Controlling False Discovery Rate Using Gaussian Mirrors

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ABSTRACT

Simultaneously, finding multiple influential variables and controlling the false discovery rate (FDR) for linear regression models is a fundamental problem. We here propose the Gaussian Mirror (GM) method, which creates for each predictor variable a pair of mirror variables by adding and subtracting a randomly generated Gaussian perturbation, and proceeds with a certain regression method, such as the ordinary least-square or the Lasso (the mirror variables can also be created after selection). The mirror variables naturally lead to test statistics effective for controlling the FDR. Under a mild assumption on the dependence among the covariates, we show that the FDR can be controlled at any designated level asymptotically. We also demonstrate through extensive numerical studies that the GM method is more powerful than many existing methods for selecting relevant variables subject to FDR control, especially for cases when the covariates are highly correlated and the influential variables are not overly sparse.

1. Introduction

Linear regression, which dates back to the beginning of the 19th century, is one of the most important statistical tools for practitioners. The theoretical research addressing various issues arising from big data analyses has gained much attention in the last decade. One important problem is to determine which covariates (aka “predictors”) are “relevant” or “important” in a linear regression. In early days (before 1970s), people often rely on the t-test to assess the importance of each individual predictor in a regression model, although the method is known to be problematic due to the existence of high multicollinearity. A greedy stepwise regression method was later proposed in Efroymson (1960) to alleviate some of the flaws. Good criterion, such as Akaike information criteria (AIC, Akaike 1978) and Bayesian information criteria (BIC, Schwarz 1978), for directing the model search were developed later. In recent years, due to the advance of data-generating technologies in both science and industry, researchers discovered that various regularization-based regression methods, such as Lasso (Tibshirani 1996), SCAD (Fan and Li 2001), elastic net (Zou and Hastie 2005), and many others, are quite effective in dealing with high-dimensional data and selecting relevant covariates with certain guaranteed theoretical properties, such as the selection consistency and the oracle property.

For the linear regression model, $y = x_1 \beta_1 + \cdots + x_p \beta_p + \epsilon$, we are interested in testing $p$ hypotheses: $H_j: \beta_j = 0$ for $j = 1, \ldots, p$, simultaneously and finding a statistical rule to decide which hypotheses should be rejected. Let $S_0 \subset \{1, 2, \ldots, p\}$ index the set of “null” predictors, that is, those with $\beta_j = 0$; so $S_1 = S_0^c$ indexes the set of relevant predictors. Let $\hat{S}_1$ be the set selected based on a statistical rule. The FDR for quantifying the Type I error for this statistical rule is defined as

$$FDR = \mathbb{E}[\text{FDP}], \text{ where } \text{FDP} = \frac{\# \{i \mid i \in S_0, i \in \hat{S}_1\}}{\# \{i \mid i \in \hat{S}_1\} \lor 1}.$$

Controlling the FDR is useful when the number of features is large. For example, modern gene expression studies usually involve thousands of genes; genome-wide association studies (GWAS) routinely examine tens of thousands to millions of single nucleotide polymorphisms (SNPs); and financial data often contain many features of thousands of companies. It is of practical importance to select a small set of the features for follow-up experimental validations and testings or future predictions, which requires the researchers to have reliable FDR control.

The task of controlling the FDR at a designated level, say $q$, is challenging in two aspects: (i) the test statistic and the corresponding distribution under the null hypothesis is not easily available for high-dimensional problems; and (ii) the dependence structure of the covariates induces a complex dependence structure among the estimated regression coefficients. A heuristic method based on permutation tests was introduced by Chung and Romano (2016), but it fails to yield valid FDR control unless $S_1$ is empty. Starting with $p$-values based on the marginal regression, Fan, Han, and Gu (2012) proposed a novel way to estimate the false discovery proportion (FDP) when the test statistic follows a multivariate normal distribution. However, the consideration of the marginal regression deviates from the original purpose of the study in many cases.

Barber and Candès (2015) introduced an innovative approach, the knockoff filter, which provides provable FDR control for cases with an arbitrary design matrix when $p < n/2$.

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2p − n predictors unchanged and constructed the knockoffs only for the remaining n − p variables. By introducing knockoffs, they obtained a test statistic that (i) are symmetric about the mean, and (ii) have independent signs, for the null variables. To this end, each column \( \tilde{X}_j \) of the knockoff matrix \( \tilde{X} \) needs to be exchangeable with the corresponding column \( X_j \) in \( X \). To gain more power, however, they want \( X \) and \( \tilde{X} \) as dissimilar as possible. When correlations or conditional correlations among the predictors are high and dense, there is little room for one to choose a good knockoff. This leads to a substantial decrease in power (see Section 6 for more details).

The knockoff method was later extended to deal with high-dimensional problems via either the screening+knockoffs strategy (Barber et al. 2020) or the model-X knockoff approach (Candes et al. 2018). In the model-X framework, Candes et al. (2018) relaxed the linear assumption by considering the joint distribution of the response \( Y \) and the predictors \( X \). The goal is to find the Markov blanket, a minimal set \( S \) such that \( Y \) is independent of all the others when conditioning on \( X_S \). Although the model-X knockoff method can control the FDR, this construct relies heavily on the assumption that the distribution of \( X \) is completely known, which is generally unrealistic except for some special scenarios. Barber et al. (2020) constructed a robust version of model-X knockoffs based on an estimated joint distribution of \( (X_1, \ldots, X_p) \). However, estimating the joint distribution in a high-dimensional setting is not only challenging even for the multivariate Gaussian case, but also leads to inaccurate FDR control. Huang and Janson (2019) further relaxed the requirement of Model-X Knockoffs by allowing the joint distribution of \( (X_1, \ldots, X_p) \) to belong to a prespecified exponential family with unknown parameters.

For high-dimensional data, another line of work is the post-selection inference, which aims at making inference conditional on the selection (Berk et al. 2013; Lee et al. 2016). In Lee et al. (2016), the selection event of LASSO is shown to be a union of polyhedra. Tibshirani et al. (2016) provided analogous results for the forward stepwise regression and the least angle regression. Taylor and Tibshirani (2018) extended these results to \( L_1 \) penalized likelihood models including generalized regression model.

In this article, we propose the Gaussian Mirror (GM) method, which constructs the test statistic marginally. Namely, for each variable \( x_j \), we create a pair of “mirror variables,” \( x_j^+ = x_j + \epsilon_j z_j \) and \( x_j^- = x_j - \epsilon_j z_j \), where \( \epsilon_j \) is a scalar and \( z_j \sim N(0, I_p) \). This construct can be viewed as a quantifiable way of perturbing the feature, and is equivalent to treating \( c_j z_j \) as a “knockoff” variable of \( x_j \) if OLS is used for the model fitting. The perturbation magnitude is chosen according to an explicit strategy (Barber et al. 2020) or the model-X knockoff approach (Candes et al. 2018). In the model-X framework, Candes et al. (2018) relaxed the linear assumption by considering the joint distribution of \( (X_1, \ldots, X_p) \), and is thus more applicable in real-data applications, such as GWAS studies where each feature takes value in \( \{0, 1, 2\} \), representing the number of minor-allele mutations of a single-nucleotide polymorphism (SNP).

In addition, practitioners often have a limited budget to verify the discoveries. For example, if the budget only allows a scientist to do 100 validation tests, a natural question is how many false discoveries (FDs) they expect to have in a top-100 list and what is an uncertainty measure for the estimated FDs. To answer these questions, we provide an estimate and confidence interval for the expectation of FDs by using the bootstrap method.

The article is organized as follows. In Section 2, we describe the general GM idea and a GM algorithm for the ordinary least-square (OLS) estimation in the low-dimensional case \( p < n \). In Section 3, we discuss how to employ the post-selection adjustment strategy to extend the GM construction for Lasso, which handles the case with \( p \geq n \). In Section 4, we investigate theoretical properties of the GM procedure. In Section 5, we introduce an estimator of the number of FDs and build its confidence interval using nonparametric bootstrap. In Section 6, we provide numerical evidence showing the advantage of GM to its competitors via simulations and real data analysis. In Section 7, we conclude the article with a short discussion. All the technical proofs of all the lemmas and theorems stated in the article are put in the appendix. The R-code for the GM procedure is publicly available at https://github.com/BioAlgs/GM.

Notations: To ease the readability, we summarize some notations used frequently in this article. Let \( X \) be the design matrix, \( x_j = (x_{j1}, \ldots, x_{jp})^T \) be the \( j \)th column of \( X \), and \( X_{-j} \) be the submatrix of \( X \) with the \( j \)th column removed. Without loss of generality, we assume that \( X \) is normalized so that \( \sum_{j=1}^{n} x_{ij} = 0 \) and \( \frac{1}{n} \| x_j \|_2 = 1, j = 1, \ldots, p \). Let \( X' = (x_1^+, x_1^-, X_{-j}) \), where \( x_j^+ = x_j + c_j z_j, x_j^- = x_j - c_j z_j \sim N(0, I_p) \), and \( c_j \) is a scalar. Let \( \beta \) be the vector of coefficients and let \( \beta_{-j} \) be the subvector with the \( j \)th entry removed. Let \( \beta^j = (\beta_j^+ \beta_j^-)^T \), where \( \beta_j^+ \) and \( \beta_j^- \) denote the coefficients of the mirror variable pair, and \( \hat{\beta}^j \) be an estimate of \( \beta^j \). Let \( S_0 = \{ j : \beta_j = 0 \} \), \( S_1 = \{ j : \beta_j \neq 0 \} \), \( p_0 = |S_0| \), and \( p_1 = |S_1| \). The designed FDR level to be controlled at is \( q \).
2. The GM Methodology for OLS

2.1. The GM

Suppose the data are generated from the following linear regression model:

\[ y = X\beta + \epsilon, \]

where \( y \in \mathbb{R}^n \) is the response vector, \( X = (X_1, \ldots, X_p) \in \mathbb{R}^{n \times p} \) is the design matrix, and \( \epsilon = (\epsilon_1, \ldots, \epsilon_n) \) is a vector of iid draws from \( N(0, \sigma^2) \). We begin with the low-dimensional case with \( p < n \) and focus on the OLS estimator. The high-dimensional case with \( p > n \) is deferred to the next section. As shown in Figure 1, we construct the \( j \)-th GM by replacing \( X_j \) with a pair of variables \((X_j^+, X_j^-)\) with \( X_j^+ = X_j + cz_j \) and \( X_j^- = X_j - cz_j \), where \( z_j \) is an independently simulated Gaussian random vector with mean 0 and covariance \( I_n \) and \( c \) is a scalar which depends on \( X \) and \( z_j \).

Note that \( \beta_j^+ = \beta_j^- = 0 \) when \( j \in S_0 \) and \( \beta_j^+ = \beta_j^- = \beta_j/2 \) when \( j \in S_1 \). Let \( GM_j \) be the design matrix with the \( j \)-th Gaussian mirror, that is,

\[ GM_j := X_j' = (X_j^+, X_j^-, X_{-j}). \quad (2) \]

Fit the model \( y = X'\beta' + \epsilon \) and estimate the coefficients by the least square

\[ \hat{\beta}' = \arg\min_{\beta'} \| y - X'\beta' \|_2^2. \quad (3) \]

The mirror statistic for the \( j \)-th variable is constructed as

\[ M_j = |\hat{\beta}_j^+ + \hat{\beta}_j^-| - |\hat{\beta}_j^+ - \hat{\beta}_j^-|. \quad (4) \]

Another possible construct is the “signed-max” statistic as suggested in Barber and Candès (2015) and studied more carefully in Ke, Liu, and Ma (2020). The mirror statistic \( M_j \) has two parts: the first part reflects the importance of the \( j \)-th predictor; and the second part captures the noise cancellation effect. Intuitively, when \( j \in S_0 \), the coefficients \( \hat{\beta}_j^+ \) and \( \hat{\beta}_j^- \) are due to noise and the mirror statistic \( M_j \) should center around zero; when \( j \in S_1 \), \( \hat{\beta}_j^+ + \hat{\beta}_j^- \) reflects the signal, whereas \( \hat{\beta}_j^+ - \hat{\beta}_j^- \) cancels out the signal and only reflects the noise effect. Based on this observation, we would declare a variable \( X_j \) as “significant” if \( M_j \geq t \) for some threshold \( t > 0 \). The choice of \( t \) depends on the number of false positives and the associated FDP. If we can choose GM properly such that \( M_j \) follows a distribution symmetric about zero, that is, \( P(M_j \geq s) = P(M_j \leq -s), \forall s \). Then, the number of false positive \( |\{j \in S_0 | M_j \geq t\}| \) can be approximated by \( \#\{j \in S_0 | M_j \leq -t\} \). The FDP can be estimated by

\[ \text{FDP}(t) = \frac{|\{j | M_j \leq -t\}|}{|\{j | M_j \geq t\}| + 1}. \quad (5) \]

For any designated FDR level \( q \), we could choose \( \tau_q \) such that

\[ \tau_q = \min_t \{\text{FDP}(t) \leq q\}, \quad (6) \]

and reject the \( j \)-th hypothesis if \( M_j \geq \tau_q \).

The next subsection explains how to construct GMs in the low-dimensional case when \( p < n \) such that the mirror statistics for the null variables are symmetric about zero. Section 3 extends the GM construct to the Lasso estimates for the high-dimensional case.

2.2. GMs for the OLS Estimator

The \( j \)-th GM design \((j = 1, \ldots, p)\) for the OLS estimate leads to the following quantity:

\[ \hat{\beta}' := (\hat{\beta}_j^+, \hat{\beta}_j^-) = \arg\min_{\beta} \| y - X'\beta' \|_2^2, \]

which has an explicit expression as \( \hat{\beta}' = (X')^{-1}X'y \). It is known that \((\hat{\beta}_j^+, \hat{\beta}_j^-)\) follows a bivariate normal distribution. As a referee pointed out, when \( p < n \) and OLS is used for the fitting, the GM construct has an equivalent “knockoff form”: one can treat \( cz_j \) as a knockoff of \( X_j \); directly regress \( y \) on \((X, cz_j)\) and contrast the coefficients of \( X_j \) and \( cz_j \). This view provides a nice connection with the knockoff idea, but the equivalence no longer holds in more complex cases when OLS is not applicable. The following lemma shows why the mirror statistic \( M_j \) is symmetrically distributed about zero for \( j \in S_0. \)

![Figure 1. Flowchart of the jth Gaussian Mirror.](image-url)
Lemma 1. Suppose \((U, V)\) follows a bivariate normal distribution with mean zero. If the correlation between \(U\) and \(V\) is zero, then \(M = |U + V| - |U - V|\) follows a symmetric distribution about zero, that is, \(P(M \geq t) = P(M \leq -t), \forall t > 0.\)

The following lemma provides an explicit formula of \(c_j\) such that the correlation between \(\hat{\beta}_j^+\) and \(\hat{\beta}_j^-\) is zero, resulting in a symmetric distribution of \(M_j\).

Lemma 2. For the \(\text{GM}_j\) design in Equation (2), choose
\[
c_j = \frac{X_j^\top (I_n - X_j(X_j^\top X_j)^{-1}X_j^\top)X_j}{z_j^\top (I_n - X_j(X_j^\top X_j)^{-1}X_j^\top)z_j}.
\]
(7)

Then \(\text{corr}(\hat{\beta}_j^+, \hat{\beta}_j^- | z_j, X_{-j}) = 0\) and \(M_j\) is symmetric with respect to zero.

Definition 1. (Gaussian mirrors for OLS) For \(j = 1, \ldots, p\), one first generates an \(n\)-dimensional Gaussian random vector \(z_j \sim N(0, I_n)\), and then computes \(c_j\) based on Equation (7). The \(j\)th \(\text{GM}_j\) design is \(\text{GM}_j = \{X_j + c_jz_j, X_j - c_jz_j, X_{1,j}, \ldots, X_{j-1,j}, X_{j+1}, \ldots, X_p\}\).

According to Lemma 2, \(\text{GM}_j\) defined in Definition 1 guarantees that the covariance between \(\hat{\beta}_j^+\) and \(\hat{\beta}_j^-\) is zero. We further construct the mirror test statistic \(M_j\) as in Equation (4). The following theorem is a direct consequence of Lemma 1.

Theorem 1. Let \(M_j\)'s be the test statistics defined in Equation (4) based on \(\text{GM}_j\) in Definition 1, then
\[
P(M_j \leq -t | z_j) = P(M_j \geq t | z_j), \forall t > 0
\]
for \(j \in S_0\).

Perturbation has been widely used in statistics to ensure stability and quantify uncertainty (Yu and Kumbier 2020; Yu 2013). For example, jackknife and bootstrap (Efron 1992) are two effective data perturbation methods with broad applications. As summarized in Algorithm 1, we use data perturbations to control the FDR, which can improve both the robustness and power of the multiple testing procedure. Since GM deals with one variable at a time, the resulting algorithm can be easily parallelized. Theorem 1 guarantees that the distribution of \(M_j\) is symmetric about zero for the null variables. Therefore, for any threshold \(t > 0\), \(\hat{S}_1 = \{j : M_j \geq t\}\), a natural estimate of the FDP in \(\hat{S}_1\) is given by Equation (5) and a data-driven threshold \(\tau_q\) can be obtained as in Equation (6). In Section 4, we show that the data-driven choice of \(\tau_q\) in Algorithm 1 guarantees that FDR is controlled asymptotically under some weak dependence assumptions of the mirror statistics.

3. GMs for High-Dimensional Regression

In the high-dimensional setting when the number of features \(p\) is greater than the number of subjects \(n\), one may still create mirror variables as \(X_j^+ = X_j + c_jz_j\) and \(X_j^- = X_j - c_jz_j\), and construct the mirror statistics using the Lasso estimates in Equation (11). Although this simple extension works well empirically, the following challenges arise. First, the easy formula for \(c_j\) as in the OLS case is no longer available. We can estimate the precision matrix of \(X\) under sparsity assumptions and construct \(c_j\) to make \(X_j^+\) and \(X_j^-\) conditionally independent asymptotically. Though this approach works well in simulations, a rigorous theoretical justification is difficult to come by. Second, the Lasso estimator is biased because of the regularization via \(L_1\) penalty. This implies that \(E(\hat{\beta}_j^+) \neq 0\) and \(E(\hat{\beta}_j^-) \neq 0\) for some predictor variables in the null set. Last but not the least, the Lasso estimator is a nonlinear function of \(y\) and the Lasso variable selection process imposes nonlinear constraints on the sample space. We here propose a post-selection strategy to design mirror variables such that the resulting mirror statistic \(M_j\) satisfies the symmetric property when \(j \in S_0\).

3.1. Literature on High-Dimensional Inference

To derive a proper inferential method for high-dimensional regression post variable selection, Zhang and Zhang (2014) and Van de Geer et al. (2014) proposed de-biased Lasso, Wasserman and Roeder (2009) advocated using data splitting (Cox 1975) to overcome difficulties caused by variable selection, and Berk et al. (2013) suggested a post-selection adjustment framework conditioning on the selection. Under the post-selection framework, Lee et al. (2016) proposed a procedure that first selects variables using Lasso and then obtained the OLS estimates for the selected model. By characterizing the selection event as a series of linear constraints on the post-selection OLS estimates, they provided a valid post-selection inference method on certain linear combinations of the coefficients of the selected variables.

Our goal is to make simultaneous inference for all the parameters such that the FDR can be controlled at a designated level. We consider a post-selection procedure based on Lasso. More specifically, similar to Lee et al. (2016), we first use Lasso to
select variables and then refit the selected model with OLS
and construct mirror statistics the same way as in the low-dimen-
sional case. In the following, we explain how to construct
the mirror statistics, adjusted according to the selection, such
that the symmetric property holds asymptotically.

3.2. Post-Selection Adjustment for GMs

Recall that Lasso solves the minimization problem
\[
\hat{\beta} = \arg \min_\beta ||y - X\beta||_2^2 + \lambda_n||\beta||_1.
\] (8)

Let \( \hat{S} = \{ j : \hat{\beta}_j \neq 0 \} \) and \( \hat{s} = \text{sign}(\hat{\beta}_S) \) denote the set of selected variables and their coefficients' signs, respectively, obtained by Lasso. By Lemma 4.1 in Lee et al. (2016), the event \( (\hat{S}, \hat{s}) = (S, s) \) can be rewritten as a series of constraints on \( y \) as
\[
\{ \hat{S} = S, \hat{s} = s \} = \left\{ \begin{array}{l}
A_0(S, s) y \leq b_0(S, s), \\
A_1(S, s) y \leq b_1(S, s), \\
\end{array} \right\},
\] (9)
where \( A_0 \) and \( A_1 \) are matrices shown below, which encode the "inactive" constraints determining the selection set and the "active" constraints determining the sign of nonzero coefficients, respectively,
\[
A_0(S, s) = \frac{1}{\lambda_n} \begin{pmatrix}
X^T S (I_n - P_S) \\
- X^T S (I_n - P_S)
\end{pmatrix},
\]
\[
b_0(S, s) = \begin{pmatrix}
1 - X^T S X_S + s \\
1 + X^T S X_S - s
\end{pmatrix},
\]
\[
A_1(S, s) = -\text{diag}(s)(X^T S X_S)^{-1} X^T, \\
b_1(S, s) = -\lambda_n \text{diag}(s)(X^T S X_S)^{-1},
\] (10)
where \( P_S \) is the projection matrix of \( S \) corresponding to \( X_S \).
Let \( X_{-j|S} \) denote the submatrix of \( X_S \) by removing its \( j \)th column, and let \( c_j \) be
\[
c_j = \frac{e_j^T (I_n - X_{j|S}) (X_{-j|S} X_{-j|S})^{-1} X_{-j|S} X_j}{\sqrt{\hat{z}_j^T (I_n - X_{j|S}) (X_{-j|S} X_{-j|S})^{-1} X_{-j|S} \hat{z}_j}},
\] (11)
where \( \hat{z}_j := (I - P_S) z_j \) with \( z_j \) generated from \( N(0, I_n) \). Then, we have

Definition 2. (Post-selection GM) Given the post-selection set \( S \) and the corresponding design matrix \( X_S \) for \( j \in \{1, \ldots, |S|\} \), we generate \( n \)-dimensional random vector \( z_j \) from \( N(0, I_n) \), then compute \( c_j \) based on Equation (11). The \( j \)th GM is designed as \( X^*_j = [X_{S[j]} + c_j z_j, X_{S[-j]} - c_j z_j, X_{S[1]}, \ldots, X_{S[|S|-1]}, X_{S[j+1]}, \ldots, X_{S[|S|]}] \) where \( S[j] \) is the \( j \)th index in \( S \).

In contrast to Equation (7) in the OLS case, here \( c_j \) is constructed by first projecting \( z_j \) on the orthogonal space of \( X_S \). Let \( \psi_1^T = e_1^T ((X^T S X_S)^{-1} X^T S)^{-1} X^T S \) and \( \psi_2^T = e_j^T ((X^T S X_S)^{-1} X^T S)^{-1} X^T S \), where \( e_1 \) is the standard basis vector with the \( 1 \)th entry as one and the others as zero. Note that the first two estimated coefficients from the OLS fitting of \( y \) on \( X^*_j \) are simple
\[
\hat{\beta}_j^+ = \psi_1^T y \quad \text{and} \quad \hat{\beta}_j^- = \psi_2^T y.
\] (12)

Before deriving the joint post-selection distribution of \( \hat{\beta}_j^+ \) and \( \hat{\beta}_j^- \), we first characterize the linear constraints on \( (\hat{\beta}_j^+, \hat{\beta}_j^-) \) due to the post-selection event \( S \).

Lemma 3. Let \( \Psi = (\psi_1, \psi_2) \), \( A_0(S, s) \) and \( A_1(S, s) \) be matrices defined in Equation (10). Then, there exist \( a_0 \in \mathbb{R}^{2(|S|-|S|)} \) and \( a_1 \in \mathbb{R}^{|S|} \), such that
\[
A_0(S, s) \Psi = a_0 (1, -1) \quad \text{and} \quad A_1(S, s) \Psi = a_1 (1, 1).
\] (13)

In Equation (13), we show that \( A_0(S, s) \Psi \) and \( A_1(S, s) \Psi \) are both rank one. Write \( y = P_\Psi y + (I_n - P_\Psi) y \) and let \( r = (I_n - P_\Psi) y \). It is easy to verify that \( r \) is uncorrelated with \( \psi^T y \), hence independent of \( \psi^T y \). Let \( \alpha = \psi_1^T \psi_1 = \psi_2^T \psi_2 \). The constraint \( A_0(S, s) y \leq b_0(S, s) \) in Equation (9) is equivalent to
\[
A_0(S, s) \Psi (\psi^T y + A_0(S, s) r) = a_0 (1, -1) \text{diag}(\alpha, \alpha) (\hat{\beta}_j^+ - \hat{\beta}_j^-) + A_0(S, s) r < b_0(S, s),
\]
that is, the "inactive" constraints on \( (\hat{\beta}_j^+, \hat{\beta}_j^-) \) are applied on the direction of \([1, -1] \). Similarly, we have \( \alpha a_1 (\hat{\beta}_j^+ - \hat{\beta}_j^-) + A_1(S, s) r < b_1(S, s) \), that is, the "active" constraints are applied on the direction of \([1, 1] \). As shown in Figure 2 (left panel), the constraint regions for \( \hat{\beta}_j^+ \) and \( \hat{\beta}_j^- \) are along the line with slope 1 and \(-1 \). By rotating the coordinate system by 45°, we have the joint distribution of \( \hat{\beta}_j^+ \) and \( \hat{\beta}_j^- \) shown in Figure 2 (right panel), where the constraint regions are parallel to the \( x \)-axis and \( y \)-axis. We characterize the constraints provided by the selection event \( S \) in Lemma 4.

Lemma 4. The selection event can be written as
\[
\{Ay \leq b\} = \{A_0(S, s) y \leq b_0(S, s)\} \cap \{A_1(S, s) y \leq b_1(S, s)\} = \{\psi_1^T y \leq \hat{\beta}_j^+, \hat{\beta}_j^- \leq \psi_2^T y, \psi_1^T y > 0\} \cap \{\psi_2^T y \leq \hat{\beta}_j^+, \hat{\beta}_j^- \leq \psi_1^T y, \psi_2^T y > 0\},
\]
where
\[
\psi_1^T y := \max_{j:a_{0j}>0} \frac{b_{0j} - (A_0 r)_j}{\alpha a_{0j}},
\]
\[
\psi_2^T y := \min_{j:a_{0j}>0} \frac{b_{0j} - (A_0 r)_j}{\alpha a_{0j}}, \quad \text{and}
\]
\[
\psi_1^T y := \max_{j:a_{1j}>0} \frac{b_{1j} - (A_1 r)_j}{\alpha a_{1j}},
\]
\[
\psi_2^T y := \min_{j:a_{1j}>0} \frac{b_{1j} - (A_1 r)_j}{\alpha a_{1j}}, \quad \text{and}
\]
\[
\psi_1^T y := \min_{j:a_{1j}>0} \frac{b_{1j} - (A_1 r)_j}{\alpha a_{1j}},
\]
with \( \alpha = \psi_1^T \psi_1 = \psi_2^T \psi_2 \), \( a_{0j}, a_{1j} \) being the \( j \)th element of \( a_0, a_1 \) in Equation (13), \( b_{0j}, b_{1j} \) being the \( j \)th element of \( b_0(S, s) \) and \( b_1(S, s) \) in (10), respectively.
Note that \( \text{cov}(\hat{\beta}_j^+ + \hat{\beta}_j^-, \hat{\beta}_j^+ - \hat{\beta}_j^-) = \sigma^2(\Psi_1 + \Psi_2)^T(\Psi_1 - \Psi_2) = 0. \) Since \( (\hat{\beta}_j^+, \hat{\beta}_j^-) \) are independent of \( \Psi^T y, \) we can treat \( r \) as “fixed” quantities for the distribution of \( \hat{\beta}_j^+ + \hat{\beta}_j^- \) and \( \hat{\beta}_j^+ - \hat{\beta}_j^- \) when conditioning on \( S. \) Thus, \( \hat{\beta}_j^+ + \hat{\beta}_j^- | (Ay \leq b) \) and \( \hat{\beta}_j^+ - \hat{\beta}_j^- | (Ay \leq b) \) are two independent, truncated normal random variables. Therefore, we have the following theorem.

**Theorem 2.** Let \( P_{[\mu, \sigma^2]} \) denote the cumulative distribution function of a \( N(\mu, \sigma^2) \) random variable truncated to the interval \([a, b],\) that is,

\[
P_{[\mu, \sigma^2]}(x) = \frac{\Phi((x - \mu)/\sigma) - \Phi((a - \mu)/\sigma)}{\Phi((b - \mu)/\sigma) - \Phi((a - \mu)/\sigma)},
\]

where \( \Phi \) is the cumulative distribution function of a standard normal random variable. When \( S_1 \subseteq S \) and for any \( j \in S_0, \) we have

\[
P_{[0, \sigma^2]}[V^U_j(r), V^L_j(r)](\hat{\beta}_j^+ + \hat{\beta}_j^-) | \hat{S} = S, \hat{s} = s \sim \text{Unif}(0, 1),
\]

\[
P_{[0, \sigma^2]}[V^U_j(r), V^L_j(r)](\hat{\beta}_j^+ - \hat{\beta}_j^-) | \hat{S} = S, \hat{s} = s \sim \text{Unif}(0, 1),
\]

where \( V^U_j(r), V^L_j(r) \) are defined in Equation (14).

We define the mirror statistic \( M_j \) as

\[
M_j = |\sigma^{-1}P_{[0, \sigma^2]}[V^U_j(r), V^L_j(r)](\hat{\beta}_j^+ + \hat{\beta}_j^-)| - |\sigma^{-1}P_{[0, \sigma^2]}[V^U_j(r), V^L_j(r)](\hat{\beta}_j^+ - \hat{\beta}_j^-)|. \tag{16}
\]

For \( j \in S_0, \) \( M_j \) is symmetrically distributed about zero. When \( j \in S_1, \) as shown in Lee et al. (2016), the truncation points are different from zero. When the magnitude of \( \beta_j \) is large, the truncated distribution function is close to the nontruncated version, indicating that the \( M_j \) defined in Equation (16) is close to \(|\beta_j^+ + \beta_j^-| - |\beta_j^+ - \beta_j^-|\). In practice, the mirror statistics tend to be conservative since we use the cumulative distribution function of a normal random variable with mean zero for both null and non-null variables. For a nonnull variable, the means for \( \hat{\beta}_j^+ + \hat{\beta}_j^- \) and \( \hat{\beta}_j^+ - \hat{\beta}_j^- \) before the truncation are \( \Psi^T \mu \) and \( \Psi^T \mu, \) respectively, where \( \mu = E y. \) Numerically, we find that replacing \( \mu \) by a reasonable estimate, such as \( X_S \hat{\beta}, \) helps increase the power without losing FDR control.

We follow the selected model framework in Tibshirani (2013) and Fithian, Sun, and Taylor (2014) by assuming that \( (S_1 \subseteq \hat{S}). \) Such a property can be guaranteed by the \( L_1 \)-consistency of the Lasso procedure under certain conditions (Knight and Fu 2000; Meinshausen and Bühlmann 2006; Zhao and Yu 2006; Van de Geer 2008; Zhang and Huang 2008; Candès and Plan 2009; Meinshausen et al. 2009). Assumption 1 is from Bühlmann and Van De Geer (2011), which guarantees the \( L_1 \)-consistency.

**Assumption 1.** (a) (compatibility condition). Let \( \phi_0 > 0 \) be a constant. For a \( p \times 1 \) vector \( \alpha \) satisfying \(||\alpha S_0||_1 \leq c_0||\alpha S_1||_1,\) we assume

\[
||\alpha S_1||_1^2 \leq \frac{p_1}{\phi_0^2} \alpha^T X^T X \alpha,
\]

where the entry \( \alpha_i \in \alpha S_0, \) if \( i \in S_0, \) and \( \alpha S_1 = \alpha \setminus \alpha S_0, c_0 \) is a constant depending on the choice of \( \lambda_n, \) and \( \phi_0 \) is the compatibility constant.

(b) (signal strength). \( \min_{j \in S_1} |\beta_j| > \frac{64\log(p)}{\phi_0^2} \sqrt{\log(p)/n}. \)

**Lemma 5.** Suppose Assumption 1 holds. Consider Lasso with regularization parameter \( \lambda_n = 4\sigma \sqrt{\log(p)/n}. \) Then, we have

\[
P(S_1 \subseteq \hat{S}) \geq 1 - \frac{2}{p},
\]

where \( \hat{S} \) is the index set of the nonzero entries in the Lasso estimator \( \hat{\beta} \) in (8).

Lemma 5 follows directly from the \( L_1 \) convergence result in Bühlmann and Van De Geer (2011), Theorem 6.1, and the signal strength condition in Assumption 1(b). Based on this lemma, event \( (S_1 \subseteq \hat{S}) \) holds with high probability, implying that the Lasso estimator selects all variables in \( S_1. \) The mirror statistic \( M_j \) further helps to pick out falsely included null variables.
Algorithm 2 Gaussian mirror algorithm for Lasso.
1. Fit Lasso with respect to the original design matrix $X$, that is, 
   $$
   \hat{\beta} = \arg \min_{\beta} \|y - X\beta\|_2^2 + \lambda_n \|\beta\|_1
   $$
   by cross-validation.
2. Parallel FOR $j = 1, \ldots, \hat{S}$:
   (a) Generate $z_j$ from Gaussian distribution with mean zero and covariance matrix $I_\alpha$.
   (b) Calculate debiased $c_j$ via Equation (11).
   (c) Calculate the mirror statistic 
   $$
   M_j = |\sigma^{-1} f_{i_{0,\alpha}}^{Y_i(r)}(\hat{\beta}_j^+ + \beta_j^-)| 
   - |\sigma^{-1} f_{i_{0,\alpha}}^{Y_i(r)}(\hat{\beta}_j^+ - \beta_j^-)|,
   $$
   where $\hat{\beta}_j^+$ and $\hat{\beta}_j^-$ are defined in Equation (12) and
   $Y_0^+, Y_0^-, Y_1^+, Y_1^-$ are defined in Equation (14).
   END parallel FOR loop.
3. Calculate the cutoff to control FDR at target $q$,
   $$
   \tau_q = \min_{t} \left\{ \frac{\# \{j \mid M_j \leq -t\}}{\# \{j \mid M_j \geq t\} \vee 1} \leq q \right\}.
   $$
4. Output the index of the selected variables: $\hat{S}_1 = \{j \mid M_j \geq \tau_q\}.$

Theorem 3. Consider the GM design in Definition 2 for linear models with the Lasso estimates. Let $M_j$ be the mirror statistic defined in Equation (16) and computed using Algorithm 2. We have
   $$
   P(M_j \leq -t \mid z_j) = P(M_j \geq t \mid z_j), \quad \forall t > 0,
   $$
   for $j \in S_0$ with probability $1 - 2/p$.

Based on Theorem 3, we use $\# \{j \mid M_j \leq -t\}$ as an (over)-estimate of the number of false positive set, and define an estimate of FDP as 
   $$
   \text{FDP}(t) = \frac{\# \{j \mid M_j \leq -t, j \in \hat{S}_1\}}{\# \{j \mid M_j \geq t \cap j \in \hat{S}_1\} \vee 1}.
   $$

Algorithm 2 details the GM procedure for variable selection with FDR control in high-dimensional linear regression. Similar to the low-dimensional case in Section 2.2, the mirror statistics $M_j$’s can be computed efficiently using parallel computing.

4. Theoretical Properties of GMs

Section 2 introduces the Gaussian mirror method for estimating the FDP. We abuse the notation and use $M_j$ to indicate both the one defined in Equation (4) and the one defined in Equation (16). The key is to design the Gaussian mirror appropriately such that for $j \in S_0$, 
   $$
   P(M_j \leq -t \mid z_j) = P(M_j \geq t \mid z_j), \quad \forall t > 0.
   $$
   When we select the $j$th variable if $M_j \geq t$, the FDP satisfies 
   $$
   \frac{\# \{j \in S_0 : M_j \geq t\} \vee 1}{\# \{j \mid M_j \geq t\} \vee 1} \leq \frac{\# \{j \mid M_j \leq -t\} \vee 1}{\# \{j \mid M_j \geq t\} \vee 1},
   $$
   where the last term is $\hat{\text{FDP}}(t)$, an (over-)estimate of the FDP defined in Equation (5). As shown in Algorithms 1 and 2, a data-driven threshold $\tau_q > 0$ is chosen in Equation (6) as the smallest value such that $\text{FDP}^{(\hat{S})} \leq q$. Intuitively, for Equation (18) to hold stably, we need the following assumptions.

Assumption 2. (a) (The low-dimensional case). There exists a constant $c \in (0, 1)$ such that $p = [cn]$. Let $\Omega^0 = (X_{(S_0)}^T X_{(S_0)})^{-1}$. Then,
   $$
   \sum_{j,k \in S_0} \left| \frac{\Omega^0_{jj} \Omega^0_{kk}}{\Omega^0_{jk}} \right| < C_1 p_0^2
   $$
   holds for a constant $C_1 > 0$ and $\alpha \in (0, 2)$.
   (b) (The high-dimensional case). Let $\Sigma$ be the covariance matrix of $X$, $p = O(n^\alpha)$ with $\omega > 1$, and $p_1 = o(n)$. Then $\Sigma$ satisfies the regularity condition $1/C_2 \leq \lambda_{\text{min}}(\Sigma) \leq \lambda_{\text{max}}(\Sigma) \leq C_2$, where $C_2 > 0$ is a constant.

Assumption 2(a) requires that the sum of pairwise partial correlations of the design matrix is bounded by $C_1 p_0^2$, where $\alpha \in (0, 2)$. This requirement is satisfied by many designs such as the autoregressive and the constant-correlation design. For the high-dimensional case, we consider a bounded eigenvalue condition in Assumption 2(b), which is commonly used as a regularization condition in high-dimensional analysis (Cai et al. 2017). Additionally, assume that $p_1 = o(n)$. The following two lemmas characterize the sum of pairwise covariances of the mirror statistics, which is the key to establish asymptotic FDR control for GM. In the low-dimensional setting, the sum is taken over the null set $S_0$, whereas in the high-dimensional setting, the sum is taken over the selection set $\hat{S}$ since the mirror statistics are derived from the post-selection Lasso.

Lemma 6. Consider the low-dimensional setting in which the mirror statistics $M_j$’s are defined as in Equation (4). If Assumption 2(a) holds, then
   $$
   \sum_{j,k \in S_0} \text{cov}(\mathbb{1}(M_j \geq t), \mathbb{1}(M_k \geq t)) \leq C_1 \|S_0\|^{\alpha_1}, \quad \forall t > 0,
   $$
   where $\alpha_1 \in (0, 2)$, $C_1 > 0$ is a constant, and $\mathbb{1}(\cdot)$ is the indicator function.

Lemma 7. Consider the high-dimensional setting, in which the mirror statistics $M_j$’s are defined as in Equation (16). If Assumptions 1 and 2(b) hold, then
   $$
   \sum_{j,k \in S_\hat{S} \cap S_0} \text{cov}(\mathbb{1}(M_j \geq t), \mathbb{1}(M_k \geq t)) \leq C_2 \|\hat{S} \cap S_0\|^{\alpha_2}, \quad \forall t > 0,
   $$
   where $\alpha_2 \in (0, 2)$, $C_2 > 0$ is a constant, and $\mathbb{1}(\cdot)$ is the indicator function.

Next, we derive some asymptotic properties of the GM method. For the low-dimensional case, we define a few
quantities

\[ V(t) = \frac{\# \{ j : j \in S_0, M_j \leq t \}}{|S \cap S_0|}, \]
\[ V'(t) = \frac{\# \{ j : j \in S_0, M_j \geq t \}}{|S \cap S_0|}, \]
\[ V^1(t) = \frac{\# \{ j : j \in S_1, M_j \geq t \}}{|S \cap S_1|}, \]
\[ G_0(t) = \lim_{p} \frac{\sum_{j \in S_0} \mathbb{1}(M_j \leq t)}{|S \cap S_0|}, \]
\[ G_1(t) = \lim_{p} \frac{\sum_{j \in S_1} \mathbb{1}(M_j \geq t)}{|S \cap S_1|}, \]

and

\[ \text{FDP}(t) := \frac{V'(t)}{(V' + r_p V^1(t)) \vee 1/p}, \]
\[ \text{FDP}^\infty(t) := \lim_{p} \frac{V'(t)}{(V' + r_p V^1(t)) \vee 1/p}, \]

where \( r_p = p_0/p_1 \) and \( \text{FDP}^\infty(t) \) is the pointwise limit of \( \text{FDP}(t) \).

With a slight abuse of the notation, we define a similar set of quantities for the high-dimensional setting as follows:

\[ V(t) = \frac{\# \{ j : j \in S_0, M_j \leq t \}}{|\hat{S} \cap S_0|}, \]
\[ V'(t) = \frac{\# \{ j : j \in S_0, M_j \geq t \}}{|\hat{S} \cap S_0|}, \]
\[ V^1(t) = \frac{\# \{ j : j \in S_1, M_j \geq t \}}{|\hat{S} \cap S_1|}, \]
\[ G_0(t) = \lim_{p} \frac{\sum_{j \in S_0} \mathbb{1}(M_j \leq t)}{|\hat{S} \cap S_0|}, \]
\[ G_1(t) = \lim_{p} \frac{\sum_{j \in S_1} \mathbb{1}(M_j \geq t)}{|\hat{S} \cap S_1|}, \]

and

\[ \text{FDP}(t) := \frac{V'(t)}{(V' + r_p V^1(t)) \vee 1/|\hat{S}|}, \]
\[ \text{FDP}^\infty(t) := \lim_{p} \frac{V'(t)}{(V' + r_p V^1(t)) \vee 1/|\hat{S}|}, \]

where \( r_p = |\hat{S} \cap S_0| / |\hat{S} \cap S_1| \). We have the following results.

**Lemma 8.** Suppose Assumption 2(a) holds for the low-dimensional case, Assumptions 1 and 2(b) hold for the high-dimensional case, and \( G_0(t) \) is a continuous function. Then, we have

\[ \sup_t [V(t) - G_0(t)] \overset{p}{\to} 0, \quad \sup_t [V'(t) - G_0(t)] \overset{p}{\to} 0, \quad \text{and} \]
\[ \sup_t [V^1(t) - G_1(t)] \overset{p}{\to} 0. \]

With the aid of this lemma, we show that the proposed GM method controls the FDR asymptotically for linear models in both low- (Theorem 4) and high (Theorem 5)-dimensional cases.

**Theorem 4.** Let \( M_j \)'s be the mirror statistics calculated in Algorithm 1 for the low-dimensional setting. For any given \( q \in (0, 1) \), we choose \( \tau_q > 0 \) according to Equation (6). If Assumption 2(a) holds and there exists \( t > 0 \) such that \( \text{FDP}^\infty(t) < q \), then, as \( p \to \infty \),

\[ \mathbb{E} \left[ \frac{\# \{ j : j \in S_0, and \ j \in \hat{S}_1 \}}{\# \{ j : j \in \hat{S}_1 \} \vee 1} \right] \leq q + o(1). \]

**Theorem 5.** Let \( M_j \)'s be the mirror statistics calculated using Algorithm 2 for the high-dimensional setting. For any given \( q \in (0, 1) \), we choose \( \tau_q > 0 \) according to Equation (17). If Assumptions 1 and 2(b) hold and there is a \( t > 0 \) such that \( \text{FDP}^\infty(t) < q \), then, as \( p \to \infty \),

\[ \mathbb{E} \left[ \frac{\# \{ j : j \in S_0, and \ j \in \hat{S}_1 \}}{\# \{ j : j \in \hat{S}_1 \} \vee 1} \right] \leq q + o(1). \]

When conditioning on the event \( \{ \hat{S}_1 \subseteq \hat{S} \} \), we can follow the proof of Theorem 4 to show that FDR conditioning on the selection is less than or equal to \( q \) asymptotically. According to Lemma 5, the probability that \( \hat{S}_1 \subseteq \hat{S} \) is greater than \( 1 - \frac{2}{p} \). Consequently, as \( p \to \infty \), the FDR is less than or equal to \( q + o(1) \), which concludes the proof of the theorem.

### 5. Estimating the Number of FDs

The GM approach introduced in Section 2 provides a way to select significant features subject to FDR control at a designated level. Next, we address a related problem that is of interest to some practitioners. Suppose a scientist is only allowed to explore no more than 100 selected features due to a limited budget, then the following questions are of immediate concerns: (i) How should they select the list of top 100? (ii) How many FDs do they expect to have? (iii) Can statisticians provide an uncertainty measure for the estimated FDs?

The first question is easy to address based on the mirror statistic \( \{ M_j \} (j = 1, \ldots, p) \). We order the mirror statistics decreasingly as \( M_{(1)} \geq \ldots \geq M_{(p)} \) and choose the top \( k \) features as those corresponding to the set of the top-\( k \) mirror statistics. Let the selected set be \( \mathcal{I}_k \), that is,

\[ \mathcal{I}_k = \{ j : M_j \in \{ M_{(1)}, \ldots, M_{(k)} \} \}, \]

where \( k \leq \# \{ j : M_j > 0 \} \) since the GM procedure does not select variables with negative mirror statistics. Let \( \text{FD}(k) = |\mathcal{I}_k \cap S_0| \) denote the true number of FDs in the top-\( k \) list and let \( \mathbb{E}[\text{FD}(k)] \) denote the expected number of FDs. Since the mirror statistics are distributed symmetrically for the null variables, we estimate \( \mathbb{E}[\text{FD}(k)] \) as

\[ \hat{\text{FD}}(k) = \# \{ M_j < -M_{(k)} \}. \]

Under high-dimensional settings, Theorem 6 shows that the error bound between \( \hat{\text{FD}}(k) \) and \( \mathbb{E}[\text{FD}(k)] \) is \( r_p(k) \). As \( k \) increases, the error bound also increases although the relative error gets smaller. Theorem 7 states that \( \hat{\text{FD}}(k) \) is an unbiased estimator of \( \mathbb{E}[\text{FD}(k)] \) with high probability.
Theorem 6. Suppose that Assumptions 1 and 2(b) hold, \( p/n \to \infty, k \leq \#(j \mid M_j > 0) \), and \( k/p_1 = O(1) \). Let \( M_j \) be the mirror statistic calculated from Algorithm 2. We have

\[
\lim_{n \to \infty} P \left( \frac{1}{k} |\hat{F}D(k) - E[FD(k)]| > \epsilon \right) = 0,
\]

for any \( \epsilon > 0 \).

Theorem 7. Suppose that Assumptions 1 and 2(b) hold, \( k \leq \#(j \mid M_j > 0) \). Let \( M_j \) be the mirror statistic calculated from Algorithm 2. We have

\[
P \left( E[FD(k)] = E[FD(k)] \right) > 1 - \frac{2}{p}.
\]

Next, we describe a bootstrap method to construct a confidence interval for \( E[FD(k)] \). The method sets by fitting the regression model based on the original design matrix using either the least-square (if \( p < n \)) or the Lasso method, and obtaining the fitted values \( \hat{y} = (\hat{y}_1, \ldots, \hat{y}_n) \) as well as the residuals \( y = y - \hat{y} \). Then, for \( b = 1, \ldots, B \), we generate independently the \( b \)-th “bootstrap sample” \( y^{(b)} = \hat{y} + \gamma^{(b)} \), where the \( y^{(b)} \) is drawn randomly from \( y \) with replacement. With the bootstrapped “observations” \( y^{(b)} \), we calculate the mirror statistics \( \{M_1^{(b)}, \ldots, M_p^{(b)}\} \) using Algorithm 1 (Algorithm 2 for Lasso). The \( B \) sets of bootstrap mirror statistics are denoted as \( \{M_1^{(1)}, M_2^{(1)}, \ldots, M_p^{(1)}\}_{b=1}^B \), which give rise to a set of \( B \) bootstrap estimates of \( FD(k) \) : \( B_{FD} = \{\hat{FD}^{(1)}(k), \ldots, \hat{FD}^{(B)}(k)\} \). A bootstrap confidence interval for \( E[FD(k)] \) can be constructed as the upper and lower \( \alpha/2 \) quantiles of the sample \( B_{FD} \), denoted as \( \hat{FD}_{(\alpha/2)}(k) \) and \( \hat{FD}_{(1-\alpha/2)}(k) \), respectively. We may also first recenter the set \( B_{FD} \) to have mean \( \hat{FD}(k) \) and then use the corresponding quantiles. If a budget-sensitive domain scientist is only interested in a budget-sensitive domain scientist, \( \epsilon < 0.1 \), then she/he can use \( \hat{FD}_{(1-\alpha)}(k) \).

6. Numerical Studies

In this section, we compare numerical performances of various multiple testing methods for regression models. The first class of methods is based on the procedure of Benjamini and Hochberg (1995), abbreviated as BH. As shown in the following two subsections, the test statistics are calculated differently depending on \( p \) and \( n \). The second class of methods is based on knockoffs, including the knockoff filter when \( p < n/2 \) (Barber and Candès 2015), and the model-X knockoff when \( p \) is large (Candes et al. 2018). For the model-X knockoff, we construct knockoffs with both a known covariance matrix (model-X-true) and a second-order estimate of the covariance matrix (model-X-est). To our surprise, we observe that the knockoff method based on the known covariance matrix becomes extremely conservative for the constant correlation setting with correlation coefficient larger than 0.5. We implement a modified version of model-X knockoff (model-X-fix), which significantly improves the power. In all simulation settings, we set the designated FDR level \( q \) as 0.1.

6.1. Low-Dimensional Case \((p < n)\)

We set \( n = 1000 \) and \( p = 300 \). For the GM approach, we calculate the mirror statistics based on Algorithm 1. For the BH method, we calculate the \( z \)-statistics \( z_1, \ldots, z_p \) for the OLS estimates, that is, \( z_i = \beta_i/(\sigma_i \sqrt{(X'X)_i^{-1}}) \). The \( j \)-th variable is selected if \( |z_j| > \tau^{BH}_j \), where \( \tau^{BH}_j \) is chosen as

\[
\tau^{BH}_j \equiv \min \left\{ \frac{P(N(0,1)) \geq t}{\#(\{j \mid |z_j| \geq t\})} \leq \frac{q}{p} \right\}.
\]

The knockoff and model-X knockoff statistics are calculated based on the Lasso estimators. For different methods, we calculate the FDR and the power based on 100 replications. In each of the following settings, we randomly set 240 coefficients of \( \beta_i \)’s as zero and generate the remaining 60 nonzero coefficients independently from \( N(0, (20/\sqrt{n})^2) \). The response variable \( y \) is generated according to Equation (1) with \( \sigma = 1 \). The design matrix is composed of iid rows with each row generated from \( N(0, \Sigma) \).

(i) Power decay correlation. The covariance matrix \( \Sigma \) is autoregressive, that is, \( \sigma_{ij} \), the element at the \( i \)-th row and \( j \)-th column is \( \kappa^{i-j} \), where \( \kappa \) is taken among 0, 0.2, 0.4, 0.6, and 0.8, respectively. Figure 3 (a1)−(a2) show plots of FDPs and proportions of true rejections of these five methods. Note that the middle bar in the box is the mean of these FDPs and proportions, a.k.a., the FDR and power. As shown in Figure 3 (a1), the FDPs of the five methods are all around the targeted value 0.1. Figure 3 (a2) shows that the GM method has the highest power among these five methods; and the discrepancies between the GM and other methods increase with respect to \( \kappa \). Particularly, when \( \kappa = 0.8 \), the power of the knockoff method becomes very small with some extreme cases of having no rejections at all.

(ii) Constant positive correlation. Here, we let \( \sigma_{ij} = \rho^{i-j} \), with \( \lfloor (\cdot) \rceil \) being an indicator function. As shown in Figure 3 (b1 and b2), correlations among the \( \beta_i \)'s are small and the \( t \)-statistics are only weakly correlated because of low partial correlations. Hence, the BH method controls the FDR well and also has a good power. Model-X-est and the GM method come as the close second with the results very similar to those of the BH method. When \( \rho \geq 0.5 \), the power of Model-X-true drops to near-zero due to a numerical issue in the original Model-X software. The Model-X procedure generates knockoffs from \( N(\mu, V) \), where \( V \) is obtained via solving a semidefinite programming problem. When \( \rho \geq 0.5 \), \( V \) is nearly a rank-one matrix, which results in high collinearity among the generated knockoffs and significantly reduces the power. Dongming Huang and Lucas Jensen (personal communication) suggested a simple remedy, which is to project each variable onto the orthogonal space of the first principal component of \( \Sigma \) and add a small perturbation as

\[
\chi_{\text{new}} = \chi - \frac{1}{\delta} \chi \Sigma^{-1} \mathbf{1} + \frac{1}{\sqrt{\delta}} z_j \sim N(0, I_p).
\]

where \( \delta = (\rho - \rho^2 \mathbf{1}_p \Sigma^{-1} \mathbf{1}_p^{-1})^{-1} \) and \( z_j \sim N(0, I_p) \). Then, \( \chi_{\text{new}} = (X_{\chi_{\text{new}}}, \ldots, X_{p,\chi_{\text{new}}}) \) serves a new design matrix for constructing knockoffs via the standard Model-X procedure with the covariance matrix \( I_p \). This modification substantially improves the power (as shown in Figures 3(b1) and (b2) and 4(b1) and (b2) for large-\( \rho \) cases), but the trick cannot be
extended to general cases. In general, power decreases as $\rho$ increases for all the methods. GM appears to be affected the least.

(iii) Constant partial correlation. In this setting, the precision matrix $Q = \Sigma^{-1}$ has constant off-diagonal elements, that is, $q_{ij} = \tau 1(i \neq j)$. Correlations among the $X$ can be very small when $\tau$ is large. For example, when $\tau = 0.6$, the off-diagonal entries of $\Sigma$ is around $-0.0083$ and the diagonal entry is 2.4917. The results are reported in Figure 3(c1)–(c2). Both the GM and BH methods work well in terms of the FDR and power, while GM is slightly more powerful. When $\tau > 0$, both the knockoff filter and Model-X-est are extremely conservative. For instance, when $\tau = 0.6$, both the FDR and power of these two methods drop to zero. Mode-X-true works better, but its power decreases much faster with respect to $\rho$ than the GM and BH methods.

6.2. High-Dimensional Case ($p \geq n$)

We consider the high-dimensional case with $p = 1000$ and $n = 300$, in which Algorithm 2 is used for the GM method. Similar to Candes et al. (2018), we implement the marginal BH (henceforth, BH-ma), which is based on the $p$-values of
the marginal regression between $y$ and $X_j$, $j = 1, \ldots, p$. We also consider the data splitting BH (henceforth, BH-ds), which employs Lasso to select variables based on the first half of the data, and applies the BH method to the $p$-values of the OLS estimates obtained from the second half of the data for the selected variables. For the Model-X knockoff, we use both the Gaussian knockoffs with a known covariance matrix and the second-order knockoffs with estimated covariance matrix as implemented in the R package knockoff. Note that the original knockoff method cannot be applied when $p \geq n$.

(i) Power decay correlation. As shown in Figure 4 (a1), FDPs of GM are around 0.1 in all cases. The FDRs of Model-X-est, Model-X, BH-ds are around 0.1 when $\kappa \leq 0.6$. When $\kappa = 0.8$, the FDR of Model-X-est could be as large as 0.23. This inflation is also observed in Candès et al. (2018). The FDR of BH-ms is also inflated when $\kappa \geq 0.4$. The FDR of the GM method is controlled at the designated level well. In Figure 4 (a2), it is shown that GM and two Model-X methods have comparable powers, whereas the two BH methods do not perform well.
(ii) **Constant positive correlation.** As shown in Figure 4(b1), GM, BH-ds, Model-X-true, and Model-X-fix all control their FDR properly around 0.1, the designated level. Model-X-est is overly conservative with observed FDPs being close to zero when ρ ≥ 0.2, whereas BH-ma fails to control the FDR, especially when ρ ≥ 0.2. When ρ is larger than 0.5, we apply the same algorithmic modification as in the low-dimensional setting for Model-X, denoted as Model-X-fix, which improves the power. Figure 4(b2) shows proportions of true positives and the power. The power of Model-X-est knockoff decreases rapidly as ρ increases. Model-X-fix has a better power than Model-X-est. The power of BH-ds is low and does not change much with respect to ρ. The powers of GM are stable throughout all ρ values, decreasing moderately as ρ increases.

(iii) **Constant partial correlation.** As shown in Figure 4(c1), the FDRs of all the methods except BH-ma are controlled well. Both GM and Model-X-estimate perform better than all other methods, with GM having a slight edge.

The FDR of Model-X knockoff is slightly inflated when the correlation is high. The BH method with data splitting shows a large variation in FDRs and has the lowest power. The marginal BH method cannot control the FDR at the designated level.

(ii) **Bi-modal distribution.** The features are generated from a Gaussian mixture distribution with two components: one centered at −0.51p and the other at 0.51p. The covariance matrices of the two components are the same and are autoregressive as in the previous case. As shown in Figure 5(b1), (b2), GM controls the FDR at the designated level for all the settings and has the highest power among all the methods that control the FDR at the designated level. Being conservative with a small FDR, the Model-X knockoff has a lower average power than the GM method. Additionally, the variation of the proportion of true rejections is much higher than that of the GM method. The BH method with data splitting shows a valid FDR control, but it has the lowest power among all these methods. The marginal BH method cannot control FDR at the designated level.

### 6.3. Simulation Studies for Non-Gaussian Designs

(i) **T-distribution.** We generate the features from a centered multivariate T-distribution with 3 degrees of freedom and the covariance matrix Σ, which is set to be autoregressive (Toeplitz), that is, σij = χ[|i−j|] for χ = 0, 0.2, . . . , 0.8. As shown in Figure 5(a1, a2), the GM method controls the FDR at the designated level for all the settings and maintains the highest power among all the methods that control the FDR at the designated level.

The FDR of Model-X knockoff is slightly inflated when the correlation is high. The BH method with data splitting shows a large variation in FDRs and has the lowest power. The marginal BH method cannot control the FDR at the designated level.

### 6.4. Simulation Studies Based on a Population Genetics Dataset

GWAS have become an attractive tool for genetic research. In these studies, researchers examine a genome-wide set (tens of thousands to millions) of genetic variants of a group of individuals randomly selected from a target population to see if any variants are associated with a phenotype of interest. Genetic
variants are usually in the form of SNPs, and are often used as covariates in a linear or logistic regression model, with a main goal being to select relevant variants. Since most SNPs take on only three values, \{0, 1, 2\} (representing 0, 1, or 2 minor allele mutations, respectively), the design matrix of such an SNP-based regression model is clearly non-Gaussian.

We consider a panel of 292 tomato accessions in Bauchet et al. (2017), which is publicly available at ftp://ftp.solenomics.net/manuscripts/Bauchet_2016/ and includes breeding materials (specimens) characterized by 11,000 SNPs. Here, we are interested in examining the FDR and power of GM, BH, and Model-X knockoff by using this real-dataset to create realistic design matrices. Specifically, we randomly select 1000 SNPs as \(X\) and randomly generate 60 nonzero regression coefficients from \(N(0, \sigma^2/n)\), where \(c\) ranges from 20 to 80 representing signal strength. The response variable \(y\) is generated from Equation (1) with a standard Gaussian noise. We set the target FDR level as 0.05.

We evaluate the performance of the GM method for estimating the expected number of FDs in a top-\(k\) list, denoted as \(E[FD(k)]\), and the coverage frequency of its bootstrap confidence interval proposed in Section 5. We consider both low-dimensional (\(n = 1000, p = 300\)) and high-dimensional settings (\(n = 300, p=1000\)), in which we randomly generate 60 nonzero coefficients independently from \(N(0, (20/\sqrt{n})^2)\). We consider three types of design matrices similar to those described in Sections 6.1 and 6.2: autoregressive (Toeplitz), constant correlation, and constant partial correlation. The response \(y\) is generated according to Eq (1) with \(\sigma = 1\). We fix \(k = p = \tau = 0.2\) for these settings, and repeat 100 times for each setting.

6.5. Empirical Results on Estimating the Expected Number of FDs

We evaluate the performance of the GM method for estimating the expected number of FDs in a top-\(k\) list, denoted as \(E[FD(k)]\), and the coverage frequency of its bootstrap confidence interval proposed in Section 5. We consider both low-dimensional (\(n = 1000, p = 300\)) and high-dimensional settings (\(n = 300, p=1000\)), in which we randomly generate 60 nonzero coefficients independently from \(N(0, (20/\sqrt{n})^2)\). We consider three types of design matrices similar to those described in Sections 6.1 and 6.2: autoregressive (Toeplitz), constant correlation, and constant partial correlation. The response \(y\) is generated according to Eq (1) with \(\sigma = 1\). We fix \(k = p = \tau = 0.2\) for these settings, and repeat 100 times for each setting.

In each replication, we obtain an estimate of \(E[FD(k)]\) with \(k \in (50, 70)\). For the \(r\)th replication (\(1 \leq r \leq 100\)), we calculate \(\hat{FD}(r)(k)\) following Equation (19), and record the underlying true number of FDs as \(FD(r)(k)\). We use the sample average \(\hat{E}[FD(k)] := \frac{1}{100} \sum_{r=1}^{100} FD(r)(k)\) as an approximation to \(E[FD(k)]\) (note that each \(FD(r)(k)\) is the true number of FDs for replication \(r\) and is only available in simulations), and use \(\hat{E}[FD(k)] := \frac{1}{100} \sum_{r=1}^{100} \hat{FD}(r)(k)\) as an approximation of \(E[FD(k)]\), which should ideally track the value of \(E[FD(k)]\).

By using Algorithm 3 with \(B = 200\), we calculate the empirical coverage frequency of the proposed bootstrap confidence

---

**Algorithm 3** Bootstrap distribution of \(M_j\) and \(\hat{FD}(k)\).

1. Parallel FOR \(b = 1, \ldots, B\):
   (a) For the low-dimensional setting, fit linear regression model via OLS, that is, minimizing (3); For the high-dimensional setting, get the Lasso solution by minimizing (8). Let \(\hat{y} = (\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n)\) be the fitted values, and \(r = y - \hat{y} = (r_1, r_2, \ldots, r_n)\) be the residuals.
   (b) Sample from \(r\) with replacement to get \(r^{(b)} = (r^{(b)}_1, r^{(b)}_2, \ldots, r^{(b)}_n)\). Let \(y^{(b)} = \hat{y} + r^{(b)}\).
   (c) Apply Algorithm 1 (low-dimensional) or Algorithm 2 (high-dimensional) by replacing \(y\) with \(y^{(b)}\), and calculate the mirror statistics \(M^{(b)}_j\), for \(j = 1, \ldots, p\), accordingly.

End Parallel FOR.

2. Output the bootstrap estimate \([M^{(B)}_1, M^{(B)}_2, \ldots, M^{(B)}_p]_{b=1}\).

3. For \(b = 1, \ldots, B\), calculate the estimate of the number of FDs based on \([M^{(b)}_1, M^{(b)}_2, \ldots, M^{(b)}_p]\) as

\[\hat{FD}(k) = \#\{M^{(b)}_j < -M^{(b)}_k\},\]

where \([M^{(1)}_1, \ldots, M^{(p)}_p]\) are the decreasingly ordered mirror statistics.

4. Construct the confidence interval of \(E[FD(k)]\) as \([\hat{FD}_{(0.05/2)}(k), \hat{FD}_{(1-0.05/2)}(k)]\) and upper confidence interval as \([0, \hat{FD}_{(1-0.05)}(k)]\).
Figure 7. The low-dimensional case with \( n=1000 \) and \( p=300 \). Left panels: scatterplots of \( \hat{FD}(k) \) versus \( FD(k) \) for \( k \in (50,70) \), under three correlation structures of the design matrix, respectively. The triangles are \( \tilde{E}[FD(k)] \) versus \( \tilde{E}[\hat{FD}(k)] \) in 100 replications, and the dashed line is \( x=y \). Right panels: the coverage frequencies of the 95% bootstrap confidence interval and confidence upper bound of \( E[FD(k)] \) (approximated by \( \tilde{E}[\hat{FD}(k)] \)), respectively, for \( k \) ranging from 50 to 70. The color shading represents different values of \( k \).

interval for \( E[FD(k)] \) as

\[
\frac{1}{100} \# \{ r : \tilde{E}[FD(k)] \in [\tilde{FD}_{(\alpha/2)}(k), \tilde{FD}_{(1-\alpha/2)}(k)] \}
\]

where \( \tilde{FD}_{(\alpha/2)}(k) \) and \( \tilde{FD}_{(1-\alpha/2)}(k) \) are the \( \alpha/2 \) and \( (1-\alpha/2) \) quantiles of the bootstrap distribution of \( \tilde{FD}(k) \) in the \( r \)th replication. In addition, we evaluate the empirical coverage probability of the bootstrap \( (1-\alpha)100\% \) upper bound

\[
\frac{1}{100} \# \{ r : \tilde{E}[FD(k)] \in [0, \tilde{FD}_{(1-\alpha)}(k)] \}.
\]

We set \( \alpha = 0.05 \) for all simulation cases.

In Figures 7 (a1)–(c1), we plot \( \tilde{FD}(k) \) against \( FD(k) \), the true number of FDs with \( k \) ranging from 50 to 70. The closer the point approaches the diagonal line, the closer the two numbers are. As \( k \) increases, the estimate tends to be more dispersed as
anticipated since the error between $\hat{F}_D(k)$ and $F_D(k)$ increases as $k$ increases. In fact, $F_D(k)$ is also more variable around its mean $\mathbb{E}(F_D(k))$ as $k$ increases. Figure 7 (a2)–(c2) report the coverage probabilities of the confidence interval and upper confidence interval for $\mathbb{E}[F_D(k)]$ in all the settings. The coverage probabilities are above 0.95 when $k$ is smaller than 60. When $k$ is larger than 60, the coverage probabilities drop occasionally below 0.95 by a small amount. This is expected since the variation of $\hat{F}_D(k)$ increases as $k$ increases.

In Figure 8, we show the simulation results for the high-dimensional settings. For the Toeplitz structure, the scatter-plot in Figure 8 (a1) shows that our proposed estimate tends to underestimate its target slightly when $k$ is large. For the constant correlation structure and constant partial correlation structure (Figure 8 (b1), (c1)), however, the proposed estimate slightly overestimates its target. Similar to the low-dimensional case, the points become more dispersed from the diagonal line as $k$ increases. In Figures 8 (a2)–(c2), we show the coverage probability of the two-sided confidence interval and confidence upper bound for $\mathbb{E}[F_D(k)]$. The coverage probabilities of the confidence upper bound of $\mathbb{E}[F_D(k)]$ were over 0.95 for all cases, and that for confidence interval are also mostly above 0.95.
except for the constant partial correlation case with \( k > 65 \). This slight under-coverage appears to be a consequence of overestimation of the number of FDs.

7. Discussion

We introduce the GM method for controlling the FDR in high-dimensional regression models. Intuitively, to test if a variable \( X_j \) is truly informative, GM constructs a pair of variables mirroring each other at \( X_j \). The scale of the mirror can be computed explicitly and easily as a function of the design matrix so as to guarantee that the distribution of the mirror statistics is symmetric about zero under the null. With this construct, we developed a testing method such that the FDR is controlled at any designated level asymptotically. We have further proposed a way to assess the variance of the number of estimated FDs in a top-k list, providing extra information about the reliability of the reported FDP results. Through empirical studies we find that GM is not sensitive to the scale of the mirror, making the method more broadly applicable.

A distinctive advantage of GM is that it can be applied to both low or high-dimensional regression problems without requiring any distributional assumption or knowledge on the design matrix, which is common in many applications. Furthermore, since each Gaussian mirror is constructed marginally for each covariate, it brings two advantages: (i) the mirror construction introduces only a small and controllable additive “disturbance,” which not only alleviates possible high correlations among the original covariates, but also gains in power; (ii) the computation in GM can be parallelized, and the method is easily scalable to handle large datasets with the deployment of a GPU-based computational infrastructure.

The GM design introduced in this article is a general framework based on the idea of marginally perturbing the predictor variables one at a time. Such a construct can be generalized to handle more complex statistical and machine-learning models such as generalized linear models, index models, additive models, and neural networks. In linear models, we choose the scale of the mirror \( \psi_j \) to annihilate the partial correlation between the mirrored variables \( X^+_j \) and \( X^-_j \) so that the mirror statistic is symmetric under the null. A natural generalization for more complex models is to choose \( \psi_j \) to minimize a dependence measure of \( X^+_j \) and \( X^-_j \) conditional on the remaining variables. Our preliminary results show that a modified GM method works well for selecting important variables in neural network models (see the appendix for a detailed example).

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Appendix

A.1. Proofs

Proof of Lemma 1. Note that \((U + V, U - V)\) also follows a bivariate normal distribution. Since the correlation between \(U\) and \(V\) is zero, \(\text{var}(U + V) = \text{var}(U - V)\). Furthermore, \(E(U + V) = E(U - V) = 0\).

Therefore, the joint distribution of \((U + V, U - V)\) is the same as the joint distribution of \((U - V, U + V)\). As a result,

\[
P(M > t) = P((U + V) - |U - V| > t)
\]

\[
= P((U - V) - |U + V| > t) = P(M < -t).
\]

Proof of Lemma 2. Note that \(\hat{\beta}^+\) is an OLS estimator based on \(X^+\), then

\[
\frac{1}{n} \text{Cov}(\hat{\beta}^+ | X^+) = \sigma^2 \begin{bmatrix}
1 + v_j^+/2 + 2 \rho(x_j x_j) & 1 - v_j^+
1 + v_j^-/2 + 2 \rho(x_j x_j) & \rho(x_j x_j)
\end{bmatrix}^{-1}
\]

\[
\rho(x_j x_j) = \frac{(\rho(x_j x_j) + \rho(x_j x_j))}{(\rho(x_j x_j) - \rho(x_j x_j))},
\]

where \(v_j^+ = \frac{1}{n} \sum_{i=1}^{n} (x_i^+ - \mu)^2\) and \(v_j^- = \frac{1}{n} \sum_{i=1}^{n} (x_i^- - \mu)^2\).

Proof of Lemma 3. Let \(A_0\) represent the “inactive” constraint defined in (10) and \(\psi = (\psi_1, \psi_2)\). We have

\[
A_0(S, s) \psi = A_0(S, s)(\psi_1, \psi_2)
\]

\[
= A_0(S, s)(\psi_1 + \psi_2, \psi_1 - \psi_2, 1/2, 1/2, 1/2, -1/2)
\]

By the definition of \(\tilde{z}_j = (I - P_S)z_j\), where \(z_j\) is defined in Equation (11), we have \(A_0(S, s)(\psi_1 + \psi_2) = 0\). Then, we have

\[
A_0(S, s) \psi = A_0(S, s)(\psi_1 - \psi_2) / 2(1, -1).
\]

Setting \(a_0 = A_0(S, s)(\psi_1 - \psi_2) / 2\), we have \(A_0(S, s) \psi = a_0(1, -1)\).

Proof of Lemma 4. We first derive the constraints \(A_0(S, s) y \leq b_0(S, s)\) and \(A_1(S, s) y \leq b_1(S, s)\) in (10) separately. Plugging in \(y = P \psi y + (I - P \psi) y\) and \(r = (I - P \psi) y\), we have

\[
A_0(S, s) \psi = a_0(\psi_1 - \psi_2),
\]

\[
A_0(S, s) r = a_0(1, -1) \text{diag}(\alpha, \alpha)(\hat{\beta}_j^+, \hat{\beta}_j^-) + A_0(S, s) r
\]

\[
= a_0(\hat{\beta}_j^+ - \hat{\beta}_j^-) + A_0(S, s) r < b_0(S, s).
\]
Then, \( \{A_0(S, s) y \leq b_0(S, s)\} \) can be written as \( \{V^0_0(r) \leq \hat{\beta}^+_{ij} - \hat{\beta}^-_{ij} \leq V^U_0(r), V^N_0(r) > 0\} \), where

\[
V^0_0(r) := \max_{j a_i \leq 0} \frac{b_{ij} - (A_0 r)_{ij}}{\alpha_{aij}}, \\
V^U_0(r) := \min_{j a_i > 0} \frac{b_{ij} - (A_0 r)_{ij}}{\alpha_{aij}}, \\
V^N_0(r) := \min_{j a_i = 0} b_{ij} - (A_0 r)_{ij}.
\]

Similarly, we have

\[
A_1(S, s) \psi(\psi^T \psi)^{-1} \psi^T y + A_1(S, s) r = a_1(1, 1) \text{diag}(\alpha, \alpha)(\hat{\beta}^+_{ij} + \hat{\beta}^-_{ij}) + A_1(S, s) r = \alpha a_1(\hat{\beta}^+_{ij} + \hat{\beta}^-_{ij}) + A_1(S, s) r < b_1(S, s).
\]

Then, \( \{A_1(S, s) y \leq b_1(S, s)\} \) can be written as \( \{V^1_1(r) \leq \hat{\beta}^+_{ij} + \hat{\beta}^-_{ij} \leq V^U_1(r), V^N_1(r) > 0\} \), where

\[
V^1_1(r) := \max_{j a_i \leq 0} b_{ij} - (A_1 r)_{ij}, \\
V^U_1(r) := \min_{j a_i > 0} b_{ij} - (A_1 r)_{ij}, \\
V^N_1(r) := \min_{j a_i = 0} b_{ij} - (A_1 r)_{ij}.
\]

Thus, we have

\[
\{A y \leq b\} = \{A_0(S, s) y \leq b_0(S, s)\} \cap \{A_1(S, s) y \leq b_1(S, s)\} = \{V^0_0(r) \leq \hat{\beta}^+_{ij} - \hat{\beta}^-_{ij} \leq V^U_0(r), V^N_0(r) > 0\} \cap \{V^1_1(r) \leq \hat{\beta}^+_{ij} + \hat{\beta}^-_{ij} \leq V^U_1(r), V^N_1(r) > 0\}.  
\]

**Proof of Theorem 2.** By Lemma 4, we know that \( \{A y \leq b\} \) imposes a rectangle region in the subspace of \( (\hat{\beta}^+_{ij}, \hat{\beta}^-_{ij}) \) with the boundaries being parallel to \( (\hat{\beta}^+_{ij}, \hat{\beta}^+_{ij}, \hat{\beta}^-_{ij}, \hat{\beta}^-_{ij}) \). The truncation points of the region are only related to \( r \), which are independent of \( (\hat{\beta}^+_{ij}, \hat{\beta}^-_{ij}, \hat{\beta}^+_{ij}, \hat{\beta}^-_{ij}) \). Thus, through a transformation using the cumulative distribution function of a truncated normal distribution, we have

\[
F_{\hat{\beta}^+_{ij}, \hat{\beta}^-_{ij}}(\hat{\beta}^+_{ij}, \hat{\beta}^-_{ij}) \mid \hat{S} = \bar{s}, \hat{S} \sim \text{Unif}(0, 1), \\
F_{\hat{\beta}^+_{ij}, \hat{\beta}^-_{ij}}(\hat{\beta}^+_{ij}, \hat{\beta}^-_{ij}) \mid \hat{S} = \bar{s}, \hat{S} \sim \text{Unif}(0, 1),
\]

where \( F_{\hat{\beta}^+_{ij}, \hat{\beta}^-_{ij}}(x) \) is the cumulative distribution function of the truncated normal distribution defined in Equation (15).

**Proof of Lemma 6.** Let \( \eta_j = \hat{\beta}^+_{ij} + \hat{\beta}^-_{ij} \) and \( \theta_j = \hat{\beta}^+_{ij} - \hat{\beta}^-_{ij} \), and we have

\[
\sum_{j, k \in S_0} \text{cov}(1(M_j \geq t), 1(M_k \geq t)) = \sum_{j, k \in S_0} E[\text{cov}(1(|\eta_j| - |\theta_j| > t), 1(|\eta_k| - |\theta_k| > t)|\theta_j, \theta_k)] + \sum_{j, k \in S_0} \text{cov}(P(|\eta_j| > t | \theta_j, \theta_k)P(|\eta_k| > t | \theta_j, \theta_k)) = I_1 + I_2.
\]
Thus, the conditions in Meinshausen et al. (2009, Lemm. 5) hold with probability approaching 1, which further implies that $|\hat{S}| = O(|S_1|)$. We have
\[
1 - C - o_p(1) \leq \lambda_{\min}(\Omega^0) \leq \lambda_{\max}(\Omega^0) \leq C + o_p(1).
\]
Then we have
\[
R(\hat{S} \cap S_0) \leq \frac{\|\Omega_1\|_{1,2}}{\lambda_{\min}(\Omega^0)} \leq \frac{\sqrt{|\hat{S} \cap S_0|}\|\Omega^0\|_{2}}{\lambda_{\min}(\Omega^0)} = O_p((|\hat{S} \cap S_0|)^{1/2}),
\]
where the first inequality follows from the fact that for any positive-definite matrix $A \in \mathbb{R}^{m \times m}$, $\lambda_{\min}(A) \leq A_{ii} \leq \lambda_{\max}(A)$ for $i \in [m]$. The second inequality follows from the Cauchy–Schwarz inequality. The third equality is based on the following fact:
\[
\sum_{i,j} A_{ij}^2 = \text{tr}(A^TA) = \sum_{i=1}^{m} \lambda_i^2(A).
\]
Second, we characterize the sum of all pairwise correlations of the $M_j$'s. Let $\eta_j = \tilde{\beta}_j^\top + \tilde{\beta}_j^{-1}$, $\theta_j = \tilde{\beta}_j^{-1} - \tilde{\beta}_j$, where $\tilde{\beta}_j^\top$ and $\tilde{\beta}_j$ are defined in Equation (12). We define $\bar{\eta}_j = F_{\omega,\sigma_2}^{-1}F_{\omega,\sigma_2}^{-1}(\psi_{\nu}(\theta_j))$ and $\bar{\theta}_j = F_{\omega,\sigma_2}^{-1}F_{\omega,\sigma_2}^{-1}(\psi_{\nu}(\theta_j))$. Then, we have
\[
\sum_{j,k \in \hat{S} \cap S_0} \text{cov}(1(M_j \geq t), 1(M_k \geq t)) = \sum_{j,k \in \hat{S} \cap S_0} \text{cov}(1(\bar{\eta}_j - |\bar{\theta}_j| > t), 1(\bar{\eta}_k - |\bar{\theta}_k| > t) | \theta_j, \theta_k)) + \sum_{j,k \in \hat{S} \cap S_0} \text{cov}(P(\bar{\eta}_j - |\bar{\theta}_j| > t) | \theta_j, \theta_k)P(\bar{\eta}_k - |\bar{\theta}_k| > t) | \theta_j, \theta_k))
\]
\[
= I_1 + I_2.
\]
Here, $\bar{\eta}_j$ and $\bar{\theta}_j$ are truncated Gaussian with truncation intervals defined in Equation (14). We define the maximum correlation coefficient between $\bar{\eta}_j$ and $\bar{\theta}_j$ as
\[
\rho_{\max}(\bar{\eta}_j, \bar{\theta}_j) = \sup_{f \in \mathcal{F}, \tilde{\theta} \in \mathcal{F}_k} E[f(\bar{\eta}_j)f(\tilde{\theta})]
\]
where $\mathcal{F}_k = \{f_1: \varepsilon_{\nu}(\tilde{\theta}) = 0, \text{var}(f_1(\tilde{\theta})) = 1\}$ and $\mathcal{F}_k = \{f_1: \varepsilon_{\nu}(\tilde{\theta}) = 0, \text{var}(f_1(\tilde{\theta})) = 1\}$. For given $\theta_j$ and $\theta_k$, we have $\text{var}(1(\bar{\eta}_j - |\bar{\theta}_j| > t)) \leq 1$ and $\text{var}(1(\bar{\eta}_k - |\bar{\theta}_k| > t)) \leq 1$. Then, similar to the proof of Lemma 6, we can bound each term in $I_1$ by the corresponding maximum correlation so that
\[
I_1 \leq \sum_{j,k \in \hat{S} \cap S_1} \rho_{\max}(\bar{\eta}_j, \bar{\theta}_j) \leq \sum_{j,k \in \hat{S} \cap S_1} |\rho(\eta_j, \eta_k)|.
\]
Similar to the definition of $\tilde{\xi}_j$ in Equation (11), we choose $z_j$ in the orthogonal space of $X_j$ which makes $\theta_j, \theta_k$ independent of $\eta_j, \eta_k$. By condition Equation (A.9), we have
\[
I_1 \leq \sum_{j,k \in \hat{S} \cap S_1} \rho_{\max}(\bar{\eta}_j, \bar{\theta}_j) \leq \sum_{j,k \in \hat{S} \cap S_1} |\rho(\eta_j, \eta_k)|.
\]
Combining Equations (A.6) and (A.7), we know that there exists $\alpha_2 \in (0, 2)$ such that
\[
\sum_{j,k \in \hat{S} \cap S_1} \text{cov}(1(M_j \geq t), 1(M_k \geq t)) \leq C_1(|\hat{S} \cap S_0|^{\alpha_2}), \forall t.
\]
This concludes the proof. \(\square\)

**Proof of Lemma 8.** For any $\epsilon \in (0, 1)$ and $N_\epsilon = [2/\epsilon]$, let $-\infty < a_0 < a_1 < \cdots < a_{N_\epsilon} = \infty$ such that $G_0(a_{k-1}) - G_0(a_k) \leq \epsilon/2$ for $k \in [N_\epsilon]$. Such a sequence $\{a_k\}_{k=0}^{N_\epsilon}$ exists since $G_0(t)$ is a continuous function with respect to $t \in \mathbb{R}$. We have
\[
P\left(\sup_{t \in \mathbb{R}} V(t) - G_0(t) > \epsilon \right) \leq \mathbb{P}\left(\bigcup_{k=1}^{N_\epsilon} \sup_{t \in \left[a_{k-1}^+, a_k^+\right]} V(t) - G_0(t) > \epsilon \right) \leq \sum_{k=1}^{N_\epsilon} \mathbb{P}\left(\sup_{t \in \left[a_{k-1}^+, a_k^+\right]} V(t) - G_0(t) > \epsilon \right).
\]
Since $V(t)$ and $G_0(t)$ are both monotonically decreasing functions, for any $k \in [N_\epsilon]$, we have
\[
\sup_{t \in \left[a_{k-1}^+, a_k^+\right]} V(t) - G_0(t) \leq V(a_{k-1}^+) - G_0(a_k^+) + \epsilon/2.
\]
For the low-dimensional case, based on Equation (A.8), Assumption 2(a), Lemma 6, and the Chebyshev inequality, it follows that
\[
P\left(\sup_{t \in \mathbb{R}} V_\rho(t) - G_0(t) > \epsilon \right) \leq \mathbb{P}\left(\inf_{t \in \mathbb{R}} V(t) - G_0(t) < -\epsilon \right) \leq \frac{4C_{N_\epsilon}}{|S_0|^{2-\alpha_1\epsilon^2}} \to 0, \text{ as } p \to \infty.
\]
Similarly, we show that
\[
P\left(\inf_{t \in \mathbb{R}} V(t) - G_0(t) < -\epsilon \right) \leq \frac{4C_{N_\epsilon}}{|S_0|^{2-\alpha_1\epsilon^2}} \to 0, \text{ as } p \to \infty.
\]
For the high-dimensional case, based on Equation (A.8), Assumption 2(b), Lemma 7, and the Chebyshev inequality, it follows that
\[
P\left(\sup_{t \in \mathbb{R}} V_\rho(t) - G_0(t) > \epsilon \right) \leq \mathbb{P}\left(\inf_{t \in \mathbb{R}} V(t) - G_0(t) < -\epsilon \right) \leq \frac{4C_{N_\epsilon}}{|S_0|^{2-\alpha_1\epsilon^2}} \to 0, \text{ as } p \to \infty.
\]
Similarly, we show that
\[
P\left(\inf_{t \in \mathbb{R}} V(t) - G_0(t) < -\epsilon \right) \leq \frac{4C_{N_\epsilon}}{|S_0|^{2-\alpha_1\epsilon^2}} \to 0, \text{ as } p \to \infty.
\]
This concludes the proof that $\sup_{t \in \mathbb{R}} |V(t) - G_0(t)| \to 0$ in probability. The convergence of $\sup_{t \in \mathbb{R}} |V(t) - G_0(t)|$ can be shown similarly using the symmetric assumption of the mirror statistics $M_j$ for $j \in S_0$. Similarly, we have
\[
\sup_t |V(t) - G_0(t)| \overset{p}{\to} 0, \quad \sup_t |V(t) - G_1(t)| \overset{p}{\to} 0.
\]
Proof of Theorem 4. We denote
\[
\text{FDP}' = \frac{V'(t)}{(V'(t) + t^p V^1(t)) \lor 1/p}.
\]
Suppose Assumption 2 holds. By Lemma 8 and the definition of FDP∞, we have \( \forall t > 0 \),
\[
|\text{FDP}'(t) - \text{FDP}^\infty(t)| \xrightarrow{p} 0.
\]
For any \( \epsilon > 0 \), we choose \( t_q \sim \epsilon \) such that \( \text{FDP}^\infty(t_q) < \epsilon - \epsilon \). Then, \( \exists \bar{p} > p \) such that \( \forall \rho > \bar{p} \),
\[
P(|\text{FDP}'(t_q) - \text{FDP}^\infty(t_q)|) \geq 1 - \epsilon.
\]
Then we have
\[
P(t_q \leq t_q - \epsilon) \geq P(\text{FDP}'(t_q) - \epsilon) \geq P(\text{FDP}^\infty(t_q) - \epsilon) \geq 1 - \epsilon.
\]
We denote
\[
\text{FDP}(t) = \frac{G_0(t)}{G_0(t) + t^p G_1(t)}.
\]
Based on Lemma 8, for any fixed \( t \), we have
\[
|\text{FDP}'(t) - \text{FDP}(t)| \xrightarrow{p} 0, \quad |\text{FDP}(t) - \text{FDP}(t)| \xrightarrow{p} 0.
\]
Then we have
\[
\sup_{0 < t \leq t_q - \epsilon} |\text{FDP}(t) - \text{FDP}(t)| \xrightarrow{p} 0, \quad \sup_{0 < t \leq t_q - \epsilon} |\text{FDP}'(t) - \text{FDP}(t)| \xrightarrow{p} 0. \quad (A.9)
\]
Now, we are ready to derive the upper bound for \( \lim_{p \to \infty} \mathbb{E} \left[ \text{FDP} \left( t_q \right) \right] \).
\[
\lim_{p \to \infty} \sup \mathbb{E} \left[ \text{FDP} \left( t_q \right) \right]
\]
because of \( \text{FDP}' \) and \( \text{FDP} \) dominating convergence theorem (Klenke (2013, coro. 6.26)). For the last term, we have \( \text{FDP}' \sim \text{FDP} \) almost surely based on the definition of \( t_q \). This concludes the proof of Theorem 4.

Proof of Theorem 6. Suppose Assumption 1 holds. Using the i1-convergence results in Van de Geer et al. (2014), we have
\[
P(M_j > 0) = P(\text{sign}(\hat{\beta}_j) = \text{sign}(\hat{\gamma}_j)) > 1 - \frac{2}{p},
\]
for \( j \in S_0 \). By Equation (2), we have
\[
\tilde{F}_{\text{D}}(k) = \#(M_j \leq -M(k)) = \#(j \in S_0 : M_j < -M(k)) = V(M(k)),
\]
where \( V(\cdot) \) is defined in Lemma 8. Also, \( \text{FD}(k) \) can be written as
\[
\text{FD}(k) = \#(j \in S_0 : M_j > t).
\]
The exception of \( \text{FD}(k) \) is
\[
\frac{1}{k} \sum_{j=1}^{k} \text{FDP}(k) = \sum_{j \in \delta_0} \mathbb{E}(M_j) = \sum_{j \in \delta_0} \mathbb{E}(M_j \leq -M(k)),
\]
where the second equality holds by the symmetric property of \( M_j \) for \( j \in S_0 \). By Lemma 8, conditioned on \( |S_1| \leq \delta \), we have
\[
\mathbb{E}(V(t) - \sum_{j=1}^{k} \mathbb{E}(j \in S_0, M_j \leq -t)) \xrightarrow{p} 0.
\]
Since the event \( |S_1| \leq \delta \) holds with probability \( 1 - \frac{1}{\delta} \), we have
\[
\mathbb{E}(V(t) - \sum_{j=1}^{k} \mathbb{E}(j \in S_0, M_j \leq -t)) \xrightarrow{p} 0.
\]

Proof of Theorem 7. By the same argument as in the proof of Theorem 6, we have that
\[
\tilde{F}_{\text{D}}(k) = \#(M_j \leq -M(k)) = \#(j \in S_0 : M_j < -M(k)),
\]
holds with probability at least \( 1 - \frac{1}{\delta} \). Thus, we have that
\[
\mathbb{E}(\tilde{F}_{\text{D}}(k)) = \mathbb{E}(j \in S_0, M_j \leq -M(k)) = \mathbb{E}(j \in S_0, M_j \geq -M(k)) = \mathbb{E}(\text{FD}(k)),
\]
holds with probability at least \( 1 - \frac{1}{\delta} \).

A.2. GMs for Neural Networks

To examine its generalizability, we apply the GM method, termed as NGM, to select features in neural networks. Similar to the GM construction for linear models, for each feature \( X_j \) of the input of a neural network model, we create its mirror variables \( X_j^+ \) and \( X_j^- \) the same way as in Equation (2), by choosing constant \( \epsilon_j \) to minimize a nonparametric measure of conditional mutual information (equivalent to partial correlation in Gaussian models). The pair of variables are then connected to all the internal nodes of the network in the same way as \( X_j \). The mirror statistic is constructed using influence measures (such as the multiplication of the all weights connecting from the output node to each mirror feature). To save computing time, we can also create such mirrors for all or a subset of features simultaneously, so as to obtain multiple mirror statistics in one run. More details can be found in Xing et al. (2020).

We compare the performances of NGM with DeepPINK, which is a generalization of the Model-X knockoff for neural network models, for variable selection in nonlinear models: \( y_i = f(x_i) + \epsilon_i, \epsilon_i \sim N(0,1), \) for \( i = 1, \ldots, n \). We choose three nonlinear link functions: \( f_1(t) = t + \sin(t), f_2(t) = 0.5t^3 \) and \( f_3(t) = 0.1t^2 \). We randomly set \( k = 30 \) elements in \( \beta \) to be nonzero and generated from \( N(0, (20/\sqrt{\log(p)/n})^2) \) to mimic various signal strengths in real applications. The FDR level is set at \( q = 0.1 \). Both NGM and DeepPINK are applied to the same three-layer perceptron model, which has two hidden layers with \( N_1 = 20 \log(p) \) nodes for the first layer and \( N_2 = 10 \log(p) \) nodes for the second layer.

As shown in Table 1, NGMs and DeepPINK all performed well for the case with \( f_1 = t + \sin(t) \). However, in the latter two cases where \( f \) is a polynomial, DeepPINK appears to have a significant lower power than NGM. In all the three cases, NGMs are capable of maintaining the FDR below the designated level.
Table 1. Neural network fitting for single-index relationships.

| n = 1000 | Link function | FDR   | Power | FDR   | Power |
|----------|---------------|-------|-------|-------|-------|
| p = 500  | \( f_1(t) = t + \sin(t) \) | 0.045 | 0.857 | 0.085 | 0.900 |
|          | \( f_2(t) = 0.5t^2 \)       | 0.080 | 0.843 | 0.155 | 0.413 |
|          | \( f_3(t) = 0.1t^2 \)       | 0.071 | 0.847 | 0.148 | 0.333 |

| p = 2000 | \( f_1(t) = t + \sin(t) \) | 0.081 | 0.820 | 0.126 | 0.817 |
|          | \( f_2(t) = 0.5t^2 \)       | 0.082 | 0.587 | 0.149 | 0.320 |
|          | \( f_3(t) = 0.1t^2 \)       | 0.108 | 0.530 | 0.477 | 0.053 |

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