ones in the future.

Examples include but are not limited to Genome-Wide Association Study (GWAS) and deep sequencing study, where we are in the so-called “large-p small-n” paradigm, with \( p \) being the number of SNPs and \( n \) being the number of subjects. As technology on data acquisition advances, we are able to measure increasingly more features per subject. However, the number of relevant features do not grow proportionally, so the relevant effects are sparse; in addition, since \( n \) is usually not as large as we wish, the effect sizes of the relevant features (in the summary statistics, e.g., two-sample t-tests) are individually small.

Effect rarity is a useful hypothesis proposed as early as 1980’s by Box and Meyer [9]. Later, this hypothesis was found to be valid in many applications (e.g., wavelet image processing [26], cosmology and astronomy [61], genetics and genomics [82]) and had inspired a long line of researches, where the common theme is to exploit sparsity (e.g., [26, 27]).

However, these works have been largely focused on the regime where the effects are rare but are individually strong (Rare/Strong), with limited attention to the more challenging Rare/Weak regime; the latter contains many new phenomena which we have not seen in the Rare/Strong regime, to discover which, we need new methods and new theoretic frameworks.

Call a relevant feature a signal and an irrelevant feature a noise. In this paper, we investigate two interconnected LSI problems in the Rare/Weak regime.

- **Sparse signal detection.** Given two groups of subjects, a treatment group and a control group, each subject is measured on the same set of features. We are interested in deciding whether there is any difference between two groups. In the Rare/Weak setting, the inter-group difference for any single relevant feature is not significant enough, so we have to combine the strengths of these features.

- **Sparse signal recovery.** We have the same setting as above, but the interest is to separate relevant features from the overwhelmingly more irrelevant ones. In the literature, this problem is known as variable selection.

Higher Criticism (HC) and Graphlet Screening (GS) are two recent classes of methods, specifically designed for Rare/Weak settings, focusing on detecting and recovering sparse signals, respectively.

HC can be viewed as an approach to combining different \( P \)-values. It was originally proposed as a method to detect sparse signals in the presence of uncorrelated noise. It was then improved to a more sophisticated form called Innovated HC, to deal with the case of correlated noise, where the new ingredient is to exploit graphic structure of the noise terms. More recently, HC was applied to classification, where it provides a way to select useful predictive features for trained classification rules.

HC is closely related to the better known methods of controlling False Discovery Rate (FDR) [5]. However, the target of the FDR-controlling methods is signal recovery in the Rare/Strong regime, and the target of HC is signal detection in the Rare/Weak regime, where signals are so rare and weak that they are inseparable from the noise terms.

GS is a graph-guided multivariate screening procedure, originally proposed as an approach to variable selection. GS can be viewed as an extension of the better known method of Univariate Screening (US) (also called marginal regression or Sure Screening [42, 34]), where the innovation is to provide a way to overcome the so-called challenge of ‘signal cancellation’ [78] by exploiting the graphic structures of the data. In the simplest case where
different features are uncorrelated, both GS and US reduce to the classical method of Hard Thresholding \[87\].

GS can also be viewed as an approach to evaluating the significance of several correlated features: recently, it was found to provide a new approach to feature ranking. In many LSI problems (e.g., multiple testing, classification, spectral clustering), feature ranking plays a pivotal role, and GS is potentially useful.

GS is very different from better known variable selection methods of $L^0/L^1$-penalizations, the goal of which is usually to fully recover Rare/Strong signals. GS focuses on Rare/Weak signals, where full recovery is usually impossible, so we must develop methods and theory different from those on $L^0/L^1$-penalizations.

Despite that their goals are seemingly very different, Innovated HC and GS are closely related to each other, and the main strategies of both methods are to exploit the graphic structures.

We review the basics of HC and GS and illustrate possible variations and extensions. We evaluate HC and GS by developing a theoretic framework using the Asymptotic Rare and Weak (ARW) model, simultaneously controlling the signal prevalence and signal strengths. We show that HC and GS offer theoretical optimality in the ARW model, and have advantages over existing methods.

We visualize the ARW model with the phase diagrams. The phase space refers to the two-dimensional space with axes simultaneously quantifying the signal prevalence and signal strengths. It partitions into several subregions, where the desired inference (signal detection, variable selection, etc.) is distinctly different; because of the partition of the phase space, we call it the phase diagram.

Phase diagram can be viewed as a new criterion for evaluating optimality which is particularly appropriate for the ARW model. Given a problem, different methods may also have different phase diagrams, characterizing the subregions where they succeed and where they fail. When a method partitions the phase diagram in exactly the same way as the optimal methods, we say it achieves the optimal phase diagram.

We show that in a wide variety of settings, HC and GS achieve the optimal phase diagrams for signal detection and signal recovery, respectively. In many of such settings, other methods (such as FDR-controlling methods \[5\], $L^0/L^1$-penalization methods \[29, 81\]) do not achieve the optimal phase diagrams.

Note that, however, HC and GS are flexible ideas and can be applied to many interesting settings. They are not tied to the ARW model and their advantages over existing methods remain in much broader settings.

### 1.1 Roadmap and highlights

In Section 2, we introduce the ARW model and the watershed phenomena associated with the problems of sparse signal detection and sparse signal recovery, respectively, and visualize them with the phase diagrams.

Section 2 does not address the achievability: which methods (presumably easy-to-use) achieve the optimal phase diagrams. The achievability is addressed in Sections 3-4, focusing on the cases of uncorrelated noise and correlated noise, respectively. In Section 3, we first review the basics of the HC and show that it achieves the optimal phase diagram for signal detection. We then show that the well-known method of Hard Thresholding achieves the optimal phase diagram for signal recovery. We also review the recent literature on the idea of HC. Section 4 discusses the case of correlated noise. For signal detection, we develop
HC into the more sophisticated Innovated HC, and for signal recovery, we use GS. Phase diagrams and optimality of HC and GS are also investigated.

In Section 5, we suggest some new applications of HC and GS, supported by some preliminary numeric studies. In Section 6, we extend HC as a feature selection method in the context of classification. We address the classification phase diagram as well as the optimality of HC.

The development of HC and GS exposes several noteworthy ideas; we provide a road map to highlight these ideas, with details later.

- Innovated Transformation (IT) is the key to many methods (e.g., Innovated HC, GS, and the classification rule in Fan et al. (2013) [36]) that incorporate correlation structures of the noise terms for inference. Compared to Whitened Transformation (WT) which attempts to create uncorrelated noise terms by transformations, IT—though counterintuitive—yields larger (post-transformation) Signal-to-Noise Ratios (SNR) than WT, simultaneously at all (pre-transformation) signal sites, and so it is preferred. See Section 4.1 for details.

- While it is expected that the optimal phase diagrams critically depend on the local graphic structures, it is not the case, and most parts of the phase diagrams remain the same across a range of very different local graphic structures. On the other hand, for optimal procedures (e.g., GS), we must exploit local graphic structures. The well-known $L^0/L^1$-penalization methods do not adequately exploit local graphic structures, so they do not achieve the optimal phase diagram, even in very simple settings and even when the tuning parameters are ideally set. See Sections 4.2-4.4 for details.

- In classification, a prevailing idea is to select a few important predictive features so that the (feature) FDR [5] is small. Recent studies reveal something very different: in some Rare/Weak settings, we must select features in a way so that the FDR is very high, so that we are able to include almost all useful features for classification. See Section 6.

Other small but noteworthy items include Lemma 2.1 and Remarks 4, 12.

2 The ARW model and phase diagrams

In this section, we introduce the ARW model. We discuss the watershed phenomena associated with signal detection and signal recovery, respectively, and visualize them with the phase diagrams. Discussions on the achievability are long and deferred to Sections 3-4; we explain our plan for the discussions on the achievability in Section 2.4.

The ARW model was first proposed by Donoho and Jin (2004) [23] for sparse signal detection. More recently, it was extended to more complicated forms [45] and to different settings including classification [25, 51, 60], variable selection [57, 63], and spectral clustering [62]; see also [3, 69, 71].

In this paper, we focus on a version of the ARW model that is simple for presentation, yet contains all important ingredients associated with the major insights exposed in the above references.

In such a spirit, we consider a Stein’s $p$-normal means model

$$Y = \beta + z, \quad z \sim N(0, \Sigma),$$

(2.1)
where $\Sigma = \Sigma_{p,p}$ is the covariance matrix. Denote the precision matrix by

$$\Omega = \Omega_{p,p} = \Sigma_{p,p}^{-1}.$$  

For simplicity, we usually drop subscripts ‘$p,p$’. We assume $\Omega$ is sparse in the (strict) sense that each row of $\Omega$ has relatively few nonzeros. Such an assumption is only for simplicity in presentation; see [45, 63] for discussions on more general $\Omega$. Model (2.1) may arise from many applications, including the following.

- **Two-group study.** In the aforementioned two-group study, $Y_j$, $1 \leq j \leq p$, can be viewed as the two-sample $t$-statistic associated with the $j$-th feature. In many such studies (e.g., Genetic Regulatory Network (GRN)), the precision matrix is sparse [76].

- **Linear models with random designs.** Given $W \sim N(X\tilde{\beta}, I_n)$, where the rows of $X$ are iid samples from the $p$-dimensional distribution $N(0, \Omega)$, where $\Omega$ is sparse. Such settings can be found in Compressive Sensing [22, 28] or Computer Security [21, 37], where $\Omega = I_p$. Letting $\tilde{W} = (1/\sqrt{n})X'W$ and $\beta = \sqrt{n}\tilde{\beta}$, then approximately $\tilde{W} \sim N(\Omega\beta, \Omega)$, which is equivalent to model (2.1); the connection is solidified in Jin et al. (2012) [63].

We assume $\Omega$ is known, as our primary goal is to investigate how the graphic structures of $\Omega$ affect the constructions of the optimal methods and optimal phase diagrams. Such an assumption is valid in many applications. For example, in the above linear model, $\Omega$ plays the role of the Gram matrix which is known to us. When $\Omega$ is unknown but is sparse, it can be estimated by many recent algorithms, such as the glasso [38]. The gained insight here is readily extendable to the case where $\Omega$ is unknown but can be estimated reasonably well, as only large entries of $\Omega$ have a major influence on the problems we are interested in.

We choose a somewhat unconventional normalization such that

$$\Omega(i,i) = 1, \quad 1 \leq i \leq p. \tag{2.2}$$

Denote $d_p^*$ by the maximum number of nonzeros in the rows of $\Omega$:

$$d_p^* = d_p^*(\Omega) = \max_{1 \leq i \leq p} \{ \# \{ 1 \leq j \leq p : \Omega(i,j) \neq 0 \} \}.$$  

We assume $d_p^*(\Omega)$ grows slowly enough:

$$d_p^*(\Omega)p^{-\delta} \to 0, \quad \text{for any fixed } \delta > 0. \tag{2.3}$$

At the same time, fixing $\epsilon \in (0, 1)$ and $\tau > 0$, we model the vector $\beta$ by

$$\beta_i \overset{iid}{\sim} (1 - \epsilon)\nu_0 + \epsilon\nu_{\tau}, \quad 1 \leq i \leq p, \tag{2.4}$$

where $\nu_a$ is the point mass at $a$. We are primarily interested in the case where $\epsilon$ is small and $\tau$ is small or moderately large, so that the signals (i.e., nonzero entries of $\beta$) are Rare and Weak.

In our asymptotic framework, we let $p$ be the driving asymptotic parameter, and tie $(\epsilon, \tau)$ to $p$ through fixed parameters $\vartheta$ and $r$:

$$\epsilon = \epsilon_p = p^{-\vartheta}, \quad 0 < \vartheta < 1, \quad \tag{2.5}$$

$$\tau = \tau_p = \sqrt{2r\log(p)}, \quad r > 0. \tag{2.6}$$

Note that as $p$ grows, the signals become increasingly sparser. To counter this effect, we have to let the signal strength parameter $\tau$ grows to $\infty$ slowly, so that the testing problem is non-trivial.
Definition 1. We call model (2.1)–(2.6) the Asymptotic Rare and Weak model $ARW(\vartheta,r,\Omega)$. See [42, 44, 45, 57, 63, 64] for the ARW model in more general forms. The ARW model is subtle even in the case where $\Omega = I_p$; see [23] for example.

2.1 Detecting Rare and Weak signals

We formulate the sparse signal detection problem as a hypothesis testing problem, where we test a joint null hypothesis that all $\beta_i$’s are 0:

$$H_0^{(p)} : \beta = 0$$

against a specific complement of the joint null:

$$H_1^{(p)} : \beta \text{ satisfies a Rare and Weak model (2.4)-(2.6).}$$

Note that $Y_i \iid \mathcal{N}(0,1)$ and $Y_i \iid (1-\epsilon_p)\mathcal{N}(0,1) + \epsilon_p\mathcal{N}(\tau_p,1)$ under $H_0^{(p)}$ and $H_1^{(p)}$, respectively, so the testing problem (2.7)-(2.8) is also the problem of detecting Gaussian mixtures [23].

It turns out that there is a watershed phenomenon, meaning that in the two-dimensional phase space \{$(\vartheta,r) : 0 < \vartheta < 1, r > 0$\}, there is a curve that partitions the whole phase space into two regions where the testing problem (2.7)-(2.8) is distinctly different. Presumably, the curve should depend on the off-diagonals of $\Omega$ in a complicated way. Somewhat surprisingly, this is not the case, and the off-diagonals of $\Omega$ do not have a major influence on the partition.

In detail, define the standard phase function for detection

$$\rho^*(\vartheta) = \begin{cases} 0, & 0 < \vartheta \leq 1/2, \\ \vartheta - 1/2, & 1/2 < \vartheta \leq 3/4, \\ (1-\sqrt{1-\vartheta})^2, & 3/4 < \vartheta < 1. \end{cases}$$ (2.9)

We have the following theorem.

Theorem 2.1. Fixing $\vartheta \in (0,1)$ and $r > 0$, consider a sequence of $ARW(\vartheta,r,\Omega)$ indexed by $p$. If $r < \rho^*(\vartheta)$, then for any sequence of tests that test $H_1^{(p)}$ against $H_0^{(p)}$, the sum of Type I and Type II errors tends to 1 as $p \to \infty$. If $r > \rho^*(\vartheta)$, then there is a test the sum of Type I and Type II errors of which tends to 0 as $p \to \infty$.

In the simplest case of $\Omega = I_p$, Theorem 2.1 was proved in Donoho and Jin (2004) [23], and also in [49, 50]. For general cases $\Omega \neq I_p$, the second claim follows from Theorem 4.1 on Innovated HC below, and the proof of the first claim is similar to that in [36, Theorem 1.1] so we skip it; at the heart of the proof is subtle analysis of the Hellinger distance associated with the testing problem, as well as the following lemma.

Lemma 2.1. (Chromatic Number). Fixing $p$ and $K$ such that $1 \leq K < p$, consider a $p \times p$ matrix $\Omega$. If each row of $\Omega$ has no more than $K$ nonzeros, then we can color indices $1,2,\ldots,p$ in no more than $K$ different colors, so that for any pair of indices $i,j$ with the same color, $\Omega(i,j) = 0$.

Remark 1. In (2.9), $\rho^*(\vartheta) = 0$ when $0 < \vartheta < 1/2$. This does not mean that two hypotheses $H_0^{(p)}$ and $H_1^{(p)}$ are asymptotically separable for any $(\epsilon_p,\tau_p)$; it only means that two hypotheses can be asymptotically separated even when $\tau_p \ll \sqrt{\log(p)}$. See [23] for more discussions.
2.2 Recovering Rare and Weak signals

Consider again the ARW model where
\[ Y = \beta + z, \quad z \sim N(0, \Sigma), \]
and \((\beta, \Omega)\) satisfy (2.2)-(2.6). Now, the main interest is to separate the nonzero entries of \(\beta\) from the zero ones (i.e., signal recovery or variable selection). For any estimator \(\hat{\beta}\), we measure the errors by the Hamming distance:
\[ h_p(\hat{\beta}, \beta) = E \sum_{i=1}^{p} 1\{\operatorname{sgn}(\hat{\beta}_i) \neq \operatorname{sgn}(\beta_i)\}, \]
where \(\operatorname{sgn}(u)\) denotes the sign of \(u\) taking values 0, ±1 and the expectation is taken over the randomness of \(\beta\) and \(Y\). Hamming distance is approximately the expected sum of the number of signals that have been classified as noise and the number of noise that have been classified as signals. The minimax Hamming distance is then
\[ \operatorname{Hamm}_p^*(\vartheta, r; \Omega) = \inf_{\hat{\beta}} \{h_p(\hat{\beta}, \beta)\}. \quad (2.10) \]

The following short-hand term is frequently used in the paper.

**Definition 2.** \(L_p > 0\) denotes a generic multi-log\((p)\) term which may change from occurrence to occurrence and satisfies that \(L_p p^{\delta} \to \infty\) and \(L_p p^{-\delta} \to 0\) for any \(\delta > 0\), as \(p \to \infty\).

The following theorem is proved by Ji and Jin (2011) [57] (see also [63, 64]).

**Theorem 2.2.** (Lower bound). Fixing \(\vartheta \in (0, 1)\) and \(r > 0\), consider a sequence of ARW\((\vartheta, r, \Omega)\) indexed by \(p\). As \(p \to \infty\),
\[ \operatorname{Hamm}_p^*(\vartheta, r; \Omega) \begin{cases} \geq L_p p^{1-(\vartheta+r)^2/(4r)}, & r > \vartheta, \\ \sim p^{1-\vartheta}, & 0 < r < \vartheta. \end{cases} \quad (2.11) \]

Similarly, there is a watershed phenomenon associated with the problem of signal recovery. This phenomenon can be most conveniently described in the case \(\Omega = I_p\), but it holds much more broadly.

When \(\Omega = I_p\), it is shown in Section 3 below that the lower bound in (2.11) is tight and can be achieved by Hard Thresholding:
\[ \operatorname{Hamm}_p^*(\vartheta, r; I_p) \begin{cases} = L_p p^{1-(\vartheta+r)^2/(4r)}, & r > \vartheta, \\ \sim p^{1-\vartheta}, & 0 < r < \vartheta. \end{cases} \quad (2.12) \]

Define the standard phase function for exact recovery:
\[ \rho_{\text{exact}}^*(\vartheta; I_p) = (1 + \sqrt{1 - \vartheta})^2, \quad 0 < \vartheta < 1. \quad (2.13) \]

Let
\[ S_p(\beta) = \{1 \leq i \leq p : \beta_i \neq 0\}, \quad s_p(\beta) = |S_p(\beta)|. \]
In the ARW model, with overwhelming probability,
\[ s_p(\beta) \sim p \epsilon_p = p^{1-\vartheta}. \quad (2.14) \]
For any fixed \((\vartheta, r)\), by (2.13)-(2.14) and basic algebra, it follows that
Figure 1: Phase diagrams ($\Omega = I_p$). Left: curves in red, green, and blue are $r = \rho^{*\text{exact}}(\vartheta; I_p)$, $r = \vartheta$, and $r = \rho^{*}(\vartheta)$, correspondingly. Right: enlargement of the region bounded by the dashed lines in the left panel.

- when $r > \rho^{*\text{exact}}(\vartheta; I_p)$, $\text{Hammm}_{p}^{*}(\vartheta, r; \Omega) = o(1)$, and it is possible to fully recover $S(\beta)$—the support of $\beta$—with overwhelming probabilities.

- when $\vartheta < r < \rho^{*\text{exact}}(\vartheta; I_p)$, $1 \ll \text{Hammm}_{p}^{*}(\vartheta, r; I_p) \ll p^{1-\vartheta}$; it is possible to recover most of the signals, but it is impossible to fully recover $S(\beta)$.

- when $0 < r < \vartheta$, $\text{Hammm}_{p}^{*}(\vartheta, r; I_p) \sim p^{1-\vartheta}$, and signals and noise are merely inseparable.

The case $\Omega \neq I_p$ is the same, except for one difference, that we have to replace the function $\rho^{*\text{exact}}(\vartheta; I_p)$ by a more general function

$$\rho^{*\text{exact}}(\vartheta; \Omega).$$

We address this case in Section 4 where we attack the problem by Graphlet Screening (GS). We derive the optimal rate of convergence of the minimax Hamming distance $\text{Hammm}_{p}^{*}(\vartheta, r; \Omega)$, and show that GS is asymptotically minimax.

In principle, $\text{Hammm}_{p}^{*}(\vartheta, r; \Omega)$ may depend on $\Omega$ in a complicate way. Still, for many sequences of $\Omega = \Omega_{p,p}$ (with careful calibrations, possibly), there is a constant $c = c(\vartheta, r; \Omega)$ depending on $(\vartheta, r)$ and the calibrations we choose for $\Omega$ such that

$$\text{Hammm}_{p}^{*}(\vartheta, r; \Omega) = L_{p}p^{1-c(\vartheta, r; \Omega)},$$

and equating $c(\vartheta, r; \Omega) = 1$ gives $r = \rho^{*\text{exact}}(\vartheta; \Omega)$. Examples of such sequences include that of $\Omega = I_p$ for all $p$, a diagonal block-wise example to be discussed in Section 4.4 and the long-memory time series model and the change point model discussed in Ke et al (2012) [64] as well as in Remark 10. In all these cases, we have explicit formulas for $\rho^{*\text{exact}}(\vartheta; \Omega)$. See details therein.

2.3 Phase diagrams

The preceding results can be visualized with the phase diagrams. The two-dimensional phase space $\{(\vartheta, r) : 0 < \vartheta < 1, r > 0\}$ is partitioned by the three curves

$$r = \rho^{*}(\vartheta), \quad r = \vartheta, \quad r = \rho^{*\text{exact}}(\vartheta; \Omega)$$
into four different subregions, where the inference is distinctly different.

- **Region of Undetectable**: \( \{(\vartheta, r) : 0 < \vartheta < 1, r < \rho^*(\vartheta)\} \). The signals are so rare and weak that it is impossible to detect their existence: the two hypotheses \( H_1^{(p)} \) and \( H_0^{(p)} \) are merely inseparable; for any test, the sum of Type I and Type II errors tends to 1 as \( p \to \infty \).

- **Region of Not Recoverable but Detectable**: \( \{(\vartheta, r) : 0 < \vartheta < 1, \rho^*(\vartheta) < r < \vartheta\} \). It is possible to have a test such that the sum of Type I and Type II errors tends to 0 as \( p \to \infty \). However, it is impossible to separate the signals from the noise: as \( \text{Hamm}_p^*(\vartheta, r; \Omega) \gtrsim p^{1-\theta} \), the expected Hamming distance of any estimator is comparable to the total number of signals.

- **Region of Almost Fully Recoverable**: \( \{(\vartheta, r) : 0 < \vartheta < 1, \vartheta < r < \rho^*_\text{exact}(\vartheta; \Omega)\} \). It is possible to recover almost all signals but not all of them; the Hamming distance is much smaller than \( p^{1-\theta} \), but is also much larger than 1.

- **Region of Exactly Recoverable**: \( \{(\vartheta, r) : 0 < \vartheta < 1, r > \rho^*_\text{exact}(\vartheta; \Omega)\} \). The signals are sufficiently strong so that \( \text{Hamm}_p^*(\vartheta, r; \Omega) = o(1) \), and it is possible to have exact recovery with overwhelming probabilities.

In the last two sub-regions, it is clearly detectable; we call the following region

\( \{(\vartheta, r) : 0 < \vartheta < 1, r > \rho^*(\vartheta)\} \)  \hspace{1cm} (2.15)

the **Region of Detectable**. Also, note that among these four subregions, only the last two depend on \( \Omega \). In Figure 1, we plot the phase diagrams in the case of \( \Omega = I_p \). Phase diagrams for more general cases are discussed in Section 4.

Phase diagram can be viewed as a new criterion for measuring performances that is particularly appropriate for Rare/Weak settings. Phase diagram is a flexible idea, which has been extended recently to many different settings, including large-scale multiple testing [3, 45, 53], variable selection [57, 63, 64], classification [25, 36, 51, 60], spectral clustering and low-rank matrix recovery [62], and computer privacy and security [37]. See sections below for more discussions.

### 2.4 Achievability of the phase diagrams

In the preceding section, we have only said that the optimal phase diagrams are achievable, without referencing to any specific methods. It is of primary interest to develop methods—preferably easy-to-implement and is not tied to the ARW model—to achieve the optimal phase diagrams:

- We say a testing procedure achieves the **optimal phase diagram for detection** if for any \((\vartheta, r)\) in the interior of Region of Detectable, the power of the procedure tends to 1 as \( p \to \infty \).

- We say a variable selection procedure \( \hat{\beta} \) achieves the **optimal phase diagram for recovery** if \( h_p(\hat{\beta}, \beta) \leq L_p \cdot \text{Hamm}_p^*(\vartheta, r; \Omega) \) for sufficiently large \( p \), where \( L_p \) is the generic multi-log\((p)\) term as in Definition 2.
If a testing procedure and a variable selection procedure achieve the optimal phase diagrams for detection and recovery, respectively, then they partition the phase space in exactly the same way as in Section 2.3.

In Section 3, we address the achievability for the case $\Omega = I_p$, and show that Orthodox Higher Criticism (OHC) and Hard Thresholding achieve the optimal phase diagrams for detection and recovery, respectively. In Section 4, we address the achievable for more genera $\Omega$, and show that Innovated HC and GS achieve the optimal phase diagrams for detection and recovery, respectively. Combining these with Theorems 2.1-2.2 gives the phase diagrams presented in Section 2.3.

3 Detecting and recovering signals in white noise

We revisit the problems of signal detection and signal recovery, and show that when $\Omega = I_p$, HC and Hard Thresholding achieve the optimal phase diagrams for detection and recovery, respectively. We also review the recent applications and extensions of the HC idea. Discussions on general $\Omega$ is in Section 4.

3.1 Higher Criticism basics and optimal signal detection (white noise)

Higher Criticism (HC) is a notion that goes back to John Tukey [83, 84, 85]. Donoho and Jin (2004) [23] developed HC into a method of combining $P$-values, and used it to resolve the testing problem (2.7)-(2.8). HC consists of three steps.

- For each $1 \leq i \leq p$, obtain a $P$-value by $\pi_i = P(N(0,1) \geq Y_i)$.
- Sort the $P$-values in the ascending order: $\pi(1) < \pi(2) < \ldots < \pi(p)$.
- The Higher Criticism statistic is then

$$HC_p^* = \max_{\{1 \leq i \leq p/2\}} HC_{p,i}, \quad \text{where} \quad HC_{p,i} = \sqrt{p} \left( \frac{(i/p) - \pi(i)}{\pi(i)(1 - \pi(i))} \right).$$

(3.16)

In this paper, we will discuss several variants of HC. To distinguish one from the other, we call the version in (3.16) the Orthodox HC (OHC).

Fix $0 < \alpha < 1$. To use the HC for a level-$\alpha$ test for the testing problem (2.7)-(2.8), we must find the critical value $h(p, \alpha)$ defined by

$$P_{H_0(p)}\{HC_p^* > h(p, \alpha)\} = \alpha.$$

Asymptotically, it is known that for any fixed $\alpha \in (0,1)$,

$$h(p, \alpha) = \sqrt{2 \log \log(p)}(1 + o(1)),$$

(3.17)

so an approximation of $h(p, \alpha)$ is $\sqrt{2 \log \log(p)}$. We say $\alpha = \alpha_p$ tends to 0 slowly enough if

$$h(p, \alpha_p) \sim \sqrt{2 \log \log(p)}.$$

Consider the HC-test where we reject $H_0(p)$ if and only if

$$HC_p^* \geq h(p, \alpha_p).$$

Recall that $\rho^*(\vartheta)$ is the standard phase function defined in (2.9). The following theorem is proved by Donoho and Jin (2004) [23].
**Theorem 3.1.** Fix \((\vartheta, r)\) in the phase space such that \( r > \rho^*(\vartheta)\). Suppose as \( p \to \infty\), the level \( \alpha_p\) of the HC-test tend to 0 slowly enough, then the power of the HC-test tends to 1.

Combining this with Theorem 2.1 (not requiring \( \Omega = I_p\)), for any fixed \((\vartheta, r)\) in Region of Detectable (see (2.15)), OHC yields an asymptotically full power test when \( \Omega = I_p\). Therefore, OHC achieves the optimal phase diagram for detection.

**Remark 2.** The approximation of \( h(p, \alpha)\) in (3.17) is largely asymptotic, so it is not very accurate for finite \( p\); our recommendation is to approximate \( h(p, \alpha)\) by simulations.

**Remark 3.** For small \( i\), \( HC_{p,i}\) is slightly heavy-tailed, so OHC is also heavy-tailed. To alleviate the problem, we recommend the following modified version:

\[
HC_{p,i}^+ = \max_{\{1 \leq i \leq \alpha_p p^\pi(i) > 1/p\}} HC_{p,i}.
\]

Similarly, we can define \( h^+(p, \alpha)\) as the critical value such that \( P_{H_0^{(p)}}(HC_{p}^+ \geq h(p, \alpha)) = \alpha\). See Donoho and Jin (2004) [23] for details.

**Remark 4.** One advantage of OHC-test is that we only need \( P\)-values to use it, without any knowledge of the parameters \((\epsilon_p, \tau_p)\), so the test is not tied to the specific model in (2.7)-(2.8). On the other hand, in the idealized case where \((\epsilon_p, \tau_p)\) are known, the optimal test is the Neyman-Pearson Likelihood Ratio Test (LRT). There is an interesting phase transition associated with the limiting distribution of LRT. Write the log-likelihood ratio associated with (2.7)-(2.8) as

\[
LR_p(\epsilon_p, \tau_p) = LR_p(\epsilon_p, \tau_p; Y) = \sum_{i=1}^{p} \log((1 - \epsilon_p) + \epsilon_p e^{\tau_p Y_i - \tau_p^2/2}).
\]

With the calibrations in (2.5)-(2.6), \( LR_p\) can have non-degenerate limits only when \((\vartheta, r)\) fall exactly onto the phase boundary \( r = \rho^*(\vartheta)\); still, this alone is inadequate, and we must modify the calibrations slightly. In detail, we let

\[
\begin{align*}
    r &= \rho^*(\vartheta), \\
    \tau_p &= \sqrt{2r \log(p)}, \\
    \epsilon_p &= \begin{cases} 
        p^{-\vartheta}, & \text{if } 1/2 < \vartheta \leq 3/4, \\
        \tau_p^{2\sqrt{\vartheta}} p^{-\vartheta}, & \text{if } 3/4 < \vartheta < 1.
    \end{cases}
\end{align*}
\]

As \( p \to \infty\), if (3.19) holds, then \( LR_p\) has weak limits as follows [38]:

\[
LR_p \longrightarrow \begin{cases} 
    N(\frac{1}{2}, 1), & \text{if } 1/2 < \vartheta < 3/4, \\
    N(\frac{1}{2}, \frac{1}{2}), & \text{if } \vartheta = 3/4, \\
    \nu_{\vartheta}^{(\vartheta)}, & \text{if } 3/4 < \vartheta < 1,
\end{cases}
\]

under \( H_0^{(p)} \) and \( H_1^{(p)} \), respectively. Here, \( \nu_{\vartheta}^{(\vartheta)} \) are the distributions with the characteristic functions \( \psi_{\vartheta}^{(\vartheta)} \) given by \( \psi_{\vartheta}^{(\vartheta)}(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[ e^{(t+1)e^{\vartheta}-\vartheta(1+\sqrt{1-\vartheta})} - 1 \right] e^{-\vartheta(1-\vartheta+\sqrt{1-\vartheta})} dz \) and \( \psi_{\vartheta}^{(\vartheta)}(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[ e^{(t+1)e^{\vartheta}-\vartheta(1+\sqrt{1-\vartheta})} - 1 \right] e^{-\vartheta(1-\vartheta+\sqrt{1-\vartheta})} dz \), respectively.

### 3.2 Optimal signal recovery by Hard Thresholding (white noise)

We now consider the problem of signal recovery in the case of \( \Omega = I_p\). In this simple setting,

\[
Y_i \overset{iid}{\sim} (1 - \epsilon_p)N(0, 1) + \epsilon_p N(\tau_p, 1),
\]
and a conventional approach to estimating $\beta$ is to use Hard Thresholding (HT). Fix a threshold $t > 0$. The HT estimator $\hat{\beta}_{t,i}^{HT}$ is given by

$$
\hat{\beta}_{t,i}^{HT} = \begin{cases} 
Y_i, & \text{if } |Y_i| \geq t, \\
0, & \text{otherwise.}
\end{cases}
$$

It is convenient to choose thresholds having the form of

$$
t_q(p) = \sqrt{2q \log p}, \quad \text{where } 0 < q < 1 \text{ is a fixed parameter.}
$$

Ideally, when $(\vartheta, r)$ are given, we choose $q$ as follows:

$$
q_{\text{ideal}} = \begin{cases} 
(\vartheta + r)^2/(4r), & r > \vartheta, \\
\vartheta, & 0 < r < \vartheta,
\end{cases} \quad (3.20)
$$

and let $t_{\text{ideal}}^p = \sqrt{2q_{\text{ideal}}^p \log p}$. By direct calculations and Mills’ ratio [87],

$$
h_p(\hat{\beta}_{t_{\text{ideal}}^p}^{HT}, \beta) = \begin{cases} 
L_p p^{1-(\vartheta+r)^2/(4r)}, & r > \vartheta, \\
\sim p^{1-\vartheta}, & 0 < r < \vartheta.
\end{cases}
$$

Combining this with Theorem 2.2 (which is for more general $\Omega$), we conclude that when $\Omega = I_p$, HT achieves the minimax Hamming distance, up to a multi-log$(p)$ factor; so it achieves the optimal phase diagram for recovery given in Section 2.3.

**Remark 5.** The ideal choice of $q$ in (3.20) depends on $(\vartheta, r)$ and it is hard to set them in a data driven fashion. On the other hand, a convenient choice is $q = 1$, corresponding to the universal threshold $t_p^* = \sqrt{2 \log(p)}$ [87]. Note that when $r > \rho^*_{\text{exact}}(\vartheta; I_p)$, $\text{Hamm}_p(\hat{\beta}_{t_{\text{ideal}}^p}^{HT}, \beta) \leq C(\log(p))^{-1/2}$ (and so exact recovery is achieved).

**Remark 6.** When a method yields exact recovery with overwhelming probabilities, we say it has the *Oracle Property*, a well-known notion in the variable selection literature [33]. In such a framework, we are using $P(\text{sgn}(\hat{\beta}) \neq \text{sgn}(\beta))$ as the measure of loss. Seemingly, such a measure is only appropriate for Rare/Strong signals. When signals are Rare and Weak, exact recovery is usually impossible, and the Hamming distance is a more appropriate measure of loss.

### 3.3 Applications

HC (and its variants) has found applications in GWAS and DNA Copy Number Variation (CNV), where the genetic effects are believed to be rare and weak. Parkhomenko et al. [75] used HC to detect modest genetic effects in a genome-wide study of rheumatoid arthritis. Sabatti et al. [79] used HC to quantify the strength of the overall genetic signals for each of the nine traits they were interested in. De la Cruz et al. [17] used HC to test whether there are associated markers in a given set of markers, with applications to Crohn’s disease. Jeng et al. [55, 56] proposed a variant of HC called *Proportion Adaptive Segment Selection (PASS)*, which can be viewed as a two-way screening process (across different SNPs and across different subjects), simultaneously dealing with the rare genetic effects and rare genomic variation. See also [48, 68, 71, 78, 89].

HC has also found applications in several modern experiments in Cosmology and Astronomy—another important source of rare and weak signals. Jin et al. [61] and Cayon et al. [15]
(see also [16, 14]) applied HC to standardized wavelet coefficients of Wilkinson Microwave Anisotropy Probe (WMAP), addressing the problem of non-Gaussianity detection in the Cosmic Microwave Background (CMB). Compared to the widely used kurtosis-based non-Gaussianity detector, HC showed superior power and sensitivity, and pointed to the cold spot centered at galactic coordinate (longitude, latitude) = (207.8°, −56.3°) (see [86] for more discussions on HC and the cold spot). Pires et al. [77] applied many non-Gaussianity detectors to gravitational weak lensing data and showed that HC is competitive, being more specifically focused on excess of observations in the tails of the distribution. Bennett et al. [6] applied the HC ideas to the problem of Gravitational Wave detection for a monochromatic periodic source in a binary system. They use a modified form of HC which offers a noticeable increase in the detection power, and yet is robust.

HC has also been applied to disease surveillance for early detection of disease outbreak (Neill and Lingwall [72, 73]) and to local anomaly detection in a graph (Saligrama and Zhao [80]), where it is found to have competitive powers.

3.4 Connections and extensions

In model (2.7)–(2.8), the noise entries are iid samples from a distribution $F$ which is known to be $N(0, 1)$. Delaigle and Hall [18] and Delaigle et al. [19] address the more realistic setting where $F$ is unknown and is probably non-Gaussian. They consider a two group model (a control group and a case group) and compute $P$-values for each individual feature using bootstrapped Student’s $t$-scores. The problem is also addressed by [43, 67], using very different approaches.

The testing problem (2.7)–(2.8) is a special case of the problem of testing $H_0^{(p)}$ of $X_i \overset{iid}{\sim} F$ versus $H_1^{(p)}$ of $X_i \overset{iid}{\sim} (1 - \epsilon)F + \epsilon G$, where $\epsilon \in (0, 1)$ is small, $F$ and $G$ are two different distributions, and $(\epsilon, F, G)$ may depend on $p$. Cai et al. [10] considers the case where $F = N(0, 1)$ and $G = N(\tau, \sigma^2)$; see also [7, 8]. Park and Ghosh [74] gave a nice review on large-scale multiple testing with a detailed discussion on HC. Cai and Wu [13] considers the extension where $F = N(0, 1)$ and $G$ is a Gaussian location mixture with a general mixing distribution, and Arias-Castro and Wang [4] investigate the case where $F$ is unknown but symmetric. In a closely related setting, Laurent et al. [66] considers the problem of testing whether the samples $X_i$ are iid samples from a single normal, or a mixture of two normals with different (but unknown) means. Addario-Berry et al. [1] and Arias-Castro et al. [2] consider a setting similar to (2.7)–(2.8) but where the signals are structured, forming clusters in (unknown) geometric shapes; the work is closely related to that in [45, Section 6].

Gayraud and Ingster [40] show that HC statistic continues to be successful in detecting very sparse mixtures in a functional setting. Haupt et al. [46, 47] consider the setting where adaptive sample scheme is available so that we can do inference and collect data in an alternating order.

HC can also be viewed as a measure for goodness-of-fit. Jager and Wellner [54] introduced a new family of goodness-of-fit tests based on the $\phi$-divergence, including HC as a special case. Wellner and Koltchinskii [88] further investigated the Berk-Jones statistic, which is closely related to HC, and derive the limiting distribution of the Berk-Jones statistic. In Jager and Wellner (2004) [53], they further investigated the limiting distribution of a class of weighted Kolmogorov statistics, including HC as a special case. The pontogram of Kendall and Kendall [65] is an instance of HC, applied to a special set of $P$-values.

HC is closely related to the False Discovery Rate (FDR) controlling procedure by Ben-
jamini and Hochberg (BH) [5], but it is different in important ways. The BH procedure targets on Rare/Strong signals, and the main goal to select the few strong signals embedded in a long list of noise, without making too many false selections. HC targets the more delicate Rare/Weak regime, where the signals and noise are hard to distinguishable. In such settings, while the BH procedure still controls the FDR, it yields very few discoveries. In this case, a more reasonable goal is to test whether any signals exist without demanding that we properly identify them all; this is what HC is specifically designed for.

HC is also intimately connected to the problem of constructing confidence bands for the False Discovery Proportion (FDP). See [11, 20, 41]. Motivated by a study of Kuiper Belt Objects (KBO) (e.g., [70]), Cai et al. [11] develop HC into an estimator for the proportion of non-null effects, a problem that has attracted substantial attention in the area of large-scale multiple testing in the past decade. The literature along this line connects to [5] on controlling FDR, as well as Efron [30] on controlling the local FDR in gene microarray studies.

4 Detecting and recovering signals in colored noise

In this section, we extend the discussions in Section 3 to the case of \( \Omega \neq I_p \). For optimal procedures in the current case, the key is to exploit the graphic structure of \( \Omega \). We propose Innovated Higher Criticism (IHC) for signal detection and Graphlet Screening (GS) for signal recovery. IHC and GS can be viewed as \( \Omega \)-aware Higher Criticism and \( \Omega \)-aware Hard Thresholding, respectively.

4.1 Innovated Higher Criticism and its optimality in signal detection

We revisit the testing problem (2.7)-(2.8), where we recall that

\[ Y = \beta + z, \quad z \sim N(0, \Sigma). \] (4.21)

Recall that HC is a method of combining \( P \)-values. We are interested in adapting HC for general sparse precision matrix \( \Omega \), and there are three perceivable ways of combining the \( P \)-values.

In the first one, we obtain individual \( P \)-values marginally in a brute-force fashion:

\[ \pi_i = P(|N(0, 1)| \geq |Y_i|/(\Sigma(i, i))^{1/2}). \]

We call the HC applied to these \( P \)-values the Brute-force HC (BHC). BHC neglects the correlation structure, so we expect some room for improvement.

For an alternative, denoting the unique square root of \( \Omega \) by \( \Omega^{1/2} \), it is tempting to use the Whitened Transformation \( Y \mapsto \Omega^{1/2} Y \sim N(\Omega^{1/2} \beta, I_p) \), so that the noise is whitened. We then obtain individual \( P \)-values by

\[ \pi_i = P(|N(0, 1)| \geq |(\Omega^{1/2} Y)_i|), \quad 1 \leq i \leq p. \]

We call the resultant HC the Whitened HC.

Our proposal is Innovated HC (IHC). Underlying IHC is the idea to find a transformation \( Y \mapsto MY = M\beta + Mz \) (\( M = M_{p,p} \), may depend on \( \Omega \)) so that

- **Preserving sparsity**: most entries of the vector \( M\beta \) are zero; this is important since the strength of HC lies in detecting very sparse signals.
Simultaneously maximizing SNR: to maximize the Signal-to-Noise Ratio for all \( i \) at which \( \beta_i \neq 0 \), defined by \( (M\beta)_i/\sqrt{(M\beta')_i(i,i)} \) (since \( MY \sim N(M\beta, MM') \)).

The best choice turns out to be \( M = \Omega \), associated with which is Innovated Transformation (IT)

\[
Y \mapsto \Omega Y \sim N(\Omega\beta, \Omega).
\]

This is related to the notion of innovation in time series literature and so the name of IT. See [36, Section 1.2] for detailed discussion on why \( M = \Omega \) is the best choice.

Now, first, IT preserves the sparsity of \( \beta \). Second, for most \( i \) at which \( \beta_i \neq 0 \), among three choices of \( M \), \( M = I_p \) (corresponding to model (4.21)), \( M = \Omega^{1/2} \), and \( M = \Omega \), the SNR are

\[
(\Sigma(i,i))^{-1/2}\beta_i, \quad ((\Omega^{1/2})(i,i))\beta_i, \quad \beta_i
\]
correspondingly, where in the last term, we have used the assumption of \( \Omega(i,i) = 1 \). See [45] for the insight underlying these results and proofs, where the key is to combine the sparsity of \( \Omega \) and the ARW model of \( \beta \). Note that by basic algebra,

\[
\Sigma(i,i)^{-1/2} \leq (\Omega^{1/2})(i,i) \leq 1,
\]

so IT has the largest SNR, simultaneously at all \( i \) such that \( \beta_i \neq 0 \).

It is particularly interesting that, while WT yields uncorrelated noise, it does not yield the largest possible SNR, so WT is not the best choice. For the current setting where signals are Rare and Weak and \( \Omega \) is sparse, larger SNR out-weights sparse correlations among the noise, so we prefer IHC to WHC. Similarly, we prefer WHC to BHC.

**Example 1.** Suppose \( \Omega \) is block-wise diagonal and satisfies \( \Omega(i,j) = 1 \{ i = j \} + h_{0} \cdot 1 \{ |i-j| = 1 \} \), \( \max \{i,j\} \) is even}, \( -1 < h_{0} < 1 \), \( 1 \leq i,j \leq p \). For all \( 1 \leq i \leq p \), \( (\Sigma(i,i))^{-1/2} = \sqrt{1-h_{0}^2} \) and \( (\Omega^{1/2})(i,i) = \frac{1}{2} [ \sqrt{1+h_{0}^2 + \sqrt{1-h_{0}^2}} ] \), and so \( (\Sigma(i,i))^{-1/2} \leq (\Omega^{1/2})(i,i) \leq 1 \); IT yields larger SNR than that of WT, and WT yields larger SNR than that of model (4.21).

**Remark 7.** At the heart of IHC is entry-wise thresholding applied to the vector \( \Omega Y \). This is equivalent to the Univariate Screening (US) [34, 42]. In detail, we can rewrite model (4.21) as a regression model \( W \sim N(X\beta, I_p) \), with \( W = \Omega^{1/2} Y \) and \( X = \Omega^{1/2} \). US thresholds the vector \( X'W \) entry-wise; note \( X'W = \Omega Y \).

Similarly, IHC consists of three simple steps (the last two are the same as in OHC).

- Obtain two-sided \( P \)-values by \( \pi_{i} = P(|N(0,1)| \geq |(\Omega Y)_{i}|), 1 \leq i \leq p \).
- Sort \( P \)-values: \( \pi_{(1)} < \pi_{(2)} < \ldots < \pi_{(p)} \).
- Innovated Higher Criticism statistic is then \( IHC_{p}^* = \max_{1 \leq i \leq p/2} IHC_{p,i} \), where \( IHC_{p,i} = \sqrt{p(i/p - \pi(i))/\sqrt{\pi(i)(1-\pi(i))}} \).

Consider the IHC test where we reject \( H_{0}^{(p)} \) if and only if \( IHC_{p}^* \geq d_{p}^*(\Omega) h(p, \alpha) \), where \( d_{p}^*(\Omega) \) is as in (2.3) and \( h(p, \alpha) \) is as in Section 3.1. It is seen that

\[
P_{H_{0}^{(p)}}(\text{reject } H_{0}^{(p)}) \leq \alpha.
\]

Moreover, we have the following theorem, which extends Theorem 3.1 from the case of \( \Omega = I_p \) to the case of more general \( \Omega \).
Theorem 4.1. Fix $(\vartheta, r)$ in the phase space. If $r > \rho^*(\vartheta)$ and as $p \to \infty$, $\alpha = \alpha_p$ tends to 0 slowly enough, then the power of the IHC-test tends to 1. If $r < \rho^*(\vartheta)$, then for any tests, the sum of Type I and Type II testing errors tends to 1 as $p \to \infty$.

Combining this with Theorem 2.1 for any $(\vartheta, r)$ in the Region of Detectable, IHC provides an asymptotically full power test, so it achieves the optimal phase diagram for detection given in Section 2.3.

The proof of Theorem 4.1 has two new ingredients, additional to that of Theorem 3.1. The first ingredient is Lemma 2.1 in Section 2.1. The second one is the similarity between $\beta$ and $\Omega^{\beta}$. Note that the most interesting region for signal detection is when $1/2 < \vartheta < 1/2$. For $\vartheta$ in this range, $\varepsilon_p \ll 1/\sqrt{p}$, so $\beta$ has about $p\varepsilon_p$ nonzeros, each equals $\tau_p$, and $\Omega^{\beta}$ has $\lesssim d^*_p(\Omega) \cdot p\varepsilon_p$ nonzeros, where about $p\varepsilon_p$ of them equals to $\tau_p$, and all others do not exceed $\tau_p$ in magnitude. Since $d^*_p(\Omega)$ does not exceed a multi-log($p$) term, we do not expect any difference between the detection boundary of $\Omega$ and that of $I_p$; both are $r = \rho^*(\vartheta)$.

4.2 Graphlet Screening and its optimality in variable selection

For signal recovery, we rewrite model (2.1) as a linear regression model

$$W \sim N(X\beta, I_p), \quad W \equiv \Omega^{1/2}Y, \quad X \equiv \Omega^{1/2}. \quad (4.22)$$

Our proposal is to use Graphlet Screening (GS), an idea developed recently by [63, 64]. At the heart of GS is graph-guided multivariate screening, which intends to overcome the shortcomings of the well-known method Univariate Screening (US) (also called marginal regression [42], Sure Screening [34]), without much increase in computational complexity. Write

$$X = [x_1, x_2, \ldots, x_p].$$

To use US, we project $W$ to the columns of $X$, one at a time, and then apply Hard Thresholding:

$$\hat{\beta}_j = <x_j, W> \cdot 1\{|<x_j, W>| \geq t\}, \quad 1 \leq j \leq p, \quad t > 0: \text{a threshold.}$$

The major challenge US faces is signal cancellation [78], meaning that due to the correlations among the design variables, the SNR of $<x_j, W>$ (which is $E[<x_j, W>] = \sum_\ell <x_j, x_\ell>\beta_\ell$ in the current setting) could be substantially smaller in magnitude than that in the case of orthogonal design.

To alleviate ‘signal cancellation’, an alternative is to use Exhaustive Multivariate Screening (EMS). Fixing a small integer $m_0$, for any $1 \leq m \leq m_0$ and a subset $\{i_1, i_2, \ldots, i_m\}$, $1 \leq i_1 < i_2 < \ldots < i_m \leq p$, we project $W$ to $\{x_{i_1}, x_{i_2}, \ldots, x_{i_m}\}$, and conduct a screening using a $\chi^2$-test with $df = m$. Unfortunately, EMS is neither computationally feasible nor efficient: it screens $\sum_{m=1}^{m_0} \binom{p}{m}$ different subsets of variables, which is hard to handle computationally; also, when we include too many subsets for screening, we need signals stronger than necessary for successful screening.

GS recognizes that in EMS, many subsets of variables can be safely skipped for screening, and the key innovation is to use a sparse graph to guide the screening. In detail, let $\mathcal{G} = (V, E)$ be the graph where $V = \{1, 2, \ldots, p\}$ and there is an edge between nodes $i$ and $j$ if and only if $\Omega(i, j) \neq 0$. Let

$$\mathcal{A}(m_0) = \{\text{all connected subgraphs of } \mathcal{G} \text{ with size } \leq m_0\}. \quad 16$$
Compared to EMS, the difference is that GS only applies $\chi^2$-screening to those subsets in $A(m_0)$. Note that when $\Omega = I_p$, GS reduces to Hard Thresholding, so it can be viewed as an $\Omega$-aware Hard Thresholding.

By a well-known result in graph theory \cite{40},

$$|A(m_0)| \leq CP(c d_p^*(G)) m_0,$$

where $d_p^*(G)$ is the maximum degree of $G$. By the definition and \cite{2.3}, $d_p^*(G) = d_p^*(\Omega)$, and does not exceed a multi-log($p$) term. As a result, GS has a much smaller computational cost than that of EMS (in fact, it is only larger than that of US by a multi-log($p$) factor for fixed $m_0$), and also requires much weaker signals than EMS does for successful screening.

**Remark 8.** GS is a flexible idea and can be adapted to many different settings, where the implementation may vary from occurrence to occurrence. It is a screening method and it has been applied to variable selection \cite{63, 64}, which includes model \cite{4.22} as a special case. It can also been viewed as a way to evaluate the combined significance of (a small number of) features, so it can be used for feature ranking; see Section 5 for more discussions.

We now describe how to apply GS to model \cite{4.22} for signal recovery. List all elements in $A(m_0)$ in the order of sizes, with ties breaking lexicographically,

$$\mathcal{I}_1, \mathcal{I}_2, \ldots, \mathcal{I}_N, \quad N \equiv |A(m_0)|.$$

Our proposal is a two-step procedure, containing a Screen step and Clean step. Fix positive tuning parameters $(u, v, q)$. In the Screen step, initialize with $S_0 = \emptyset$. For $i = 1, 2, \ldots, N$, letting $S_{i-1}$ be the set of all retained indices up to stage $i - 1$, we update $S_i$ by

$$S_i = \begin{cases} S_{i-1} \cup \mathcal{I}_i, & \text{if } \|P_{\mathcal{I}_i}Y\|^2 - \|P_{\mathcal{I}_i \cap S_{i-1}}Y\|^2 \geq 2q \log(p), \\ S_{i-1}, & \text{otherwise} \end{cases}$$

where for any $\mathcal{I} \subset \{1, 2, \ldots, p\}$, $P_{\mathcal{I}}$ is the projection matrix from $R^n$ to $\{x_j : j \in \mathcal{I}\}$. The set of all retained nodes in the Screen step is then $S_N$.

In the Clean step, when $j \notin S_N$, we set $\beta_{j}^g = 0$. When $j \in S_N$, let $G_{S_N}$ be the subgraph of $G$ formed by restricting all nodes to $S_N$. We decompose

$$G_{S_N} = G_{S_N,1} \cup G_{S_N,2} \cup \ldots \cup G_{S_N,L},$$

and estimate $\{\beta_j : j \in G_{S_N,\ell}, 1 \leq \ell \leq L\}$, by minimizing

$$\|P_{G_{S_N,\ell}}(Y - \sum_{j \in G_{S_N,\ell}} \beta_j x_j)\|^2 + u^2 \|\beta\|_0,$$

subject to the constraint that either $\beta_j = 0$ or $|\beta_j| \geq v$. Putting these together gives the final estimate, denoted by $\hat{\beta} = \hat{\beta}^{gs}(m_0, u, v, q)$.

**Theorem 4.2.** Fix $(m_0, \vartheta, r)$ such that $1 < r/\vartheta < 3 + 2\sqrt{2} \approx 5.828$ and $m_0 \geq (r - \vartheta)^2/(4 r v)$. Suppose $\vartheta \leq 2.3$ hold, the spectral norm of $\Omega^{-1}$ is bounded by $C$, and for some constants $\gamma \in (0, 1)$ and $C > 0$. Also, suppose $|\Omega(i,j)| \leq 4\sqrt{2} - 5 \approx 0.6569$ for all $1 \leq i, j \leq p, i \neq j$. If we set the tuning parameters $(u, v, q)$ in GS by $u = \sqrt{2\gamma \log(p)}$, $v = \sqrt{2r \log(p)}$ and $q$ an appropriately small constant, then as $p \to \infty$, $h_p(\beta^{gs}, \hat{\beta}) \leq L_p \text{Hamm}_p^{\vartheta}(\vartheta, r; \Omega) = L_p p^{1-(\vartheta+r)^2/(44r) + o(1)}.$
Recall that $\text{Ham}_p^*(\theta, r; \Omega)$ is the minimax Hamming distance as in (2.10). This says that for all $\Omega$ considered in Theorem 4.2, GS achieves the optimal phase diagram for recovery; see Section 2.3.

Theorem 4.2 was proved in Jin et al (2012) [63, Section 2.6], as a special example. The conditions on $r/\theta$ and off-diagonals of $\Omega$ are not necessary for GS to achieve the minimax Hamming distance. In fact, $h_p(\hat{\beta}^{gs}, \beta) \leq L_p \text{Ham}_p^*(\theta, r; \Omega) + o(1)$ holds in much broader settings, but $\text{Ham}_p^*(\theta, r; \Omega)$ can not have such a simple expression. See more discussions in [63] for the asymptotic minimaxity of GS in more general settings.

Remark 9. For the tuning parameters, $m_0$ is usually chosen for the computational capacity. The choice of $q$ is relatively flexible, as long as it falls into certain ranges. The choice of $u$ is harder, but the best $u$ is a function of $\epsilon_p$; in some settings (e.g., [11]), we can estimate $\epsilon_p$ consistently, and we know how to choose the best $u$. For these reasons, we essentially only have one tuning parameter $v$, which is connected to the tuning parameter in the subset selection and that of the lasso. See [63] for more discussions.

4.3 Phase diagrams (colored noise)

Recall that the optimal phase diagram for general $\Omega$ consists of four subregions separated by three curves $r = \rho^*(\theta)$, $r = \theta$ and $r = \rho^*_\text{exact}(\theta; \Omega)$. The conditions on $r/\theta$ may depend on the off-diagonals of $\Omega$ in a complicated way, but we always have

$$\rho^*_\text{exact}(\theta; \Omega) \geq \rho^*_\text{exact}(\theta; I_p),$$

since $\Omega = I_p$ is the easiest case for exact recovery.

For $\Omega$ satisfying conditions of Theorem 4.2 and for $(\theta, r)$ such that $1 < r/\theta < 3 + 2\sqrt{2}$, the minimax Hamming distance for $\Omega$ has the same convergence rate as that for the case of $\Omega = I_p$. Note that in the phase space, the curve $r = \rho^*_\text{exact}(\theta; I_p)$ and the line $r/\theta = 3 + 2\sqrt{2}$ intersect at the point $(\theta, r) = (1/2, (3 + 2\sqrt{2})/2)$. Therefore,

$$\rho^*_\text{exact}(\theta; \Omega) = \rho^*_\text{exact}(\theta; I_p), \quad \text{for all } 1/2 < \theta < 1.$$

Consequently, the right half of the curve $r = \rho^*_\text{exact}(\theta; \Omega)$ coincides with the right half of the curve $r = \rho^*_\text{exact}(\theta; I_p)$. See [63] for discussion in more general settings.

By Theorems 2.1-2.2 and Theorems 4.1-4.2, the optimal phase diagram for detection is achieved by IHC, and the optimal phase diagram for recovery is achieved by GS for a wide range of $\Omega$, including but are not limited to those satisfying the conditions of Theorem 4.2. See [63] for details.

4.4 An example, and comparisons with $L^0/L^1$-penalization methods

In general, it is hard to derive an explicit form for $r = \rho^*_\text{exact}(\theta; \Omega)$ for the whole range of $\theta$. Still, examples for some $\Omega \neq I_p$ would shed light on how this curve depends on the off-diagonal entries of $\Omega$.

We revisit Example 1 in Section 4.1, where $\Omega$ is block-wise diagonal, and each diagonal block is the $2 \times 2$ matrix with 1 on the diagonals and $h_0$ on the off-diagonals. It was shown in [63] that $\text{Ham}_p^*(\theta, r, \Omega) = L_p F^{1-c(\theta, r; h_0)}$, where

$$c(\theta, r; h_0) = \min \left\{ \frac{(\theta + r)^2}{4r}, \theta^2, \frac{1}{2} \left( (1-h_0^2)(r-\theta) + \frac{1}{2} \right)^2 \right\}, \quad (4.24)$$

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The curve $\rho_{\text{exact}}^*(\vartheta; \Omega)$ is then the solution of $c(\vartheta, r; h_0) = 1$, which depends on $h_0$. The top left panel of Figure 2 displays the phase diagram for $h_0 = 0.5$.

Somewhat surprisingly, even for very simple $\Omega$ such as the block-wise diagonal example above and even when the tuning parameters are ideally set, subset selection ($L^0$-penalization) and the lasso have non-optimal phase diagrams; in particular, their Region of Exactly Recoverable is smaller than that of GS. Figure 2 shows phase diagrams associate with GS, $L^0/L^1$-penalization methods for the block-wise diagonal example, where the tuning parameters are set ideally to minimize the Hamming distance; see Ji and Jin (2010) [57] and Jin et al. (2012) [63]. Given the non-optimality of $L^0/L^1$-penalization methods in such a simple $\Omega$, we do not expect that for more general $\Omega$ they could be optimal.

We must note that the optimalities of $L^0/L^1$-penalization methods in the literature are largely limited to settings different from here, where they usually have Rare/Strong signals, and either $\ell^2$-loss or $P(\text{sgn}(\hat{\beta}) \neq \text{sgn}(\beta))$ is frequently used as the measure of loss. However, $\ell^2$-loss is more appropriate for prediction setting, not for variable selection, and $P(\text{sgn}(\hat{\beta}) \neq \text{sgn}(\beta))$ is more appropriate for Rare/Strong signals, not for Rare/Weak signals where it is merely impossible to fully recover the support of $\beta$. Since $L^0$-penalization method is the target of many penalization methods, including the lasso, SCAD [33], MC+ [90], we should not expect these penalization methods to be optimal as well.

**Remark 10.** Ke et al. (2012) [64] studied a more complicate setting than that in Theorem 4.2 or that in [63], where the Gram matrix is not sparse but is sparsifiable. They derived the phase diagrams for a case that $\Omega$ is the correlation matrix of a long-memory time series and for a change-point model. The change-point model is a special case of model (4.22) where $X$ is an upper triangular matrix of 1’s (therefore, $X\beta$ is piece-wise constant). For the change-point model, the phase space partitions into only 2 regions, separating by the curve $r = \rho_{\text{exact}}^*(\vartheta)$, where $\rho_{\text{exact}}^*(\vartheta) = \max\{4(1 - \vartheta), (4 - 10\vartheta) + 2\sqrt{[(2 - 5\vartheta)^2 - \vartheta^2]}\}_+$.

### 4.5 Connections to the literature

Model (4.21) is closely related to the linear model $W = N(X\beta, I_n)$, where the Innovated Transformation reduces that of $W \mapsto X'W$. Arias-Castro et al. (2011) [3] applied HC to $X'W$ for signal detection, which is similar to IHC. Ingster et al. (2009) [52] considered a
case that \( W \sim N(X\beta, \sigma^2 I_p) \) for an unknown \( \sigma \) and \( X_i \)'s are iid samples from \( N(0, (1/n)I_p) \). They proposed a modified IT, \( W \mapsto \|W\|^{-1}X'W \), to adapt to the unknown \( \sigma \). Mukherjee et al. (2013) [71] considered the binary-response logistic regression. They proposed HC-like statistics for signal detection and exposed interesting dependence of the detection boundary on the design matrix.

Another related setting is that the data are iid samples \( Y_1, \ldots, Y_n \) of \( N(\beta, \Sigma) \). This reduces to model (4.21) noting that \( (1/\sqrt{n})\sum_{i=1}^n Y_i \sim N(\beta, \Sigma) \) is the vector of sufficient statistics of \( \beta \). When the data are nonGaussian, Zhong et al. [92] proposed an “\( L_\gamma \)-thresholding test” which takes BHC as a special case of \( \gamma = 0 \).

GS, as a method to improve US, is different from the Iterative Sure Independence Screening (ISIS) [34, 35]. ISIS first applies US to select a small set of variables \( M_1 \). In the second step, for each \( j /\in M_1 \), it runs a least-square algorithm on the model \( M_1 \cup \{j\} \) and records the coefficient of \( j \). These coefficients are then used to rank variables and expand \( M_1 \) to a set \( M_2 \). This procedure runs iteratively. ISIS alleviates ‘signal cancellation’ between variables in \( M_1 \) and those in \( \{1, \ldots, p\} \setminus M_1 \), but unlike GS, it does not deal with ‘signal cancellation’ among variables in \( \{1, \ldots, p\} \setminus M_1 \).

GS is closely related to LARS [32] and forward-backward greedy algorithm [91] in utilizing local graphic structure of variables. The Screen step of GS is a step-wise forward algorithm and the Clean step is a backward algorithm.

5 Stylized applications

HC and GS are flexible ideas that can be adapted to a broad set of problems and settings. In this section, we outline some potential applications of HC and GS.

5.1 Higher Criticism for estimating the bandwidth of a matrix

The HC idea, although still in its early stage of development, is seeing increasing interest both in practice and in theory. In Section 3.3-3.4 we have reviewed applications and extensions of HC in many different settings. In this section, we illustrate a new application of HC.

Suppose we have samples \( X_i \in R^p \) from a Gaussian distribution

\[
X_i \overset{iid}{\sim} N(0, \Sigma), \quad 1 \leq i \leq n.
\]

The Gaussian assumption is not critical and is only for simplicity. In many applications, with the Linkage Disequilibrium (LD) matrix being an iconic example, \( \Sigma \) is unknown but is banded; denote the bandwidth by \( b = b(\Sigma) \) so that \( b \) is the smallest integer such that \( \Sigma(i, j) = 0 \) for all \( i, j \) with \( |i - j| \geq b + 1 \).

We adapt HC to estimate \( b(\Sigma) \). HC can also be adapted to test whether \( b(\Sigma) \leq k_0 \) or \( b(\Sigma) > k_0 \) for a given small integer \( k_0 \); the discussion is similar so we omit it to save space.

Let the empirical covariance matrix be \( S_n = \frac{1}{n} \sum_{i=1}^n X_iX_i' \). For \( 1 \leq k \leq p - 1 \), let \( \xi^{(k)} \) and \( \hat{\xi}^{(k)} \) be the \((p-k) \times 1 \) vectors formed by the \( k \)-th (upper) off-diagonal of \( \Sigma \) and \( S_n \), respectively:

\[
\xi^{(k)} = (\Sigma(1, 1+k), \ldots, \Sigma(p-k,p))', \quad \hat{\xi}^{(k)} = (S_n(1, 1+k), \ldots, S_n(p-k,p))'.
\]

We consider a Rare/Weak setting where each \( \xi^{(k)} \) has a small fraction of nonzeros, and each nonzero is relatively small. By elementary statistics, for any \( i, j \) such that \( \Sigma(i, j) = 0 \), we have that approximately, \( \sqrt{n}S_n(i, j) \sim N(0, 1) \).
We propose the following HC estimator for \( b(\Sigma) \). Fix an integer \( b_0 \) (a relatively small but conservative upper bound for \( b(\Sigma) \)) and a level \( \alpha \in (0,1) \),

- For \( k = 1, \ldots, b_0 \), apply \( HC_p^+ \) in (3.18) to \( \hat{\xi}^{(k)} \), where the individual \( P \)-values associated with the entries of \( \hat{\xi}^{(k)} \) are computed by \( P(|N(0,1)| \geq \sqrt{n} \hat{\xi}_i^{(k)}) \), \( 1 \leq i \leq p - k \).

Denote the resultant HC scores by \( HC^{(1)}, \ldots, HC^{(b_0)} \), correspondingly.

- Estimate \( b(\Sigma) \) by \( \hat{b}^{HC} = \hat{b}^{HC}(S_n; n, p, t_n, b_0) = \max\{1 \leq k \leq b_0 : HC^{(k)} \geq h^+(p, \alpha/b_0)\} \).

Recall that \( h^+(p, \alpha) \) is as in Section 3.1 which can be computed by simulations.

We conducted a small-scale simulation, where \( (p, n, b(\Sigma), b_0, \alpha) = (5000, 200, 2, 10, 0.05) \). For \( k = 1, 2 \), and fixed \((\epsilon, \tau)\), we generate the entries of \( \xi^{(k)} \) randomly from \((1-\epsilon)\nu_0 + \nu_\tau \). We then apply the above procedure and repeat the whole simulation processes independently for 200 times, and recorded the error rates (the fraction of simulations where \( \hat{b}^{HC} \neq b(\Sigma) \)).

We have investigated 6 different combinations of \((\epsilon, \tau)\): \((.01,.175), (.01,.2), (.01,.225), (.005,.225), (.005,.25) \) and \((.01,.275)\); and the corresponding error rates of \( \hat{b}^{HC} \) are 6.5%, 0.5%, 0%, 8.5%, 3% and 2%.

**Remark 11.** The choice of \( h^+(p, \alpha/N) \) is based on Bonferroni correction which is acceptable for relatively small \( N \). For large \( N \), we may need to adjust the threshold, say, with Benjamini and Hochberg’s FDR-controlling method [5].

### 5.2 Ranking features by Graphlet Screening

Consider a linear regression of \( n \) samples and \( p \) features (or variables):

\[
W = X\beta + z, \quad X = X_{n,p} = [x_1, x_2, \ldots, x_p], \quad z \sim N(0, I_n).
\] (5.25)

Denote the Gram matrix by

\[
G = X'X.
\]

We assume \( X \) is normalized so that \( G \) has unit diagonals. We are primarily interested in the case where \( G \) is approximately sparse in the sense that each row of \( G \) has relatively few large entries. At the same time, we assume the feature vector \( \beta \) is sparse in the sense that it only has a small fraction of nonzeros. We are interested in ranking the features in a way to have a competitive Receiver Operating Curve Characteristic (ROC) curve.

Conventionally, we rank the features by US: we project \( W \) to the columns of \( X \), one at a time, and rank their significances according to \(|(x_j, W)|\). The challenge of this approach is, again, ‘signal cancellation’; see Section 4.2 for discussions. When ‘signal cancelation’ presents, there is room for improvement.

We propose to rank the features by GS. Fixing a threshold \( \delta > 0 \), introduce a graph \( G^{*,\delta} = (V, E) \) where \( V = \{1, 2, \ldots, p\} \) and there is an edge between \( i \) and \( j \) if and only if \( |G(i,j)| \geq \delta \); since \( G \) is approximately sparse, \( G^{*,\delta} \) is sparse in that the maximum degree is small, given an appropriate choice of \( \delta \). Fixing \( m_0 > 1 \), we similarly define

\[
A^{*,\delta}(m_0) = A^{*,\delta}(m_0, G) = \{ \text{all connected subgraphs of } G^{*,\delta} \text{ with size } \leq m_0 \},
\]

Similarly to (4.23),

\[
|A^{*,\delta}(m_0)| \leq Cp(d^\ast_p)^{m_0}, \quad \text{where } d^\ast_p = d^\ast_p(\delta, G) \text{ is the maximal degree of } G^{*,\delta}.
\]

Our procedure consists of the following steps.
Feature ranking is of interest in many high dimensional problems, including but are not limited to (a) large-scale multiple testing, where it is of interest to develop methods that control the FDR while maximizing the power of multiple tests, (b) cancer classification where it is desirable to select a small fraction of features for the trained classification decision \([24, 25, 60]\), and spectral clustering where it is desirable to perform a dimension reduction before we apply Principle Component Analysis (PCA) \([62]\). As GS provides a better strategy in feature ranking than US, it is potentially useful in attacking all the problems above.

6 Feature selection by Higher Criticism for classification

Among many uses of Higher Criticism, one that is particularly interesting is to set thresholds for feature selection in the context of classification.

Consider a two-class classification setting where \((Y^{(i)}, \ell_i), 1 \leq i \leq n, \) are measurements from two different classes. Here, \(Y^{(i)} \in \mathbb{R}^p\) are the feature vectors and \(\ell_i \in \{-1, 1\}\) are
the class labels. We assume two classes are equally likely, so that after a standardizing transformation,

\[ Y^{(i)} \sim N(\ell_i \cdot \mu, \Sigma), \]

with \( \mu \in \mathbb{R}^p \) the contrast mean vector and \( \Sigma \) the \( p \times p \) covariance matrix; such an assumption is only for simplicity in presentations. Given a fresh feature vector \( Y \), the primary interest is to predict the associated class label \( \ell \in \{-1, 1\} \).

For simplicity, we assume \( \Sigma \) is known and the precision matrix \( \Omega = \Sigma^{-1} \) is sparse. The case \( \Sigma \) is unknown (but \( \Omega \) is sparse) is discussed in Fan et al. (2013) \[36\]; see details therein. Fisher’s linear discriminant analysis (LDA) is a classical approach to classification. Let \( w = (w_1, w_2, \ldots, w_p)' \) be a \( p \times 1 \) feature weight vector. For a fresh feature vector \( Y = (Y_1, \cdots, Y_p)' \), Fisher’s LDA takes the form

\[ L(Y) = \sum_{i=1}^{p} w_i Y_i, \]

and classifies \( \ell = \pm 1 \) according to \( L(Y) \gtrless 0 \). When \( (\Sigma, \mu) \) are known, it is known that the optimal weight vector satisfies \( w \propto \Omega \mu \).

To adapt Fisher’s LDA to the current setting, the key is to estimate \( \mu \). We are primarily interested in the Rare/Weak setting where only a small fraction of the entries of \( \mu \) is nonzero and the nonzero entries are individually small. Define the feature \( z \)-vector

\[ Z = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\ell_i \cdot Y^{(i)}) \sim N(\sqrt{n} \mu, \Sigma). \]  

(6.26)

A standard approach to estimating \( \mu \) is by some sort of thresholding scheme. For any \( t > 0 \), denote by \( \eta_t(z) \) the clipping thresholding function \( \eta_t(z) = \text{sgn}(z)1\{|z| \geq t\} \) \[24, 36\]. Our proposal is to use Innovated Thresholding which thresholds \( \Omega Z \) coordinate-wise:

\[ \hat{\mu}^{IT}_{t,i} = \eta_t((\Omega Z)_i), \quad 1 \leq i \leq p. \]

(6.27)

One may also use Brute-force Thresholding which thresholds \( Z \) coordinate-wise, or the Whitened Thresholding which thresholds \( \Omega^{1/2} Z \) coordinate-wise. However, these schemes are inferior to Innovated Thresholding, for Innovated Transformation yields larger Signal-to-Noise Ratio than Brute-force Transformation and Whitened Transformation; see Section 4.1 for details. Also, in [6.27], we have used the clipping thresholding rule. Alternatively, one may use hard-thresholding or soft-thresholding, but the difference is usually not significant. See [24, 36] for more discussions.

We now modify Fisher’s LDA by

\[ L^{IT}_t(Y; \Omega) = (\hat{\mu}_t^{IT})' \Omega Y, \quad \text{where} \quad \hat{\mu}^{IT}_t = (\hat{\mu}^{IT}_{t,1}, \hat{\mu}^{IT}_{t,2}, \ldots, \hat{\mu}^{IT}_{t,p})'. \]

and classify \( \ell \) as \( \pm 1 \) according to \( L^{IT}_t(Y; \Omega) \gtrless 0 \). This is related to the modified HC in [92], but the focus there is on signal detection, not feature selection.

Seemingly, an important issue is how to set the threshold \( t \). We propose to set the threshold by Higher Criticism Thresholding (HCT), a variant of OHC. Fix \( \alpha_0 \in (0, 1/2] \).

- Calculate (two-sided) \( P \)-values \( \pi_i = P\{|N(0,1)| \geq |(\Omega Z)_i|\}, \ 1 \leq i \leq p. \)
- Sort the \( P \)-values into ascending order: \( \pi_{(1)} < \pi_{(2)} < \ldots < \pi_{(p)} \).
We introduce the ARW model for classification:

6.1 Phase diagram for classification

suggested by Fisher’s LDA. Note that this also suggests the (one-sided) clipping hard thresholding, similar to that of (2.7)-(2.8), although in a similar spirit. See \[25\] for explanations.

In practice, we set \(\alpha_0 = 0.10\); HCT is relatively insensitive to different choices of \(\alpha_0\). In (6.28), the denominator of the HC objective function is different from that of OHC we used for testing problems (2.7)-(2.8), although in a similar spirit. See \[25\] for explanations.

Once the threshold is decided, the associated Fisher’s LDA is then

\[
\hat{\mu}_{HC} = \hat{\mu}_{HC}(Z_1, Z_2, \ldots, Z_p; \alpha_0) = |Z|_{HC}. 
\] (6.29)

The HCT trained classification rule classifies \(\ell = \pm 1\) according to \(L_{HC}^{IT}(Y) \geq 0\).

Remark 12. The classification problem is closely connected to the testing problem (2.7)-(2.8). For illustration, assume \(\Omega = I_p\) and \(\sqrt{n} \mu_i \sim (1 - \epsilon) \nu_0 + \epsilon \nu_\tau\). Given a test feature \(Y \sim N(\ell \cdot \mu, I_p)\), the classification problem can be viewed as the problem of testing \(H_1^{(\mu)}\) of \(Y \sim N(\mu, I_p)\). Despite this, there is a major difference. In (2.7)-(2.8), we don’t have any information additional to the prior distribution on \(\mu\), so all features are equally likely to be useful. In the classification problem, however, the training \(z\)-vector \(Z \sim N(\sqrt{n} \mu, I_p)\) contains additional information about \(\mu\); for feature \(i\), \(1 \leq i \leq p\), the posterior probability that it is a useful feature is given by \(P(\mu_i \neq 0 | Z) = e^{(1 - \epsilon)\sqrt{n}Z_i - \tau^2/2}/[(1 - \epsilon) + e^{(1 - \epsilon)\sqrt{n}Z_i - \tau^2/2}]\), which \(\approx 1\) if \(Z_i\) is large and positive and \(\approx 0\) if \(Z_i\) is large and negative. Seemingly, the posterior distribution contains much more information on inference than the prior distribution does. Note that this also suggests the (one-sided) clipping hard thresholding, similar to that suggested by Fisher’s LDA.

6.1 Phase diagram for classification

We introduce the ARW model for classification:

\[
\sqrt{n} \mu_i \sim (1 - \epsilon) \nu_0 + \epsilon \nu_\tau, \quad 1 \leq i \leq p.
\]

Fix \((\vartheta, r, \theta)\) such that \(r > 0\), \(0 < \theta < 1\) and \(0 < \vartheta < 1 - \theta\). Similarly, we let \(\epsilon = \epsilon_p = p^{-\vartheta}\), \(\tau = \tau_p = \sqrt{2r \log(p)}\) and \(n = n_p = p^\theta\).

It was noted in \[60, 36\] that for any fixed \(\theta \in (0, 1)\), the most interesting range for \(\vartheta\) is \(0 < \vartheta < (1 - \theta)\). When \(\vartheta > (1 - \theta)\), for successful classification, we need \(\tau_p \gg \log(p)\), but this corresponds to Rare/Strong regime, which is relatively easy, for we can separate the nonzero entries of \(\mu\) from zero ones by simple thresholding. For \(\rho^*(\cdot)\) be as in (2.9), let

\[
\rho^*_\vartheta(\vartheta) = (1 - \theta)\rho^*(\frac{\vartheta}{1 - \theta}), \quad 0 < \vartheta < (1 - \theta).
\]

The following theorem is proved in Fan et al (2013) \[36\].
Figure 4: Left: curves $r = \rho^*_\theta(\vartheta)$ for $\theta = 0, 0.2, 0.4$. Right: enlargement the rectangular region bounded by dashed lines in the left panel. It partitions into three regions, where in the yellow region, it is not only possible to have successful classifications, but is also possible to separate useful features from useless ones.

**Theorem 6.1.** Fixing $(\vartheta, \theta, r) \in (0,1)^3$ such that $0 < \vartheta < (1 - \theta)$, and suppose $\Omega = \Sigma^{-1}$ satisfies (2.2)-(2.3), and that the spectral norm of $\Sigma$ is bounded by a constant $C > 0$. If $r > \rho^*_\theta(\vartheta)$, then the classification error of the trained HCT classification rule in (6.29) tends to 0 as $p \to \infty$. If $0 < r < \rho^*_\theta(\vartheta)$, then the classification error of any trained classification rule is no less than $1/2 + o(1)$, where $o(1) \to 0$ as $p \to \infty$.

There is a similar phase diagram associated with the classification problem.

- **Region of Classifiable**: $\{(\vartheta, r) : 0 < \vartheta < (1 - \theta), r > \rho^*_\theta(\vartheta)\}$. In this region, the HC threshold $\hat{t}_{\text{HC}}$ satisfies $\hat{t}_{\text{HC}}/t_{\text{ideal}} \to 1$ in probability, where $t_{\text{ideal}}$ is the ideal threshold that one would choose if the underlying parameters $(\vartheta, r, \Omega)$ are known. Also, the classification error of HCT-trained classification rule tends to 0 as $p \to \infty$.

- **Region of Unclassifiable**: $\{(\vartheta, r) : 0 < \vartheta < (1 - \theta), r < \rho^*_\theta(\vartheta)\}$. In this region, the classification error of any trained classification rule can not be substantially smaller than $1/2$.

See more discussion in [24, 25, 60]. Ingster et al. (2009) [51] derived independently the classification boundary in a broader setting, but they didn’t discuss HC. In Figure 4 we plot the phase diagrams for $\theta = 0, 2, 4$.

The advantage of HC is its optimality in the ARW model. Note that HCT is a data-driven non-parametric statistic the use of which does not require the knowledge of the ARW parameters. HC is not tied to the idealized model we discussed here, and can be useful for more general settings. See [24] for applications of HC to cancer classification with microarray data sets.

Our proposal of threshold choice by HC is very different from Benjamini-Hochberg’s FDR-controlling method (or Efron’s local FDR approach), where the philosophy is to control the feature FDR (i.e., the expected fraction of falsely selected features out of all selected features) by a small number (e.g., 5%). However, this is not necessarily the right strategy when signals are Rare/Weak. Donoho and Jin (2009) [25] identified a sub-region of Region of Classifiable where to obtain optimal classification behavior, we must set the feature se-
lection threshold very low so that we include most of the useful features; but when we do this, we must include many useless features and the feature FDR is approximately 1.

References


