Bayesian Knockoff Filter Using Gibbs Sampler

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Abstract

In many fields, researchers are interested in discovering features with substantial effect on the response from a large number of features and controlling the proportion of false discoveries. By incorporating the knockoff procedure in the Bayesian framework, we develop the Bayesian knockoff filter (BKF) for selecting features that have important effect on the response. In contrast to the fixed knockoff variables in the frequentist procedures, we allow the knockoff variables to be continuously updated in the Markov chain Monte Carlo. Based on the posterior samples and elaborated greedy selection procedures, our method can distinguish the truly important features as well as controlling the Bayesian false discovery rate at a desirable level. Numerical experiments on both synthetic and real data demonstrate the advantages of our method over existing knockoff methods and Bayesian variable selection approaches, i.e., the BKF possesses higher power and yields a lower false discovery rate.

Keywords: Bayesian false discovery rate, feature selection, generalized linear model, knockoff filter, Markov chain Monte Carlo.

1 Introduction

Identifying important features that have substantial effect on a response variable is one of the most common problems in both machine learning and statistics. Traditionally, the importance of a feature can be measured by the value of the fitted regression coefficient or \( p \)-value from hypothesis testing of a parameter under a statistical model. Recent decades have witnessed the emergence of vast data of high dimensionality, and extensive research has been carried out for feature selection. Taking the generalized linear model (GLM) as an example, variable selection methods (Efroymson, 1960; Mitchell and Beauchamp, 1988; Tibshirani, 1996; Fan and Li, 2001; Park and Casella, 2008; Carvalho et al., 2010), and multiple
testing procedures (Benjamini and Hochberg, 1995; Sarkar and Chang, 1997; Yekutieli and Benjamini, 2001; Storey, 2002; Leek and Storey, 2008; Whittemore, 2007; Blanchard and Roquain, 2009) represent the two main classes of approaches to learning important features with respect to the response.

However, the aforementioned methods have several limitations. For variable selection methods, the false discovery rate (FDR) is not controlled and thus their reliability is questionable. Spurious features with no effect on response might be falsely selected because they are correlated to some important features. Although multiple testing procedures (Blanchard and Roquain, 2009) can be incorporated to control FDR under an arbitrary dependency structure of features, it tends to be conservative for practical use. To overcome such limitations, a new powerful method called the knockoff filter (Barber and Candès, 2015) has been developed recently. By introducing the knockoff variables which mimic the dependency structure of original features and act as control variables as well as a statistic that overestimates the FDR for arbitrary dependency structures among features, the knockoff filter is able to conduct feature selection with a well-controlled FDR. Inspired by this idea, a series of knockoff methods have been developed (Dai and Barber, 2016; Candès et al., 2018; Gimenez et al., 2019; Gimenez and Zou, 2019; Katsevich and Sabatti, 2019; Barber and Candès, 2019; Sesia et al., 2019; Bates et al., 2020), which however are all frequentist approaches and their inferences heavily rely upon the quality of the sole set of generated knockoff variables. To control the FDR under a desired level, the existing methods sacrifice their ability to distinguish the truly important features if a set of poor-quality knockoff variables is generated or the number of truly important features is small, and this would further cause power loss. Up to now, these two problems have only been partly solved by multi-knockoffs (Gimenez and Zou, 2019) at the cost of power loss in the optimal cases.

In the Bayesian paradigm, we restate the concepts of knockoff variables and FDR and develop the Bayesian knockoff filter (BKF). With the Markov chain Monte Carlo (MCMC) algorithm and elaborated selection procedures, our method outperforms existing knockoff methods in distinguishing important (non-null) features when the FDR is controlled under the same target level, while existing Bayesian variable selection approaches are unable to control FDR when sample size is small.

The rest of this article is organized as follows. In Section 2, we formulate the feature selection problem in GLMs and briefly introduce existing knockoff procedures. Details of the BKF, including the Bayesian model, definition of Bayesian FDR, FDR-controlled selection procedure and MCMC algorithm, are provided in Section 3. We conduct experiments on synthetic and real data respectively in Sections 4 and 5 to investigate performance of the BKF under different circumstances and compare it with existing methods in terms of both statistical power and the ability to mitigate false discoveries. Section 6 concludes with discussions.
2 Background

2.1 Problem Setup

Consider a dataset $D$ with $n$ independent and identically distributed (i.i.d.) observations $(x_1, y_1), \ldots, (x_n, y_n)$, where $x_i$ and $y_i$ are copies of feature vector $X = (X_1, \ldots, X_p)^T \in \mathbb{R}^p$ and response variable $Y \in \mathbb{R}$ respectively. It is assumed that responses $y_1, \ldots, y_n$ only depend on a relatively small subset of features. Conditional on this subset of important features, responses are independent of the remaining features. Mathematically speaking, there are two disjoint subsets of features, $H_0$ and $H_1$, satisfying that

- $H_0 \cup H_1 = \{1, \ldots, p\}$;
- $\forall j \in H_0$, $X_j \perp Y|X_{-j}$, where $\perp$ represents independence between two variables;
- $\forall j \in H_1$, $X_j \not\perp Y|X_{-j}$, where $\not\perp$ represents dependence between two variables;

where $X_{-j} = (X_1, \ldots, X_{j-1}, X_{j+1}, \ldots, X_p)^T$. The set $H_1$ contains all the non-null features that have important effects on response $Y$, while all the null features in $H_0$ are irrelevant to the response given the other features. Our goal is to obtain an estimator $\hat{S}$ of the set $H_1$ based on the observed data $D = \{(x_i, y_i) : i = 1, \ldots, n\}$. Our goal is to achieve two objectives simultaneously:

- Controlling the false discovery rate (FDR),

$$\text{FDR} = \mathbb{E}\left(\frac{|\hat{S} \cap H_0|}{|\hat{S}| \lor 1}\right),$$

under a desired level $\alpha$.

- Making the number of true discoveries, $|\hat{S} \cap H_1|$, as large as possible.

In the aspect of hypothesis testing, we are interested in testing the null hypotheses

$$H_{0j} : X_j \perp Y|X_{-j}, \quad j = 1, \ldots, p,$$

by constructing a multiple testing procedure on $H_{01}, \ldots, H_{0p}$ with a controlled FDR. The FDR is analogous to the type I error rate in traditional single hypothesis testing, while a larger size of $\hat{S} \cap H_1$ implies higher power in testing hypotheses (2). In practice, if a GLM is used to approximate the conditional distribution $f(Y|X)$ with

$$E(Y|X) = g^{-1}(\eta), \quad \eta = \sum_{j=1}^{p} X_j \beta_j,$$
where \( g(\cdot) \) is a link function, the null hypothesis \( H_{0j} \) is equivalent to \( H_{0j}^* : \beta_j = 0 \) for \( j = 1, \ldots, p \). Thus, estimating \( \mathcal{H}_1 \) or multiple testing on (2) is equivalent to conducting variable selection on features \( X_1, \ldots, X_p \) under the GLM approximation (3) (Candès et al., 2018).

Various methods have been proposed in the literature for multiple testing on hypotheses \( H_{01}, \ldots, H_{0p} \) under GLMs (3). Existing methods can be classified into two popular paradigms. One is variable selection in regression analysis under both frequentist and Bayesian frameworks. Frequentist methods in this class include step-wise regression (Efroymson, 1960) and penalized regression methods with different penalty functions, such as ridge regression, Lasso (Tibshirani, 1996), SCAD (Fan and Li, 2001) and their variants. By fitting a GLM on \((X, Y)\) with penalties or step-wise selection procedures to promote sparsity in coefficients \( \beta_1, \ldots, \beta_p \), we can obtain the estimator \( \hat{S} = \{ j : \hat{\beta}_j \neq 0 \} \) for the set of non-null features. Although the asymptotic guarantees of these methods such as model selection consistency have been established even under high-dimensional settings, they still suffer from an uncontrollable FDR with finite sample size.

Bayesian variable selection approaches, such as the spike-and-slab regression (Mitchell and Beauchamp, 1988), Bayesian Lasso (Park and Casella, 2008), the horseshoe estimator (Carvalho et al., 2010) and the recent iterative Bayesian stepwise selection (IBSS) procedure (Wang et al., 2020), compute the posterior distribution of \( \mathcal{H}_1 \), which yields the Bayesain estimator \( \hat{S} \) by minimizing the expected posterior loss. However, commonly used Bayesian estimators \( \hat{S} \), including the highest probability model and the median probability model, do not take the FDR into consideration and hence their control of false discoveries are questionable.

Following the multiple testing procedure (Benjamini and Hochberg, 1995), another class of approaches (Sarkar and Chang, 1997; Yekutieli and Benjamini, 2001; Leek and Storey, 2008) calculate \( p \)-value for each hypothesis \( H_{0j} \) (\( j = 1, \ldots, p \)) or equivalently \( H_{0j}^* \), which is only feasible under low-dimensional GLMs. Moreover, these methods can only control FDR theoretically when these \( p \)-values possess an independent property or positive regression dependency on a subset (Yekutieli and Benjamini, 2001), which is difficult to verify under GLMs. To overcome such shortcomings of frequentist multiple testing procedures, Bayesian methods have been developed with control of the Bayesian FDR (Storey, 2002; Whittemore, 2007) for multiple comparisons (Scott and Berger, 2006; Miranda-Moreno et al., 2007; Efron, 2008). We incorporate the recently developed knockoff methods (Barber and Candès, 2015; Candès et al., 2018) to Bayesian multiple testing procedures and develop a fully Bayesian approach with Gibbs sampled knockoffs for feature selection.
2.2 Knockoffs

To control the finite-sample FDR in feature selection, Barber and Candès (2015) propose a (fixed-X) knockoff filter to estimate $H_1$ without imposing any assumptions on dependency structures among features $X_1, \ldots, X_p$ under a linear model:

$$Y = \sum_{j=1}^{p} X_j \beta_j + \epsilon, \quad \epsilon \sim N(0, \sigma^2),$$

(4)

where features are assumed to be fixed. In contrast, the model-X knockoff filter (Candès et al., 2018) makes an extension by assuming the distribution $f(X)$ to be known but $f(Y|X)$ unknown. With the distribution of features $f(X)$, a joint model $f(X, \tilde{X})$ satisfying Definition 1 is constructed and the model-X knockoff variables $\tilde{X} = (\tilde{x}_1, \ldots, \tilde{x}_n)^T$ are generated conditional on the observed features $X = (x_1, \ldots, x_n)^T$.

**Definition 1. Model-X knockoff** (Candès et al., 2018): For random variables $X = (X_1, \ldots, X_p)^T$ of any families and response $Y$, the random variables $\tilde{X} = (\tilde{X}_1, \ldots, \tilde{X}_p)^T$ are the model-X knockoff variables for $X$ if

1. for any subset $S \subset \{1, \ldots, p\}$,
   $$\mathcal{D}(X, \tilde{X})_{\text{Swap}(S)} \overset{d}{=} \mathcal{D}(X, \tilde{X}),$$

   (5)

   where $\mathcal{D}(X, \tilde{X})_{\text{Swap}(S)}$ is obtained by swapping elements $X_j$ and $\tilde{X}_j$ of $(X, \tilde{X})$ for all $j \in S$;

2. $\tilde{X} \perp Y | X$.

If $f(X)$ is unknown, Candès et al. (2018) provide an approximate construction on the basis of the first two moments of features with a graphical Lasso estimator of the covariance matrix. That is, a Gaussian graphical model is fitted on features $X = (x_1, \ldots, x_n)^T$ and the joint model $f(X, \tilde{X})$ is constructed based on the fitted graphical model. Barber and Candès (2019) further incorporate a screening procedure prior to implementation of the knockoff filter to make it feasible in high-dimensional settings. Dai and Barber (2016); Katsevich and Sabatti (2019) extend the knockoff method in a way that prior knowledge of group structures among features can be utilized in feature selection and FDR can be controlled at both the feature level and group level.

With the knockoff sample $\tilde{X}$, the model-X knockoff filter computes feature statistics $W_1, \ldots, W_p$ to evaluate the evidence in $D$ against hypotheses $H_{01}, \ldots, H_{0p}$. As suggested by Candès et al. (2018), $W_j$ should satisfy the flip-sign property under swapping of the $j$-th feature with its knockoff. Typical ways to construct feature statistics $W_1, \ldots, W_p$ include the Lasso signed max (Barber and Candès, 2015) and Lasso
coefficient-difference (Candès et al., 2018) statistic. A large value of $W_j$ usually implies strong evidence in $D$ against $H_{0j}$. The estimator $\hat{S}$ is then obtained as $\{j : W_j > \tau\}$ where the threshold $\tau$ is chosen as

$$\tau = \min\{t > 0 : \hat{\text{FDP}}(t) \leq \alpha\},$$

(6)

where the estimator of the false discovery proportion

$$\hat{\text{FDP}}(t) = \frac{1 + |\{j : W_j < -t\}|}{|\{j : W_j > t\}| \vee 1}$$

is shown to overestimate the overall FDR for all $t \in (0, \infty)$ (Candès et al., 2018).

However, all the aforementioned knockoff filters are frequentist methods and their inferences are based on one knockoff sample $\tilde{X}$ only. Because $\hat{\text{FDP}}(t)$ overestimates FDR, it is a conservative way to control the overall FDR by adopting the estimator of FDP, and the inference is highly dependent on the quality of the generated knockoff sample. With a low-quality $\tilde{X}$, such procedures may lead to power loss. In addition, all the methods rely on the assumption that the dimension of the feature vector ($p$) is large, so that the selection procedures force the size of $\hat{S}$ to be zero or not smaller than $\lfloor 1/\alpha \rfloor$ if nonzero. This property results in power loss when the size of the true $H_1$ is small. Up to now, the two problems have only been partly solved by multi-knockoffs (Gimenez and Zou, 2019) at the cost of power loss for large $H_1$.

3 Bayesian Knockoff Filter

3.1 Bayesian Model

To overcome the weaknesses of existing knockoff filters, we develop the Bayesian knockoff filter (BKF). Similar to the model-$X$ knockoff filter, we assume the distribution $f(X)$ is known and establish the joint distribution $f(X, \tilde{X})$ which is invariant to swaps for all subsets $S \subset \{1, \ldots, p\}$. For example, if the original $X$ follows a multivariate Gaussian distribution $\text{MVN}(0, \Sigma)$, the joint distribution $f(X, \tilde{X})$ satisfying Definition 1 is

$$\begin{pmatrix} X \\ \tilde{X} \end{pmatrix} \sim \text{MVN} \left[ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, G \right],$$

with $G = \begin{bmatrix} \Sigma & \Sigma - \text{diag}\{s\} \\ \text{diag}\{s\} & \Sigma \end{bmatrix}$,

(7)

where the diagonal matrix $\text{diag}\{s\}$ satisfies the condition $2\text{diag}\{s\} - \text{diag}\{s\} \Sigma \text{diag}\{s\} \geq 0$ (Barber and Candès, 2015).

In the case of Gaussian covariates, (7) can be used to construct knockoff variables. However, if covariates
are non-Gaussian or even not continuous, it is challenging to deduce the joint distribution $f(X, \tilde{X})$. Although there are several existing methods to generate $\tilde{X}$ without an explicit expression of $f(X, \tilde{X})$ (Sesia et al., 2019; Bates et al., 2020), they rely on either a specific structure of $f(X)$ (e.g., hidden Markov models or graphical models) or an intense computational strategy (multiple-try Metropolis). If the distribution of the original $X$ is unknown, we require $(X, \tilde{X})_{\text{Swap}(S)}$ and $(X, \tilde{X})$ to have the same first two moments rather than the same distribution for any subset $S$. We adopt the second-order approximation construction in Candès et al. (2018) to approximate $f(X)$ with a Gaussian model $\text{MVN}(\hat{\mu}, \hat{\Sigma})$ with the estimated mean $\hat{\mu}$ and covariance matrix $\hat{\Sigma}$ to construct the joint distribution $f(X, \tilde{X})$. As a result, the conditional generative model $f(\tilde{X}|X)$ can be deduced, from which $\tilde{X}$ is generated.

Similar to the work of Candès et al. (2018), we do not assume any parametric model for the conditional distribution $f(Y|X, \tilde{X})$. We may use the distribution $h(Y|X, \tilde{X}; \beta, \tilde{\beta}, \phi)$ under the GLM to approximate $f(Y|X, \tilde{X})$, with

$$E(Y|X, \tilde{X}; \beta, \tilde{\beta}, \phi) = g^{-1}(\eta), \quad \eta = \sum_{j=1}^{p} (X_j \beta_j + \tilde{X}_j \tilde{\beta}_j),$$

(8)

where $\phi$ represents nuisance parameters; for example, the variance parameter $\sigma^2$ in a normal distribution or the dispersion parameter in an over-dispersed Poisson distribution (Nelder and Wedderburn, 1972). If the prior is denoted by $f(\beta, \tilde{\beta}, \phi)$, the joint posterior density of knockoff variables and parameters under model (8) is

$$f(\tilde{x}_1, \ldots, \tilde{x}_n, \beta, \tilde{\beta}, \phi|D) \propto f(\beta, \tilde{\beta}, \phi) \prod_{i=1}^{n} h(y_i|x_i, \tilde{x}_i; \beta, \tilde{\beta}, \phi) f(\tilde{x}_i|x_i).$$

(9)

### 3.2 Feature Selection with Bayesian FDR

Analogous to the existing frequentist work, our goal is to obtain a Bayesian estimator $\hat{S}$ for the set of non-null features $H_1$ with the Bayesian FDR controlled and the posterior expected number of true discoveries as large as possible. In the Bayesian paradigm, the set $H_1$ is assumed to be random and the Bayesian FDR of any subset $S$ is defined as follows.

**Definition 2. Bayesian FDR** (Storey, 2002; Whittemore, 2007): For all possible subsets $S \subset \{1, \ldots, p\}$, the Bayesian false discovery rate (BFDR) with regard to $H_1$ is

$$BFDR(S) = \mathbb{E}\left(\frac{|S - H_1|}{|S| \lor 1} | D\right).$$

(10)
If posterior probabilities $P(H_0_j|D) \ (j = 1, \ldots, p)$ are known, it is clear that

$$\mathbb{E}(|S - H_1||D|) = \mathbb{E}\left(\sum_{j \in S} I[j \notin H_1]\right) = \sum_{j \in S} P(H_0_j|D).$$

As a result, we can obtain an equivalent definition of Bayesian FDR for all possible $S \subset \{1, \ldots, p\}$ as

$$BFDR(S) = \frac{1}{|S|} \sum_{j \in S} P(H_0_j|D). \quad (11)$$

Thus, our estimation of $H_1$ can be translated into a decision problem to select a subset,

$$\hat{S} = \arg \min_{S \in \{1, \ldots, p\}} E[L(H_1, S)|D], \quad \text{s.t.} \quad BFDR(S) \leq \alpha, \quad (12)$$

where the loss function $L(H_1, S) = -|S \cap H_1|$. Under the Bayesian paradigm, the importance of feature $X_j$ is depicted by the posterior probability $P(H_1_j|D)$, and minimizing the expected posterior loss $E[L(H_1, S)|D] = -\sum_{j \in S} P(H_1_j|D)$ is equivalent to maximizing the overall importance of features in the subset $S$. Following the equivalent definition (11) and $P(H_{1j}|D) = 1 - P(H_{0j}|D)$, when posterior probabilities $P(H_{0j}|D) \ (j = 1, \ldots, p)$ are known, the constrained optimization problem can be solved as a knapsack problem to include as many features in $\hat{S}$ as possible while keeping $BFDR(S) \leq \alpha$. The solution can be easily computed via a greedy algorithm described as follows:

1. Set $S_0 = \emptyset$ and $BFDR(S_0) = 0$.
2. Sort $P(H_{01}|D), \ldots, P(H_{0p}|D)$ in an increasing order: $P(H_{0(1)}|D) \leq \cdots \leq P(H_{0(p)}|D)$.
3. For $j = 1, \ldots, p$, calculate $BFDR(S_j)$ by (11) where $S_j = \{j' : P(H_{0j'}|D) \leq P(H_{0(j)}|D)\}$.
4. Let $\hat{S} = S_k$ where $k = \max\{j : BFDR(S_j) \leq \alpha\}$.

As shown by Müller et al. (2004), such a decision rule is optimal in the sense that it maximizes the statistical power while controlling the Bayesian FDR under $\alpha$.

However, posterior probabilities $P(H_{0j}|D) \ (j = 1, \ldots, p)$ cannot be directly derived from the posterior density (9), especially when the prior does not possess a point mass at $\beta_j = 0$. To link posterior density (9) with posterior probabilities $P(H_{0j}|D) \ (j = 1, \ldots, p)$, we use a set of random variables with the flip-sign property to compute the approximated upper bounds of $P(H_{0j}|D) \ (j = 1, \ldots, p)$. We restate the flip-sign property in the Bayesian framework.
Definition 3. The flip-sign property: A family of random variables \( \{W_j : j = 1, \ldots, p\} \) are said to obey the flip-sign property if for all subsets \( S \subset H_0 \), the posterior distribution of \( W = (W_1, \ldots, W_p)^T \) satisfies

\[
  f(W|D) = f(W_S|D)
\]

where \( W_S = (W_{1,S}, \ldots, W_{p,S})^T \) and

\[
  W_{j,S} = \begin{cases} 
  W_j, & j \notin S, \\
  -W_j, & j \in S.
  \end{cases}
\]

Given the definition of subset \( H_0 \) and model-\( X \) knockoff, Theorem 1 offers us a way to construct a family of random variables which obey the flip-sign property.

Theorem 1. If the marginal prior \( f(\beta, \tilde{\beta}) \) is invariant to swaps for any subset \( S \subset \{1, \ldots, p\} \), the feature statistics \( W = (W_1, \ldots, W_p)^T \) obey the flip-sign property as long as \( W_j \) is antisymmetric with respect to \( \beta_j \) and \( \tilde{\beta}_j \), \( j = 1, \ldots, p \).

The proof of Theorem 1 is provided in the Appendix. When the marginal prior \( f(\beta, \tilde{\beta}) \) is invariant to swaps, the posterior distribution of antisymmetric \( W_j \) is symmetric with respect to 0 if \( H_{0j} \) holds and thus

\[
  P(W_j < 0|D, H_{0j}) = P(W_j > 0|D, H_{0j}).
\]

By the law of total probability where

\[
  P(W_j < 0|D) = P(W_j < 0|D, H_{0j})P(H_{0j}|D) + P(W_j < 0|D, H_{1j})P(H_{1j}|D),
\]

\[
  P(W_j > 0|D) = P(W_j > 0|D, H_{0j})P(H_{0j}|D) + P(W_j > 0|D, H_{1j})P(H_{1j}|D),
\]

if antisymmetric \( W_j \) is well defined so that \( P(W_j > 0|D, H_{1j}) > P(W_j < 0|D, H_{1j}) \) and (14) holds, we can subtract (15a) from (15b), leading to

\[
  P(W_j > 0|D) - P(W_j < 0|D) = P(H_{1j}|D) \left\{ P(W_j > 0|D, H_{1j}) - P(W_j < 0|D, H_{1j}) \right\}.
\]

Due to the fact that \( 0 < P(W_j > 0|D, H_{1j}) - P(W_j < 0|D, H_{1j}) \leq 1 \), an upper bound of \( P(H_{0j}|D) \) can be obtained as

\[
  P(H_{0j}|D) = 1 - P(H_{1j}|D) \leq 1 - P(W_j > 0|D) + P(W_j < 0|D).
\]

Examples of marginal priors invariant to swaps and antisymmetric \( W_j \) which satisfies that \( P(W_j > 0|D, H_{1j}) > P(W_j < 0|D, H_{1j}) \) and leads to inequality (17) include
- Invariant prior:
  1. Flat prior: \( f(\beta, \tilde{\beta}) \propto 1; \)
  2. Normal prior: \( f(\beta, \tilde{\beta}) \propto \prod_{j=1}^{p} \exp\{-\beta_j^2 - \tilde{\beta}_j^2/(2\sigma_j^2)\}; \)
  3. Laplacian prior: \( f(\beta, \tilde{\beta}) \propto \prod_{j=1}^{p} \exp\{-\lambda_j |\beta_j| - \lambda_j |\tilde{\beta}_j|\}; \)
  4. Modified spike-and-slab prior (Candès et al., 2018):

\[
f(\beta, \tilde{\beta}) = \prod_{j=1}^{p} f(\beta_j, \tilde{\beta}_j), \quad \text{where } f(\beta_j, \tilde{\beta}_j) = \begin{cases} I[\beta_j = \tilde{\beta}_j = 0] & \text{w.p. } (1 - \xi), \\ \phi(\beta_j; 0, \tau^2)I[\tilde{\beta}_j = 0] & \text{w.p. } \xi/2, \\ \phi(\tilde{\beta}_j; 0, \tau^2)I[\beta_j = 0] & \text{w.p. } \xi/2. \end{cases}
\]

- Antisymmetric \( W_j \):
  1. \( W_j = |\beta_j| - |\tilde{\beta}_j| \) or \( W_j = |\beta_j|^2 - |\tilde{\beta}_j|^2; \)
  2. \( W_j = |\beta_j + \tilde{\beta}_j| \cdot \text{sign}(|\beta_j| - |\tilde{\beta}_j|). \)

In practice, with posterior samples \((\tilde{\mathbf{X}}^{(t)}, \mathbf{\beta}^{(t)}, \tilde{\mathbf{\beta}}^{(t)}, \phi^{(t)})\), \( \mathbf{W}^{(t)} = (W_1^{(t)}, \ldots, W_p^{(t)})^T \) can be computed for \( t = 1, \ldots, T \) and thus upper bounds (17) can be estimated by

\[
\hat{P}(H_0|D) = \frac{2}{T} \sum_{t=1}^{T} I(W_j^{(t)} < 0), \quad j = 1, \ldots, p.
\]

As a result, we can substitute \( P(H_0|D) \) in the greedy algorithm by the estimated upper bound \( \hat{P}(H_0|D) \) to select the subset \( \hat{S} \) which minimizes the expected posterior loss in (12).

### 3.3 Markov Chain Monte Carlo

Following (9), Algorithm 1 provides a Gibbs sampling framework to draw posterior samples \( \{\tilde{\mathbf{X}}^{(t)}, \mathbf{\beta}^{(t)}, \tilde{\mathbf{\beta}}^{(t)}, \phi^{(t)}\} : t = 1, \ldots, T \}, \) from the full conditional distributions.

In practice, the sampling of \( (\mathbf{\beta}, \tilde{\mathbf{\beta}}), \phi \) and \( \tilde{\mathbf{x}} \), corresponding to steps 4–7 can be implemented by existing computational methods, such as Metropolis–Hasting or rejection sampling algorithms (Sesia et al., 2019; Bates et al., 2020).

To investigate whether posterior samples \( \mathbf{\tilde{X}}^{(1)}, \ldots, \mathbf{\tilde{X}}^{(T)} \) generated by Algorithm 1 satisfy Definition 1, we apply Algorithm 1 to the data generated under settings in Section 4.1.1 (with sample size \( n = 1000 \).
Algorithm 1: Gibbs sampler

1: **Input:** Observed data $D$.
2: Initialize $\tilde{x}_i \sim f(\tilde{x}_i | x_i)$ for $i = 1, \ldots, n$.
3: repeat
4: Sample $(\beta, \tilde{\beta}) \sim f(\beta, \tilde{\beta} | \tilde{x}_1, \ldots, \tilde{x}_n, \phi, D)$;
5: Sample $\phi \sim f(\phi | \tilde{x}_1, \ldots, \tilde{x}_n, \beta, \tilde{\beta}, D)$;
6: for $i = 1, \ldots, n$ do
7: Sample $\tilde{x}_i \sim f(\tilde{x}_i | \beta, \tilde{\beta}, \phi, x_i, y_i)$.
8: end for
9: until convergence

and signal strength $a = 4$) and use the statistic

$$\Delta(\tilde{X}) = \frac{1}{n} \sum_{j \neq k} \sum_{i=1}^{n} (\tilde{x}_{ij} \tilde{x}_{ik} + 2x_{ij} \tilde{x}_{ik} - 3x_{ij}x_{ik})$$  \hspace{1cm} (19)

to examine whether augmented knockoff variables satisfy Definition 1. As it is required $E[\Delta(\tilde{X})] = 0$ for valid knockoffs, $\Delta(\tilde{X})$ would fluctuate around 0 if Algorithm 1 generates valid knockoff variables $\tilde{X}$. In our experiments, we keep $T = 10,000$ posterior samples after 1,000 burn-in iterations. As shown in Figure 1, the Markov chains are stable, well mixed and $\Delta(\tilde{X})$ fluctuates around 0, which indicate $\tilde{X}^{(1)}, \ldots, \tilde{X}^{(T)}$ are valid knockoff variables.

3.4 Relationships with Existing Methods

Although the BKF is developed along the inspiring idea of knockoffs (Barber and Candès, 2015), we elaborate on its differences from existing related methods as follows.

- **Model-X knockoff** (Candès et al., 2018): In contrast to the fixed-X knockoff (Barber and Candès, 2015), our method follows a similar setup of the model-X knockoff where no assumption is made on the conditional distribution $f(Y|X, \tilde{X})$. Similar to the way of computing Bayesian variable selection knockoff statistics in Candès et al. (2018), a GLM $h(Y|X, \tilde{X}; \beta, \tilde{\beta}, \phi)$ is imposed as a data-driven approximation of $f(Y|X, \tilde{X})$ for inference. However, there are fundamental differences between the model-X knockoff and our BKF. The model-X knockoff is a frequentist method, which relies upon only one set of knockoff variables. It uses the Bayesian variable selection (BVS) method as one of possible ways to compute feature statistics and still controls the frequentist FDR in feature selection. When BVS feature statistics are used, it can leverage prior knowledge via the probability point mass at $\beta_j = 0$ in the prior specification. In contrast, our BKF is a fully Bayesian data augmentation approach where knockoffs $\tilde{x}_1, \ldots, \tilde{x}_n$ and parameters $\beta, \tilde{\beta}, \phi$ are treated as random.
Incorporating the knockoffs as missing data and FDR into a Bayesian framework, our BKF repeatedly samples knockoff variables in MCMC for more stable inference and conducts feature selection based on the Bayesian FDR control, no matter whether priors have a point mass at $\beta_j = 0$.

- **Metropolized knockoff sampling** (Bates et al., 2020): Although Bates et al. (2020) use MCMC as a mechanism to generate knockoff variables, the Metropolized knockoff sampling is still a frequentist method, relying upon only one set of knockoff variables for inference. In contrast, our BKF treats knockoff variables as missing data and continuously samples them via data augmentation in MCMC for stable Bayesian inference.

- **Multiple knockoffs** (Gimenez and Zou, 2019): The multiple knockoffs generate more than one set of knockoff variables. Taking the 2 multi-knockoffs under a Gaussian case as an example, the
joint model of original features $X$ and knockoff features ($\tilde{X}_1, \tilde{X}_2$) in Gimenez and Zou (2019) is exchangeable for any generalized swaps among the three sets of features. In contrast, we only define the joint model of original features $X$ and each set of knockoff features, which is exchangeable for any swaps between original features and each set of knockoff features. As a result, the difference between original features and knockoff features would be greater in BKF, leading to higher power especially when strong correlations exist among original features.

4 Numerical Experiments

We conduct numerical experiments on synthetic data: (i) to evaluate the performance of BKF in controlling FDR and detecting true discoveries (power) under various data generation settings; (ii) to compare BKF with existing frequentist knockoff methods on power and FDR; and (iii) to illustrate the advantage of BKF in controlling false discoveries over existing Bayesian feature selection approaches. We also apply our method to real data to demonstrate the practical performance of BKF. All of our experiments are implemented with R codes which are included in the supplementary materials.

4.1 Comparisons with Existing Knockoffs

We first compare the performances of BKF with three existing knockoff methods including the fixed-$X$ knockoff (Barber and Candès, 2015), the model-$X$ knockoff (Candès et al., 2018) and the multi-knockoffs (Gimenez and Zou, 2019). For multi-knockoffs, we use the 2 multi-knockoffs in the experiments. For all the existing methods, we use their SDP (semidefinite program) constructions of knockoff and the Lasso coefficient difference as the importance statistic for inference. To evaluate the performances of different methods, two criteria are considered: (a) the overall FDR defined by (1); and (b) statistical power $|\hat{S} \cap H_1|/|H_1|$, where $\hat{S}$ corresponds to the estimator obtained by each of the knockoff methods in each replication. We consider different settings to examine the effects of sample size, signal strength, variance structures among features, dimensionality and the size of $H_1$.

For fair comparison between our BKF with existing frequentist methods, we use the flat prior in the implementation of BKF. We discard the first 500 iterations as burn-ins and keep $T = 2,000$ posterior samples for inference.

4.1.1 Sample Size and Signal Strength

To examine how BKF performs under different sample sizes and signal strengths, we simulate 100 datasets $D = \{(x_i, y_i) : i = 1, \ldots, n\}$ with a fixed number of features $p = 30$. For each dataset, features
Figure 2: FDR, power and the standard deviation (SD) of power for the BKF and other knockoffs under different sample sizes $n$ and signal strengths $a$. Each point is averaged over 100 replications.
\( \mathbf{x}_1, \ldots, \mathbf{x}_n \) are generated as i.i.d. samples from \( \text{MVN}(\mathbf{0}, \mathbf{I}) \) and responses \( y_1, \ldots, y_n \) are generated from a Gaussian linear model (4) with coefficients \( \beta_1, \ldots, \beta_p \). The true non-null features in subset \( \mathcal{H}_1 \) of size 10 are randomly chosen with \( \beta_j \sim \text{Unif}[-a, a] \) if \( j \in \mathcal{H}_1 \) and \( \beta_j = 0 \) otherwise. By varying the sample size \( n \in \{100, 200, 500, 1000\} \) and signal strength \( a \in \{0.2, 0.4, \ldots, 4\} \) with a fixed noise level \( \sigma^2 = 4 \), we can evaluate the effects of sample size and signal strengths on the performances of BKF and other existing methods. In our experiments, we use model (7) for knockoffs, and the desired level of FDR is \( \alpha = 0.1 \).

Figure 2 shows that similar to other knockoff methods, the power of BKF grows as the signal strength \( a \) or sample size \( n \) increases. At the same time, the overall FDR of BKF is controlled under the desired level, indicating BKF is valid for multiple testing on hypotheses (2). Compared with existing knockoff methods, the overall FDR of BKF is significantly lower, implying that our method is more reliable in avoiding discovery of false signals. Similar to the 2 multi-knockoffs, the capability of BKF to distinguish the true \( H_{ij} \) grows much faster and becomes more stable as the signal strength or sample size increases than the single knockoff methods (i.e., fixed-\( \mathbf{X} \) knockoff and model-\( \mathbf{X} \) knockoff). For example, when \( a = 2 \), the power of BKF reaches 0.8 with sample size \( n = 500 \), while the single knockoff methods can only distinguish about 60% of the true signals even when the sample size is doubled. At the same time, the robustness of its power is comparable to the 2 multi-knockoffs and better than the other two methods. As a summary, BKF performs well and stable at detecting important signals yet with smaller chance of making false discoveries.

4.1.2 Variance Structure

We also investigate the impact of the variance structure among features \( X_1, \ldots, X_p \) on the performance of BKF. Toward this goal, we apply BKF to obtain \( \hat{\mathbf{S}} \) for datasets from model (4) with dimension \( p = 30 \). We consider two cases for the variance-covariance matrix. Features \( \mathbf{x}_1, \ldots, \mathbf{x}_n \) are generated from \( \text{MVN}(\mathbf{0}, \Sigma_\rho) \) where

\[
\Sigma_\rho = [\sigma_{\rho,ij}]_{p \times p} \quad \text{and} \quad \sigma_{\rho,ij} = \begin{cases} 
\rho^{\lvert i-j \rvert}, & \text{Case (i)}, \\
\rho^{\lvert i \neq j \rvert}, & \text{Case (ii)}. 
\end{cases}
\]

Case (i) corresponds to the situation where features are sampled from an autocorrelated time series and Case (ii) indicates an equal correlation among all features. Given features \( \mathbf{x}_1, \ldots, \mathbf{x}_n \), responses \( y_1, \ldots, y_n \) are generated from model (4). For each dataset, the true non-null features in subset \( \mathcal{H}_1 \) of size 10 are randomly chosen with \( \beta_j \sim \text{Unif}[-4, 4] \) if \( j \in \mathcal{H}_1 \) and \( \beta_j = 0 \) otherwise. For each combination of sample size \( n \in \{100, 200, 500, 1000\} \) and the Case (i) and (ii) variance structures, 100 datasets are simulated for each value of the correlation coefficient \( \rho \in \{0, \ldots, 0.9\} \).
Figure 3: FDR, power and the standard deviation (SD) of power for the BKF and other knockoffs under different sample sizes $n$ and correlations $\rho$ in Case (i). Each point is averaged over 100 replications.
Figure 4: FDR, power and the standard deviation (SD) of power for the BKF and other knockoffs under different sample sizes $n$ and correlations $\rho$ in Case (ii). Each point is averaged over 100 replications.
The power and overall FDR of our BKF as well as those of existing methods are presented in Figures 3 and 4. It can be observed that correlations among features would lower the power of all methods. With the overall FDR under control, the power of all methods decreases as the correlation $\rho$ increases for both covariance structures. In all scenarios, both BKF and the 2 multi-knockoffs possess higher power than the fixed-$X$ knockoff and the model-$X$ knockoff with the overall FDR controlled under $\alpha = 0.1$. However, there are still differences between BKF and the 2 multi-knockoffs. When features are generated under Case (i), the power of BKF is between the 2 multi-knockoffs and other single knockoff methods. As $\rho$ increases, the power of BKF is closer to the single knockoff methods. However, when correlations among features are the same, i.e., Case (ii), BKF is more powerful than the 2 multi-knockoffs, especially when $\rho$ is large. Therefore, BKF is more powerful to identify false $H_{0j}$ in the case of equal correlations (Case (ii)) while the 2 multi-knockoffs method has higher power in autocorrelated cases (Case (i)). The reason is that in the case of equal correlations, the difference between the 2 multi-knockoffs and original variables diminishes much faster than BKF as $\rho$ increases, leading to higher power of BKF for large $\rho$. In contrast, the quality of the 2 multi-knockoffs does not decrease vastly in autocorrelated cases and thus the 2 multi-knockoffs performs slightly better.

4.1.3 Dimensionality and Size of $\mathcal{H}_1$

Single knockoff methods, including the fixed-$X$ knockoff and the model-$X$ knockoff, rely their inferences on only one knockoff sample $\tilde{X}$. As a result, these methods would lose power and stability when the size of $\mathcal{H}_1$ is small. The multi-knockoffs method (Gimenez and Zou, 2019), on the other hand, makes inference based on more than one knockoff samples. However, as the number of knockoff samples grows, the difference between the original features and the knockoffs would diminish, leading to power loss when the size of $\mathcal{H}_1$ is large. To demonstrate the robustness of BKF with respect to both the size of $\mathcal{H}_1$ (denoted as $v$) and the number of features ($p$), we compare the performances of BKF with the model-$X$ knockoff filter and 2 multi-knockoffs on datasets with different numbers of features and different sizes of $\mathcal{H}_1$. In all datasets, the sample size is fixed as $n = 200$ and vectors $x_1, \ldots, x_n$ are generated under the setup of Section 4.1.1 and Case (i) of Section 4.1.2 with $\rho = 0.6$. With $p \in \{100, 200, 500, 1000\}$ and $v \in \{1, \ldots, 30\}$, responses $y_1, \ldots, y_n$ of each dataset are generated from model (4) with randomly chosen true non-null features in subset $\mathcal{H}_1$ of size $v$ where $\beta_j \sim \text{Unif}[-4, 4]$ if $j \in \mathcal{H}_1$ and $\beta_j = 0$ otherwise. Since the flat prior would make the joint posterior density (9) degenerated, the modified spike-and-slab prior (Candès et al., 2018) is used for the BKF where $\xi = 0.1$ and $\tau = 1$. The full conditionals under the modified spike-and-slab prior is given in Appendix B.

As $p$ and $v$ vary, the performances of the BKF, model-$X$ knockoff and 2 multi-knockoffs are exhibited
Figure 5: Power of the BKF, model-X knockoff and 2 multi-knockoffs under different numbers of features ($p$) and different sizes of $\mathcal{H}_1 (v)$. Each point is averaged over 100 replications. The left column corresponds to the cases of independent features while the right column corresponds to autocorrelated features.
in Figure 5, where we omit the plots of FDR as all methods can control the FDR under $\alpha = 0.1$. For all three methods, power incurs slight loss when the number of features ($p$) is large. However, there exist substantial differences in their ability to detect false $H_{0j}$ when $v$ decreases. As discussed in Section 2.2, the selection procedure of model-X knockoff forces $|\hat{S}|$ to be zero or not smaller than $\lfloor 1/\alpha \rfloor$ if nonzero. This can be reflected by the phenomenon that it possesses comparable power only when $v$ is larger than $\lfloor 1/\alpha \rfloor = 10$. Although the 2 multi-knockoffs method improves the power when $v$ is between 5 and 10, it still suffers from power loss for extremely small $v$. The improvement in power is achieved at the sacrifice of the ability to detect false $H_{0j}$ when the true $\mathcal{H}_1$ is large. In addition, the performance would deteriorate if features are correlated. In contrast, BKF maintains its power above 80% for all values of $v$ and both covariance structures of features, indicating that it is not susceptible to power loss caused by the small size of $\mathcal{H}_1$ as well as dependency among features.

4.2 Comparisons with Bayesian Variable Selection Approaches

As our BKF is a Bayesian approach for feature selection, we also compare it with existing Bayesian variable selection approaches, including the commonly used spike-and-slab regression, Bayesian Lasso, horseshoe estimator and recent IBSS procedure (Wang et al., 2020), to demonstrate the advantage of our method in controlling the proportion of false discoveries. In particular, for the spike-and-slab regression, Bayesian Lasso and horseshoe estimator, we compute the estimator $\hat{S}$ using the thresholding procedure with threshold 0.5. For IBSS, the estimator $\hat{S}$ is obtained via the greedy algorithm in Section 3.2 by substituting posterior probabilities $P(H_{0j}|D)$ with $1 - \text{PIP}_j$, where $\text{PIP}_j$ follows Definition 3.12 in Wang et al. (2020).

Figures 6–7 display the performances of all Bayesian approaches in low-dimensional settings, where only BKF can control FDR under the desired level $\alpha = 0.1$. The IBSS procedure would reduce the proportion of false discoveries as sample size increases, signal strength amplifies or feature correlation decreases, while FDRs of the Bayesian Lasso and horseshoe estimator are always out of control. Although the performance of IBSS is acceptable in low-dimensional settings, its estimator deteriorates for high-dimensional data, as shown in Figure 7. The IBSS procedure possesses lower power and larger FDR, suggesting its weakness in FDR control for high-dimensional settings. On the other hand, our BKF is robust in FDR control and true signal discovery regardless of the dimensionality and the number of non-null features.
Figure 6: FDRs of the BKF and existing Bayesian methods in low-dimensional settings. The left, middle and right panels correspond to cases of independent, auto-correlated and equal-correlated features respectively. Each point is averaged over 100 replications (SS: spike-and-slab regression; BL: Bayesian Lasso; HS: horseshoe estimator; IBSS: the iterative Bayesian stepwise selection procedure).
Figure 7: Performances of the BKF and IBSS procedures under different numbers of features \( (p) \) and different sizes of \( H_1 (v) \). Each point is averaged over 100 replications. The left two columns correspond to the FDR and power under independent features while the right column corresponds to the power under autocorrelated features.
5 Real Data Analysis

To illustrate its empirical performance, we apply our BKF to the League of Legends 2020 Esports Match Data\(^1\) from Kaggle. The League of Legends (LOL) is a multiplayer online battle arena video game between two teams. In each game, 10 players are assigned to different positions (“top”, “jungle”, “mid”, “adc” and “support”) in two teams labeled as “blue” and “red”. Players are asked to select champions with unique abilities and different attributes to battle against the other team. This dataset records the selection of champions and results of all games of LOL matches in the year of 2020 as well as 18 attributes of each selected champion. As a result, each game record consists of 180 attributes in different positions as features \(X\). We extract all of 726 records of the LOL Pro League in China to investigate which attributes in different positions would substantially affect the results of games.

Given that all the attributes are continuous-valued, we standardize all of the 180 features among 726 records and approximate the joint distribution of original features and knockoff features \(f(X, \tilde{X})\). Taking the binary game result (equals 1 when the blue team wins and 0 when the red team wins) as the response, we impose a probit model for approximate inference on the conditional distribution \(f(Y|X, \tilde{X})\) and apply our BKF with flat priors as well as other knockoff methods to conduct multiple hypotheses testing (2) on all the features. The full conditionals under the probit model is given in Appendix C. We control the FDR at the desired level \(\alpha = 0.1\) and show the results in Table 1 and Figure 8, where we only display 30 features with the lowest \(\hat{P}(H_0|D)\).

From Table 1, we can see one obvious pattern that the posterior means of \(\beta_j\) are all positive (negative) for attributes corresponding to the blue (red) team. This is consistent with the common sense that attributes corresponding to the blue (red) team would make the blue team more (less) likely to win, suggesting the validity of our analysis. Fifteen features are chosen in the estimator \(\hat{S}\), most of which are attributes in the positions “adc” and “support”. This result is consistent with the consensus among pro players that the strength of the bottom duo (“adc” and “support”) is more decisive to match results in 2020. In contrast, when we apply the model-X knockoff procedure to the same data, no features are selected. This indicates that our BKF is more powerful in detecting non-null features under the same FDR-controlling level.

6 Conclusion

The knockoff procedure is a powerful tool to select important features with a control over the FDR. We incorporate the knockoff method into the Bayesian framework and propose a more powerful BKF, where the knockoff variables, instead of being generated only once and fixed, are also updated in the Gibbs sampling

\(^1\)https://www.kaggle.com/xmorra/lol2020esports
Table 1: Posterior means and standard deviations (in parentheses) of coefficients $\beta_j$ and $\tilde{\beta}_j$ for analysis of the League of Legends 2020 Esports Match Data. Features selected by BKF are bold.

| Features                          | $\beta_j$  | $\tilde{\beta}_j$ | $\hat{P}(H_0|D)$ |
|-----------------------------------|------------|-------------------|------------------|
| Blue top mp per level             | 1.841 (0.481) | -0.114 (0.457) | 0.016            |
| Blue adc spell block per level    | 2.070 (0.612) | -0.007 (0.439) | 0.040            |
| Blue adc armor                    | 1.888 (0.615) | -0.054 (0.421) | 0.045            |
| Red adc attack speed              | -2.546 (0.825) | 0.012 (0.458) | 0.046            |
| Red adc hp per level              | -1.818 (0.548) | 0.016 (0.452) | 0.063            |
| Blue support armor                | 1.463 (0.476) | 0.016 (0.420) | 0.068            |
| Red adc attack damage per level   | -2.145 (0.735) | 0.165 (0.544) | 0.071            |
| Red support spell block per level | -2.632 (1.289) | 0.087 (0.596) | 0.076            |
| Red adc mp per level              | -2.852 (1.242) | -0.002 (0.462) | 0.096            |
| Red support spell block           | -1.264 (0.554) | 0.003 (0.391) | 0.121            |
| Blue adc mp                       | 1.326 (0.547) | -0.088 (0.452) | 0.122            |
| Red adc armor per level           | -2.138 (1.210) | 0.142 (0.481) | 0.135            |
| Blue adc attack speed             | 1.353 (0.707) | -0.120 (0.465) | 0.152            |
| Red adc attack speed per level    | -2.070 (1.431) | -0.038 (0.424) | 0.165            |
| Red adc hp                        | -1.647 (0.901) | 0.043 (0.415) | 0.168            |
| Red jungle move speed             | -0.935 (0.446) | 0.086 (0.417) | 0.217            |
| Blue adc attack range             | 1.078 (0.505) | 0.060 (0.423) | 0.220            |
| Red adc hp recovery per level     | -1.353 (0.864) | 0.087 (0.415) | 0.224            |
| Red jungle mp per level           | -1.205 (0.893) | -0.124 (0.457) | 0.231            |
| Blue adc hp recovery              | 1.040 (0.542) | 0.048 (0.449) | 0.238            |
| Blue adc hp recovery per level    | 1.176 (0.738) | 0.022 (0.467) | 0.255            |
| Blue top attack damage per level  | 0.858 (0.425) | -0.014 (0.395) | 0.262            |
| Blue top hp per level             | 0.945 (0.461) | 0.017 (0.442) | 0.270            |
| Blue top mp recovery per level    | 0.938 (0.437) | -0.097 (0.462) | 0.277            |
| Blue adc attack speed per level   | 1.132 (0.800) | 0.082 (0.451) | 0.281            |
| Red support hp per level          | -0.776 (0.450) | -0.055 (0.381) | 0.285            |
| Red jungle mp                     | -1.094 (0.749) | -0.029 (0.411) | 0.296            |
| Blue top attack range             | 0.802 (0.418) | -0.005 (0.398) | 0.302            |
| Red support attack damage per level| -0.953 (0.721) | -0.007 (0.405) | 0.303            |
| Red jungle mp recovery            | -0.822 (0.481) | -0.027 (0.403) | 0.305            |
Figure 8: Values of $\hat{P}(H_0|D)$ and $\widehat{\text{BFDR}}(S_j)$ corresponding to all features sorted by $\hat{P}(H_0|D)$. 
steps. Under the Bayesian model, we develop an MCMC data augmentation algorithm to obtain posterior samples of knockoff variables and parameters. Based on a probability inequality deduced from the flip-sign property of feature statistics and the equivalent definition of the Bayesian FDR, we are able to estimate the upper bound of the Bayesian FDR for any sets of features. As a result, the estimation of the non-null feature set is translated to a knapsack problem and we develop a greedy selection procedure with control of the Bayesian FDR. Experiments show that BKF generally possesses higher power in identifying non-null features and lower probability of making false discoveries than existing knockoff filters and Bayesian approaches, especially in the extreme case where sample size is not large, the true number of non-null features is small and the correlations among original features are strong. In real data analysis, it is shown that BKF yields reasonable results which can be clearly visualized, allowing easier interpretations and decision making than existing knockoff filters.

Appendices

Appendix A  Proof of Theorem 1

For any $S \in \mathcal{H}_0$, we assume without loss of generality that $S = \{1, \ldots, m\}$ and $\mathcal{H}_0 = \{1, \ldots, v\}$ and $m \leq v$. Let $(\beta_{\text{Swap}(S)}, \tilde{\beta}_{\text{Swap}(S)})$ denote $(\beta, \tilde{\beta})$ by swapping elements $\beta_j$ and $\tilde{\beta}_j$ for all $j \in S$. Similarly, $(X_{\text{Swap}(S)}, \tilde{X}_{\text{Swap}(S)})$ are also obtained by swapping elements $X_j$ and $\tilde{X}_j$ of $(X, \tilde{X})$ for all $j \in S$. Since for all $j \in S$, $X_j \perp Y | X_{-j}$, we have $X_S \perp Y | X_{-S}$ where $X_S$ and $X_{-S}$ are the subvectors of $X$ corresponding to indices in and not in the set $S$. Thus, we have $X_S \perp Y | X_{-S}, \tilde{X}$. Under Definition 1, it is also true that $\tilde{X}_S \perp Y | \tilde{X}_{-S}, X$. As a result, it is clear that

$$f(Y|X, \tilde{X}) = f(Y|X_{\text{Swap}(S)}, \tilde{X}_{\text{Swap}(S)}).$$  \hfill (20)

Suppose a generalized linear model with density $h(Y|X, \tilde{X}; \beta, \tilde{\beta}, \phi)$ in (8) is imposed to approximate the conditional distribution $f(Y|X, \tilde{X})$:

$$E[Y|X, \tilde{X}; \beta, \tilde{\beta}, \phi] = g^{-1}(\eta), \quad \eta = \sum_{j=1}^{p} (X_j\beta_j + \tilde{X}_j\tilde{\beta}_j).$$

By (20), we can deduce that

$$h(Y|X, \tilde{X}; \beta, \tilde{\beta}, \phi) = h(Y|X_{\text{Swap}(S)}, \tilde{X}_{\text{Swap}(S)}; \beta, \tilde{\beta}, \phi).$$  \hfill (21)
Since in the approximate model \( h(Y|X, \tilde{X}; \beta, \tilde{\beta}, \phi) \) the response is related to original and knockoff features only via the conditional mean \( g^{-1}(\eta) \), we have that

\[
h(Y|X_{\text{Swap}(S)}, \tilde{X}_{\text{Swap}(S)}; \beta, \tilde{\beta}, \phi) = h(Y|X, \tilde{X}; \beta_{\text{Swap}(S)}, \tilde{\beta}_{\text{Swap}(S)}, \phi). \tag{22}
\]

If \( f(\beta, \tilde{\beta}) \) is invariant to swapping for \( S \), i.e., \( f(\beta, \tilde{\beta}) = f(\beta_{\text{Swap}(S)}, \tilde{\beta}_{\text{Swap}(S)}) \), it is clear that by (21)–(22),

\[
f(\beta, \tilde{\beta}|\tilde{x}_1, \ldots, \tilde{x}_n, \sigma^2, D) = f(\beta_{\text{Swap}(S)}, \tilde{\beta}_{\text{Swap}(S)}|\tilde{x}_1, \ldots, \tilde{x}_n, \sigma^2, D),
\]

and

\[
f(\beta, \tilde{\beta}|D) = \int f(\beta, \tilde{\beta}|\tilde{x}_1, \ldots, \tilde{x}_n, \sigma^2, D)f(\tilde{x}_1, \ldots, \tilde{x}_n, \sigma^2|D)d\tilde{x}_1 \cdots d\tilde{x}_n d\sigma^2
\]

\[
= \int f(\beta_{\text{Swap}(S)}, \tilde{\beta}_{\text{Swap}(S)}|\tilde{x}_1, \ldots, \tilde{x}_n, \sigma^2, D)f(\tilde{x}_1, \ldots, \tilde{x}_n, \sigma^2|D)d\tilde{x}_1 \cdots d\tilde{x}_n d\sigma^2
\]

\[
= f(\beta_{\text{Swap}(S)}, \tilde{\beta}_{\text{Swap}(S)}|D).
\]

As long as \( W_j \) is antisymmetric with respect to \( \beta_j \) and \( \tilde{\beta}_j \), \( j = 1, \ldots, p \), the feature statistics \( W = (W_1, \ldots, W_p)^T \) obey the flip-sign property because

\[
f(W|D) = \int_{\Theta_W} f(\beta_{\text{Swap}(S)}, \tilde{\beta}_{\text{Swap}(S)}|D)d\beta_{\text{Swap}(S)}d\tilde{\beta}_{\text{Swap}(S)}
\]

\[
= \int_{\Theta_W} f(\beta, \tilde{\beta}|D)d\beta d\tilde{\beta}
\]

\[
=f(W|D),
\]

where \( W_S \) is defined in Definition 3 and \( \Theta_W \) is the subspace of all possible values of \( (\beta, \tilde{\beta}) \) corresponding to the value of \( W \).

Appendix B  Full Conditionals under the Modified Spike-and-Slab Prior

Suppose the joint distribution \( f(X, \tilde{X}) \) is (7) and the distribution

\[
h(Y|X, \tilde{X}; \beta, \tilde{\beta}, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left\{ -\frac{1}{2\sigma^2}(Y - X^T \beta - \tilde{X}^T \tilde{\beta})^2 \right\}
\]

27
is imposed to approximate \( f(Y|X, \hat{X}) \). Let \( x_i = (x_{i1}, \ldots, x_{ip})^T \), \( \tilde{x}_i = (\tilde{x}_{i1}, \ldots, \tilde{x}_{ip})^T \) \((i = 1, \ldots, n)\), the joint posterior distribution (9) is

\[
\begin{align*}
&f(\tilde{x}_1, \ldots, \tilde{x}_n, \beta, \tilde{\beta}, \sigma^2|D) \propto f(\beta, \tilde{\beta}, \sigma^2) \prod_{i=1}^{n} h(y_i|x_i, \tilde{x}_i; \beta, \tilde{\beta}, \sigma^2) f(\tilde{x}_i|x_i) \\
&\quad \propto f(\beta, \tilde{\beta}, \sigma^2) \frac{1}{\sigma^n} \exp \left\{ -\frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - x_i^T \beta - \tilde{x}_i^T \tilde{\beta})^2 - \frac{1}{2} \sum_{i=1}^{n} (x_i^T, \tilde{x}_i^T) G^{-1} \left( x_i \right) \right\}.
\end{align*}
\]

\( \text{(23)} \)

Let \( \beta_{-j} = (\beta_1, \ldots, \beta_{j-1}, \beta_{j+1}, \ldots, \beta_p)^T \), \( \tilde{\beta}_{-j} = (\tilde{\beta}_1, \ldots, \tilde{\beta}_{j-1}, \tilde{\beta}_{j+1}, \ldots, \tilde{\beta}_p)^T \) \((j = 1, \ldots, p)\). When the modified spike-and-slab prior (18) is used, the full conditional distributions of joint posterior density (23) are given as follows,

- For \( j = 1, \ldots, p \), let \( z_{ij} = y_i - \sum_{j' \neq j} x_{ij'} \beta_{j'} - \sum_{j' \neq j} \tilde{x}_{ij'} \tilde{\beta}_{j'} \) \((i = 1, \ldots, n)\) and we have

\[
\begin{align*}
&f(\beta_j, \tilde{\beta}_j|x_1, \ldots, x_n, \beta_{-j}, \tilde{\beta}_{-j}, \sigma^2, D) = \begin{cases} 
I[\beta_j = \tilde{\beta}_j = 0] & \text{w.p. } (1 - \xi_j - \tilde{\xi}_j), \\
\phi(\beta_j; \mu_j, \tau^2_j)I[\beta_j = 0] & \text{w.p. } \xi_j, \\
\phi(\tilde{\beta}_j; \tilde{\mu}_j, \tilde{\tau}^2_j)I[\beta_j = 0] & \text{w.p. } \tilde{\xi}_j,
\end{cases}
\end{align*}
\]

where

\[
\begin{align*}
\tau^2_j &= (1/\tau^2 + \sum_{i=1}^{n} x_{ij}^2/\sigma^2)^{-1}, \\
\tilde{\tau}^2_j &= (1/\tau^2 + \sum_{i=1}^{n} \tilde{x}_{ij}^2/\sigma^2)^{-1}, \\
\mu_j^2 &= \tau^2_j \sum_{i=1}^{n} x_{ij} z_{ij}/\sigma^2, \\
\tilde{\mu}_j^2 &= \tilde{\tau}^2_j \sum_{i=1}^{n} \tilde{x}_{ij} z_{ij}/\sigma^2, \\
\xi_j &= \frac{\xi \sqrt{2\pi \tau^2_j} \exp \{ \mu_j^2/(2\tau^2_j) \}}{2(1 - \xi) + \xi \sqrt{2\pi \tau^2_j} \exp \{ \mu_j^2/(2\tau^2_j) \} + \xi \sqrt{2\pi \tilde{\tau}^2_j} \exp \{ \tilde{\mu}_j^2/(2\tilde{\tau}^2_j) \}},
\end{align*}
\]

\[
\tilde{\xi}_j = \frac{\xi \sqrt{2\pi \tilde{\tau}^2_j} \exp \{ \tilde{\mu}_j^2/(2\tilde{\tau}^2_j) \}}{2(1 - \xi) + \xi \sqrt{2\pi \tau^2_j} \exp \{ \mu_j^2/(2\tau^2_j) \} + \xi \sqrt{2\pi \tilde{\tau}^2_j} \exp \{ \tilde{\mu}_j^2/(2\tilde{\tau}^2_j) \}}.
\]

- \( \sigma^2|x_1, \ldots, x_n, \beta, \tilde{\beta}, D \sim IG\left( n/2, \sum_{i=1}^{n} (y_i - x_i^T \beta - \tilde{x}_i^T \tilde{\beta})^2/2 \right) \).
For $i = 1, \ldots, n$, $\tilde{x}_i | \beta, \tilde{\beta}, \sigma^2, x_i, y_i \sim \text{MVN}(\tilde{\mu}_i, \tilde{\Sigma})$ where

\[
\tilde{\Sigma} = \left( A + \frac{1}{\sigma^2} \tilde{\beta} \beta^T \right)^{-1}, \\
\tilde{\mu}_i = \tilde{\Sigma} \left[ \left( \text{diag}\{s\}^{-1} - A - \frac{1}{\sigma^2} \beta \beta^T \right) x_i + \frac{1}{\sigma^2} \beta y_i \right], \\
A = \left( 2 \text{diag}\{s\} - \text{diag}\{s\} \Sigma^{-1} \text{diag}\{s\} \right)^{-1}.
\]

**Appendix C  Full Conditionals under Probit Model**

In our real data analysis, the joint distribution $f(X, \tilde{X})$ is (7) and the probit model

\[
h(Y | X, \tilde{X}; \beta, \tilde{\beta}) = \begin{cases} 
\Phi(X^T \beta + \tilde{X}^T \tilde{\beta}), & Y = 1, \\
1 - \Phi(X^T \beta + \tilde{X}^T \tilde{\beta}), & Y = 0,
\end{cases}
\]

is imposed to approximate $f(Y | X, \tilde{X})$. We augment variables $u_i$ ($i = 1, \ldots, n$), leading to the augmented probit model as follows,

\[
y_i = \begin{cases} 
1, & \text{if } u_i > 0, \\
0, & \text{if } u_i \leq 0,
\end{cases}
\]

$u_i \sim N(x_i^T \beta + \tilde{x}_i^T \tilde{\beta}, 1)$.

The joint posterior distribution under the augmented probit model is

\[
f(\tilde{x}_1, \ldots, \tilde{x}_n, u_1, \ldots, u_n, \beta, \tilde{\beta} | D) \propto f(\beta, \tilde{\beta}) \prod_{i=1}^n p(y_i | u_i)p(u_i | x_i, \tilde{x}_i; \beta, \tilde{\beta}) f(\tilde{x}_i | x_i)
\]

\[
\propto f(\beta, \tilde{\beta}) \exp \left\{ -\frac{1}{2} \sum_{i=1}^n (u_i - x_i^T \beta - \tilde{x}_i^T \tilde{\beta})^2 - \frac{1}{2} \sum_{i=1}^n (x_i^T, \tilde{x}_i^T) G^{-1} \begin{pmatrix} x_i \\ \tilde{x}_i \end{pmatrix} \right\}
\]

\[
\times \prod_{i=1}^n \left[ I\{y_i = 1\} I\{u_i > 0\} + I\{y_i = 0\} I\{u_i \leq 0\} \right].
\]

(24)

Under the flat prior, the full conditional distributions are given as follows,
• Conditional on \( \tilde{x}_1, \ldots, \tilde{x}_n, u_1, \ldots, u_n, D, \)

\[
\begin{pmatrix} \beta \\ \tilde{\beta} \end{pmatrix} \sim \text{MVN}(\mu_{\beta, \tilde{\beta}}, \Sigma_{\beta, \tilde{\beta}}),
\]

with \( \Sigma_{\beta, \tilde{\beta}} = \left\{ \sum_{i=1}^{n} \begin{pmatrix} x_i x_i^T & x_i \tilde{x}_i^T \\ \tilde{x}_i x_i^T & \tilde{x}_i \tilde{x}_i^T \end{pmatrix} \right\}^{-1}, \)

\[
\mu_{\beta, \tilde{\beta}} = \Sigma_{\beta, \tilde{\beta}} \left\{ \sum_{i=1}^{n} u_i \begin{pmatrix} x_i \\ \tilde{x}_i \end{pmatrix} \right\}.
\]

• For \( i = 1, \ldots, n, \) \( \tilde{x}_i|\beta, \tilde{\beta}, x_i, y_i, u_i \sim \text{MVN}(\tilde{\mu}_i, \tilde{\Sigma}) \) where

\[
\tilde{\Sigma} = (A + \tilde{\beta} \tilde{\beta}^T)^{-1},
\]

\[
\tilde{\mu}_i = \tilde{\Sigma} \left[ (\text{diag}\{s\})^{-1} - \tilde{\beta} \beta^T \right] x_i + \tilde{\beta} u_i,
\]

\[
A = (2\text{diag}\{s\} - \text{diag}\{s\} \Sigma^{-1} \text{diag}\{s\})^{-1}.
\]

• For \( i = 1, \ldots, n, \)

\[
f(u_i|\beta, \tilde{\beta}, x_i, \tilde{x}_i, y_i) \sim \begin{cases} 
\text{TN}_{(0,\infty)}(x_i^T \beta + \tilde{x}_i^T \tilde{\beta}, 1), & \text{if } y_i = 1, \\
\text{TN}_{(-\infty,0)}(x_i^T \beta + \tilde{x}_i^T \tilde{\beta}, 1), & \text{if } y_i = 0,
\end{cases}
\]

where \( \text{TN} \) stands for truncated normal distribution.

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