On the Computational Complexity of High-Dimensional Bayesian Variable Selection

Yun Yang\textsuperscript{1} Martin J. Wainwright\textsuperscript{1,2} Michael I. Jordan\textsuperscript{1,2}

University of California, Berkeley
\textsuperscript{1}Department of Electrical Engineering and Computer Science \textsuperscript{2}Department of Statistics

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Abstract

We study the computational complexity of Markov chain Monte Carlo (MCMC) methods for high-dimensional Bayesian linear regression under sparsity constraints. We first show that a Bayesian approach can achieve variable-selection consistency under relatively mild conditions on the design matrix. We then demonstrate that the statistical criterion of posterior concentration need not imply the computational desideratum of rapid mixing of the MCMC algorithm. By introducing a truncated sparsity prior for variable selection, we provide a set of conditions that guarantee both variable-selection consistency and rapid mixing of a particular Metropolis-Hastings algorithm. The mixing time is linear in the number of covariates up to a logarithmic factor. Our proof controls the spectral gap of the Markov chain by constructing a canonical path ensemble that is inspired by the steps taken by greedy algorithms for variable selection.

1 Introduction

In many areas of science and engineering, it is common to collect a very large number of covariates $X_1, \ldots, X_p$ in order predict a response variable $Y$. We are thus led to instances of high-dimensional regression, in which the number of covariates $p$ exceed the sample size $n$. A large literature has emerged to address problems in the regime $p \gg n$, where the ill-posed nature of the problem is addressed by imposing sparsity conditions—namely, that the response $Y$ depends only on a small subset of the covariates. Much of this literature is based on optimization methods, where penalty terms are incorporated that yield both convex \cite{9} and nonconvex\cite{39} optimization problems. Theoretical analysis is based on general properties of the design matrix and the penalty function.

Alternatively, one can take a Bayesian point of view on high-dimensional regression, placing a prior on the model space and performing the necessary integration so as to obtain a posterior distribution \cite{12, 16, 5}. Obtaining such a posterior allows one to report a subset of possible models along with their posterior probabilities as opposed to a single model. One can also report the marginal posterior probability of including each covariate. Some recent work has provided some theoretical understanding of the performance of Bayesian approaches to variable selection. In the moderate-dimension scenario (in which $p$ is allowed to grow with $n$ but $p \leq n$), Shang and Clayton \cite{28} establish posterior consistency for variable selection.
in a Bayesian linear model, meaning that the posterior probability of the true model that contains all influential covariates tends to one as \( n \) grows. Narisetty and He \[26\] consider a high-dimensional scenario in which \( p \) can grow nearly exponentially with \( n \); in this setting, they show the Bayesian spike-and-slab variable-selection method achieves variable-selection consistency. Since this particular Bayesian method resembles a randomized version of \( \ell_0 \)-penalized methods, it could have better performance than \( \ell_1 \)-penalized methods for variable selection under high-dimensional settings \[26, 29\]. Empirical evidence for this conjecture is provided by Guan et al. \[13\] for SNP selection in genome-wide association studies, but it has not been confirmed theoretically.

The most widely used tool for fitting Bayesian models are sampling techniques based on Markov chain Monte Carlo (MCMC), in which a Markov chain is designed over the parameter space so that its stationary distribution matches the posterior distribution. Despite its popularity, the theoretical analysis of the computational efficiency of MCMC algorithms lags that of optimization-based methods. In particular, the central object of interest is the mixing time of the Markov chain, which characterizes the number of iterations required to converge to an \( \epsilon \)-distance of stationary distribution from any initial configuration. In order for MCMC algorithms to be controlled approximations, one must provide meaningful bounds on the mixing time as a function of problem parameters such as the number of observations and the dimensionality. Of particular interest is determining whether the chain is rapidly mixing—meaning that the mixing time grows at most polynomially in the problem parameters—or slowly mixing meaning that the mixing time grows exponentially in the problem parameters. In the latter case, one cannot hope to obtain approximate samples from the posterior in any reasonable amount of time for large models.

Unfortunately, theoretical analysis of mixing time is comparatively rare in the Bayesian literature, with a larger number of negative results. On the positive side, Jones and Hobert \[17\] consider a Bayesian hierarchical version of the one-way random effects model, and obtain upper bounds on the mixing time of Gibbs and block Gibbs samplers as a function of the initial values, data and hyperparameters. Belloni and Chernozhukov \[4\] show that a Metropolis random walk is rapidly mixing in the dimension for regular parametric models in which the posterior converges to a normal limit. It is more common to find negative results in the literature. Examples include Mossel and Vigoda \[25\], who show that the MCMC algorithm for Bayesian phylogenetics takes exponentially long to reach the stationary distribution as data accumulates, and Woodard and Rosenthal \[37\], who analyze a Gibbs sampler used for genomic motif discovery and show that the mixing time increases exponentially as a function of the length of the DNA sequence.

The goal of the current paper is to study the computational complexity of Metropolis-Hastings procedures for high-dimensional Bayesian variable selection. For concreteness, we focus our analysis on a specific hierarchical Bayesian model for sparse linear regression, and an associated Metropolis-Hastings random walk, but these choices should be viewed as representative of a broader family of methods. In particular, we study the well-known Zellner \( g \)-prior for linear regression \[38\]. The main advantage of this prior is the simple expression that it yields for the marginal likelihood, which is convenient in our theoretical investigations. As in past analyses \[26\], we consider the marginal probability of including each covariate into the model as being on the order of \( p^{-\Omega(1)} \). Moreover, we restrict the support of the prior to rule out unrealistically large models. As a specific computational methodology, we focus on an iterative, local-move and neighborhood-based procedure for sampling from the model space, which is motivated by the shotgun stochastic search \[14\].

Our main contribution is to provide conditions under which Bayesian posterior consistency
holds, and moreover, the mixing time grows linearly in $p$ (up to logarithmic factor), implying that the chain is rapidly mixing. As a by-product, we provide conditions on the hyperparameter $g$ to achieve model-selection consistency. We also provide a counter-example to illustrate that although ruling out unrealistically large models is not necessary for achieving variable-selection consistency, it is necessary in order that the Metropolis-Hastings random walk is rapidly mixing. To be clear, while our analysis applies to a fully Bayesian procedure for variable selection, it is based on a frequentist point of view in assuming that the data are generated according to a true model.

There are a number of challenges associated with characterizing the computational complexity of Markov chain methods for Bayesian models. First, the posterior distribution of a Bayesian model is usually a much more complex object than the highly structured distributions in statistical physics for which meaningful bounds on the Markov chain mixing times are often obtained (e.g. [6], [23, 21]). Second, the transition probabilities of the Markov chain are themselves stochastic, since they depend on the underlying data-generating process. In order to address these challenges, our analysis exploits asymptotic properties of the Bayesian model to characterize the typical behavior of the Markov chain. We show that under conditions leading to Bayesian variable-selection consistency, the Markov chain over the model space has a global tendency of moving towards the true data-generating model, even though the posterior distribution can be highly irregular. In order to bound the mixing time, we make use of the canonical path technique developed by Sinclair [31, 30] and Diaconis and Stroock [8]. More precisely, the particular canonical path construction used in our proof is motivated by examining the solution path of stepwise regression procedures for linear model selection (e.g., [40, 2]), where a greedy criterion is used to decide at each step whether a covariate is to be included or deleted from the current model.

Overall, our results reveal that there is a delicate interplay between the statistical and computational properties of Bayesian models for variable selection. On the one hand, we show that concentration of the posterior is not only useful in guaranteeing desirable statistical properties such as parameter estimation or model-selection consistency, but they also have algorithmic benefits in certifying the rapid mixing of the Markov chain methods designed to draw samples from the posterior. On the other hand, we show that posterior consistency on its own is not sufficient for rapid mixing, so that algorithmic efficiency requires somewhat stronger conditions.

The remainder of this paper is organized as follows. Section 2 provides background on the Bayesian approach to variable selection, as well as Markov chain algorithms for sampling and techniques for analysis of mixing times. In Section 3, we state our two main results (Theorems 1 and 2) for a class of Bayesian models for variable selection, along with simulations that illustrate the predictions of our theory. Section 4 is devoted to the proofs of our results, with many of the technical details deferred to the appendices. We conclude in Section 5 with a discussion.

## 2 Background and problem formulation

In this section, we introduce some background on the Bayesian approach to variable selection, as well some background on Markov chain algorithms for sampling, and techniques for analyzing their mixing times.
2.1 Variable selection in the Bayesian setting

Consider a response vector \( Y \in \mathbb{R}^n \) and a design matrix \( X \in \mathbb{R}^{n \times p} \) that are linked by the standard linear model

\[
Y = X\beta^* + w, \quad \text{where } w \sim \mathcal{N}(0, \sigma^2 I_n),
\]

and \( \beta^* \in \mathbb{R}^p \) is the unknown regression vector. Based on observing the pair \((Y, X)\), our goal is to recover the support set of \( \beta^* \)—that is, to select the subset of covariates with non-zero regression weights, or more generally, a subset of covariates with absolute regression weights above some threshold.

In generic terms, a Bayesian approach to variable selection is based on first imposing a prior over the set of binary indicator vectors, and then using the induced posterior (denoted by \( \pi(\gamma | Y) \)) to perform variable selection. Here each binary vector \( \gamma \in \{0, 1\}^p \) should be thought of as indexing the model which involves only the covariates indexed by \( \gamma \). We make use of the shorthand \( |\gamma| = \sum_{j=1}^p \gamma_j \) corresponding to the number of non-zero entries in \( \gamma \), or the number of active covariates in the associated model. It will be convenient to adopt a dualistic view of \( \gamma \) as both a binary indicator vector, and as a subset of \( \{1, \ldots, p\} \). Under this identification, the expression \( \gamma \subset \gamma' \) for a pair of inclusion vectors \((\gamma, \gamma')\) can be understood as that the subset of variables selected by \( \gamma \) is contained in the subset of variables selected by \( \gamma' \). Similarly, it will be legitimate to use set operators on those indicator vectors, such as \( \gamma \cap \gamma' \), \( \gamma \cup \gamma' \) and \( \gamma \setminus \gamma' \). Using the set interpretation, we let \( X_\gamma \in \mathbb{R}^{n \times |\gamma|} \) denote the submatrix formed of the columns indexed by \( \gamma \), and we define the subvector \( \beta_\gamma \in \mathbb{R}^{|\gamma|} \) in an analogous manner. We make use of this notation in defining the specific hierarchical Bayesian model analyzed in this paper, defined precisely in Section 3.1 to follow.

2.2 MCMC algorithms for Bayesian variable selection

Past work on MCMC algorithms for Bayesian variable selection can be divided into two main classes—Gibbs samplers (e.g., [12, 16, 26]) and Metropolis-Hastings random walks (e.g., [14, 13]). In this paper, we focus on a particular form of Metropolis-Hastings updates.

In general terms, a Metropolis-Hastings random walk is an iterative and local-move based procedure involving three steps:

**Step 1:** Use the current state \( \gamma \) to define a neighborhood \( \mathcal{N}(\gamma) \) of proposal states.

**Step 2:** Choose a proposal state \( \gamma' \) in \( \mathcal{N}(\gamma) \) according to some probability distribution \( S(\gamma, \cdot) \) over the neighborhood, e.g. the uniform distribution.

**Step 3:** Move to the new state \( \gamma' \) with probability \( R(\gamma, \gamma') \), and stay in the original state \( \gamma \) with probability \( 1 - R(\gamma, \gamma') \), where the acceptance ratio is given by

\[
R(\gamma, \gamma') : = \min \left\{ 1, \frac{\pi_n(\gamma' | Y) S(\gamma', \gamma)}{\pi_n(\gamma | Y) S(\gamma, \gamma')} \right\}.
\]

In this way, for any fixed choice of the neighborhood structure \( \mathcal{N}(\gamma) \), we obtain a Markov chain with transition probability given by

\[
P_{\text{MH}}(\gamma, \gamma') = \begin{cases} 
S(\gamma, \gamma') R(\gamma, \gamma') & \text{if } \gamma' \in \mathcal{N}(\gamma), \\
0 & \text{if } \gamma' \notin \mathcal{N}(\gamma) \cup \{\gamma\}, \\
1 - \sum_{\gamma' \neq \gamma} P_{\text{MH}}(\gamma, \gamma') & \text{if } \gamma' = \gamma.
\end{cases}
\]
The specific form of Metropolis-Hastings update analyzed in this paper is obtained by randomly selecting one of the following two schemes to update \( \gamma \), each with probability 0.5.

**Single flip update:** Choose an index \( j \in [p] \) uniformly at random, and form the new state \( \gamma' \) by setting \( \gamma'_j = 1 - \gamma_j \).

**Double flip update:** Define the subsets \( S(\gamma) = \{ j \in [p] \mid \gamma_j = 1 \} \) and let \( S^c(\gamma) = \{ j \in [p] \mid \gamma_j = 0 \} \). Choose an index pair \( (k, \ell) \in S(\gamma) \times S^c(\gamma) \) uniformly at random, and form the new state \( \gamma' \) by flipping \( \gamma_k \) from 1 to 0 and \( \gamma_\ell \) from 0 to 1. (If the set \( S(\gamma) \) is empty, then we do nothing.)

This scheme can be understood as a particular of the general Metropolis-Hastings scheme in terms of a neighborhood \( \mathcal{N}(\gamma) \) to be all models \( \gamma' \) that can be obtained from \( \gamma \) by either changing one component to its opposite (i.e., from 0 to 1, or from 1 to 0) or switching the values of two components with different values.

Letting \( d_H(\gamma, \gamma') = \sum_{j=1}^{p} I(\gamma_j \neq \gamma'_j) \) denote the Hamming distance between \( \gamma \) and \( \gamma' \). the overall neighborhood is given by the union \( \mathcal{N}(\gamma) := \mathcal{N}_1(\gamma) \cup \mathcal{N}_2(\gamma) \), where

\[
\mathcal{N}_1(\gamma) := \{ \gamma' \mid d_H(\gamma', \gamma) = 1 \}, \quad \text{and} \quad \mathcal{N}_2(\gamma) := \{ \gamma' \mid d_H(\gamma', \gamma) = 2, \text{ and } \exists (k, \ell) \in S(\gamma) \times S^c(\gamma) \text{ s.t. } \gamma'_k = 1 - \gamma_k \text{ and } \gamma'_\ell = 1 - \gamma_\ell \}.
\]

With these definitions, the transition matrix of the previously described Metropolis-Hastings scheme takes the form

\[
P_{\text{MH}}(\gamma, \gamma') = \begin{cases} \frac{1}{2p} \min \left\{ 1, \frac{\pi_n(\gamma'|Y)}{\pi_n(\gamma|Y)} \right\}, & \text{if } \gamma' \in \mathcal{N}_1(\gamma) \\ \frac{1}{2|S(\gamma)||S^c(\gamma)|} \min \left\{ 1, \frac{\pi_n(\gamma'|Y)}{\pi_n(\gamma|Y)} \right\}, & \text{if } \gamma' \in \mathcal{N}_2(\gamma) \\ 0, & \text{if } d_H(\gamma', \gamma) > 2, \text{ and} \\ 1 - \sum_{\gamma' \neq \gamma} P_{\text{MH}}(\gamma, \gamma'), & \text{if } \gamma' = \gamma. \end{cases}
\]

### 2.3 Background on mixing times

Let \( \mathcal{C} \) be an irreducible, aperiodic Markov chain on the discrete state space \( \mathcal{M} \), and described by the transition probability matrix \( P \in \mathbb{R}^{\left| \mathcal{M} \right| \times \left| \mathcal{M} \right|} \) with stationary distribution \( \pi \). We assume throughout that \( \mathcal{C} \) is reversible; i.e., it satisfies the detailed balance condition \( \pi(\gamma)P(\gamma, \gamma') = \pi(\gamma')P(\gamma', \gamma) \) for all \( \gamma, \gamma' \in \mathcal{M} \). It is easy to see that the previously described Metropolis-Hastings matrix \( P_{\text{MH}} \) satisfies this reversibility condition. It is convenient to identify a reversible chain with a weighted undirected graph \( G \) on the vertex set \( \mathcal{M} \), where two vertices \( \gamma \) and \( \gamma' \) are connected if and only if the edge weight \( Q(\gamma, \gamma') := \pi(\gamma)P(\gamma, \gamma') \) is strictly positive.

For \( \gamma \in \mathcal{M} \) and any subset \( S \subseteq \mathcal{M} \), we write \( P(\gamma, S) = \sum_{\gamma' \in S} P(\gamma, \gamma') \). If \( \gamma \) is the initial state of the chain, then the total variation distance to the stationary distribution after \( t \) iterations is

\[
\Delta_\gamma(t) = \|P^n(\gamma, \cdot) - \pi(\cdot)\|_{TV} := \max_{S \subseteq \mathcal{M}} \left| P^n(\gamma, S) - \pi(S) \right|.
\]

The \( \epsilon \)-mixing time is given by

\[
\tau_\epsilon := \max_{\gamma \in \mathcal{M}} \min \left\{ t \in \mathbb{N} \mid \Delta_\gamma(t') \leq \epsilon \text{ for all } t' \geq t \right\},
\]

(4)
which measures the number of iterations required for the chain to be within distance $\epsilon \in (0, 1)$ of stationarity. The efficiency of the Markov chain can be measured by the dependence of $\tau_\epsilon$ on the difficulty of the problem, for example, the dimension of the parameter space and the sample size. In our case, we are interested in the dependence of $\tau_\epsilon$ on the covariate dimension $p$ and the sample size $n$. Of particular interest is whether the chain is rapidly mixing, meaning that the mixing time grows at most polynomially in the pair $(p, n)$, or slowly mixing, meaning that the mixing time grows exponentially.

3 Main results and their consequences

The analysis of this paper applies to a particular family of hierarchical Bayes models for variable selection. Accordingly, we begin by giving a precise description of this family of models, before turning to statements of our main results and a discussion of their consequences. Our first result (Theorem 1) provides sufficient conditions for posterior concentration, whereas our second result (Theorem 2) provides sufficient conditions for rapid mixing of the Metropolis-Hastings updates.

3.1 Bayesian hierarchical model for variable selection

In addition to the standard linear model (1), the Bayesian hierarchical model analyzed in this paper involves three other ingredients: a prior over the precision parameter $\phi$ (or inverse noise variance) in the linear observation model, a prior on the regression coefficients, and a prior over the binary indicator vectors. More precisely, it is given by

$$ M_\gamma : \quad \text{Linear model: } \quad Y = X_\gamma \beta_\gamma + w, \quad w \sim \mathcal{N}(0, \phi^{-1} I_n) \quad (5a) $$

$$ \text{Precision prior } \quad \pi(\phi) \propto \frac{1}{\phi} \quad (5b) $$

$$ \text{Regression prior } \quad (\beta_\gamma \mid \gamma) \sim \mathcal{N}(0, g \phi^{-1}(X_\gamma^T X_\gamma)^{-1}) \quad (5c) $$

$$ \text{Sparsity prior } \quad \pi(\gamma) \propto \left(\frac{1}{p}\right)^{\kappa|\gamma|} \mathbb{1}[|\gamma| \leq s_0]. \quad (5d) $$

For each model $M_\gamma$, there are three parameters to be specified: the integer $s_0 < n$ is a prespecified upper bound on the maximum number of important covariates, the hyperparameter $g > 0$ controls the degree of dispersion in the regression prior, and the hyperparameter $\kappa > 0$ penalizes models with large size. For a given integer $s_0 \in \{1, \ldots, p\}$, we let $\mathcal{M}(s_0) = \{M_\gamma \mid |\gamma| \leq s_0\}$ the class of all models involving at most $s_0$ covariates.

Let us make a few remarks on our choice of Bayesian model. First, the choice of covariance matrix in the regression prior—namely, involving $X_\gamma^T X_\gamma$—is made for analytical convenience, in particular in simplifying the posterior. A more realistic choice would be the independent prior

$$ \beta_\gamma \mid \gamma \sim \mathcal{N}(0, g \phi^{-1} I_{|\gamma|}). $$

However, the difference between these choices will be negligible when $g \gg n$, which, as shown by our theoretical analysis, is the regime under which the posterior is well-behaved. Another popular choice for the prior of $\beta_\gamma$ is the spike-and-slab prior [10], where for each covariate $X_j$, one specifies the marginal prior for $\beta_j$ as a mixture of two normal distributions, one with a substantially larger variance than the other, and $\gamma_j$ can be viewed as the latent class indicator.
for this mixture prior. Our primary motivation in imposing Zellner’s $g$-prior is in order to streamline the theoretical analysis: it leads to an especially simple form of the marginal likelihood function. However, we note that our conclusions remain valid under essentially the same conditions when the independent prior or the spike-and-slab prior is used, but with much longer proofs. The sparsity prior on $\gamma$ is similar to the prior considered by Narisetty and He [26] and Castillo et al. [7]. The $p^{-\kappa}$ decay rate for the marginal probability of including each covariate imposes a vanishing prior probability on the models of diverging sizes. The only difference is that we put a constraint $|\gamma| \leq s_0$ to rule out models with too many covariates.

As will be clarified in the sequel, while this additional constraint is not needed for Bayesian variable-selection consistency, it is necessary for rapid mixing of the MCMC algorithm that we analyze.

Recall from our earlier set-up that the response vector $Y \in \mathbb{R}^n$ is generated from the standard linear model $Y = X\beta^* + w$, where $w \sim \mathcal{N}(0, \sigma_0^2 I_n)$, $\beta^* \in \mathbb{R}^p$ is the unknown regression vector, and $\sigma_0$ the unknown noise standard deviation. In rough terms, the goal of variable selection is to determine the subset $S$ of "influential" covariates. In order to formalize this notion, let us fix a constant $C_\beta > 0$ depending on $(\sigma_0, n, p)$ that quantifies the minimal signal size requirement for a covariate to be "influential". We then define $S = S(C_\beta)$ to consist of the indices with relatively large signal—namely

$$S := \{ j \in [p] \mid |\beta^*_j| \geq C_\beta \},$$

and our goal is to recover this subset. Thus, the “non-influential” coefficients $\beta^*_{S^c}$ are allowed to be non-zero, but their magnitudes are constrained.

We let $\gamma^*$ be the indicator vector that selects the influential covariates, and let $s^* := |\gamma^*|$ be the size of the corresponding “true” model $M_{\gamma^*}$. Without loss of generality, we may assume that the first $s^*$ components of $\gamma^*$ are ones, and the rest are zeros. We assume throughout this section that we are in the high-dimensional regime where $p \geq n$, since the low-dimensional regime where $n < p$ is easier to analyze. For any symmetric matrix $Q$, let $\lambda_{\min}(Q)$ and $\lambda_{\max}(Q)$ denote its smallest and largest eigenvalues. Our analysis involves the following assumptions:

**Assumption A (Conditions on $\beta^*$):** The true regression vector has components $\beta^* = (\beta_{S^c}^*, \beta_{S^*}^*)$ that satisfy the bounds

$$\text{Full $\beta^*$ condition: } \frac{1}{\sqrt{n}} \| X \beta^* \|_2^2 \leq g \sigma_0^2 \frac{\log p}{n},$$

$$\text{Off-support $S^c$ condition: } \frac{1}{\sqrt{n}} \| X_{S^c} \beta_{S^c}^* \|_2^2 \leq \tilde{L} \sigma_0^2 \frac{\log p}{n},$$

for some universal constant $\tilde{L}$.

In the simplest case, the true regression vector $\beta^*$ is $S$-sparse (meaning that $\beta_{S^c}^* = 0$), so that the off-support condition holds trivially. As for the full $\beta^*$ condition, it is known [28] that some form of upper bound on the norm $\| \beta^* \|_2$ in terms of the $g$-hyperparameter is required in order to prove Bayesian model selection consistency [28]. The necessity of such a condition is a manifestation of the so-called information paradox of $g$-priors [22].

Our next assumption involves an integer parameter $s$, which is set either to a multiple of the true sparsity $s^*$ (in order to prove posterior concentration) or the truncated sparsity $s_0$ (in order to prove rapid mixing).
In the low-dimensional regime \( p \) regime where \( g \) design matrix \( X \) the sparse projection condition always holds with \( L \) conditions holds:

For a constant \( \hat{\gamma} \) Assumption D (Sparsity control): \( g \) consideraions motivate us to choose the hyperparameter for the high-dimensional setting as \( L \) to the same argument, the sparse projection condition holds with \( L \). Assumption C (Choices of prior hyperparameters): \( \kappa \) sparsity penalty hyperparameter \( \kappa \) neither on \( p \) are at most \( L \) be satisfied by choosing \( L \). Assumption B (Conditions on the design matrix): \( \nu \) constants \( \nu > 0 \) and \( L < \infty \) such that

Lower restricted eigenvalue (RE(\( s \))): \( \min_{|\gamma| \leq s} \lambda_{\min} \left( \frac{1}{n} X_\gamma^T X_\gamma \right) \geq \nu \), and

Sparse projection condition (SI(\( s \))):

\[
\mathbb{E}_Z \left[ \max_{|\gamma| \leq s} \max_{k \in [p] \setminus \gamma} \frac{1}{\sqrt{n}} \sqrt{\nu} \| (I - \Phi_\gamma) X_k, Z) \| \right] \leq \frac{1}{2} \sqrt{L \nu \log p},
\]

(7b)

where \( \Phi_\gamma \) denotes projection onto the span of \( \{X_j, j \in \gamma\} \). The lower restricted eigenvalue condition is a mild requirement, and one that plays a role in the information-theoretic limitations of variable selection [31]. On the other hand, the sparse projection condition can always be satisfied by choosing \( L = O(s_0) \). To see this, notice that \( \frac{1}{\sqrt{n}} \| (I - \Phi_\gamma) X_k \| \leq 1 \) and there are at most \( p^{s_0} \) different choice of distinct pair \((\gamma, k)\). Therefore, by the Gaussianity of \( q_\gamma \), the sparse projection condition always holds with \( L = 4\nu^{-1}s_0 \). On the other extreme, if the design matrix \( X \) has orthogonal columns, then \((I - \Phi_\gamma) X_k = X_k \). As a consequence, due to the same argument, the sparse projection condition holds with \( L = 4\nu^{-1} \), which depends neither on \( s^* \) nor on \( s_0 \).

Assumption C (Choices of prior hyperparameters): The noise hyperparameter \( g \) and sparsity penalty hyperparameter \( \kappa > 0 \) are chosen such that

\[
g \asymp p^{2\alpha} \quad \text{for some } \alpha > 0, \quad \text{and} \quad \kappa + \alpha \geq C_1 (L + \bar{L}) + 2 \quad \text{for some universal constant } C_1 > 0.
\]

(7c)

In the low-dimensional regime \( p = o(n) \), the \( g \)-prior with either the unit information prior \( g = n \), or the choice \( g = \max\{n, p^2\} \) have been recommended [18, 10, 32]. In the intermediate regime where \( p = O(n) \), Sparks et al. [32] show that \( g \) must grow faster than \( pn^{-1} \log p \) for the Bayesian linear model without variable selection to achieve posterior consistency. These considerations motivate us to choose the hyperparameter for the high-dimensional setting as \( g \asymp p^{2\alpha} \) for some \( \alpha > 0 \), and our theory establishes the utility of this choice.

Assumption D (Sparsity control): For a constant \( C_0 > 4 \), one of the following conditions holds:

Version D(\( s^* \)): We set \( s_0 := p \) in the sparsity prior (5d), and the true sparsity \( s^* \) is bounded as \( s^* \leq \frac{1}{8C_0 K} \left\{ \frac{n}{\log p} - 16\bar{L}^2 \right\} \) for some constant \( K \geq 4 + \alpha + c\bar{L} \).

Version D(\( s_0 \)): The sparsity parameter \( s_0 \) in the prior (5d) satisfies the sandwich relation

\[
(2\nu^{-2} \omega(X) + 1) s^* \leq s_0 \leq \frac{1}{8C_0 K} \left\{ \frac{n}{\log p} - 16\bar{L}^2 \right\};
\]

(7d)

where \( \omega(X) := \max_{\gamma \in \Psi} \| (X_\gamma^T X_\gamma)^{-1} X_\gamma^T X_{\gamma^* \setminus \gamma} \|_{op}^2 \).

Assumptions A, B, C and D are a common set of conditions assumed in the existing literature (e.g., [28, 26]) for establishing Bayesian variable-selection consistency; i.e., that the posterior probability of the true model \( \pi_n(\gamma^* | Y) \to 1 \) as \( n \to \infty \).
3.2 Sufficient conditions for posterior consistency

Our first result characterizes the behavior of the (random) posterior $\pi_n(\cdot \mid Y)$. As we mentioned in Section 2.1, Bayesian variable-selection consistency does not require that the sparsity prior ($5d$) be truncated at some sparsity level much less than $p$, so that we analyze the hierarchical model with $s_0 = p$, and use the milder Assumption $D(s^*)$. The reader should recall from equation (6) the threshold parameter $C_\beta$ that defines the subset $S = S(C_\beta)$ of influential covariates.

**Theorem 1** (Posterior concentration). Suppose that Assumption A, Assumption B with $s = Ks^*$, Assumption C, and Assumption $D(s^*)$ hold. If the threshold $C_\beta$ satisfies

$$C_\beta^2 \geq c_0(L + \tilde{L} + \alpha + \kappa) \sigma_0^2 \frac{\log p}{n},$$

then we have $\pi_n(\gamma^* \mid Y) \geq 1 - c_1 p^{-1}$ with probability at least $1 - c_2 p^{-c_3}$.

The threshold condition (8) requires the set of influential covariates to have reasonably large magnitudes; this type of signal-to-noise condition is needed for establishing variable selection consistency of any procedure [34]. We refer to it as the $\beta_{\min}$-condition in the rest of the paper. Due to the mildness of Assumption A (conditions on $\beta^*$), the claim in the theorem holds even when the true model is not exactly sparse: Assumption A allows the residual $\beta^*_S$ to be nonzero as long as it has small magnitude.

It is worth noting that the result of Theorem 1 covers two regimes, corresponding to different levels of signal-to-noise ratio. More precisely, it is useful to isolate the following two mutually exclusive possibilities:

**High SNR:** $S = \{j \in [p] \mid \beta^*_j \neq 0\}$ and $\min_{j \in S} |\beta^*_j|^2 \geq c_0(\alpha + \kappa + L) \sigma_0^2 \frac{\log p}{n}$, (9a)

**Low SNR:** $S = \emptyset$ and $\frac{1}{\sqrt{n}} X \beta^* \|_2^2 \leq \left(\frac{\alpha + \kappa - 2}{C_1} - L\right) \sigma_0^2 \frac{\log p}{n}$. (9b)

In terms of the parameter $\tilde{L}$ in Assumption A, The high SNR regime corresponds to $\tilde{L} = 0$, whereas the low SNR regime corresponds to $\tilde{L} = \frac{\alpha + \kappa - 2}{C_1} - L$. The intuition for the low SNR setting is that the signal in every component is so weak that the “penalty” induced by hyperparameters $(g, \kappa)$ completely overwhelms it. Theorem 1 guarantees that the posterior concentrates around the model $M_{\gamma^*}$ under the high SNR condition, and under the null model $M_{\gamma_0}$ under the low SNR condition. More precisely, we have:

**Corollary 1.** Under the conditions of Theorem 1 with probability at least $1 - c_2 p^{-c_3}$:

(a) Under the high SNR condition (9a), we have $\pi_n(\gamma^* \mid Y) \geq 1 - c_1 p^{-1}$.

(b) Conversely, under the low SNR condition (9b), we have $\pi_n(\gamma_0 \mid Y) \geq 1 - c_1 p^{-1}$.

Corollary 1 provides a complete characterization of the high or low SNR regimes, but it does not cover the intermediate regime, in which some component $\beta^*_j$ of $\beta^*$ is sandwiched as

$$\left(\frac{\alpha + \kappa - 2}{C_1} - L\right) \sigma_0^2 \frac{\log p}{n} \leq |\beta^*_j|^2 \leq c_0(\alpha + \kappa + L) \sigma_0^2 \frac{\log p}{n}. \quad (10)$$

On one hand, Theorem 1 still guarantees a form of Bayesian variable selection consistency in this regime. However, the MCMC algorithm for sampling from the posterior can exhibit
slow mixing due to multimodality in the posterior. In Appendix A.2 we provide a simple example that satisfies the conditions of Theorem 1 so that posterior consistency holds, but the Metropolis-Hastings updates have mixing time growing exponentially in \( p \). This example reveals a phenomenon that might seem counter-intuitive at first sight: sharp concentration of the posterior distribution need not lead to rapid mixing of the MCMC algorithm.

### 3.3 Sufficient conditions for rapid mixing

With this distinction in mind, we now turn to developing sufficient conditions for Metropolis-Hastings scheme (3) to be rapidly mixing. As discussed in Section 2, this rapid mixing ensures that the number of iterations required to converge to an \( \epsilon \)-ball of the stationary distribution grows only polynomially in the problem parameters. The main difference in the conditions is that we now require Assumption B—the RE and sparse projection conditions—to hold with parameter \( s = s_0 \), as opposed to with the smaller parameter \( s = Ks^* \ll s_0 \) involved in Theorem 1.

**Theorem 2** (Rapid mixing guarantee). Suppose that Assumption A, Assumption B with \( s = s_0 \), Assumption C, and Assumption D(\( s_0 \)) all hold. Then under either the high SNR condition (9a) or the low SNR condition (9b), there are universal constants \( c_1, c_2 \) such that, for any \( \epsilon \in (0, 1) \), the \( \epsilon \)-mixing time of the Metropolis-Hastings chain (3) is upper bounded as

\[
\tau_\epsilon \leq c_1 p s_0^2 (c_2 \alpha (n + s_0) \log p + \log(1/\epsilon) + 2)
\]

with probability at least \( 1 - 4p^{-c_1} \).

According to our previous definition (4) of the mixing time, Theorem 2 characterizes the worst case mixing time, meaning the number of iterations when starting from the worst possible initialization. If we start with a good intial state—for example, the true model \( \gamma^* \) would be a nice though impractical choice—then we can remove the \( n \) term in the upper bound (11). In this way, the term \( c_1c_2\alpha nps_0^2 \log p \) can be understood as the worst-case number of iterations required in the burn-in period of the MCMC algorithm.

Theorems 1 and Theorem 2 lead to the following corollary, stating that after \( O(\alpha nps_0^2 \log p) \) iterations, the MCMC algorithm will output \( \gamma^* \) with high probability.

**Corollary 2.** Under the conditions of Theorem 2, for any fixed iterate \( t \) such that

\[
t \geq c_1 p s_0^2 (c_2 \alpha (n + s_0) \log p + \log p + 2),
\]

the iterate \( \gamma_t \) from the MCMC algorithm matches \( \gamma^* \) with probability at least \( 1 - c_2 p^{-c_1} \).

As with Corollary 1, Theorem 2 does not characterize the intermediate regime in which some component \( \beta^*_j \) of \( \beta^* \) satisfies the sandwich inequality (10). Based on our simulations, we suspect that the Markov chain might be slowly mixing in this regime, but we do not have a proof of this statement.

### 3.4 Illustrative simulations

In order to illustrate the predictions of Theorem 2, we conducted some simulations. We also provide an example for which a frequentist method such as the Lasso fails to perform correct variable selection while our Bayesian method succeeds.
3.4.1 Comparison of mixing times

In order to study mixing times and their dependence on the model structure, we performed simulations for linear models with random design matrices, formed by choosing row $x_i \in \mathbb{R}^p$ i.i.d. from a multivariate Gaussian distribution. In detail, setting the noise variance $\sigma^2 = 1$, we considered two classes of linear models with random design matrices $X \in \mathbb{R}^{n \times p}$, in each case formed with i.i.d. rows $x_i \in \mathbb{R}^p$:

- **Independent design:** $Y \sim \mathcal{N}(X\beta^*, \sigma^2 I_n)$ with $x_i \sim \mathcal{N}(0, I_p)$ i.i.d.;
- **Correlated design:** $Y \sim \mathcal{N}(X\beta^*, \sigma^2 I_n)$ with $x_i \sim \mathcal{N}(0, \Sigma)$ i.i.d. and $\Sigma_{jk} = e^{-|j-k|}$.

In all cases, we choose a design vector $\beta^* \in \mathbb{R}^p$ with true sparsity $s^* = 10$, taking the form

$$\beta^* = \text{SNR} \sqrt{\frac{\sigma^2 \log p}{n}} (2, -3, 2, 2, -3, 3, -2, 3, 0, \ldots, 0)^T \in \mathbb{R}^p,$$

where $\text{SNR} > 0$ is a signal-to-noise parameter. Varying the parameter SNR allows us to explore the behavior of the chains when the model lies on the boundary of the $\beta_{\text{min}}$-condition. We performed simulations for the SNR parameter $\text{SNR} \in \{0.5, 1, 2, 3\}$, sample sizes $n \in \{300, 900\}$, and number of covariates $p \in \{500, 5000\}$. In all cases, we specify our prior model by setting the dispersion hyperparameter $g = p^3$ and the expected maximum model size $s_0 = 100$.

Figure 1 plots the typical trajectories of log-posterior probability versus the number of iterations of the Markov chain under the independent design. In the strong signal regime ($\text{SNR} = 3$), the true model receives the highest posterior probability, and moreover the Metropolis-Hastings chain converges rapidly to stationarity, typically within $3p$ iterations. This observation is confirmation of our theoretical prediction of the behavior when all nonzero components in $\beta^*$ have relative high signal-to-noise ratio ($S = \{j : \beta_j \neq 0\}$). In the intermediate signal regime ($\text{SNR} = 1$), Bayesian variable-selection consistency typically fails to hold, and here, we find that the chain converges even more quickly to stationarity, typically within $1.5p$ iterations. This observation cannot be fully explained by our theory. A simulation to follow using a correlated design shows that it is not a robust phenomenon: the chain can have poor mixing performance in this intermediate signal regime when the design is sufficiently correlated.

In order to gain further insight into the algorithm’s performance, for each pair $\{X, Y\}$ we ran the Metropolis-Hastings random walk based on six initializations: the first three of them are random perturbations of the null model, whereas the remaining three are the true model. We made these choices of initialization because our empirical observations suggest that the null model and the true model tend to be near local modes of the posterior distribution. We run the Markov chain for $20p$ iterations and use the Gelman-Rubin (GR) scale factor [11] to detect whether the chains have reached stationarity. More precisely, we calculate the GR scale factor for the coefficient of determination summary statistics

$$R^2_\gamma = \frac{Y^T \Phi_\gamma Y}{\|Y\|_2^2}, \quad \text{for } \gamma \in \{0, 1\}^p,$$

where $\Phi_\gamma$ denotes the projection matrix onto the span of $\{X_j, j \in \gamma\}$. Since the typical failing of convergence to stationarity is due to the multimodality of the posterior distribution, the GR scale factor can effectively detect the problem. If the chains fail to converge, then the GR scale factor will be much larger than 2; otherwise, the scale factor should be close to 1.
Figure 1. Log-posterior probability versus the number of iterations (divided by the number of covariates $p$) of 100 randomly initialized Markov chains with $n = 500$, $p = 1000$ and SNR $\in \{1, 3\}$ in the independent design. In all cases, each grey curve corresponds to one trajectory of the chain (100 chains in total). Half of the chains are initialized at perturbations of the null model and half the true model. (a) Weak signal case: SNR = 1. (b) Strong signal case: SNR = 3 (the posterior probability of the true model coincides with that of the highest probability model).

Convergence of the chain within at most $20p$ iterations provides empirical confirmation of our theoretical prediction that the mixing time grows at most linearly in the covariate dimension $p$. (As will be seen in our empirical studies, the sample size $n$ and $s_0$ have little impact on the mixing time, as long as $s_0$ remains small compared to $n$.)

We report the percentage of simulated datasets for which the GR scale factor from six Markov chains is less than 1.5 (success). Moreover, to see whether the variable-selection procedure based on the posterior is consistent, we also compute the difference between the highest posterior probability found during the Markov chain iterations and the posterior probability of the true model (H-T) and the difference in posterior probabilities between the null model and the true model (N-T). If the true model receives the highest posterior probability, then H-T would be 0; if the null model receives the highest posterior probability, then N-T would be the same as H-T.

Table 1 shows the results for design matrices drawn from the independent ensemble. In this case, the Markov chain method has fast convergence in all settings (it converges within $20p$ iterations). From the table, the setting SNR = 0.5 (respectively SNR $\geq 2$) corresponds to the weak (respectively strong) signal regime, while SNR = 1 is in the intermediate regime where neither the null model nor the true model receives the highest posterior probability. Table 2 shows the results for design matrices drawn from the correlated ensemble. Now the Markov chain method exhibits poor convergence behavior in the intermediate regime SNR = 1 with $n = 500$, but still has fast convergence in the weak and strong signal regimes. However, with larger sample size $n = 1000$, the Markov chain has fast convergence in all settings on $p$ and SNR. Comparing the results under the two different designs, we find that correlations among the covariates increases the difficulty of variable-selection tasks when Markov chain methods are used. Moreover, the results under the correlated design suggest that there exists a regime, characterized by $n$, $p$ and SNR, in which the Markov chain is slowly mixing. It would be interesting to see whether or not this regime characterizes some type of fundamental
Table 1. Convergence behaviors of the Markov chain methods with sample sizes \( n \in \{500, 1000\} \), ambient dimensions \( p \in \{1000, 5000\} \), and SNR \( \in \{0.5, 1, 2, 3\} \) in the independent design. SP: proportion of successful trials (in which GR \( \leq 1.5 \)); H-T: log posterior probability difference between the highest probability model and the true model; N-T: log posterior probability difference between the null model and the true model. Each quantity is computed based on 20 simulated datasets.

| (\( n, p \)) | SNR = 0.5 | SNR = 1 | SNR = 2 | SNR = 3 |
|------------|---------|---------|---------|---------|
| (500, 1000) | SP | 100 | 100 | 100 | 100 |
|             | H-T  | 113.4 | 24.6 | 0 | 0 |
|             | N-T  | 113.4 | 11.4 | -210.9 | -383.6 |
| (500, 5000) | SP | 100 | 100 | 100 | 100 |
|             | H-T  | 148.7 | 33.2 | 0 | 0 |
|             | N-T  | 148.7 | 17.4 | -216.6 | -395.9 |
| (1000, 1000) | SP | 100 | 100 | 100 | 100 |
|             | H-T  | 117.1 | 34.8 | 0 | 0 |
|             | N-T  | 117.1 | -6.9 | -342.4 | -649.5 |
| (1000, 5000) | SP | 100 | 100 | 100 | 100 |
|             | H-T  | 160.4 | 32.8 | 0 | 0 |
|             | N-T  | 160.4 | -4.2 | -377.6 | -743.4 |

limit on computationally efficient procedures for variable selection. We leave this question open as a possible future direction.

3.4.2 Bayesian methods versus the Lasso

Our analysis reveals one possible benefit of a Bayesian approach as opposed to \( \ell_1 \)-based approaches such as the Lasso. It is well known that the performance of the Lasso and related \( \ell_1 \)-relaxations depends critically on fairly restrictive incoherence conditions on the design matrix. Here we provide an example of an ensemble of linear regression problems for which the Lasso fails to perform correct variable selection whereas the Bayesian approach succeeds with high probability.

For Lasso-based methods, the irrepresentable condition

\[
\max_{|\gamma|=s^*} \max_{k \not\in \gamma} \|X_k^T X_\gamma (X_\gamma^T X_\gamma)^{-1}\|_1 < 1
\]

is both sufficient and necessary for variable-selection consistency [24, 41, 33]. In our theory for the Bayesian approach, the analogous conditions are the upper bound in Assumption D(\( s_0 \)) on the maximum model size, namely

\[
s_0 \geq (2\nu^{-2} \omega(X) + 1)s^*,
\]

as well as the sparse projection condition in Assumption B. Roughly speaking, the first condition is needed to ensure that saturated models, i.e., models with size \( s_0 \), receive negligible posterior probability, such that if too many unimportant covariates are included the removal of some of them does not hurt the goodness of fit (see Lemma 8 in the Appendix). This condition is weaker than the irrepresentable condition since we can always choose \( s_0 \) large enough so that \( s_0 \geq (2\nu^{-2} \omega(X) + 1)s^* \) holds, as long as Assumption B is not violated.
Table 2. Convergence behavior of the Markov chain methods with sample size \(n \in \{500, 1000\}\), ambient dimension \(p \in \{1000, 5000\}\), and parameter \(\text{SNR} \in \{0.5, 1, 2, 3\}\) for the case of correlated design. SP: proportion of successful trials (in which \(\text{GR} \leq 1.5\)); H-T: log posterior probability difference between the highest probability model and the true model; N-T: log posterior probability difference between the null model and the true model. Each quantity is computed based on 20 simulated datasets.

| \((n, p)\)        | \(\text{SNR} = 0.5\) | \(\text{SNR} = 1\) | \(\text{SNR} = 2\) | \(\text{SNR} = 3\) |
|-------------------|-----------------------|---------------------|---------------------|---------------------|
| \((500, 1000)\)   | SP 100                | 95                  | 80                  | 100                 |
|                   | H-T 123.4             | 75.2                | 0                   | 0                   |
|                   | N-T 123.4             | 71.2                | -107.3              | -275.8              |
| \((500, 5000)\)   | SP 100                | 15                  | 100                 | 100                 |
|                   | H-T 170.0             | 81.0                | 0                   | 0                   |
|                   | N-T 170.0             | 78.7                | -102.1              | -288.9              |
| \((1000, 1000)\)  | SP 100                | 100                 | 100                 | 100                 |
|                   | H-T 138.7             | 75.1                | 0                   | 0                   |
|                   | N-T 138.7             | -67.0               | -180.8              | -431.7              |
| \((1000, 5000)\)  | SP 100                | 100                 | 100                 | 100                 |
|                   | H-T 161.8             | 61.9                | 0                   | 0                   |
|                   | N-T 161.8             | -58.8               | -204.2              | -445.4              |

As an example, consider a design matrix \(X \in \mathbb{R}^{n \times p}\) that satisfies

\[
\frac{1}{n} X^T X = \Sigma_{\text{bad}} := \begin{bmatrix} 1 & \mu & \cdots & \cdots & \mu \\ \mu & 1 & 0 & \cdots & \cdots \\ \mu & 0 & 1 & \cdots & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mu & 0 & 0 & \cdots & 1 \end{bmatrix} \in \mathbb{R}^{p \times p},
\]

with \(\mu = (2\sqrt{p})^{-1}\). (When \(p > n\), we may consider instead a random design \(X\) where the rows of \(X\) are generated i.i.d. from the \(p\)-variate normal distribution \(\mathcal{N}(0, \Sigma_{\text{bad}})\).) This example was previously analyzed by Wainwright [34], who shows that it is an interesting case in which there is a gap between the performance of \(\ell_1\)-based variable-selection recovery and that of an optimal (but computationally intractable) method based on searching over all subsets. For a design matrix of this form, we have \(\max_{|\gamma| = s^*} \|X_k^T X\gamma(X_k^T X\gamma)^{-1}\|_1 \geq s^* \mu\), so that the irrepresentable condition fails if \(s^* > 2\sqrt{p}\). Consequently, by known results on the necessity of the irrepresentable condition for Lasso [41, 35], it will fail in performing variable selection for this ensemble.

On the other hand, for this example, it can be verified that Assumption D(\(s_0\)) is satisfied with \(s_0 \geq 13s^*\), and moreover, that the the RE(\(s\)) condition in Assumption B holds with \(\nu = 1/2\), whereas the sparse projection condition is satisfied with \(L = 16(1 + s_0^2 \mu^2) = 16 + \frac{4s_0^2}{\mu^2}\). The only consequence for taking larger values of \(L\) is in the \(\beta_{\min}\)-condition: in particular, the threshold \(C_\beta\) is always lower bounded by \(L \frac{\log p}{n}\). Consequently, our theory shows that the Bayesian procedure will perform correct variable selection with high probability for this ensemble.

To compare the performance of the Bayesian approach and the Lasso under this setup, we generate our design matrix from a Gaussian version of this ensemble; i.e., the rows of \(X\) are generated i.i.d. from the \(p\)-variate normal distribution \(\mathcal{N}(0, \Sigma_{\text{bad}})\). We choose \((n, p, s^*) = (300, 80, 20)\) so that \(s^* \mu = 10/\sqrt{80} \approx 1.1 > 1\), i.e. the irrepresentable condition
Figure 2. Boxplots indicating variable-selection performance of the Bayesian approach (BVS) and the Lasso. The boxplots are based on the logarithms of the ratio between the posterior probability of the selected model and the true model over 100 replicates. The model selected by the Bayesian approach is the median probability model \cite{1} and the regularization parameter of the Lasso is chosen by cross-validation.

fails. Figure 2 shows the variable-selection performance for the Bayesian approach and the Lasso over 100 replicates. We report the logarithm of the ratio between the posterior probability (see equation (42)) of the selected model and the true model, where we use the median probability model \cite{1} as the selected model of the Bayesian approach. If a variable-selection approach has good performance, then we will expect this logarithm to be close to zero. Figure 2 shows that the Bayesian approach almost always selects the true model while the Lasso fails most of the time, which is consistent with the theory.

4 Proofs

We now turn to the proofs of our main results, beginning with the rapid mixing guarantee in Theorem 2, which is the most involved technically. We then use some of the machinery developed in Theorem 2 to prove the posterior consistency guarantee in Theorem 1. Finally, by combining these two theorems we prove Corollary 2. In order to promote readability, we defer the proofs of certain more technical results to the appendices.

4.1 Proof of Theorem 2

For the purposes of this proof, let \( \tilde{P} \) denote the transition matrix of the original Metropolis-Hastings sampler \cite{3}. Now consider instead the transition matrix \( P := \tilde{P}/2 + I/2 \), corresponding to a lazy random walk that has a probability of at least 1/2 in staying in its current state. By construction, the smallest eigenvalue of \( P \) will always be nonnegative, and as a consequence, the mixing time of the Markov chain \( \mathcal{C} \) is completely determined by the second largest eigenvalue \( \lambda_2 \) of \( P \). The difference \( \text{Gap}(P) := 1 - \lambda_2 \) is known as the spectral gap, and for any
lazy Markov chain, we have the sandwich relation
\[
\frac{1}{2} \left( 1 - \text{Gap}(P) \right) \log \left[ \frac{1}{2(2\epsilon)} \right] \leq \tau_\epsilon \leq \frac{\left( \log \left[ \frac{1}{\min_{\gamma \in \mathcal{M}} \pi(\gamma)} + \log(1/\epsilon) \right] \right)}{\text{Gap}(P)}.
\] (14)

See the papers [30, 37] for bounds of this form.

Using this sandwich relation, we claim that it suffices to show that there are universal constants \((c_1, c_2)\) such that with probability at least \(1 - 4p^{-c_1}\), the spectral gap of the lazy transition matrix \(P\) is lower bounded as
\[
\text{Gap}(P) \geq \frac{c_2}{ps_0^2}.
\] (15)

To establish the sufficiency of this intermediate claim, we apply Theorem 1 and make use of the expression (42) for the posterior distribution, thereby obtaining that for \(\gamma \in \mathcal{M}\), the posterior probability is lower bounded as
\[
\pi_n(\gamma | Y) = \pi_n(\gamma^* | Y) \cdot \frac{\pi_n(\gamma | Y)}{\pi_n(\gamma^* | Y)} \geq e^{-2/p} \cdot (p\sqrt{1 + g})^{-(|\gamma| - |\gamma'|)} \cdot \frac{(1 + g(1 - R_{\gamma^*}^2))^n/2}{(1 + g(1 - R_{\gamma}^2))^n/2} \geq e^{-2/p} \cdot p^{-(1+\alpha/2)s_0} \cdot p^{-\alpha n/2}
\]
with probability at least \(1 - 4p^{-c_1}\). Combining the above two displays with the sandwich relation (14), we obtain that there exist constants \((c_1', c_2')\) such that for \(\epsilon \in (0, 1)\),
\[
\tau_\epsilon \leq c_1' ps_0^2 \left( c_2' \alpha (n + s_0) \log p + \log(1/\epsilon) + 2 \right)
\]
with probability at least \(1 - 4p^{-c_1}\).

Accordingly, the remainder of our proof is devoted to establishing the spectral gap bound (15), and we do so via a version of the canonical path argument [30]. Let us begin by describing the idea of a canonical path ensemble associated with a Markov chain. Given a Markov chain \(C\) with state space \(\mathcal{M}\), consider the weighted directed graph \(G(C) = (V, E)\) with vertex set \(V = \mathcal{M}\) and edge set \(E\) in which an ordered pair \(e = (\gamma, \gamma')\) is included as an edge with weight \(Q(e) = Q(\gamma, \gamma') = \pi(\gamma)P(\gamma, \gamma')\) if and only if \(P(\gamma, \gamma') > 0\). A canonical path ensemble \(\mathcal{T}\) for \(C\) is a collection of paths that contains, for each ordered pair \((\gamma, \gamma')\) of distinct vertices, a unique simple path \(T_{\gamma, \gamma'}\) in the graph that connects \(\gamma\) and \(\gamma'\). We refer to any path in the ensemble \(\mathcal{T}\) as a canonical path.

In terms of this notation, Sinclair [30] shows that for any reversible Markov chain and any choice of canonical path \(T\), the spectral gap of \(P\) is lower bounded as
\[
\frac{\text{Gap}(P)}{1 - \lambda_2} \geq \frac{1}{\rho(T)\ell(T)},
\] (16)
where \(\ell(T)\) corresponds to the length of a longest path in the ensemble \(\mathcal{T}\), and the quantity \(\rho(T) := \max_{e \in E} \frac{1}{Q(e)} \sum_{T_{\gamma, \gamma'} \ni e} \pi(\gamma)\pi(\gamma')\) is known as the path congestion parameter.

In order to apply this approach to our problem, we need to construct a suitable canonical path ensemble \(\mathcal{T}\). To begin with, let us introduce some notation for operations on simple paths. For two given paths \(T_1\) and \(T_2\):
• Their intersection $T_1 \cap T_2$ corresponds to the subset of overlapping edges. (For instance, if $T_1 = (1, 1, 1) \rightarrow (0, 1, 1) \rightarrow (0, 0, 1)$ and $T_2 = (0, 0, 1) \rightarrow (0, 0, 0)$, then $T_1 \cap T_2 = (0, 0, 0)$.)

• If $T_2 \subset T_1$, then $T_1 \setminus T_2$ denotes the path obtained by removing all edges in $T_2$ from $T_1$. (With the same specific choices of $(T_1, T_2)$ as above, we have $T_1 \setminus T_2 = (1, 1, 1) \rightarrow (0, 1, 1) \rightarrow (0, 0, 1)$.)

• We use $\bar{T}_1$ to denote the reverse of $T_1$. (With the choice of $T_1$ as above, we have $\bar{T}_1 = (0, 0, 0) \rightarrow (0, 0, 1) \rightarrow (0, 1, 1) \rightarrow (1, 1, 1)$.)

• If the endpoint of $T_1$ and the starting point of $T_2$ are the same, then we define the union $T_1 \cup T_2$ as the path that connects $T_1$ and $T_2$ together. (If $T_1 = (0, 0, 0) \rightarrow (0, 0, 1)$ and $T_2 = (0, 0, 1) \rightarrow (0, 0, 1)$, then their union is given by $T_1 \cup T_2 = (0, 0, 0) \rightarrow (0, 0, 1) \rightarrow (0, 1, 1)$.)

We now turn to the construction of our canonical path ensemble. At a high level, our construction is inspired by the variable-selection paths carved out by greedy stepwise variable-selection procedures (e.g., [20][2]).

**Canonical path ensemble construction for $\mathcal{M}$:** First, we construct the canonical path $T_{\gamma, \gamma^*}$ from any $\gamma \in \mathcal{M}$ to the true model $\gamma^*$. The following construction will prove helpful. We call a set $\mathcal{R}$ of canonical paths memoryless with respect to the central state $\gamma^*$ if: (1) for any state $\gamma \in \mathcal{M}$ satisfying $\gamma \neq \gamma^*$, there exists a unique simple path $T_{\gamma, \gamma^*}$ in $\mathcal{R}$ that connects $\gamma$ and $\gamma^*$; (2) for any intermediate state $\bar{\gamma} \in \mathcal{M}$ on any path $T_{\gamma^*, \gamma^*}$ in $\mathcal{R}$, the unique path $T_{\bar{\gamma}, \gamma^*}$ in $\mathcal{R}$ that connects $\bar{\gamma}$ and $\gamma^*$ is the sub-path of $T_{\gamma^*, \gamma^*}$ starting from $\bar{\gamma}$ and ending at $\gamma^*$. Intuitively, this memoryless property means that for any intermediate state on any canonical path towards the central state, the next move from this intermediate state towards the central state does not depend on the history. A memoryless canonical path ensemble has the property that in order to specify the canonical path connecting any state $\gamma \in \mathcal{M}$ and the central state $\gamma^*$, we only need to specify which state to move to from any $\gamma \neq \gamma^*$ in $\mathcal{M}$; i.e., we need a transition function $\mathcal{G} : \mathcal{M} \setminus \{\gamma^*\} \rightarrow \mathcal{M}$ that maps the current state $\gamma \in \mathcal{M}$ to a next state $\mathcal{G}(\gamma) \in \mathcal{M}$. For simplicity, we define $\mathcal{G}(\gamma^*) = \gamma^*$ to make $\mathcal{M}$ as the domain of $\mathcal{G}$. Clearly, each memoryless canonical path ensemble with respect to a central state $\gamma^*$ corresponds to a transition function $\mathcal{G}$ with $\mathcal{G}(\gamma^*) = \gamma^*$, but the converse is not true. For example, if there exist two states $\gamma$ and $\gamma'$ so that $\mathcal{G}(\gamma) = \gamma'$ and $\mathcal{G}(\gamma') = \gamma$, then $\mathcal{G}$ is not the transition function corresponding to any memoryless canonical path ensemble. However, every valid transition function $\mathcal{G}$ gives rise to a unique memoryless canonical path set consisting of paths connecting any $\gamma \in \mathcal{M}$ to $\gamma^*$, with $\gamma^*$ corresponding to the fixed point of $\mathcal{G}$. We call function $\mathcal{G}$ a valid transition function if there exists a memoryless canonical path set for which $\mathcal{G}$ is the corresponding transition function. The next lemma provides a sufficient condition for a function $\mathcal{G} : \mathcal{M} \setminus \{\gamma^*\} \rightarrow \mathcal{M}$ to be valid, which motivates our construction to follow. Recall that $d_H$ denotes the Hamming metric between a pair of binary strings.

**Lemma 1.** If a function $\mathcal{G} : \mathcal{M} \setminus \{\gamma^*\} \rightarrow \mathcal{M}$ satisfies that for any state $\gamma \in \mathcal{M} \setminus \gamma^*$, the Hamming distance between $\mathcal{G}(\gamma)$ and $\gamma^*$ is strictly less than the Hamming distance between $\gamma$ and $\gamma^*$, then $\mathcal{G}$ is a valid transition function.

**Proof.** Based on this function $\mathcal{G}$, we can construct the canonical path $T_{\gamma, \gamma^*}$ from any state $\gamma \in \mathcal{M}$ to $\gamma^*$ by defining $T_{\gamma, \gamma^*}$ as $\gamma \rightarrow \mathcal{G}(\gamma) \rightarrow \mathcal{G}^2(\gamma) \rightarrow \ldots \rightarrow \mathcal{G}^k(\gamma)$, where $\mathcal{G}^k := \mathcal{G} \circ \ldots \circ \mathcal{G}$.
denotes the \(k\)-fold self-composition of \(G\) for any \(k \in \mathbb{N}\) and \(k_\gamma := \min_k \{G^k(\gamma) = \gamma^*\}\). In order to show that the set \(\{T_{\gamma, \gamma^*} : \gamma \in \mathcal{M}, \gamma \neq \gamma^*\}\) is a memoryless canonical path set, we only need to verify two things:

(a) for any \(\gamma \neq \gamma^*\), \(T_{\gamma, \gamma^*}\) is a well-defined path; i.e., it has finite length and ends at \(\gamma^*\), and

(b) for any \(\gamma \neq \gamma^*\), \(T_{\gamma, \gamma^*}\) is a simple path.

By our assumption, the function \(F : \mathcal{M} \to \mathbb{R}\) defined by \(F(\gamma) = d_H(\gamma, \gamma^*)\) is strictly decreasing along the path \(T_{\gamma, \gamma^*}\) for \(\gamma \neq \gamma^*\). Because \(F\) only attains a finite number of values, there exists a smallest \(k_\gamma\) such that \(G^{k_\gamma+1}(\gamma) = G^k(\gamma)\) for each \(k \geq k_\gamma\), implying that \(G^{k_\gamma}(\gamma)\) is a fixed point of \(G\). Since \(\gamma^*\) is the unique fixed point of \(G\), we must have \(G^{k_\gamma}(\gamma) = \gamma^*\), which proves the first claim. The second claim is obvious since the function \(F\) defined above is strictly decreasing along the path \(T_{\gamma, \gamma^*}\), which means that the states on the path \(T_{\gamma, \gamma^*}\) are all distinct. \(\square\)

Equipped with this lemma, we start constructing a memoryless set of canonical paths from any state \(\gamma \in \mathcal{M}\) to \(\gamma^*\) by specifying a valid \(G\) function. First, we introduce some definitions on the states. A state \(\gamma \neq \gamma^*\) is called saturated if \(|\gamma| = s_0\) and unsaturated if \(|\gamma| < s_0\). We call a state \(\gamma \neq \gamma^*\) overfitted if it contains all influential covariates, i.e. \(\gamma^* \subset \gamma\), and underfitted if it does not contain at least one influential covariate. Recall the two updating schemes in our Metropolis-Hastings (MH) sampler: single flip and double flips. We accordingly construct the transition function \(G\) as follows.

(i) If \(\gamma \neq \gamma^*\) is overfitted, then we define \(G(\gamma)\) to be \(\gamma'\), which is formed by deleting the least influential covariate from \(\gamma\), i.e. \(\gamma'_j = \gamma_j\) for any \(j \notin \ell_\gamma\) and \(\gamma'_{\ell_\gamma} = 0\), where \(\ell_\gamma\) is the index from the set \(\gamma \setminus \gamma^*\) of uninfluential covariates that minimizes the difference

\[
\|\Phi_\gamma X_{\gamma^*} \beta^*_{\gamma^*} \|^2 - \|\Phi_\gamma X_{\gamma^* \setminus \ell_\gamma} \beta^*_{\gamma^*} \|^2,
\]

where \(\Phi_\gamma\) denotes the projection onto the span of \(\{X_j, j \in \gamma\}\). This transition resembles the backward deletion step in the stepwise variable-selection procedure and involves the single flip updating scheme of the MH algorithm. By construction, if \(\gamma \neq \gamma^*\) is overfitted, then \(d_H(G(\gamma), \gamma^* ) = d_H(G(\gamma), \gamma^* ) - 1\).

(ii) If \(\gamma \neq \gamma^*\) is underfitted and unsaturated, then we define \(G(\gamma)\) to be \(\gamma'\), which is formed by adding the influential covariate from \(\gamma^* \setminus \gamma\) that explains the most signal variation, i.e. \(\gamma'_j = \gamma_j\) for any \(j \notin \gamma\) and \(\gamma'_{\gamma\setminus j} = 1\), where \(j_\gamma\) is defined as the \(j \in \gamma^* \setminus \gamma\) that maximizes the quantity \(\|\Phi_{\gamma \setminus \{j\}} X_{\gamma^*} \beta^*_{\gamma^*} \|^2\). This transition resembles the forward selection step in the stepwise variable selection procedure and involves the single flip updating scheme of the MH algorithm. By construction, if \(\gamma \neq \gamma^*\) is underfitted and unsaturated, then \(d_H(G(\gamma), \gamma^* ) = d_H(G(\gamma), \gamma^* ) - 1\).

(iii) If \(\gamma \neq \gamma^*\) is underfitted and saturated, then we define \(G(\gamma)\) to be \(\gamma'\), which is formed by replacing the least influential unimportant covariate in \(\gamma\) with the most influential covariate from \(\gamma^* \setminus \gamma\), i.e. \(\gamma'_j = \gamma_j\) for any \(j \notin \{j_\gamma, k_\gamma\}\), \(\gamma'_{j_\gamma} = 1\) and \(\gamma'_{k_\gamma} = 0\), where \(j_\gamma\) is defined in case 2 and \(k_\gamma \in \gamma \setminus \gamma^*\) minimizes \(\|\Phi_{\gamma \cup \{j\}} X_{\gamma^*} \beta^*_{\gamma^*} \|^2 - \|\Phi_{\gamma \cup \{j\} \setminus \{k\}} X_{\gamma^*} \beta^*_{\gamma^*} \|^2\). This transition step involves the double-flip updating scheme of the MH algorithm. By construction, if \(\gamma \neq \gamma^*\) is underfitted and saturated, then \(d_H(G(\gamma), \gamma^* ) = d_H(G(\gamma), \gamma^* ) - 2\).
Figure 3. Illustration of the construction of the canonical path ensemble. In the plot, $\gamma^*$ is the central state, $G$ is the transition function, and solid blue arrows indicate canonical paths $T_{\gamma_2, \gamma^*}$ and $T_{\gamma_3, \gamma_4}$.

By Lemma 1, this transition function $G$ is valid and gives rise to a unique memoryless set of canonical paths from any state $\gamma \in \mathcal{M}$ to $\gamma^*$. For example, Fig. 3 shows such a memoryless set of canonical paths for $\mathcal{M}$ consisting of 14 states, where $T_{\gamma_2, \gamma^*}$ corresponds to the canonical path from state $\gamma_2$ to the central state $\gamma^*$.

Based on this memoryless canonical path set, we can finish constructing the canonical path ensemble $\mathcal{T}$ by specifying the path $T_{\gamma, \gamma'}$ connecting any distinct pair $(\gamma, \gamma') \in \mathcal{M} \times \mathcal{M}$. More specifically, by the memoryless property, the two simple paths $T_{\gamma, \gamma^*}$ and $T_{\gamma', \gamma^*}$ share an identical subpath towards $\gamma^*$ from their first common intermediate state. Let $T_{\gamma} \cap \gamma'$ denote this common subpath $T_{\gamma} \cap T_{\gamma'}$, and $T_{\gamma} \setminus \gamma' := T_{\gamma} \setminus T_{\gamma} \cap \gamma'$ denote the remaining path of $T_{\gamma}$ after removing the segment $T_{\gamma} \cap \gamma'$. Then it is easy to see that the two remaining paths $T_{\gamma} \setminus \gamma'$ and $T_{\gamma'} \setminus \gamma$ share the same endpoint. Therefore, it is valid to define the path $T_{\gamma, \gamma'}$ as $T_{\gamma} \setminus \gamma' \cup T_{\gamma'} \setminus \gamma$. To understand this construction, let us consider an example where $T_{\gamma, \gamma^*} = (0, 1, 1, 1) \rightarrow (1, 1, 0, 1) \rightarrow (1, 1, 0, 0)$ and $T_{\gamma', \gamma^*} = (1, 0, 0, 1) \rightarrow (1, 1, 0, 1) \rightarrow (1, 1, 0, 0)$. Their intersection is $T_{\gamma} \cap \gamma' = (1, 1, 1, 1) \rightarrow (1, 1, 0, 1)$ and $T_{\gamma'} \setminus \gamma = (1, 0, 0, 1) \rightarrow (1, 1, 0, 1)$. Consequently, the path $T_{\gamma, \gamma'}$ from $\gamma$ to $\gamma'$ is $(0, 1, 1, 1) \rightarrow (1, 1, 0, 1) \rightarrow (1, 0, 0, 1)$ by our construction. For example, path $T_{\gamma_3, \gamma_4}$ in Fig. 3 illustrates the construction of the path connecting $(\gamma_3, \gamma_4)$ when $\mathcal{M}$ is composed of 14 states.

We call $\gamma$ a *precedent* of $\gamma'$ if $\gamma'$ is on the canonical path $T_{\gamma, \gamma^*} \in \mathcal{T}$, and a pair of states $\gamma, \gamma'$ *adjacent* if the canonical path $T_{\gamma, \gamma'}$ is $e_{\gamma, \gamma'}$, the edge in $E$ connecting $\gamma$ and $\gamma'$. For $\gamma \in \mathcal{M}$, let

$$\Lambda(\gamma) := \{ \bar{\gamma} \mid \gamma \in T_{\bar{\gamma}, \gamma^*}\}$$

(17)

denote the set of all its precedents. Use the notation $|T|$ to denote the length of a path $T$. The following lemma provides some important properties of the constructed canonical path ensemble that will be used later.
Lemma 2. For any distinct pair \((\gamma, \gamma') \in \mathcal{M} \times \mathcal{M}\):

(a) We have

\[
|T_{\gamma, \gamma'}| \leq d_H(\gamma, \gamma^*) \leq s_0, \quad \text{and} \quad |T_{\gamma, \gamma'}| \leq d_H(\gamma, \gamma^*) + d_H(\gamma', \gamma^*) \leq 2s_0.
\] (18a)

(b) If \(\gamma\) and \(\gamma'\) are adjacent (joined by edge \(e_{\gamma, \gamma'}\)) and \(\gamma\) is a precedent of \(\gamma'\), then

\[
\{(\tilde{\gamma}, \tilde{\gamma}') \mid T_{\tilde{\gamma}, \tilde{\gamma}'} \supset e_{\gamma, \gamma'}\} \subseteq \Lambda(\gamma) \times \mathcal{M},
\]

Proof. The first claim follows since the function \(F : \mathcal{M} \to \mathbb{R}\) defined by \(F(\gamma) = d_H(\gamma, \gamma^*)\) is strictly decreasing along the path \(T_{\gamma, \gamma^*}\) for \(\gamma \neq \gamma^*\). Now we prove the second claim. For any pair \((\tilde{\gamma}, \tilde{\gamma}')\) such that \(T_{\tilde{\gamma}, \tilde{\gamma}'} \supset e_{\gamma, \gamma'}\), either \(e_{\gamma, \gamma'} \in T_{\gamma, \gamma'}\) or \(e_{\gamma, \gamma'} \in T'_{\gamma, \gamma'}\) should be satisfied since \(T_{\gamma, \gamma'} = T_{\gamma, \gamma'} \cup T'_{\gamma, \gamma'}\) by our construction. Because \(\gamma\) is a precedent of \(\gamma'\), we can only have \(e_{\gamma, \gamma'} \in T'_{\gamma, \gamma'}\). This shows that \(\gamma\) is on the path \(T_{\gamma, \gamma^*}\) and \(\tilde{\gamma} \in \Lambda(\gamma)\).

According to Lemma 2(b), the path congestion parameter \(\rho(T)\) of the canonical path \(T\) satisfies

\[
\rho(T) \leq \max_{(\gamma, \gamma') \in \Gamma^*} \frac{1}{Q(\gamma, \gamma')} \sum_{\tilde{\gamma} \in \Lambda(\gamma), \tilde{\gamma}' \in \mathcal{M}} \pi(\tilde{\gamma}) \pi(\tilde{\gamma}') = \max_{(\gamma, \gamma') \in \Gamma^*} \frac{\pi[\Lambda(\gamma)]}{Q(\gamma, \gamma')} ,
\] (19)

where the maximum is taken over the set

\[
\Gamma^* := \left\{(\gamma, \gamma') \in \mathcal{M} \times \mathcal{M} \mid T_{\gamma, \gamma'} = e_{\gamma, \gamma'} \text{ and } \gamma \in \Lambda(\gamma')\right\}.
\]

Here we used the fact that the weight function \(Q\) of a reversible chain satisfies \(Q(\gamma, \gamma') = Q(\gamma', \gamma)\) so as to be able to restrict the range of the maximum to pairs \((\gamma, \gamma')\) where \(\gamma \in \Lambda(\gamma')\).

For the lazy form of the Metropolis-Hastings walk [5], given any pair \((\gamma, \gamma')\) such that \(P(\gamma, \gamma') > 0\), we have

\[
Q(\gamma, \gamma') = \frac{1}{2} \pi_n(\gamma \mid Y) P(\gamma, \gamma') \\
\quad \geq \frac{1}{2p_{s_0}} \pi_n(\gamma \mid Y) \min \left\{1, \frac{\pi_n(\gamma' \mid Y)}{\pi_n(\gamma \mid Y)}\right\} = \frac{1}{2p_{s_0}} \min \left\{\frac{\pi_n(\gamma' \mid Y)}{\pi_n(\gamma \mid Y)}, \pi_n(\gamma \mid Y)\right\}.
\]

Substituting this lower bound into our upper bound (19) on the path congestion parameter yields

\[
\rho(T) \leq 2ps_0 \max_{(\gamma, \gamma') \in \Gamma^*} \frac{\pi_n[\Lambda(\gamma) \mid Y]}{\min \left\{\pi_n(\gamma \mid Y), \pi_n(\gamma' \mid Y)\right\}} \\
= 2ps_0 \max_{(\gamma, \gamma') \in \Gamma^*} \left\{\max \left\{1, \frac{\pi_n(\gamma \mid Y)}{\pi_n(\gamma' \mid Y)}\right\} \cdot \frac{\pi_n[\Lambda(\gamma) \mid Y]}{\pi_n(\gamma \mid Y)}\right\}.
\] (20)

In order to prove that \(\rho(T) = \mathcal{O}(ps_0)\) with high probability, it suffices to show that the two terms inside the maximum are \(\mathcal{O}(1)\) with high probability. In order to do so, we make use of two auxiliary lemmas.
Given the constant $C_0 \geq 4$ and the noise vector $w \sim \mathcal{N}(0, \sigma_0^2 I_n)$, consider the following events

\begin{align*}
A_n &:= \left\{ \max_{\gamma_1, \gamma_2 \in \mathcal{M}} \frac{w^T (\Phi_{\gamma_1} - \Phi_{\gamma_2}) w}{|\gamma_1| - |\gamma_2|} \leq L\sigma_0^2 \log p \right\}, & (21a) \\
B_n &:= \left\{ \max_{\gamma \in \mathcal{M}} \frac{w^T \Phi_{\gamma} w}{|\gamma|} \leq r\sigma_0^2 \log p \right\}, \text{ and} & (21b) \\
C_n &:= \left\{ \frac{\|w\|^2}{n\sigma_0^2} - 1 \leq \frac{1}{2} \right\}, \text{ and } D_n := \left\{ \frac{\|Y\|^2}{g} \leq \frac{5n\sigma_0^2}{s^*} \right\}. & (21c)
\end{align*}

Our first auxiliary lemma guarantees that, under the stated assumptions of our theorem, the intersection of these events holds with high probability:

**Lemma 3.** Under the conditions of Theorem 2, we have

$$\mathbb{P}(A_n \cap B_n \cap C_n \cap D_n) \geq 1 - 6p^{-c}. \quad (22)$$

We prove this lemma in Section 4.2 to follow.

Our second auxiliary lemma ensures that when these four events hold, then the two terms on the right-hand side of the upper bound (20) are controlled.

**Lemma 4.** Suppose that, in addition to the conditions of Theorem 2, the compound event $A_n \cap B_n \cap C_n \cap D_n$ holds. Then for all $\gamma \neq \gamma^*$, we have

$$\frac{\pi_n(\gamma \mid Y)}{\pi_n(G(\gamma) \mid Y)} \leq \begin{cases} p^{-2}, & \text{if } \gamma \text{ is overfitted}, \\ p^{-3}, & \text{if } \gamma \text{ is underfitted}, \end{cases} \quad (23a)$$

and moreover, for all $\gamma$,

$$\frac{\pi_n[ \Lambda(\gamma) \mid Y]}{\pi_n(\gamma \mid Y)} \leq c \quad \text{for some universal constant } c. \quad (23b)$$

We prove this lemma in Section 4.3 to follow.

Combining Lemmas 3 and 4 with our earlier bound (20), we conclude that $\rho(T) \leq 2cp s_0$. By Lemma 2(a), our path ensemble $T$ has maximal length $\ell(T) \leq 2s_0$, and hence the canonical path lower bound (16) implies that $\text{Gap}(P) \geq \frac{1}{4cp s_0}$, as claimed in inequality (15). This completes the proof of the theorem.

The only remaining detail is to prove Lemmas 3 and 4 and we do so in the following two subsections.

### 4.2 Proof of Lemma 3

We split the proof up into separate parts, one for each of the events $A_n, B_n, C_n$ and $D_n$.

**Bound on $\mathbb{P}[C_n]$:** Since $\|w\|^2/\sigma_0^2 \sim \chi_n^2$, a standard tail bound for the $\chi_n^2$ distribution (e.g., [19], Lemma 1) yields

$$\mathbb{P}[C_n] \geq 1 - 2e^{-\frac{\alpha}{2}}. \quad (24)$$
Bound on $\mathbb{P}[B_n]$: For each state $\gamma \in \mathcal{M}$, the random variable $w^T \Phi \gamma w / \sigma_0^2$ follows a chi-squared distribution with $|\gamma|$ degrees of freedom. For each integer $\ell \in \{1, \ldots, s_0\}$, the model space $\mathcal{M}$ contains $(p_{\ell})$ models of size $\ell$. Therefore, by a union bound, we find that

$$
\mathbb{P}[B_n] \geq 1 - \sum_{\ell=1}^{s_0} \left( \frac{p_{\ell}}{\ell} \right) \mathbb{P}(\chi_{\ell}^2 \geq C_0 \ell \log p) \geq 1 - \sum_{\ell=1}^{s_0} e^{-(C_0/4-1) \ell \log p} \geq 1 - 2e^{-(C_0/4-1) \log p} = 1 - 2p^{-(C_0/4-1)}.
$$

(25)

Bound on $\mathbb{P}[D_n]$: Given the linear observation model, we have

$$
\|Y\|_2^2 = \|X\beta^* + w\|_2^2 \leq 2\|X\beta^*\|^2 + 2\|w\|_2^2.
$$

Combining this with inequality (24), we obtain

$$
\mathbb{P}[\|Y\|_2^2 \geq 2\|X\beta^*\|_2^2 + 3n\sigma_0^2] \leq 2e^{-\frac{n}{k}} \leq p^{-s_0(r/4-1)}
$$

for large $n$ and some constant $C > 0$, where we have used Assumption D. By Assumptions A and D, we have $\|X\beta^*\|_2^2 \leq 2n\sigma_0^2 g/s^*$, implying that

$$
\mathbb{P}[D_n^c] \leq \mathbb{P}[\|Y\|_2^2 \geq 2\|X\beta^*\|_2^2 + 3n\sigma_0^2] \leq p^{-s_0(r/4-1)}.
$$

(26)

Bound on $\mathbb{P}[A_n]$: To control this probability, we require two auxiliary lemmas.

Lemma 5. Under Assumption B, for any distinct pair $(\gamma, \bar{\gamma}) \in \mathcal{M} \times \mathcal{M}$ satisfying $\gamma \subset \bar{\gamma}$, we have

$$
\lambda_{\text{min}} \left( \frac{1}{n} X_{\bar{\gamma}\setminus\gamma}^T (I_n - \Phi_\gamma) X_{\bar{\gamma}\setminus\gamma} \right) \geq \nu.
$$

Proof. By partitioning the matrix $X_\gamma$ into a block form $(X_\gamma, X_{\bar{\gamma}\setminus\gamma})$ and using the formula for the inverse of block matrices, one can show that the lower right corner of $(n^{-1}X_\gamma^T X_\gamma)^{-1}$ is $(n^{-1}X_{\bar{\gamma}\setminus\gamma}^T (I_n - \Phi_\gamma) X_{\bar{\gamma}\setminus\gamma})^{-1}$, which implies the claimed bound.

$\square$

Lemma 6. For $\gamma \in \mathcal{M}$ and $k \notin \gamma$, we have

$$
\Phi_{\gamma\cup\{k\}} - \Phi_\gamma = \frac{(I - \Phi_\gamma) X_k X_k^T (I - \Phi_\gamma)}{X_k^T (I - \Phi_\gamma) X_k}.
$$

Proof. By the block matrix inversion formula [15], we have

$$
\begin{bmatrix}
X_\gamma^T X_\gamma & X_\gamma^T X_k \\
X_k^T X_\gamma & X_k^T X_k
\end{bmatrix}^{-1} = \begin{bmatrix}
B + a X_\gamma^T X_k X_k^T X \gamma & -a X_\gamma^T X_k \\
-a X_k^T X_\gamma B & a
\end{bmatrix},
$$

where $B = (X_\gamma^T X_\gamma)^{-1} \in \mathbb{R}^{\|\gamma\| \times \|\gamma\|}$ and $a = (X_k^T (I - \Phi_\gamma) X_k)^{-1} \in \mathbb{R}$. Then simple linear algebra yields

$$
\Phi_{\gamma\cup\{k\}} - \Phi_\gamma = \begin{bmatrix}
X_\gamma & X_k
\end{bmatrix} \begin{bmatrix}
X_\gamma^T X_\gamma & X_\gamma^T X_k \\
X_k^T X_\gamma & X_k^T X_k
\end{bmatrix}^{-1} \begin{bmatrix}
X_\gamma^T \\
X_k^T
\end{bmatrix} - \Phi_\gamma
$$

$$
= a(I - \Phi_\gamma) X_k X_k^T (I - \Phi_\gamma),
$$

which is the claimed decomposition.

$\square$
Returning to our main task, let us define the event
\[ A'_n := \left\{ \max_{\gamma \in \mathcal{M}, k \in \{1, \ldots, p\}} w^T (\Phi_{\gamma \cup \{k\}} - \Phi_\gamma) w \leq L\sigma_0^2 \log p \right\}. \]

By construction, we have \( A'_n \subseteq A_n \) so that it suffices to lower bound \( \mathbb{P}(A'_n) \). Lemma 6 implies that
\[ w^T (\Phi_{\gamma \cup \{k\}} - \Phi_\gamma) w = \frac{\left| \langle (I - \Phi_\gamma) X_k, w \rangle \right|^2}{X_k^T (I - \Phi_\gamma) X_k / n}. \]

Now we show that with probability at least \( 1 - p^{-c} \), the above quantity is uniformly bounded by \( L\sigma_0^2 \log p \) over all \((\gamma, k) \in \mathcal{M} \times \{1, \ldots, p\}\) satisfying \(|\gamma| \leq s_0\) and \( k \notin \gamma \), which yields the intermediate result
\[ \mathbb{P}(A_n) \geq \mathbb{P}(A'_n) \geq 1 - p^{-c}. \]

Now Lemma 5 implies that
\[ \frac{1}{n} X_k^T (I - \Phi_\gamma) X_k \geq \nu, \]
and therefore, if we define the random variable
\[ V(Z) := \max_{\gamma \in \mathcal{M}, k \in \{1, \ldots, p\}} \frac{1}{\sqrt{n}} \left| \langle (I - \Phi_\gamma) X_k, Z \rangle \right|, \quad \text{where } Z \sim N(0, I_n), \]
then it suffices to show that \( V(Z) \leq \sqrt{L\nu \log p} \) with probability at least \( 1 - p^{-c} \). For any two vectors \( Z, Z' \in \mathbb{R}^n \), we have
\[ |V(Z) - V(Z')| \leq \max_{\gamma \in \mathcal{M}, k \in \{1, \ldots, p\}} \frac{1}{\sqrt{n}} \left| \langle (I - \Phi_\gamma) X_k, Z - Z' \rangle \right| \leq \frac{1}{\sqrt{n}} \| (I - \Phi_\gamma) X_k \|_2 \| Z - Z' \|_2 \leq \| Z - Z' \|_2, \]
where we have used the normalization condition of Assumption B in the last inequality. Consequently, by concentration of measure for Lipschitz functions of Gaussian random variables [20], we have
\[ \mathbb{P}[V(Z) \geq \mathbb{E}[V(Z)] + t] \leq e^{-\frac{t^2}{2}}. \]

By the sparse projection condition in Assumption B, the expectation satisfies \( \mathbb{E}[V(Z)] \leq \sqrt{L\nu \log p} / 2 \), which combined with (29) yields the claimed bound (28) with \( c \leq L\nu / 8 \).

4.3 Proof of Lemma 4

We defer the proof of the claim (23a) to Appendix B as it is somewhat technically involved. It is worth mentioning that its proof uses some auxiliary results in Lemma 8 in Appendix B which characterizes some key properties of the state \( G(\gamma) \) selected by the transition function \( G \) via the greedy criterion.

It remains to prove the second bound (23b) in Lemma 4 and we split our analysis into two cases, depending on whether \( \gamma \) is underfitted or overfitted.
4.3.1 Case \( \gamma \) is underfitted

In this case, the bound \( p_{(23a)} \) implies that \( \frac{\pi_n(\gamma|Y)}{\pi_n(\gamma|Y)} \leq p^{-3} \). For each \( \bar{\gamma} \in \Lambda(\gamma) \), where \( \Lambda(\gamma) \) is defined in Lemma \( 2(e) \), we know \( \gamma \in T_{\bar{\gamma},\gamma} \subseteq T_{\bar{\gamma},\gamma^*} \). Let the path \( T_{\bar{\gamma},\gamma} \) be \( \gamma_0 \to \gamma_1 \to \cdots \to \gamma_s \), where \( s = |T_{\bar{\gamma},\gamma}| \) is the length of \( T_{\bar{\gamma},\gamma} \), and \( \gamma_0 = \bar{\gamma} \) and \( \gamma_s = \gamma \) are the two endpoints. Since any intermediate state \( \bar{\gamma} \) on path \( T_{\bar{\gamma},\gamma} \) is also underfitted, inequality \( p_{(23a)} \) ensures that

\[
\frac{\pi_n(\bar{\gamma} | Y)}{\pi_n(\gamma | Y)} = \prod_{\ell=1}^{s} \frac{\pi_n(\gamma_{\ell-1} | Y)}{\pi_n(\bar{\gamma} | Y)} \leq p^{-3s} = p^{-3|T_{\bar{\gamma},\gamma}|}.
\]

Now for each \( s \in \{0, \ldots, s^*\} \), we count the total number of states \( \bar{\gamma} \) in \( \Lambda(\gamma) \) that satisfies \( |T_{\bar{\gamma},\gamma}| = s \). By construction, at each intermediate state in a canonical path, we either add a new influential covariate by the single flip updating scheme of the MH algorithm, or add a new influential covariate and delete an unimportant covariate by the double-flip updating scheme. As a consequence, any state in \( M \) has at most \( (s^* + 1)p \) adjacent predecessors, implying that the total number of states \( \bar{\gamma} \) in \( \Lambda(\gamma) \) with path length \( |T_{\bar{\gamma},\gamma}| = s \) is upper bounded by \((s^* + 1)^s p^s\).

Consequently, we have by the preceding display that under the event \( A_n \cap B_n \cap C_n \cap D_n \)

\[
\frac{\pi_n[\Lambda(\gamma)|Y]}{\pi_n(\gamma|Y)} = \sum_{\gamma \in f(\gamma)} \frac{\pi_n(\gamma | Y)}{\pi_n(\gamma|Y)} \leq \sum_{s=0}^{s^*} p^s (s^* + 1)^s p^{-3s} \leq \sum_{s=0}^{\infty} p^{-s} \leq \frac{1}{1 - 1/p}. \tag{30}
\]

The above argument is also valid for \( \gamma = \gamma^* \).

4.3.2 Case \( \gamma \) is overfitted

In this case, we bound the ratio \( \frac{\pi_n[\Lambda(\gamma)|Y]}{\pi_n(\gamma|Y)} \) by dividing the set \( \Lambda(\gamma) \) into two subsets:

(a) Overfitted models: \( M_1 = \{\gamma' \in \Lambda(\gamma) : \gamma' \supset \gamma^*\} \), all models in \( \Lambda(\gamma) \) that include all influential covariates.

(b) Underfitted models: \( M_2 = \{\gamma' \in \Lambda(\gamma) : \gamma' \not\supset \gamma^*\} \), all models in \( \Lambda(\gamma) \) that miss at least one influential covariate.

First, we consider the ratio \( \frac{\pi_n(M_1 \mid Y)}{\pi_n(\gamma \mid Y)} \). For each model \( \bar{\gamma} \in M_1 \), according to our construction of the canonical path, all intermediate states on path \( T_{\bar{\gamma},\gamma} = \gamma_0 \to \gamma_1 \to \cdots \to \gamma_k \) correspond to overfitted models (only involve the first flipping updating scheme of the MH algorithm), where endpoints \( \gamma_0 = \bar{\gamma} \) and \( \gamma_k = \gamma \), and \( k \) denotes the length of path \( T_{\bar{\gamma},\gamma} \). As a consequence, inequality \( p_{(23a)} \) implies that

\[
\frac{\pi_n(\bar{\gamma} | Y)}{\pi_n(\gamma | Y)} = \prod_{s=1}^{k} \frac{\pi_n(\gamma_{s-1} | Y)}{\pi_n(\bar{\gamma} | Y)} \leq p^{-2k}.
\]

Since there are at most \( p^k \) states \( \bar{\gamma} \) in \( M_1 \) satisfying \( |\bar{\gamma}| - |\gamma| = k \), we obtain that under the event \( A_n \cap B_n \cap C_n \cap D_n \)

\[
\frac{\pi_n(M_1 \mid Y)}{\pi_n(\gamma \mid Y)} \leq \sum_{k=0}^{p-|\gamma|} p^k p^{-2k} \leq \sum_{k=0}^{\infty} p^{-k} \leq \frac{1}{1 - 1/p} \leq 2. \tag{31}
\]

Second, we consider the ratio \( \frac{\pi_n(M_2 \mid Y)}{\pi_n(\gamma \mid Y)} \). For fixed \( \bar{\gamma} \in M_2 \), let \( f(\bar{\gamma}) \) be the first state along the path \( T_{\bar{\gamma},\gamma} \) that contains all influential covariates. Since the overfitted state \( \gamma \)
contains all influential covariates, \( f(\gamma) \) exists and is well-defined. Moreover, this construction ensure that \( f(\tilde{\gamma}) \in M_1 \) and \( \tilde{\gamma} \subset \Lambda f(\tilde{\gamma}) \setminus \{f(\tilde{\gamma})\} \). Applying inequality (23a) then yields

\[
\frac{\pi_n(M_2 \mid Y)}{\pi_n(\gamma \mid Y)} = \sum_{\gamma \in M_2} \frac{\pi_n(\gamma \mid Y)}{\pi_n(\gamma \mid Y)} \leq \sum_{\exists \tilde{\gamma} \in M_2 \text{ such that } \tilde{\gamma} = f(\gamma)} \frac{\pi_n(\tilde{\gamma} \mid Y)}{\pi_n(\gamma \mid Y)} \cdot \left\{ \frac{1}{1 - 1/p} - 1 \right\}
\]

Then by treating \( \tilde{\gamma} = f(\gamma) \in M_1 \) as the \( \gamma \) in inequality (30) and inequality (31), we obtain that under the event \( A_n \cap B_n \cap C_n \cap D_n \)

\[
\frac{\pi_n(M_2 \mid Y)}{\pi_n(\gamma \mid Y)} \leq \sum_{\exists \tilde{\gamma} \in M_2 \text{ such that } \tilde{\gamma} = f(\gamma)} \frac{\pi_n(\tilde{\gamma} \mid Y)}{\pi_n(\gamma \mid Y)} \cdot \left\{ \frac{1}{1 - 1/p} - 1 \right\}
\]

\[
\leq \frac{2}{p} \sum_{\tilde{\gamma} \in M_1} \frac{\pi_n(\tilde{\gamma} \mid Y)}{\pi_n(\gamma \mid Y)}
\]

\[
= \frac{2}{p} \frac{\pi_n(M_1 \mid Y)}{\pi_n(\gamma \mid Y)}
\]

\[
\leq \frac{4}{p}
\]

Combining inequality (31) and inequality (32), we obtain that that under the event \( A_n \cap B_n \cap C_n \cap D_n \), the posterior ratio is upper bounded as

\[
\frac{\pi_n(\Lambda(\gamma) \mid Y)}{\pi_n(\gamma \mid Y)} = \frac{\pi_n(M_1 \mid Y)}{\pi_n(\gamma \mid Y)} + \frac{\pi_n(M_2 \mid Y)}{\pi_n(\gamma \mid Y)} \leq 6.
\]  

The above argument is also valid for \( \gamma = \gamma^* \), and this completes the proof of inequality (23b).

### 4.4 Proof of Theorem [1]

We divide the analysis into two steps. In the first step, we show that the total posterior probability assigned to models with size \( \mathcal{O}(s^*) \) other than \( \gamma^* \) is small. In the second step, we use the fact that all large models receive small prior probabilities to show that the remaining models should also receive small posterior probability.

**Step 1:** Let \( M_S := \{\gamma \in \{0,1\}^p : |\gamma| \leq Ks^*, \gamma \neq \gamma^*\} \) denote the set of all models with moderate sizes, where \( K \geq 1 \) some constant to be determined in step 2. Consider the quantity

\[
\frac{\pi_n(M_S \mid Y)}{\pi_n(\gamma^* \mid Y)} = \sum_{\gamma \in M_S} \frac{\pi_n(\gamma \mid Y)}{\pi_n(\gamma^* \mid Y)}.
\]

Similar to Lemma [3] we modify the definition of the four events \( A_n, B_n, C_n \) and \( D_n \) by replacing \( M \) with \( M_S \). Following the proof of Lemma [3] it is straightforward to show that
these four events satisfy
\[
P \left[ A_n \cap B_n \cap C_n \cap D_n \right] \geq 1 - 6p^{-c}.
\] (35)

The following auxiliary lemma ensures that when these four events hold, then the posterior ratios on the right hand side of equation (34) are well controlled.

**Lemma 7.** Under Assumptions A–D and under the event \( A_n \cap B_n \cap C_n \cap D_n \), the posterior ratio of any \( \gamma (\neq \gamma^*) \) in \( M_S \) is bounded as
\[
\frac{\pi_n(\gamma | Y)}{\pi_n(\gamma^* | Y)} \leq \begin{cases} 
p^{-2|\gamma \setminus \gamma^*|}, & \text{if } \gamma \text{ is overfitted}, 
p^{-2|\gamma| - 2}, & \text{if } \gamma \text{ is underfitted}. \end{cases}
\]

We prove this lemma in Appendix [C].

Equipped with this lemma, a simple counting argument yields that under the event \( A_n \cap B_n \cap C_n \cap D_n \),
\[
\pi_n(\gamma | Y) \leq \sum_{k=1}^{\infty} p^k p^{-2k} + \sum_{\ell=0}^{\infty} p^\ell p^{-2\ell - 2} \leq 3p^{-1},
\] (36)

where in step (i), we used the fact that there are at most \( p^k \) overfitted models \( \gamma \) with \( |\gamma \setminus \gamma^*| = k \) and at most \( p^\ell \) underfitted models \( \gamma \) with \( |\gamma| = \ell \). Combining this with inequality (35), we obtain that with probability at least \( 1 - 6p^{-c} \),
\[
\pi_n(\gamma | Y) \leq 3p^{-1} \pi_n(\gamma^* | Y) \leq 3p^{-1}.
\]

**Step 2:** Let \( M_L := \{ \gamma \in \{0, 1\}^p : |\gamma| \geq Ks^* + 1 \} \) denote the set of large models. By Bayes’ theorem, we can express the posterior probability of \( M_L \) as
\[
\pi_n(\gamma | Y) = \frac{\sum_{\gamma \in M_L} \int \theta, \phi \frac{dP_{\beta, \phi}}{dP_0} (Y) \pi_n(d\theta, d\phi, \gamma)}{\sum_{\gamma \in \{0, 1\}^p} \int \theta, \phi \frac{dP_{\beta, \phi}}{dP_0} (Y) \pi_n(d\theta, d\phi, \gamma)},
\] (37)

where \( P_{\beta, \phi, \gamma} \) and \( P_0 \) stand for probability distribution of \( Y \) under parameters \((\beta, \phi, \gamma)\) and the true data generating model, respectively. We bound the numerator and denominator separately.

First consider the numerator. According to our specification of the sparsity prior (5d) for the binary indicator vector \( \gamma \), the prior probability of \( M_L \) satisfies
\[
\pi_n(M_L) = \sum_{\gamma : |\gamma| \geq Ks^* + 1} \pi_n(\gamma) \leq p^{-Ks^* - 1}.
\]

By Fubini’s theorem we have the following bound for the expectation of the numerator:
\[
E_0 \left[ \sum_{\gamma \in M_L} \int \theta, \phi \frac{dP_{\beta, \phi, \gamma}}{dP_0} (Y) \pi_n(d\theta, d\phi, \gamma) \right] = \sum_{\gamma \in M_L} \int \theta, \phi \left[ E_0 \left( \frac{dP_{\beta, \phi, \gamma}}{dP_0} (Y) \right) \pi_n(d\theta, d\phi, \gamma) \right] \pi_n(d\theta, d\phi, \gamma)
\]
\[
= \sum_{\gamma \in M_L} \int \theta, \phi \pi_n(d\theta, d\phi, \gamma) = \pi_n(M_L) \leq p^{-Ks^* - 1},
\]
where we have used the fact that \( \mathbb{E}_0 \left[ \frac{dP_{\beta, \phi, \gamma}}{dP_0} (Y) \right] = 1 \). Therefore, by applying Markov’s inequality we have

\[
P_0 \left[ \sum_{\gamma \in \mathcal{M}_L} \int_{\theta, \phi} \frac{dP_{\beta, \phi, \gamma}}{dP_0} (Y) \pi_n (d\theta, d\phi, \gamma) \leq p^{-Ks^*/2 - 1} \right] \geq 1 - p^{-Ks^*/2}. \tag{38}
\]

By the expression (41) of the marginal likelihood function, we can bound the denominator from below by

\[
\int_{\theta, \phi} \frac{dP_{\beta, \phi, \gamma^*}}{dP_0} (Y) \pi_n (d\theta, d\phi, \gamma^*) = \frac{\mathcal{L}_n (Y | \gamma^*) \pi_n (\gamma^*)}{dP_0 (Y)}
\]

\[
= \Gamma \left( \frac{d}{2} \right) (1 + g)^{n/2} (1 + g)^{-s^*/2} \left( \frac{1}{\mathbb{T} Y \mathbb{L} P \mathbb{D}} \right) \Gamma \left( \frac{d}{2} \right) \left( \frac{1}{\mathbb{T} Y \mathbb{L} P \mathbb{D}} \right)^{-s^*/2} \cdot c \exp \left\{ (2\sigma_0^2)^{-1} (||Y||_2^2 - ||\tilde{w}||_2^2 - ||Y||_2^2 / g) \right\} \frac{u^{-n/2} e^{u/2}}{f(u)} \frac{1}{1/f(n)}
\]

where \( \tilde{w} = w + X_{\mathcal{S}^c}^* \mathcal{S}^c \sim N(0, \sigma_0^2) \). Under the true data-generating model \( P_0 \), the density for \( Y \) is \( \sigma_0^{-n} (2\pi)^{-n/2} \exp \left\{ -\frac{1}{2} \right\} \). By applying the the lower bound \( \Gamma \left( (n-2) \right) \geq \left( (2\pi)^{-1} \right) \left( (n-2) \right)^{n/2-1} e^{-n/2+1} \) and using the fact that the projection operator \( I - \Phi_{\gamma^*} \) is non-expansive, we obtain

\[
\int_{\theta, \phi} \frac{dP_{\beta, \phi, \gamma^*}}{dP_0} (Y) \pi_n (d\theta, d\phi, \gamma^*) \geq c \exp \left\{ (2\sigma_0^2)^{-1} (||w||_2^2 - ||\tilde{w}||_2^2 - ||Y||_2^2 / g) \right\} \frac{u^{-n/2} e^{u/2}}{f(u)} \frac{1}{1/f(n)}
\]

where \( u = \sigma_0^{-2} (||\tilde{w}||_2^2 + ||Y||_2^2 / g) \). Since \( g^{-1} \leq n^{-1} \) and the function \( f(u) = u^{-n/2} e^{u/2} \) attains its minimum at \( u = n \), we further obtain

\[
\int_{\theta, \phi} \frac{dP_{\beta, \phi, \gamma^*}}{dP_0} (Y) \pi_n (d\theta, d\phi, \gamma^*) \geq c \exp \left\{ (2\sigma_0^2)^{-1} (||w||_2^2 - ||\tilde{w}||_2^2 - ||Y||_2^2 / g) \right\},
\]

with a different universal constant \( c \).

The off-support \( \mathcal{S}^c \) condition in Assumption A and the high probability bound for the event \( \mathcal{C}_n \cap \mathcal{D}_n \) in Lemma 3 imply that the last exponential term is of order \( p^{-c_1 L} \) for some universal constant \( c' \) with probability at least \( 1 - p^{-c_2} \). Therefore, for \( K \geq 4 + \alpha + 2c_1 L \), we have

\[
\int_{\theta, \phi} \frac{dP_{\beta, \phi, \gamma^*}}{dP_0} (Y) \pi_n (d\theta, d\phi, \gamma^*) \geq c \exp \left\{ (2\sigma_0^2)^{-1} (||w||_2^2 - ||\tilde{w}||_2^2 - ||Y||_2^2 / g) \right\},
\]

Combining equations (37), (38) and (39), we obtain that

\[
\pi_n (\mathcal{M}_L | Y) \leq c p^{-1} \tag{40}
\]

holds with probability at least \( 1 - 2 p^{-c'} \).

Finally, inequalities (36) and (40) in steps 1 and 2 together yield that

\[
\pi_n (\gamma^* | Y) = 1 - \pi_n (\mathcal{M}_S | Y) - \pi_n (\mathcal{M}_L | Y) \geq 1 - c_3 p^{-1},
\]

holds with probability at least \( 1 - 8 p^{-c'} \), which completes the proof.
4.5 Proof of Corollary 2

Let \( P_t \) denote the probability distribution of iterate \( \gamma_t \) in the MCMC algorithm. According to the definition of \( \epsilon \)-mixing time, for any \( t \geq \tau_{1/p} \), we are guaranteed that
\[
\left| P_t(\gamma^*) - \pi_n(\gamma^*) \right| \leq \frac{1}{p}.
\]
By Theorem 1, the posterior probability of \( \gamma^* \) satisfies \( \pi_n(\gamma^*) \geq 1 - c_1 p^{-1} \) with probability at least \( 1 - c_2 p^{-c_3} \). By Theorem 2, the \( p^{-1} \)-mixing time \( \tau_{1/p} \) satisfies
\[
\tau_{1/p} \leq c_1 p s_0^2 \left( c_2 \alpha (n + s_0) \log p + \log p + 2 \right)
\]
with probability at least \( 1 - 4p^{-c_3} \). Combining the three preceding displays, we find that
\[
P_t(\gamma^*) \geq 1 - (c_1 + 1) p^{-1},
\]
as claimed.

5 Discussion

In this paper, we studied the computational complexity of MCMC methods for high-dimensional Bayesian linear regression under a sparsity constraint. We show that under a set of conditions that guarantees Bayesian variable-selection consistency, the corresponding MCMC algorithm achieves rapid mixing. Our result on the computational complexity of Bayesian variable-selection example provides insight into the dynamics of the Markov chain methods applied to statistical models with good asymptotic properties. It suggests that contraction properties of the posterior distribution are useful not only in guaranteeing desirable statistical properties such as parameter estimation or model selection consistency, but they also have algorithmic benefits in certifying the rapid mixing of the Markov chain methods designed to draw samples from the posterior.

As a future direction, it is interesting to investigate the mixing behavior of the MCMC algorithm when Bayesian variable selection fails. For example, slow mixing behavior is observed empirically in the intermediate SNR regime in our simulated example and it would be interesting to understand this result theoretically. Another interesting direction is to consider the computational complexity of MCMC methods for models more complex than linear regression, for example, high-dimensional nonparametric additive regression. A third direction is to investigate whether the upper bound on mixing time provided in Theorem 2 is sharp up to constants.

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A Further details on Metropolis-Hastings

In Appendix A, we show that under the specified model, the maximum a posteriori solution (MAP) of the Bayesian variable-selection problem is equivalent to the following optimization problem with \( \ell_0 \)-penalty
\[
\hat{\gamma} = \arg \min_{|\gamma| \leq s_0} \left\{ \frac{n}{2} \log \left[ 1 + g \left( 1 - \frac{Y^T \Phi \gamma}{\|Y\|_2^2} \right) \right] + \lambda |\gamma| \right\},
\]
where $\Phi_\gamma = X_\gamma (X_\gamma^T X_\gamma)^{-1} X_\gamma^T$ is the projection onto the column space of $X_\gamma$, and the regularization parameter $\lambda := \frac{1}{2} \log(1 + g) + \kappa \log p$. Here the penalty $\lambda \mid \gamma$ comes from two sources: the penalty $\kappa \log p \mid \gamma$ on $\gamma$ and the Occam’s razor penalty $\frac{1}{2} \log(1 + g) \mid \gamma$ due to the integration over the model parameter $\beta_\gamma$. Therefore, choosing an appropriate hyperparameter $\kappa$ in the Bayesian approach is equivalent to choosing a corresponding regularization parameter $\lambda$ in the penalization method: a small $\kappa$ could make the posterior include uninfluential covariates due to noise; a large $\kappa$ requires the signal-to-noise ratio $\beta_\gamma / \sigma$ of influential covariates to be large enough so that they can be selected out by the posterior.

A.1 Connections to MAP estimates

Under the Bayesian model specified by equation (5), we can obtain a closed-form expression for the marginal likelihood of the indicator vector $\gamma$ by integrating out $\beta_\gamma$ and $\phi$:

$$L_n(Y \mid \gamma) := \pi_n(Y \mid \gamma) = \int dP_{\beta, \phi, \gamma}(Y) \pi_n(d\beta, d\phi \mid \gamma) = \frac{\Gamma\left(\frac{n}{2}\right) (1 + g)^{n/2}}{\pi^{n/2} \|Y\|_2^n} \frac{(1 + g)^{-|\gamma|/2}}{(1 + g(1 - R_\gamma^2))^{n/2}},$$

(41)

where $\Gamma(\cdot)$ the Gamma function, $P_{\beta, \phi, \gamma}$ is the distribution of $(\beta, \phi, \gamma)$, and $R_\gamma^2$ is the coefficient of determination for the model $M_\gamma$

$$R_\gamma^2 = \frac{Y^T \Phi_\gamma Y}{\|Y\|_2^n},$$

with $\Phi_\gamma = X_\gamma (X_\gamma^T X_\gamma)^{-1} X_\gamma^T$ the projection onto the column space of $X_\gamma$. When there is no confusion, we identify the variable inclusion vector $\gamma$ and the linear model $M_\gamma$ associated with it. Let $\mathcal{M} := \{\gamma : |\gamma| \leq s_0\}$ denote the entire model space, which is a subset of the $p$-dimensional hypercube $\{0, 1\}^p$ under our identification. Then, by Bayes’ theorem the posterior probability of $\gamma$ is given by

$$\pi_n(\gamma \mid Y) = C \cdot \frac{1}{p^{|\gamma|}} \cdot \frac{(1 + g)^{-|\gamma|/2}}{(1 + g(1 - R_\gamma^2))^{n/2}} 1[|\gamma| \in \mathcal{M}],$$

(42)

where $C$ is a normalization constant.

According to the preceding display, the maximum a posteriori (MAP) solution of the Bayesian variable-selection problem is equivalent to the following penalized optimization problem $\ell_0$-penalty

$$\hat{\gamma} = \arg \min_{|\gamma| \leq s_0} \left\{ \frac{n}{2} \log \left[ 1 + g \left( 1 - \frac{Y^T \Phi_\gamma Y}{\|Y\|_2^n} \right) \right] + \lambda |\gamma| \right\},$$

where the regularization parameter $\lambda := \frac{1}{2} \log(1 + g) + \kappa \log p$. Conversely, if we have a variable-selection procedure based on the penalization method with $\ell_0$-penalty

$$\hat{\gamma} = \arg \min_{\gamma : |\gamma| \leq s_0} \left\{ f(Y, \gamma) + \lambda |\gamma| \right\},$$

where $f(Y, \gamma)$ is some function reflecting the goodness of fit by using model $M_\gamma$, then we can construct a pseudo-posterior distribution

$$\tilde{\pi}_n(\gamma | Y) = \tilde{C} \cdot e^{-\lambda |\gamma|} \cdot e^{-f(Y, \gamma)} 1[|\gamma| \leq s_0]$$

29
with \( \tilde{C} \) is a normalization constant, and conduct Bayesian inference based on \( \tilde{\pi}_n \). For example, when \( f(Y, \gamma) \) is the negative profile log-likelihood \( \frac{n}{2} \log \left( \frac{1}{n} \| (I - \Phi_\gamma) Y \|_2^2 \right) \), where the regression coefficient \( \beta_\gamma \) and the precision parameter \( \phi \) have been profiled out from the log-likelihood given \( \gamma \) by maximization, then the choice of \( \lambda = 1 \) corresponds to the Akaike information criterion, or AIC for short [1], \( \lambda = \log n/2 \) the Bayesian information criterion, or BIC for short [27]), and \( \lambda = \alpha \log p (\alpha \geq 1) \) the high-dimensional BIC [36]. Our conclusion on the MCMC complexity of Bayesian variable selection with Zellner’s g-prior applies to BIC in the low-dimensional regime where \( p = o(n) \), and to high-dimensional BIC in the high-dimensional regime where \( p \geq n \). Because of the Bayesian interpretation for \( \pi_n(\gamma | Y) \) in equation (42), we will focus on this posterior distribution over the model space. 

A.2 Example of slow mixing

Suppose \( p = n \) and \( g = p^{2\alpha} \) with \( \alpha > 1 \). Let \( Y = w \sim \mathcal{N}(0, I_n) \). We claim that if we use the untruncated distribution \( \pi_n(\gamma) = C p^{-|\gamma|} \) as the prior for the variable-selection indicator vector over the entire space \( \{0, 1\}^p \), then the mixing time of the Markov chain with transition probability specified by formula (3) grows exponentially in \( n \) with probability \( \alpha \geq 1/2 \) with respect to the randomness of \( w \). Moreover, it is easy to check that this example satisfies the conditions in Theorem 1, which imply Bayesian variable-selection consistency. As a consequence, this example suggests that although a size constraint \( \gamma \leq s_0 \) such as the one in the sparsity prior [34], is not needed for Bayesian model selection consistency, it is necessary for MCMC to mix rapidly.

Proof of slow mixing: We use the following conductance argument: for any reversible Markov chain \( C \) over a finite state space, the spectral gap is upper bounded as

\[
1 - \lambda_2 \leq 2 \Phi_C, \tag{43}
\]

where the quantity

\[
\Phi_C := \min_{A \subseteq \mathcal{A} : 0 < \pi(B) < 1} \Phi_C(A), \quad \text{where} \quad \Phi_C(A) := \frac{\sum_{\gamma \in A} \pi(\gamma) P(\gamma, A^C)}{\pi(A) \pi(A^C)} \tag{44}
\]

is called the conductance of \( C \) [30].

Now we analyze the mixing time of the Markov chain in the previous example. Use the notation 1 to denote the full model. Under the prior choice in the theorem, the posterior has an expression as

\[
\pi_n(\gamma | Y) \propto \frac{1}{p^{|\gamma|}} \cdot \frac{(1 + g)^{-|\gamma|/2}}{(1 + g(1 - R_\gamma^2))^{n/2}} \quad \text{for} \quad \gamma \in \{0, 1\}^p. \tag{45}
\]

Now we apply inequality [43] and equation (44) with \( B = \{1\} \) to obtain

\[
1 - \lambda_2 \leq 2 \Phi_C \leq \frac{2 \sum_{i=1}^n \pi_n(1 | Y) P(1, 1-j)}{\pi_n(1 | Y) (1 - \pi_n(1 | Y))} = \frac{2 \sum_{i=1}^n P(1, 1-j)}{1 - \pi_n(1 | Y)},
\]

where we have used the fact that under the transition probability specification (3), the only “neighbor” of 1 is \( 1_j \) for \( j = 1, \ldots, n \), i.e. \( \gamma (\neq 1) \) satisfies \( P(1, \gamma) > 0 \) if and only if \( \gamma = 1_{-j} \) for some \( j \in \{1, \ldots, n\} \). Using (3) and the last display, we can further obtain

\[
1 - \lambda_2 \leq \frac{\sum_{i=1}^n \min \{1, \frac{\pi_n(1_{-j} | Y)}{\pi_n(1_{-j} | Y)}\}}{n(1 - \pi_n(1 | Y))}. \tag{46}
\]
We consider the numerator of the right-hand side in equation (46) first. Since the true model is the null model, we have

\[
\frac{\pi_n(1 - j \mid Y)}{\pi_n(1 \mid Y)} = \frac{n^\kappa(1 + g)^{1/2}}{(1 + gw^T(I - P_{-j})w/(w^Tw))^{n/2}},
\]

(47)

where \( P_{-j} \) is the projection onto \( X_{-j} \). Since \( \{w^T(I - P_{-j})w\}_{j=1}^n \) are \( \chi^2 \) random variables, by the union bound and the tail probability of \( \chi^2 \) distribution, we have that for constant \( c_1 \) sufficiently small,

\[
\mathbb{P}\left( \min_{j=1,...,n} w^T(I - P_{-j})w \leq \frac{c_1}{n^2} \right) \geq 1 - n \cdot \frac{1}{4n} = \frac{3}{4}.
\]

Moreover, by a standard tail bound for the \( \chi^2 \) distribution ([19], Lemma 1) we have

\[
\mathbb{P}\left( w^Tw \leq \frac{3}{2} \right) \geq \frac{3}{4}.
\]

Combining the last two displays, we obtain

\[
\mathbb{P}\left( \min_{j=1,...,n} \frac{w^T(I - P_{-j})w}{\|w\|^2} \geq \frac{c_2}{n^2} \right) \geq \frac{1}{2},
\]

where \( c_2 = 2c_1/3 \). Combining the above with equation (47), we obtain

\[
\mathbb{P}\left( \min_{j=1,...,n} \frac{\pi_n(1 - j \mid Y)}{\pi_n(1 \mid Y)} \leq e^{-c_3gn^{-2}} \right) \geq \frac{1}{2},
\]

(48)

where we have used the inequality \( 1 + x \leq e^x \) for \( x \in \mathbb{R} \) and \( c_3 \) is some universal constant.

Now we consider the denominator of the right-hand side in (46). Recall that \( \mathbf{0} \) denotes the indicator vector in \( \{0,1\}^p \) associated with the null model. By equation (45), we have

\[
\pi_n(1 \mid Y) = \frac{(1 + g)^{-n/2}}{n^{\kappa n}} = n^{-\kappa n} \leq \frac{1}{2},
\]

for \( n \geq 2 \). This implies

\[
\pi_n(1 \mid Y) = \frac{\pi_n(1 \mid Y)}{\sum_{\gamma \in \mathcal{M}} \pi_n(\gamma \mid Y)} \leq \frac{\pi_n(1 \mid Y)}{\pi_n(0 \mid Y)} \leq \frac{1}{2}.
\]

Combining equations (46), (48) and (49) yields

\[
\mathbb{P}\left( 1 - \lambda_2 \leq 2e^{-c_3gn^{-2}} \right) \geq \frac{1}{2},
\]

which completes the proof of the claimed result.

B Proof of inequality (23a) in Lemma 4

Since \( \gamma \neq \gamma^* \), we know that \( \gamma' := \mathcal{G}(\gamma) \neq \gamma \). We divide the proof into the following three disjoint cases:

- model \( \gamma \) is overfitted,
- model \( \gamma \) is underfitted and unsaturated,
- model \( \gamma \) is underfitted and saturated.
B.1 Case \( \gamma \) is overfitted

Let \( \ell_\gamma \) be the index selected from the set \( \gamma \setminus \gamma^* \) of uninfluential covariates in our construction of the transition function \( G \), i.e. \( \gamma' = \gamma \setminus \{ \ell_\gamma \} \). We can express the posterior probability ratio as

\[
\frac{\pi_n(\gamma | Y)}{\pi_n(\gamma' | Y)} = \frac{1}{p^n \sqrt{1 + g}} \cdot \left( \frac{1 + g(1 - R_{\gamma'}^2)}{1 + g(1 - R_\gamma^2)} \right)^{n/2}
\]

Applying the Cauchy-Schwarz inequality yields

\[
\| (I - \Phi_\gamma)(X_{(\gamma')c} \beta_{(\gamma')c}^{\gamma} + w) \|_2^2 \leq \frac{1}{2} \| (I - \Phi_\gamma)w \|_2^2 - 2\| X_{(\gamma')c} \beta_{(\gamma')c}^{\gamma} \|_2^2 \]

where in step (i) we used the fact that the projection is a non-expansive mapping and in step (ii) we used the assumption \( \| X_{(\gamma')c} \beta_{(\gamma')c}^{\gamma} \|_2^2 \leq \bar{L}\sigma_0^2 \log p \). Similarly, since \( \gamma' \subset \gamma \), we obtain the following inequality for the quantity \( R_{\gamma'}^2 - R_\gamma^2 \)

\[
R_{\gamma'}^2 - R_\gamma^2 = \frac{\| (\Phi_\gamma - \Phi_{\gamma'}) (X_{(\gamma')c} \beta_{(\gamma')c}^{\gamma} + w) \|_2^2}{\| Y \|_2^2} \leq \frac{2\| (\Phi_\gamma - \Phi_{\gamma'}) w \|_2^2}{\| Y \|_2^2} \leq 2\bar{L}\sigma_0^2 \log p.
\]

On the event \( A_n \cap B_n \cap C_n \), we have

\[
\| (I - \Phi_\gamma)w \|_2^2 \geq \frac{1}{2} n - r s_0 \log p \geq \frac{3n}{8}, \quad \text{and} \quad \| (\Phi_\gamma - \Phi_{\gamma'})w \|_2^2 \leq (|\gamma| - |\gamma'|) L\sigma_0^2 \log p = L\sigma_0^2 \log p,
\]

where we have used the assumption \( 4r s_0 \log p \leq n \). Combining these two inequalities with the preceding two displays, we obtain that the posterior probability ratio on the event \( A_n \cap B_n \cap C_n \) is bounded as

\[
\frac{\pi_n(\gamma | Y)}{\pi_n(\gamma' | Y)} \leq \frac{1}{p^n \sqrt{g}} \cdot \left( 1 + \frac{2(L + \bar{L}) \log p}{n/8} \right)^{n/2} \leq \frac{1}{p^n \sqrt{g}} \cdot \exp \left\{ \frac{16L + \bar{L}}{n} \log p \right\} = p^{8(L + \bar{L}) - 1 - \alpha - \kappa} \leq p^{-2}, \tag{50}
\]

where in step (i) we used the inequality \( 1 + x \leq e^x \) for \( x \in \mathbb{R} \) and the last step follows since \( \sqrt{g} \asymp p^\alpha \) with \( \alpha \geq 8(L + \bar{L}) + 1 - \kappa \) according to our choice of the hyperparameter, which completes the proof of the overfitted case.
B.2 Case $\gamma$ is underfitted and unsaturated

This case happens only when $s^* \geq 1$. Let $j_\gamma$ be the index in our construction of the transition function $G$, i.e. the index from the set $\gamma^* \setminus \gamma$ that maximizes $\|\Phi_{\gamma \cup \{j\}} X_{\gamma^* \setminus \gamma} \|_2^2$ over $j \in \gamma^* \setminus \gamma$. Then we have $\gamma' = \gamma \cup \{j_\gamma\}$, implying that $\Phi_{\gamma'} - \Phi_{\gamma}$ is a projection operator. Therefore, we can write

$$1 - R_{\gamma}^2 - (1 - R_{\gamma}^2) = \frac{Y^T(\Phi_{\gamma'} - \Phi_{\gamma})Y}{\|Y\|_2^2} = \frac{\| (\Phi_{\gamma'} - \Phi_{\gamma}) X_{\gamma\setminus\gamma} \beta_{\gamma^*}^* + (\Phi_{\gamma'} - \Phi_{\gamma}) X_{(\gamma^* \setminus \gamma) \setminus \gamma} \beta_{(\gamma^* \setminus \gamma)^*} + (\Phi_{\gamma'} - \Phi_{\gamma}) w \|_2^2}{\|Y\|_2^2} \geq \left( \frac{\| (\Phi_{\gamma'} - \Phi_{\gamma}) X_{\gamma\setminus\gamma} \beta_{\gamma^*}^* \|_2 - \| (\Phi_{\gamma'} - \Phi_{\gamma}) X_{(\gamma^* \setminus \gamma) \setminus \gamma} \beta_{(\gamma^* \setminus \gamma)^*} \|_2 - \| (\Phi_{\gamma'} - \Phi_{\gamma}) w \|_2^2}{\|Y\|_2^2} \right)^2.$$

By the $\beta_{\text{min}}$-condition and Lemma 8 at the end of this appendix, we have

$$\| (\Phi_{\gamma'} - \Phi_{\gamma}) X_{\gamma\setminus\gamma} \beta_{\gamma^*}^* \|_2 \geq \nu \frac{\| (I - \Phi_{\gamma}) X_{\gamma\setminus\gamma} \beta_{\gamma^*}^* \|_2^2}{\|\gamma^* \setminus \gamma\|} \geq n\nu^2 \frac{\|\beta_{\gamma^* \setminus \gamma}^*\|_2^2}{s^*} \geq \nu^2 C_{\beta} \sigma_0^2 \log p,$$

where $C_{\beta} := c_0 (L + \tilde{L} + \alpha + \kappa)$ denotes the coefficient in the $\beta_{\text{min}}$-condition of the theorem. The last display shows that at least an amount of $\nu^2 C_{\beta} \sigma_0^2 \log p$ variation in the true signal $X_{\gamma\setminus\gamma} \beta_{\gamma^*}^*$ can be explained by adding the influential covariate $X_{j_\gamma}$ into the current model $\gamma$. Combining the above two displays, we obtain that for $n$ sufficiently large, so that $\nu \sqrt{C_{\beta}} \geq 2 \sqrt{L + \tilde{L}}$, the following holds under the event $A_n$

$$1 - R_{\gamma}^2 - (1 - R_{\gamma}^2) \geq \frac{nu^2 \|\beta_{\gamma^* \setminus \gamma}^*\|_2^2}{4s^* \|Y\|_2^2}.$$

Similarly, we have that under the event $C_n$,

$$1 - R_{\gamma}^2 = \frac{Y^T(I - \Phi_{\gamma})Y}{\|Y\|_2^2} \leq \frac{\| (I - \Phi_{\gamma}) X_{\gamma\setminus\gamma} \beta_{\gamma^*}^* \|_2 + \| (\Phi_{\gamma'} - \Phi_{\gamma}) X_{(\gamma^* \setminus \gamma) \setminus \gamma} \beta_{(\gamma^* \setminus \gamma)^*} \|_2 + \| (I - \Phi_{\gamma}) w \|_2^2}{\|Y\|_2^2} \leq \frac{2 \| (I - \Phi_{\gamma}) X_{\gamma\setminus\gamma} \beta_{\gamma^*}^* \|_2^2 + 4 \| (\Phi_{\gamma'} - \Phi_{\gamma}) X_{(\gamma^* \setminus \gamma) \setminus \gamma} \beta_{(\gamma^* \setminus \gamma)^*} \|_2^2 + 4 \| (I - \Phi_{\gamma}) w \|_2^2}{\|Y\|_2^2} \leq \frac{2 \| (I - \Phi_{\gamma}) X_{\gamma\setminus\gamma} \beta_{\gamma^*}^* \|_2^2 + 4 \tilde{L} \sigma_0^2 \log p + 3n\sigma_0^2}{\|Y\|_2^2} \leq \frac{4 \| (I - \Phi_{\gamma}) X_{\gamma\setminus\gamma} \beta_{\gamma^*}^* \|_2^2}{\|Y\|_2^2}$$

where in step (i) we have used Assumption A, the fact that $\| (I - \Phi_{\gamma}) w \|_2^2 \leq \|w\|_2^2$, and the last step uses $2 \| (I - \Phi_{\gamma}) X_{\gamma\setminus\gamma} \beta_{\gamma^*}^* \|_2^2 \geq 2nu \|\beta_{\gamma^* \setminus \gamma}^*\|_2^2 \geq 4 \tilde{L} \sigma_0^2 \log p + 3n\sigma_0^2$ for $C_{\beta} \geq (4L + 3)/\nu$. Combining the above two displayed inequalities, we obtain that for $C_{\beta}$ sufficiently large, so that $\nu^2 C_{\beta} \geq 64 (\alpha + \kappa + 3)$, the posterior probability ratio $\frac{\pi_n(\gamma|Y)}{\pi_n(\gamma'|Y)}$ under the event $A_n \cap C_n \cap D_n$
satisfies
\[
\frac{\pi_n(\gamma \mid Y)}{\pi_n(\gamma' \mid Y)} = p^* \sqrt{1 + g} \cdot \left(1 - \frac{\|Y\|_2^2(1 - R_\gamma^2 - (1 - R_{\gamma'}^2))}{\|Y\|_2^2 / g + Y^T(I - \Phi_Y)Y}\right)^{n/2}
\leq p^* \sqrt{1 + g} \cdot \left(1 - \frac{\nu\| (I - \Phi_{\gamma})X_{\gamma \setminus \gamma'}\beta_{\gamma'}^* \|^2 / (4s^*)}{4n\sigma_0^2 / s^* + 4\nu\| (I - \Phi_{\gamma})X_{\gamma \setminus \gamma'}\beta_{\gamma'}^* \|^2}\right)^{n/2}
\leq p^* \sqrt{1 + g} \cdot \left(1 - \min\left\{\frac{\nu}{32s^*}, \frac{\nu^2 C_{\beta} \log p}{32n}\right\}\right)^{n/2}
\leq p^* \cdot p^{-\alpha} \cdot p^{-(\alpha + \kappa + 3)}
= p^{-3},
\] (53)
where in step (i) we have used the inequality \(a/(b + a) \geq \min\{1/2, a/(2b)\}\) for any \(a, b > 0\) and inequality (51), and step (ii) follows by our assumption on \(C_{\beta}\) and Assumption D on \(s^*\).

### B.3 Case \(\gamma\) is underfitted and saturated

This case happens only when \(s^* \geq 1\). Let \(j_\gamma\) and \(k_\gamma\) be the indices defined in the construction of \(G(\gamma)\) in the underfitted and saturated case. Then we have \(\gamma' = \gamma \cup \{j_\gamma\} \setminus \{k_\gamma\}\). Let \(v_1 = (\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_\gamma)X_{\gamma \setminus \gamma'}\beta_{\gamma'}^*\) and \(v_2 = (\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_{\gamma'})X_{\gamma \setminus \gamma'}\beta_{\gamma'}^*\). Then Lemma [B.3] stated and proved in Appendix [B.3] guarantees that
\[
\|v_1\|^2 \geq \nu\| (I - \Phi_\gamma)X_{\gamma \setminus \gamma'}\beta_{\gamma'}^* \|^2 \geq n\nu^2\| \beta_{\gamma \setminus \gamma'}^* \|^2 / s^* \quad \text{and}
\|v_2\|^2 \leq n\nu \omega(X)\| \beta_{\gamma \setminus \gamma'}^* \|^2 / s^* \leq 1/2n\nu^2\| \beta_{\gamma \setminus \gamma'}^* \|^2 / s^* \leq 1/2\nu\| (I - \Phi_\gamma)X_{\gamma \setminus \gamma'}\beta_{\gamma'}^* \|^2 / |\gamma \setminus \gamma'|, \quad \text{under Assumption D on } s_0.
\] (54)
This inequality shows that a larger proportion of the true signal \(X_{\gamma \setminus \gamma'}\beta_{\gamma'}^*\) can be explained when the unimportant covariate \(X_{k_\gamma}\) is replaced with the influential covariate \(X_{j_\gamma}\) in the current model \(\gamma\). By letting \(\tilde{w} = w + X_{(\gamma \setminus \gamma')c} \beta_{(\gamma \setminus \gamma')c}\) be the effective noise, we have
\[
1 - R_\gamma^2 - (1 - R_{\gamma'})^2 = \frac{Y^T(\Phi_{\gamma'} - \Phi_\gamma)Y}{\|Y\|_2^2} = \frac{Y^T(\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_\gamma)Y - Y^T(\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_{\gamma'})Y}{\|Y\|_2^2}
= \frac{\|v_1\|^2 + 2v_1^T \tilde{w} + \tilde{w}^T(\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_\gamma)\tilde{w} - \left\{\|v_2\|^2 + 2v_2^T \tilde{w} + \tilde{w}^T(\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_{\gamma'})\tilde{w}\right\}}{\|Y\|_2^2}
\geq \frac{1}{\|Y\|_2^2} \left\{\|v_1\|^2, \|v_1\|^2 - 2\| (\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_\gamma)\tilde{w}\|^2, \|v_2\|^2, \|v_2\|^2 - 2\| (\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_{\gamma'})\tilde{w}\|^2\right\},
\] (55)
where in the last step we applied the Cauchy-Schwarz inequality to the two cross terms \(v_1^T w = v_1^T(\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_\gamma)w\) and \(v_2^T w = v_2^T(\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_{\gamma'})w\). Note that under the event \(A_n\), the Cauchy-Schwarz inequality guarantees that
\[
\| (\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_\gamma)\tilde{w}\|^2 \leq 2\| (\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_\gamma)w\|^2 + 2\| X_{(\gamma \setminus \gamma')c}\beta_{(\gamma \setminus \gamma')c}\|^2 \leq 2(L + \bar{L})\sigma_0^2 \log p, \quad \text{and}
\| (\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_{\gamma'})\tilde{w}\|^2 \leq 2\| (\Phi_{\gamma \cup \{j_\gamma\}} - \Phi_{\gamma'})w\|^2 + 2\| X_{(\gamma \setminus \gamma')c}\beta_{(\gamma \setminus \gamma')c}\|^2 \leq 2(L + \bar{L})\sigma_0^2 \log p.
\]
Let \( A^2 = \nu \| (I - \Phi_\gamma) X_{\gamma} \beta_{\gamma}^* \|^2 \geq n \nu^2 \min_{j \in \gamma^*} |\beta_j^*|^2 \geq \nu^2 C_\beta \sigma_0^2 \log p \). Then, for \( C_\beta \) large enough so that \( \nu^2 C_\beta \geq 32(L + L) \), we have, by the \( \beta_{\min} \)-condition and the preceding display, that under the event \( A_n \)

\[
\| (\Phi_{\gamma \cup \{j\}} - \Phi_\gamma) \tilde{w} \|_2 \leq \frac{A}{4} \quad \text{and} \quad \| (\Phi_{\gamma \cup \{j\}} - \Phi_\gamma) \tilde{w} \|_2 \leq \frac{A}{4}.
\]

By the definition of \( A \), we can also write inequality (54) as

\[
\| v_1 \| \geq A \quad \text{and} \quad \| v_2 \| \leq \frac{A}{\sqrt{2}}.
\]

By plugging in the bounds (56) and (57) into inequality (55), we obtain

\[
1 - R_{\gamma}^2 - (1 - R_{\gamma'}^2) \geq \frac{A \cdot (A - A/4) - (A/\sqrt{2}) \cdot (A/\sqrt{2} + A/4) - A^2/16}{\| Y \|^2_2} \geq \frac{A^2}{8\| Y \|^2_2}.
\]

Combining this with inequality (52), we obtain that for \( C_\beta \) sufficiently large so that \( \nu^2 C_\beta \geq 192 \), the following holds under the event \( A_n \cap C_n \cap D_n \)

\[
\pi_n(\gamma | Y) = \left(1 - \frac{\| Y \|^2_2 (1 - R_{\gamma}^2 - (1 - R_{\gamma'}^2))}{\| Y \|^2_2 / g + Y^T (I - \Phi_\gamma) Y} \right)^{n/2} \\
\leq \left(1 - \frac{\nu \| (I - \Phi_\gamma) X_{\gamma} \beta_{\gamma}^* \|^2 / (8s^*)}{\| (I - \Phi_\gamma) X_{\gamma} \beta_{\gamma}^* \|^2 / 2} \right)^{n/2} \\
\leq \left(1 - \frac{3 \log p}{n/2} \right)^{n/2} \leq p^{-3},
\]

where the last two steps follows by the same argument as for the steps (i) and (ii) in inequality (52).

**B.4 Lemma 8 and its proof**

Recall the definition of \( j_\gamma, k_\gamma \) and \( \ell_\gamma \) in the construction of the transition function \( G \) after Lemma 1. The first result in following lemma shows that at least an amount of \( n \nu^2 \| \beta_{\gamma \cup \{j\}} \|^2_2 / s^* \) variation in the true signal \( X_{\gamma} \beta_{\gamma}^* \), can be explained by adding \( X_{j_\gamma} \) into the current model \( \gamma \). The second result shows that removing \( X_{k_\gamma} \) from the model \( \gamma \cup \{j_\gamma\} \) incurs a loss in the explained variation of at most \( n \omega(X) \| \beta_{\gamma \cup \{j\}} \|^2_2 / (s_0 - s^*) \). As a result, if \( s_0 \) satisfies the condition \( s_0 \geq (2 \nu^{-2} \omega(X) + 1)s^* \) in Assumption D, then it is favorable to replace the unimportant covariate \( X_{k_\gamma} \) with the influential covariate \( X_{j_\gamma} \) in the current model \( \gamma \).

**Lemma 8.** Under the conditions and notation of Lemma 4, we have:

(a) If \( \gamma \) is underfitted, then

\[
\| \Phi_{\gamma \cup \{j_\gamma\}} X_{\gamma} \beta_{\gamma}^* \|^2_2 - \| \Phi_\gamma X_{\gamma} \beta_{\gamma}^* \|^2_2 \geq n \nu^2 \frac{\| \beta_{\gamma \cup \{j\}} \|^2_2}{s^*}.
\]

(b) If \( \gamma \) is underfitted and saturated, then

\[
\| \Phi_{\gamma \cup \{j_\gamma\}} X_{\gamma} \beta_{\gamma}^* \|^2_2 - \| \Phi_{\gamma \cup \{j_\gamma\} \setminus \{k_\gamma\}} X_{\gamma} \beta_{\gamma}^* \|^2_2 \leq n \omega(X) \frac{\| \beta_{\gamma \cup \{j\}} \|^2_2}{s_0 - s^*}.
\]
Proof. For each $\ell \in \gamma^* \setminus \gamma$, Lemma 6 yields
\[
\|\Phi_{\gamma \cup \{\ell\}} X_{\gamma^* \beta_{\gamma}^*}\|_2^2 - \|\Phi_{\gamma} X_{\gamma^* \beta_{\gamma}^*}\|_2^2 = (\beta_{\gamma}^*)^T X_{\gamma^* \beta_{\gamma}^*}^T (\Phi_{\gamma \cup \{\ell\}} - \Phi_{\gamma}) X_{\gamma^* \beta_{\gamma}^*}^T
\]
\[
= (\beta_{\gamma}^*)^T X_{\gamma^* \beta_{\gamma}^*}^T (I - \Phi_{\gamma}) X_{\gamma^* \beta_{\gamma}^*}^T \frac{X_{\gamma^* \beta_{\gamma}^*}^T (I - \Phi_{\gamma}) X_{\gamma^* \beta_{\gamma}^*}}{n} \\
\geq (\beta_{\gamma}^*)^T X_{\gamma^* \beta_{\gamma}^*}^T (I - \Phi_{\gamma}) \frac{X_{\gamma^* \beta_{\gamma}^*}}{n} \frac{n}{(I - \Phi_{\gamma}) X_{\gamma^* \beta_{\gamma}^*}}
\]
where the first step follows by the idempotence of projection matrices and the last step follows by the normalization condition in Assumption B. By summing the preceding inequality over $\ell \in \gamma^* \setminus \gamma$, we obtain
\[
\sum_{\ell \in \gamma^* \setminus \gamma} (\|\Phi_{\gamma \cup \{\ell\}} X_{\gamma^* \beta_{\gamma}^*}\|_2^2 - \|\Phi_{\gamma} X_{\gamma^* \beta_{\gamma}^*}\|_2^2)
\]
\[
\geq (\beta_{\gamma}^*)^T X_{\gamma^* \beta_{\gamma}^*}^T (I - \Phi_{\gamma}) \frac{X_{\gamma^* \beta_{\gamma}^*}}{n} (I - \Phi_{\gamma}) X_{\gamma^* \beta_{\gamma}^*}^T \\
= (\beta_{\gamma}^*)^T X_{\gamma^* \beta_{\gamma}^*}^T (I - \Phi_{\gamma}) \frac{X_{\gamma^* \beta_{\gamma}^*}}{n} (I - \Phi_{\gamma}) X_{\gamma^* \beta_{\gamma}^*}^T \\
\geq \nu (\beta_{\gamma}^*)^T X_{\gamma^* \beta_{\gamma}^*}^T (I - \Phi_{\gamma}) X_{\gamma^* \beta_{\gamma}^*}^T \\
= \nu (\beta_{\gamma}^*)^T X_{\gamma^* \beta_{\gamma}^*}^T (I - \Phi_{\gamma}) X_{\gamma^* \beta_{\gamma}^*}^T \\
\]
where in step (i) we used the fact that for $k \notin \gamma^*$, $\Phi_{\gamma^*} X_{\gamma^* \setminus \gamma} = \Phi_{\gamma \setminus \{k\}} X_{\gamma \setminus \gamma}$, and step (ii) follows by equation (59). This shows that the second claimed inequality is equivalent to

$$
\|X\hat{\beta}(\hat{\gamma}) - X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma}\|^2 \leq n \omega(X) \frac{\|\hat{\beta}_{\gamma^* \setminus \gamma}\|^2}{s_0 - s^*}.
$$

We use $\hat{\beta}_j(\hat{\gamma})$ to denote the $j$th component of $\hat{\beta}(\hat{\gamma})$. By the optimality of $\hat{\beta}(\hat{\gamma})$ for the least-squares problem (58), we have

$$
X_k^T (X_{\hat{\gamma}} \hat{\beta}(\hat{\gamma}) - X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma}) = 0, \quad \text{for all } k \in \hat{\gamma}.
$$

Therefore, for each $k \in \hat{\gamma}$, we have

$$
\|X\hat{\beta}(\hat{\gamma} \setminus \{k\}) - X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma}\|^2 = \|X\hat{\beta}(\hat{\gamma}) - X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma} - X_k\hat{\beta}_k(\hat{\gamma})\|^2.
$$

In the last step we used the optimality of $\hat{\beta}(\gamma \setminus \{k\})$ and the normalization assumption $\|X_k\|^2 = n$. Then, by the definition of $k_{\gamma}$ as the index $k$ in $\gamma \setminus \gamma^*$ that minimizes $\|X_{\gamma^*} \hat{\beta}_{\gamma^*}\|^2 - \Phi_{\gamma \setminus \{k\}} X_{\gamma^*} \hat{\beta}_{\gamma^*}\|^2$, we have

$$
\|X\hat{\beta}(\hat{\gamma} \setminus \{k\}) - X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma}\|^2 = \min_{k \in \gamma \setminus \gamma^*} \|X\hat{\beta}(\hat{\gamma} \setminus \{k\}) - X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma}\|^2
$$

$$
\leq \|X\hat{\beta}(\hat{\gamma}) - X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma}\|^2 + n \min_{k \in \gamma \setminus \gamma^*} |\hat{\beta}_k(\hat{\gamma})|^2
$$

$$
\leq \|X\hat{\beta}(\hat{\gamma}) - X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma}\|^2 + 2n |\hat{\beta}(\hat{\gamma})|^2
$$

$$
= \|X\hat{\beta}(\hat{\gamma}) - X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma}\|^2 + 2n |\hat{\beta}(\hat{\gamma})|^2.
$$

where last step follows since $|\gamma \setminus \gamma^*| = s_0 - s^*$ by the saturation of $\gamma$. By our definition and Assumption D,

$$
|\hat{\beta}(\hat{\gamma})|^2 = \|X_{\hat{\gamma}}^T X_{\hat{\gamma}}\|^{-1} X_{\hat{\gamma}}^T X_{\gamma^* \setminus \gamma} \hat{\beta}_{\gamma^* \setminus \gamma}\|^2 \leq \|X_{\hat{\gamma}}^T X_{\hat{\gamma}}\|^{-1} \|X_{\hat{\gamma}}^T X_{\gamma^* \setminus \gamma}\|_F^2 \|\hat{\beta}_{\gamma^* \setminus \gamma}\|^2
$$

$$
\leq \omega(X) \|\hat{\beta}_{\gamma^* \setminus \gamma}\|^2.
$$

Combining the last two displays yields the second claimed inequality. \hfill \Box

### C  Proof of Lemma 7

We divide the proof into two cases: $\gamma$ is overfitted and underfitted.

**Case $\gamma$ is overfitted:** Let $k = |\gamma \setminus \gamma^*|$ be the number of unimportant covariates selected by $\gamma$. Since $\gamma \neq \gamma^*$, we have $k \geq 1$. Then, we can express the posterior probability ratio as

$$
\frac{\pi_n(\gamma \mid Y)}{\pi_n(\gamma^* \mid Y)} = \frac{1}{p^k (1 + g)^{k/2}} \cdot \left( \frac{1 + g (1 - R^{\gamma^*}_\gamma)}{1 + g (1 - R^\gamma_\gamma)} \right)^{n/2}
$$

$$
= \frac{1}{p^k (1 + g)^{k/2}} \cdot \left( 1 + \frac{R^\gamma_\gamma - R^{\gamma^*}_\gamma}{g^{-1} (1 - R^\gamma_\gamma)} \right)^{n/2}.
$$

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Since all influential covariates are included in models $M_\gamma$ and $M_{\gamma^*}$, we have

$$1 - R_\gamma^2 = \frac{|| (I - \Phi_\gamma)(X(\gamma^*)\beta_{(\gamma^*)}^\gamma + w) ||_2^2}{|| Y ||_2^2} \quad \text{and} \quad 1 - R_{\gamma^*}^2 = \frac{|| (I - \Phi_{\gamma^*})(X(\gamma^*)\beta_{(\gamma^*)}^{\gamma^*} + w) ||_2^2}{|| Y ||_2^2}.$$ 

Applying the Cauchy-Schwarz inequality yields

$$1 - R_\gamma^2 \geq \frac{\frac{1}{2} || (I - \Phi_\gamma) w ||_2^2 - || (I - \Phi_\gamma) X(\gamma^*)\beta_{(\gamma^*)}^\gamma ||_2^2}{|| Y ||_2^2} \geq \frac{\frac{1}{2} || (I - \Phi_\gamma) w ||_2^2 - 2 \| X(\gamma^*)\beta_{(\gamma^*)}^\gamma \|_2^2}{2 \| Y \|_2^2} \geq \frac{|| (I - \Phi_\gamma) w ||_2^2 - 2 \tilde{L} \sigma_0^2 \log p}{2 \| Y \|_2^2},$$

where in step (i) we used the fact the projection is a non-expansive mapping and in step (ii) we used the assumption $\| X(\gamma^*)\beta_{(\gamma^*)}^\gamma \|_2^2 \leq \tilde{L} \sigma_0^2 \log p$. Similarly, since $\gamma^* \subset \gamma$, we can obtain the following inequality for the quantity $R_\gamma^2 - R_{\gamma^*}^2$,

$$R_\gamma^2 - R_{\gamma^*}^2 = \frac{|| (\Phi_\gamma - \Phi_{\gamma^*})(X(\gamma^*)\beta_{(\gamma^*)}^\gamma + w) ||_2^2}{|| Y ||_2^2} \leq \frac{2 \| (\Phi_\gamma - \Phi_{\gamma^*}) w \|_2^2 + 2 \tilde{L} \sigma_0^2 \log p}{2 \| Y \|_2^2}.$$ 

Under the event $A_n \cap B_n \cap C_n$, we have $|| (I - \Phi_\gamma) w ||_2^2 \geq \frac{1}{2} n - r K s^* \log p \geq \frac{3n}{8}$ and $|| (\Phi_\gamma - \Phi_{\gamma^*}) w ||_2^2 \leq k \tilde{L} \sigma_0^2 \log p$, where we have used the assumption $4r K s^* \log p \leq n$. Combining these two inequalities with the preceding two displays, we obtain that the posterior probability ratio under the event $A_n \cap B_n \cap C_n$ is bounded as

$$\frac{\pi_n(\gamma \mid Y)}{\pi_n(\gamma^* \mid Y)} \leq \frac{1}{p^{\ell k}(1 + g)^{k/2}} \cdot \left( 1 + \frac{2(L + \tilde{L}) \log p}{n/8} \right)^{n/2} \leq \frac{1}{p^{\ell k}(1 + g)^{k/2}} \cdot \exp \left( - \frac{16(L + \tilde{L}) \log p}{n} \right) = p^{8(L + \tilde{L}) - k(\alpha + \kappa)}$$

where in step (i) we used the inequality $1 + x \leq e^x$ for $x \in \mathbb{R}$ and step (ii) follows since $\sqrt{g} \asymp p^x$ with $\alpha \geq 8(L + \tilde{L}) + 2 - \kappa$ according to our choice of the hyperparameter. This proves the first part. Now we consider the underfitted case.

**Case $\gamma$ is underfitted:** This case happens only when $s^* \geq 1$. Let $\bar{\gamma} = \gamma \cup \gamma^*$. Denote $k = |\gamma^* \backslash \gamma|$ and $\ell = |\gamma|$, then $|\bar{\gamma} \backslash \gamma| = k$, $|\bar{\gamma} \backslash \gamma^*| = k + \ell - s^*$, and $|\bar{\gamma}| = k + \ell \leq (K + 1)s^*$. Since $\gamma \subset \bar{\gamma}$, we can write

$$1 - R_\gamma^2 - (1 - R_{\bar{\gamma}}^2) = \frac{Y^T (\Phi_{\bar{\gamma}} - \Phi_\gamma) Y}{|| Y ||_2^2} = \frac{|| (\Phi_{\bar{\gamma}} - \Phi_\gamma) X_\gamma \beta_{\gamma}^\gamma + (\Phi_{\bar{\gamma}} - \Phi_\gamma) X(\gamma^*)\beta_{(\gamma^*)}^\gamma + (\Phi_{\bar{\gamma}} - \Phi_\gamma) w ||_2^2}{|| Y ||_2^2} \geq \frac{|| (\Phi_{\bar{\gamma}} - \Phi_\gamma) X_\gamma \beta_{\gamma}^\gamma ||_2 - || (\Phi_{\bar{\gamma}} - \Phi_\gamma) X(\gamma^*)\beta_{(\gamma^*)}^\gamma ||_2 - || (\Phi_{\bar{\gamma}} - \Phi_\gamma) w ||_2}{|| Y ||_2^2}.$$ 

By the $\beta_{\min}$-condition and Lemma 5 we have

$$|| (\Phi_{\bar{\gamma}} - \Phi_\gamma) X_\gamma \beta_{\gamma}^\gamma ||_2 \geq || (I - \Phi_\gamma) X_\gamma \beta_{\gamma}^\gamma ||_2 \geq n \nu^2 \| \beta_{\gamma}^\gamma \|_2 \geq \nu^2 C_\beta k \sigma_0^2 \log p, \quad (61)$$

and
where $C_\beta := c_0(L + \bar{L} + \alpha + \kappa)$ denotes the coefficient in the $\beta_{\min}$-condition of the theorem. Consequently, as long as $c_0$ is sufficiently large, we can ensure that $\nu \sqrt{C_\beta} \geq 4\sqrt{L + \bar{L}}$, and hence, under the event $\mathcal{A}_n$, we find that

$$1 - R_\gamma^2 - (1 - R_\gamma^2) \geq \frac{\| (I - \Phi_\gamma) X_{\gamma^*}\beta_{\gamma^*}^* \|^2}{4\| Y \|_2^2}.$$ 

Similarly, under the event $\mathcal{C}_n$, we have

$$1 - R_\gamma^2 = \frac{Y^T(I - \Phi_\gamma)Y}{\| Y \|_2^2} \leq \frac{\| (I - \Phi_\gamma) X_{\gamma^*}\beta_{\gamma^*}^* \|_2 + \| \Phi_\gamma^* - \Phi_\gamma \|_2 + \| (I - \Phi_\gamma)w \|_2}{\| Y \|_2^2} \leq \frac{2\| (I - \Phi_\gamma) X_{\gamma^*}\beta_{\gamma^*}^* \|_2 + 4\| \Phi_\gamma^* - \Phi_\gamma \|_2}{\| Y \|_2^2} \leq \frac{4\| (I - \Phi_\gamma) X_{\gamma^*}\beta_{\gamma^*}^* \|^2}{\| Y \|_2^2},$$

where in step (i) we have used Assumption A, the fact that $\| (I - \Phi_\gamma)w \|_2^2 \leq \| w \|_2^2$, and the last step uses $2\| (I - \Phi_\gamma) X_{\gamma^*}\beta_{\gamma^*}^* \|_2 \geq 2\nu\| \beta_{\gamma^*}^* \|_2 \geq 4L\sigma_0^2 \log p + 3n\sigma_0^2$ for $C_\beta \geq (4L + 3)/\nu$.

Consequently, as long as $C_\beta$ is large enough so that $\nu^2 C_\beta \geq 64 (\alpha + \kappa + 8(L + \bar{L}) + 2)$, the posterior probability ratio $\frac{\pi_n(\gamma | Y)}{\pi_n(\gamma^* | Y)}$ under the event $\mathcal{A}_n \cap \mathcal{C}_n \cap \mathcal{D}_n$ is upper bounded as

$$\frac{\pi_n(\gamma | Y)}{\pi_n(\gamma^* | Y)} = p_{\alpha k} (1 + g)^{k/2} \cdot (1 - \frac{\| Y \|_2^2(1 - R_\gamma^2 - (1 - R_\gamma^2))}{\| Y \|_2^2/g + Y^T(I - \Phi_\gamma)Y})^{n/2} \leq p_{\alpha k} (1 + g)^{k/2} \cdot (1 - \frac{\| (I - \Phi_\gamma) X_{\gamma^*}\beta_{\gamma^*}^* \|_2^2/4}{4n\sigma_0^2/s^* + 4\| (I - \Phi_\gamma) X_{\gamma^*}\beta_{\gamma^*}^* \|_2^2})^{n/2} \leq p_{\alpha k} (1 + g)^{k/2} \cdot (1 - \min \left\{ \frac{1}{32} \cdot \frac{\nu C_\beta s^* \log p}{32n} \right\})^{n/2} \leq p_{\alpha k} \cdot p_{\alpha k} \cdot p_{\alpha \kappa + 8(L + \bar{L}) + 2} \cdot \left( \frac{2}{n} \right)^{n/2} \leq p_{\alpha \kappa + 8(L + \bar{L}) + 2} \leq p_{\alpha \kappa + 8(L + \bar{L}) + 2},$$

where in step (i) we have used the inequality $a/(b + a) \geq \min\{1/2, a/(2b)\}$ for any $a, b > 0$ and inequality (61), and step (ii) follows by our assumption on $C_\beta$ and the assumption $s^* \geq 1$ made at the beginning of this underfitted case.

Since model $\mathcal{M}_\gamma$ is overfitted, by the intermediate result (60), we have that under the event $\mathcal{A}_n \cap \mathcal{B}_n \cap \mathcal{C}_n$

$$\frac{\pi_n(\gamma | Y)}{\pi_n(\gamma^* | Y)} \leq p_{8(L + \bar{L}) - (\alpha + \kappa) | \gamma^* |}^{8(L + \bar{L}) - (\alpha + \kappa) | k + \ell - s^* |} = p_{8(L + \bar{L}) - (\alpha + \kappa) | k + \ell - s^* |}.$$

Combining the last two displays, we obtain that under the event $\mathcal{A}_n \cap \mathcal{B}_n \cap \mathcal{C}_n \cap \mathcal{D}_n$

$$\frac{\pi_n(\gamma | Y)}{\pi_n(\gamma^* | Y)} \leq p_{-(\alpha + \kappa) \ell - 2} \leq p_{-2\ell - 2},$$

where in the last step we have used Assumption C.
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