Variable Selection Using Bayesian Additive Regression Trees

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Abstract

Variable selection is an important statistical problem. This problem becomes more challenging when the candidate predictors are of mixed type (e.g. continuous and binary) and impact the response variable in nonlinear and/or non-additive ways. In this paper, we review existing variable selection approaches for the Bayesian additive regression trees (BART) model, a nonparametric regression model, which is flexible enough to capture the interactions between predictors and nonlinear relationships with the response. An emphasis of this review is on the capability of identifying relevant predictors. We also propose two variable importance measures which can be used in a permutation-based variable selection approach, and a backward variable selection procedure for BART. We present simulations demonstrating that our approaches exhibit improved performance in terms of the ability to recover all the relevant predictors in a variety of data settings, compared to existing BART-based variable selection methods.

Keywords and phrases: Variable selection, BART, nonparametric regression.

1 Introduction

Variable selection, also known as feature selection in machine learning, is the process of selecting a subset of relevant variables for use in model construction. It has been, and continues to be a major focus of research and practice because researchers and practitioners often seek low-cost, interpretable and not overfitted models. For example, in causal inference, model-based estimation of the effects of an exposure on an outcome is generally sensitive to the choice of confounders included in the model. If there are no unmeasured confounders, the full model with all the confounders and many non-confounders generally yields an unbiased estimation, but with a large standard error (C. Wang, Parmigiani, and Dominici (2012)). On the contrary, a

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model with fewer non-confounders not only produces an unbiased estimation with a smaller standard error, but also saves computation time.

Variable selection is often carried out in parametric settings, such as the linear regression model (Efroymson (1960), Edward I George and Robert E McCulloch (1993), Tibshirani (1996), Zou and Hastie (2005), Carvalho, Polson, and Scott (2010), and Bhattacharya et al. (2015)). However, variable selection approaches based on a linear model often fail when the underlying relationship between the predictors and the response variable is nonlinear and/or non-additive, and it is generally challenging to extend them to nonparametric models, such as tree-based models which incorporate both main effects and interaction effects of varying orders.

Tree-based models have been developed from both the frequentist and Bayesian perspectives, including but not limited to random forests (Breiman (2001)), stochastic gradient boosting (Friedman (2002)), reinforcement learning trees (Zhu, Zeng, and Kosorok (2015)) and Bayesian additive regression trees (Chipman, Edward I. George, and Robert E. McCulloch (2010)), the last of which is the focus of this paper. Variable selection for the tree-based models in machine learning is often achieved through variable importance. Taking random forests as an example, there are two types of variable importance measures typically used: Gini importance (Friedman (2001)) and permutation importance (Breiman (2001)). Gini importance evaluates the importance of a variable by adding up the weighted decrease in impurity of all the nodes using the variable as a split variable, averaged over all the trees, while permutation importance evaluates the importance of a variable by adding up the difference in out-of-bag error before and after the permutation of the values of the variable in the training data, also averaged over all the trees. Though widely used, as pointed out by Strobl et al. (2007), both Gini importance and permutation importance are biased in favor of continuous and high cardinality predictors when the random forest is applied to data with mixed-type predictors. Methods such as growing unbiased trees (Strobl et al. (2007)) and partial permutations (Altmann et al. (2010)) can be used to solve this issue.

Compared to the tree-based models in machine learning, Bayesian additive regression trees (BART) not only possesses competitive predictive performance, but also enables the user to make inference on it due to its fully Bayesian construction. The original BART paper suggests using variable inclusion proportions to measure the importance of predictors and later Bleich et al. (2014) propose a principled permutation-based inferential approach to determine how large the variable inclusion proportion has to be in order to select a predictor. This approach exhibits superior performance in a variety of data settings, compared to many existing variable selection procedures including random forests with permutation importance. In fact, we
note that the variable inclusion proportion produced by BART is a special case of Gini importance, which
treats the weight and the decrease in impurity at each node to be constant. We also note that the approach
of Bleich et al. (2014) is reminiscent of the partial permutation approach of Altmann et al. (2010) which
also repeatedly permutes the response vector to estimate the distribution of the variable importance for
each predictor in a non-informative setting where the relationship between the response and predictors is
removed and the dependencies among the predictors are maintained. Though the approach of Altmann
et al. (2010) is designed for mitigating the bias of Gini importance, we find that the approach of Bleich
et al. (2014) is still biased against predictors with low cardinality, such as binary predictors, especially when
the number of predictors is not large. In addition to the approach of Bleich et al. (2014), two variable
selection approaches are proposed based on variants of the BART model. One variant of BART is DART
(Linero (2018)) which modifies BART by placing a Dirichlet hyper-prior on the splitting proportions of the
regression tree prior to encourage sparsity. To conduct variable selection, they suggest selecting predictors
in the median probability model (Barbieri and Berger (2004)), i.e., selecting predictors with a marginal
posterior variable inclusion probability at least 50%. This approach is more computationally efficient than
other BART-based variable selection methods, as it does not require fitting model multiple times. In general,
we find that DART works better than other BART-based variable selection methods, but it becomes less
stable in presence of correlated predictors and in the probit BART model. Another variant of the BART
prior is the spike-and-forest prior (Ročková and Pas (2020)) which wraps the BART prior with a spike-
and-slab prior on the model space. Liu, Ročková, and Y. Wang (2021) provide model selection consistency
results for the spike-and-forest prior and propose approximate Bayesian computation (ABC) Bayesian forest,
a modified ABC sampling method, to conduct variable selection in practice. Similar to DART, variables
are selected based on their marginal posterior variable inclusion probabilities. ABC Bayesian forest shows
good performance in terms of excluding irrelevant predictors, but its ability to include relevant predictors is
relatively poor when predictors are correlated.

The main issues of existing BART-based variable selection methods include being biased against cate-
gorical predictors with fewer levels and being conservative in terms of including relevant predictors in the
model. The goal of this paper is to develop variable selection approaches for BART to overcome these issues.
For simplicity, we assume that the possible types of potential predictors only include binary and continuous
types. This paper is organized as follows. In Section 2, we review the BART model and existing BART-based
variable selection approaches. An example where the approach of Bleich et al. (2014) fails to include rele-
vant binary predictors is also provided. In Section 3, we present the proposed variable selection approaches.
In Section 4, we compare our approaches with existing BART-based variable selection approaches through simulated examples. Finally, we conclude this paper with a discussion in Section 5.

2 Review of BART

2.1 Model Specification

Motivated by the boosting algorithm and built on the Bayesian classification and regression tree algorithm (Chipman, Edward I. George, and Robert E. McCulloch (1998)), BART (Chipman, Edward I. George, and Robert E. McCulloch (2010)) is a Bayesian approach to nonparametric function estimation and inference using a sum of trees. Consider the problem of making inference about an unknown function \( f_0 \) that predicts a continuous response \( y \) using a \( p \)-dimensional vector of predictors \( \mathbf{x} = (x_1, \ldots, x_p) \) when

\[
y = f_0(\mathbf{x}) + \epsilon, \quad \epsilon \sim N(0, \sigma^2). \tag{1}
\]

BART models \( f_0 \) by a sum of \( M \) Bayesian regression trees, i.e.,

\[
f(\mathbf{x}) = \sum_{m=1}^{M} g(\mathbf{x}; T_m, \mathbf{\mu}_m), \tag{2}
\]

where \( g(\mathbf{x}; T_m, \mathbf{\mu}_m) \) is the output of \( \mathbf{x} \) from a single regression tree. Each \( g(\mathbf{x}; T_m, \mathbf{\mu}_m) \) is determined by the binary tree structure \( T_m \) consisting of a set of splitting rules and a set of terminal nodes, and the vector of parameters \( \mathbf{\mu}_m = (\mu_{m,1}, \ldots, \mu_{m,b_m}) \) associated with the \( b_m \) terminal nodes of \( T_m \), such that \( g(\mathbf{x}; T_m, \mathbf{\mu}_m) = \mu_{m,l} \) if \( \mathbf{x} \) is associated with the \( l^{th} \) terminal node of the tree \( T_m \).

A regularization prior consisting of three components, (1) the \( M \) independent trees structures \( \{T_m\}_{m=1}^{M} \), (2) the parameters \( \{\mathbf{\mu}_m\}_{m=1}^{M} \) associated with the terminal nodes given the trees \( \{T_m\}_{m=1}^{M} \) and (3) the error variance \( \sigma^2 \) which is assumed to be independent of the former two, is specified for BART in a hierarchical manner. The posterior distribution of BART is sampled through a Metropolis-within-Gibbs algorithm (Hastings (1970), S. Geman and D. Geman (1984), and Kapelner and Bleich (2016)). The Gibbs sampler involves \( M \) successive draws of \( (T_m, \mathbf{\mu}_m) \) followed by a draw of \( \sigma^2 \). A key feature of this sampler is that it employs Bayesian backfitting (Hastie and Tibshirani (2000)) to sample each pair of \( (T_m, \mathbf{\mu}_m) \).

BART estimates \( f_0(\mathbf{x}) = E( Y \mid \mathbf{x}) \) by taking the average of the posterior samples of \( f(\mathbf{x}) \) after a burn-in period. As the trees structures are being updated through the MCMC chain, the model space is being
searched by BART. In light of this, the estimation of \( f_0(x) \) can be considered as a model averaging estimation with each posterior sample of the trees structures treated as a model and therefore BART can be regarded as a Bayesian model selection approach.

The continuous BART model (1–2) can be extend to a binary regression model for a binary response \( Y \) by specifying

\[
P(Y = 1 \mid x) = \Phi [f(x)],
\]

where \( f \) is the sum-of-trees function in (2) and \( \Phi \) is the cumulative distribution function of the standard normal distribution. Posterior sampling can be done by applying the Metropolis-within-Gibbs sampler of continuous BART to the latent variables which are obtained via the data augmentation approach of Albert and Chib (1993).

### 2.2 Existing BART-Based Variable Selection Methods

In this section, we review the BART variable inclusion proportion, a variable importance measure produced by BART, and three existing variable selection methods based on BART.

#### 2.2.1 BART variable inclusion proportions

The MCMC algorithm of BART returns posterior samples of the trees structures, from which we can obtain the variable inclusion proportion for each predictor.

**Definition 2.1 (BART Variable Inclusion Proportion).** Let \( K \) be the number of posterior samples obtained from a BART model. For each \( j = 1, \cdots, p \) and \( k = 1, \cdots, K \), let \( c_{jk} \) be the number of splitting rules using the predictor \( x_j \) as the split variable in the \( k \)th posterior sample of the trees structures and let \( c_{k} = \sum_{j=1}^{p} c_{jk} \) be the total number of splitting rules in the \( k \)th posterior sample. The BART variable inclusion proportion (VIP) for the predictor \( x_j \) is defined as

\[
v_j = \frac{1}{K} \sum_{k=1}^{K} \frac{c_{jk}}{c_{k}}.
\]

The BART VIP \( v_j \) describes the average usage per splitting rule for the predictor \( x_j \). Intuitively, a large VIP is suggestive of the predictor being an important driver of the response. Therefore, the original BART paper uses VIPs to rank predictors in terms of relative importance and recommends conducting variable selection using VIPs with a small number of trees in order to introduce competition among predictors.

We note that BART VIP is a special case of Gini importance (Louppe (2014)) which evaluates the importance of a variable by adding up the weighted decrease in impurity of all the nodes using the variable
as a split variable, averaged over all the trees in the ensemble:

\[
\text{IMP}_{\text{Gini}} (x_j) = \frac{1}{M} \sum_{m=1}^{M} \sum_{\eta \in \phi_m} \mathbb{I} (j_\eta = j) [w(\eta) \Delta i(\eta)],
\]

where \(\phi_m\) is the set of all the splitting nodes in the \(m\)th tree, \(j_\eta\) is the index of the variable used for the splitting node \(\eta\), \(w(\eta)\) is the weight of the node \(\eta\) and \(\Delta i(\eta)\) is the decrease in impurity of the node \(\eta\). In random forests, the weight \(w(\eta)\) is typically the proportion of the samples reaching the node \(\eta\) and the impurity \(i(\eta)\) is typically the variance of the observed response values of the samples reaching the node \(\eta\). BART VIP can be regarded as Gini importance with the weight \(w(\eta)\) set to \(1/c_k\) and the impurity \(i(\eta)\) set to 1 for all the nodes.

Gini importance is known to be biased against variables with low cardinality in random forests (Strobl et al. (2007)). As a variant of Gini importance, BART VIP is also a biased variable importance measure. To illustrate this, we consider the following example.

**Example 1.** For each \(i = 1, \cdots, 500\), sample \(x_{i1}, \cdots, x_{i10}\) from Bernoulli(0.5) independently, \(x_{i11}, \cdots, x_{i20}\) from Uniform(0,1) independently and \(y_i\) from Normal\((f_0(x_i), 1)\) independently, where

\[
f_0(x) = 10 \sin(\pi x_{11}) + 20(x_{13} - 0.5)^2 + 10x_2 + 5x_{12}.
\]

This example is a variant of Friedman’s example (Friedman (1991)) where the predictors impact the response in a nonlinear and non-additive way. We modify Friedman’s example by changing the predictors \(x_1\) and \(x_2\) from continuous to binary. We fit a BART model on the observations \(\{y_i, x_i\}_{i=1}^{500}\) with \(M = 20\) trees and obtain the VIPs based on 1000 posterior samples after burning in 1000 posterior samples. Since all the predictors are on the same scale [0, 1], the binary predictor \(x_1\) improves the fit of the response \(y\) the same as the continuous predictor \(x_{11}\) and the binary predictor \(x_2\) moves the response \(y\) more than the continuous predictor \(x_{12}\). However, Figure 1 shows that \(x_{11}\) and \(x_{12}\) have higher VIPs than \(x_1\) and \(x_2\) respectively, suggesting that BART VIP is biased against binary predictors. This issue occurs because a binary predictor has only one available splitting value while a continuous predictor has many more splitting values. As a result, continuous predictors appear more often in the ensemble.
Permutation-based variable selection with BART VIP

Apart from the bias issue of BART VIP, the original BART paper does not provide a complete variable selection approach in the sense that it does not provide a way of setting the threshold for BART VIPs to select predictors. In fact, Bleich et al. (2014) show that it is not possible to decide on an appropriate threshold for VIPs based on a single BART fit, because BART may fit noise due to its nonparametric flexibility. To deal with this, they develop a principled permutation-based variable selection approach which facilitates determining how large a BART VIP has to be in order to select a predictor.

Specifically, this approach first creates $L$ permutations $\{y^*_l\}_{l=1}^L$ of the response vector $y$ to form $L$ null datasets $\{y^*_l, X\}_{l=1}^L$, where $X$ is a matrix of the observed predictors with each row corresponding to an observation, and then fits a BART model on each null dataset $(y^*_l, X)$. As a result, $L$ vectors of BART VIPs $v^*_l = (v^*_l, 1, \cdots, v^*_l, p)$, $l = 1, \cdots, L$, can be obtained from the $L$ BART models. Since the null datasets delete the relationship between the response and predictors, the $L$-dimensional vector $\{v^*_1, j, \cdots, v^*_L, j\}$ can be regarded as a sample of the null distribution of the BART VIP for the predictor $x_j$, which is the distribution of the BART VIP when the predictor $x_j$ is unrelated to the response $y$. If the predictor $x_j$ is indeed not related to the response $y$, then the true BART VIP obtained from the BART model on the original dataset $(y, X)$ follows the null distribution. Hence, predictors can be selected according to the relative location of their true BART VIPs in the corresponding null distributions. Since BART may fit noise, the true VIPs
are estimated by the averaged VIPs \( \bar{v} = (\bar{v}_1, \cdots, \bar{v}_p) \) which is the mean of multiple vectors of VIPs with each obtained from a replication of BART on the original dataset \((y, X)\). Bleich et al. (2014) propose three criteria to select a subset of predictors. The least stringent one is the local threshold, i.e., the predictor \( x_j \) is selected if the averaged VIP \( \bar{v}_j \) exceeds the \( 1 - \alpha \) quantile of the corresponding empirical distribution \( \sum_{l=1}^{L} \delta v_{l,j}^*(\cdot) \) of the null distribution, where \( \delta v_{l,j}^*(\cdot) \) is a degenerate distribution at \( v_{l,j}^* \). The algorithm for a general permutation-based variable selection approach, not restricted to the one using BART VIP as the variable importance measure, is summarized in Algorithm 1.

**Algorithm 1** Permutation-based variable selection approach

**Input:** \( X \): predictors; \( y \): response; \( L \): number of permutations; \( L_{rep} \): number of repetitions; \( \alpha \): selection threshold

**Output:** A subset of predictors

1. for \( s = 1, \cdots, L_{rep} \) do
2. Run the model on the original dataset \((y, X)\) and compute the variable importance scores \( (v_{s,1}, \cdots, v_{s,p}) \)
3. end for
4. Compute the averaged variable importance scores \( \bar{v}_j = (\sum_{s=1}^{L_{rep}} v_{s,j})/L_{rep} \) for \( j = 1, \cdots, p \)
5. for \( l = 1, \cdots, L \) do
6. Run the model on the null dataset \((y_l^*, X)\) and compute the variable importance scores \( (v_{l,1}^*, \cdots, v_{l,p}^*) \)
7. end for
8. for \( j = 1, \cdots, p \) do
9. Compute the \( 1 - \alpha \) quantile \( v_j^* \) of the empirical distribution \( \sum_{l=1}^{L} \delta v_{l,j}^*(\cdot) \) for the predictor \( x_j \)
10. if \( \bar{v}_j > v_j^* \) then
11. Select \( x_j \)
12. end if
13. end for

This approach works well when all the predictors are continuous; however, it often fails to include relevant binary predictors when the predictors belong to different types and the number of predictors is small. Consider the following variant of Friedman’s example.

**Example 2.** For each \( i = 1, \cdots, 500 \), sample \( x_{i1}, \cdots, x_{i10} \) from Bernoulli(0.5) independently, \( x_{i11}, \cdots, x_{i20} \) from Uniform(0,1) independently and \( y_i \) from Normal\((f_0(x_i), 1)\) independently, where

\[
\begin{align*}
f_0(x) &= 10 \sin(\pi x_{11} x_{12}) + 20(x_{13} - 0.5)^2 + 10x_1 + 5x_2.
\end{align*}
\]

Figure S.1 of the Supplementary Material shows that both the two relevant binary predictors \( x_1 \) and \( x_2 \) are not selected by this method. Further analysis is provided in Section 3.1.
2.2.3 Variable selection with DART

DART (Linero (2018)) is a variant of BART, which replaces the discrete uniform distribution for selecting a split variable with a categorical distribution of which the event probabilities \( s_1, \ldots, s_p \) follow a Dirichlet distribution. With the Dirichlet hyper-prior, probability mass is accumulated towards the predictors that are more frequently used along the MCMC iterations, thereby inducing sparsity and improving the predictive performance in high dimensional settings.

As discussed in Section 2.1, BART can be considered as a Bayesian model selection approach, so predictors can be selected by using the marginal posterior variable inclusion probability (MPVIP)

\[
\pi_j = P(x_j \text{ in the model} \mid y).
\]

However, the model space explored by BART is not only all the possible combinations of the predictors, but also all the possible relationships that the sum-of-trees model can express using the \( p \) predictors, which implies that the cardinality of the model space is much bigger than \( 2^p \) and that the variable selection results can be susceptible to the influence of noise predictors, especially when the number of predictors is large. DART avoids the influence of noise predictors by employing the shrinkage Dirichlet hyper-prior. DART estimates the MPVIP for a predictor by the proportion of the posterior samples of the trees structures where the predictor is used as a split variable at least once, and selects predictors with MPVIP at least 0.5, yielding a median probability model. Barbieri and Berger (2004) shows that the median probability model, rather than the most probable model, is the optimal choice in the sense that the predictions for future observations are closest to the Bayesian model averaging prediction in the squared error sense. However, the assumptions for this property are quite strong and often not realistic, including the assumption of an orthogonal predictors matrix.

2.2.4 Variable selection with ABC Bayesian forest

Ročková and Pas (2020) introduce a spike-and-forest prior which wraps the BART prior with a spike-and-slab prior on the model space:

\[
S \sim \pi(S), \forall S \subseteq \{1, \ldots, p\},
\]

\[
\{T_m, \mu_m\}_{m=1}^M, \sigma^2 \mid S \sim \text{BART prior}.
\]
The tree-based model under the spike-and-forest prior can be used not only for estimation but also for variable selection, as shown in Liu, Ročková, and Y. Wang (2021). Due to the intractable marginal likelihood, they propose an approximate Bayesian computation (ABC) sampling method based on data-splitting to help sample from the model space with higher ABC acceptance rate. Specifically, at each iteration, the dataset is randomly split into a training set and a test set according to a certain split ratio. The algorithm proceeds by sampling a subset $S$ from the prior $\pi(S)$, fitting a BART model on the training set only with the predictors in $S$, and computing the root mean squared errors (RMSE) for the test set based on a posterior sample from the fitted BART model. Only those subsets that result in a low RMSE on the test set are kept for selection.

Similar to DART, ABC Bayesian forest selects predictors based on their MPVIP $\pi_j$ defined as (4) which is estimated by computing the proportion of ABC accepted BART posterior samples that use the predictor $x_j$ at least one time. Given the $\pi_j$'s, predictors with $\pi_j$ exceeding a pre-specified threshold are selected.

ABC Bayesian forest exhibits good performance in excluding irrelevant predictors, but it does not perform well in including relevant predictors in presence of correlated predictors, as shown in Section 4. One possible reason is that ABC Bayesian forest internally uses only one posterior sample after a short burn-in period and a small number of trees for BART, making it easy to miss relevant predictors. Furthermore, given that ABC Bayesian forest computes $\pi_j$ based on the ABC accepted BART posterior samples rather than the ABC accepted subsets, it appears that the good performance in excluding irrelevant predictors may be primarily due to the variable selection capability of BART itself, when the number of trees is small.

3 New Approaches

3.1 BART VIP with Type Information

In Section 2.2.2, we show an example where the approach of Bleich et al. (2014) fails to include relevant binary predictors. The intuition of this approach is that a relevant predictor is expected to appear more often in the model built on the original dataset than that built on a null dataset. In this section, we revisit Example 2 and show that the intuition does hold for both relevant continuous and relevant binary predictors, but that the increase in usage of a relevant binary predictor is often offset by the increase of relevant continuous predictors, when the number of predictors is not large, thereby making the true VIP of a relevant binary predictor insignificant with respect to (w.r.t.) the corresponding null VIPs. In light of this observation, we modify BART VIP with the type information of predictors to help identify relevant binary predictors.

Direct studying BART VIP is challenging because each $v_j$ consists of $K$ different components
\{c_{jk}/c_k\}_{k=1}^K$. To make the analysis more interpretable, we introduce an approximation of BART VIP, which only contains one component.

**Definition 3.1** (Approximation of BART VIP). Following the notation in Definition 2.1, for every $j = 1, \cdots, p$ and $k = 1, \cdots, K$, let $c_j = \sum_{k=1}^K c_{jk}$ be the number of splitting nodes using the predictor $x_j$ over all the posterior samples of the trees structures and $c_\cdot = \sum_{j,k=1}^{p,K} c_{jk}$ be the total number of splitting nodes over all the posterior samples. For each predictor $x_j$, define

$$
\tilde{v}_j = \frac{c_j}{c_\cdot}.
$$

The following lemma shows that $\tilde{v}_j$ defined above can be used to approximate BART VIP $v_j$ under mild conditions.

**Lemma 3.2.** For any $j = 1, \cdots, p$ and $k = 1, \cdots, K$, let $c_k = \sum_{j=1}^p c_{jk}$ be the total number of splitting nodes in the $k$th posterior sample and $\bar{c}_K = c_/K$ be the average number of splitting nodes in a posterior sample. If $\sum_{k=1}^K (c_{jk}/c_k)^2/K \leq \delta_1$ and $[\sum_{k=1}^K (c_{jk} - \bar{c}_k)^2/K]^{1/2}/\bar{c}_K \leq \delta_2$ for some positive numbers $\delta_1, \delta_2 > 0$, then the difference between $\tilde{v}_j$ and the corresponding BART VIP $v_j$ is bounded, i.e., $|\tilde{v}_j - v_j| \leq \delta_1^{1/2} \delta_2$.

**Remark.** The first condition above means that the variance of $c_{jk}/c_k$, the proportion of the usage of the predictor $x_j$ in an ensemble, is bounded. The second condition means that the coefficient of variation of $c_k$, the number of splitting nodes in an ensemble, is also bounded. Since Bleich et al. (2014) use posterior samples after a burn-in period, the variance of $c_{jk}/c_k$ and the coefficient of variation of $c_k$ are small (see Figure S.2 of the Supplementary Material). Hence, Lemma 3.2 implies that $\tilde{v}_j$ can be used as an alternative to the corresponding BART VIP $v_j$.

**Proof.** See Section S.1 of the Supplementary Material.

Consider the approach of Bleich et al. (2014). For every $j = 1, \cdots, p$, $k = 1, \cdots, K$, $r = 1, \cdots, L_{\text{rep}}$ and $l = 1, \cdots, L$, let $c_{l,jk}^r$ be the number of splitting nodes using the predictor $x_j$ in the $k$th posterior sample of the BART model built on the $l$th null dataset and $c_{r,jk}$ be that of the $r$th repeated BART model built on the original dataset. Following the notation in Definition 3.1, write $c_{l,.j}^r = \sum_{k=1}^K c_{l,jk}^r$, $c_{r,.j}^r = \sum_{k=1}^{p,K} c_{r,jk}$, $c_{r,.} = \sum_{j,k=1}^{p,K} c_{r,jk}$, and $c_{r,..} = \sum_{j,k=1}^{p,K} c_{r,jk}$. By Lemma 3.2, for each predictor $x_j$, we can use $\tilde{v}_{r,j} = c_{r,jk}/c_{r,.}$ to approximate $v_{r,j}$, the VIP obtained from the BART model on the $l$th null dataset, and $\bar{v}_{r,j} = c_{r,jk}/c_{r,..}$ to approximate $v_{r,j}$, the VIP obtained from the $r$th repeated BART model on the original dataset. Denote by $\bar{v}_j = (\sum_{r=1}^{L_{\text{rep}}} \bar{v}_{r,j})/L_{\text{rep}}$ the averaged approximate VIP for the predictor $x_j$ across $L_{\text{rep}}$ repetitions of BART.
on the original dataset. According to the local threshold of Bleich et al. (2014), a predictor \( x_j \) is selected only if the average VIP \( \bar{v}_j \) exceeds the \( 1 - \alpha \) quantile of the empirical distribution \( \sum_{l=1}^{L} \delta_{c_l}^{j} (...) \), i.e.,

\[
\frac{1}{L} \sum_{l=1}^{L} \mathbb{I} \left( \frac{1}{L_{\text{rep}}} \sum_{r=1}^{L_{\text{rep}}} c_{r,j} > c_{l,j}^{*} / c_{l}^{*} \right) > 1 - \alpha. \tag{5}
\]

Similar to the approximation of BART VIP, we can approximate \( (\sum_{r=1}^{L_{\text{rep}}} c_{r,j} / c_{r..}) / L_{\text{rep}} \) in (5) by \( \bar{c}_{L_{\text{rep}},j} / \bar{c}_{L_{\text{rep}},..} \) and therefore the selection criteria (5) can be rewritten as

\[
\frac{1}{L} \sum_{l=1}^{L} \mathbb{I} \left( \frac{\bar{c}_{L_{\text{rep}},j} / c_{l,j}^{*}}{\bar{c}_{L_{\text{rep}},..} / c_{l}^{*}} > 1 - \alpha, \right. \tag{6}
\]

where \( \bar{c}_{L_{\text{rep}},j} = (\sum_{r=1}^{L_{\text{rep}}} c_{r,j}) / L_{\text{rep}} \) and \( \bar{c}_{L_{\text{rep}},..} = (\sum_{r=1}^{L_{\text{rep}}} c_{r..}) / L_{\text{rep}}. \)

The ratio \( \bar{c}_{L_{\text{rep}},j} / c_{l,j}^{*} \) on the left hand side (LHS) of the inequality inside the sum of (6) represents the average increment in usage of a predictor \( x_j \) in a BART model built on the original dataset, compared to a null dataset; the ratio \( \bar{c}_{L_{\text{rep}},..} / c_{l}^{*} \) on the right hand side (RHS) represents the average increment in the total number of the splitting nodes over all the posterior samples of a BART model built on the original dataset, compared to a null dataset. Figure S.3 of the Supplementary Material shows the overall counts ratio \( \bar{c}_{L_{\text{rep}},..} / c_{l}^{*} \) and the counts ratio \( \bar{c}_{L_{\text{rep}},j} / c_{l,j}^{*} \) for each predictor in Example 2. Both relevant continuous \( (x_{11}, x_{12} \) and \( x_{13} \) and relevant binary \( (x_1 \) and \( x_2 \) predictors are indeed used more frequently in the BART model built on the original dataset, i.e., \( \bar{c}_{L_{\text{rep}},j} / c_{l,j}^{*} > 1 \), but the increment in usage of a relevant binary predictor is not always greater than the increment in the total number of splits, i.e., \( \bar{c}_{L_{\text{rep}},j} / c_{l,j}^{*} \neq \bar{c}_{L_{\text{rep}},..} / c_{l}^{*} \). A binary predictor can only be used once at most in each path of a tree because it only has one split value, and a few splits are sufficient to provide the information about a binary predictor. As a result, \( \bar{c}_{L_{\text{rep}},j} \), the number of splits using a binary predictor, is limited by its low cardinality, even if it is relevant. In addition, the number of splits \( c_{l,j}^{*} \), using a binary predictor in a BART model built on a null dataset is roughly \( 1/p \) of the total number of splits in the ensemble (Bleich et al. (2014)). As such, when the number of predictors is small, \( c_{l,j}^{*} \) is close to \( \bar{c}_{L_{\text{rep}},j} \). (see the left subfigure of Figure S.4 of the Supplementary Material), thereby making the counts ratio \( \bar{c}_{L_{\text{rep}},j} / c_{l,j}^{*} \) for a binary predictor close to 1. The overall counts ratio \( \bar{c}_{L_{\text{rep}},..} / c_{l}^{*} \) is also close to 1 because of the BART regularization prior. In fact, given a fixed number of trees in an ensemble, the total number of splits in the ensemble is controlled by the splitting probability, the probability of splitting a node into two child nodes, which is the same for BART models built on the original dataset and null datasets, so the total number of splits for the original dataset and a null dataset, \( \bar{c}_{L_{\text{rep}},..} \) and \( c_{l}^{*} \),
are of similar magnitude (see the right subfigure of Figure S.4). As such, the increment in usage of a relevant binary predictor \( \bar{c}_{L, rep, j}/c_{i, j}^* \) is easily offset by the increment in the total number of splits \( \bar{c}_{L, rep}/c_{i,..}^* \).

Figure S.4 of the Supplementary Material also shows that the increment in the total number of splits is primarily driven by those relevant continuous predictors, so essentially the increment in usage of a relevant binary predictor is offset by that of relevant continuous predictors. To alleviate this behavior, we modify Definition 2.1 using the type information of predictors.

**Definition 3.3** (BART Within-Type Variable Inclusion Proportion). Denote by \( S_{cts} \) (or \( S_{bin} \)) the set of indicators for continuous (or binary) predictors. Following the notation in Definition 2.1, for every \( k = 1, \cdots, K \), let \( c_{cts, k} = \sum_{j \in S_{cts}} c_{jk} \) (or \( c_{bin, k} = \sum_{j \in S_{bin}} c_{jk} \)) be the total number of splitting nodes using continuous (or binary) predictors in the \( k^{th} \) posterior sample. For every \( j = 1, \cdots, p \), define the BART within-type VIP for the predictor \( x_j \) as follows:

\[
v_{w.t.}^j = \frac{1}{K} \sum_{k=1}^{K} \frac{c_{jk}}{c_{cts, k} \cdot \mathbb{I}(j \in S_{cts}) + c_{bin, k} \cdot \mathbb{I}(j \in S_{bin})}.
\]

Define \( \delta_{jj'} = \mathbb{I}(x_j \text{ and } x_{j'} \text{ are of the same type}) \) for any \( j = 1, \cdots, p \) and \( j' = 1, \cdots, p \). Write \( \bar{c}_{L, rep, \text{type of } x_{j'}} = (\sum_{r=1}^{L_{rep}} \sum_{j'=1}^{p} c_{r, j'} \cdot \delta_{jj'})/L_{rep} \) and \( c_{i, \text{type of } x_{j'}} = \sum_{j'=1}^{p} c_{i, j'}^* \cdot \delta_{jj'} \). The permutation-based variable selection approach (Algorithm 1) using BART within-type VIP as the variable importance measure selects a predictor \( x_j \) only if

\[
\frac{1}{L} \sum_{l=1}^{L} \left( \frac{\bar{c}_{L, rep, j}/c_{i, j}^*}{c_{i, \text{type of } x_j}} \right) > 1 - \alpha. \tag{7}
\]

For a binary predictor, the selection criteria (7) removes the impact of continuous predictors, thereby not diluting the effect of a relevant binary predictor. Figure 2 shows the variable selection result of this approach. As opposed to the approach of Bleich et al. (2014), both the two relevant binary predictors \( x_1 \) and \( x_2 \) are clearly identified by this approach.

### 3.2 BART Variable Importance Using Metropolis Ratios

While BART within-type VIP works well in including relevant predictors in presence of a similar number of binary and continuous predictors, it becomes problematic if the number of predictors of one type is low. For example, when there are 99 continuous predictors and 1 binary predictor, the BART within-type VIP of the binary predictor is always 1 for both the original dataset and a null dataset. As such, the binary predictor is
Figure 2: Variable selection results of the permutation-based approach using BART within-type VIP as the variable importance measure for Example 2. The same setting ($L = 100$, $L_{\text{rep}} = 10$, $\alpha = 0.05$ and $M = 20$) and BART posterior samples as Figure S.1 of the Supplementary Material are used. Red (or green) dots are for continuous (or binary) predictors. Solid (or open) dots are for selected (or not selected) predictors. Each vertical grey line is the local threshold for the corresponding predictor. Both the two relevant binary predictors, $x_1$ and $x_2$, are selected and have similar variable importance to the relevant continuous ones.

never selected by the permutation-based approach, whether it is relevant or not. Furthermore, when there are more than two types of predictors, the computation of BART within-type VIP becomes complicated. Hence, we propose a new type of variable importance measure based on the Metropolis ratios calculated in the Metropolis-Hastings steps for sampling new trees, which are not affected by the issues above.

As mentioned in Section 2.1, a key feature of the Metropolis-within-Gibbs sampler is the Bayesian backfitting procedure for sampling $(T_m, \mu_m)$, $1 \leq m \leq M$, where each $T_m$ is fit iteratively using the residual response $r_m = y - \sum_{m' \neq m} g(x; T_{m'}, \mu_{m'})$, with all the other trees $T_{-m} = \{T_{m'}\}_{m' \neq m}$ held constant. Thus, each $(T_m, \mu_m)$ can be obtained in two sequential steps:

$$T_m \mid r_m, \sigma^2,$$

$$\mu_m \mid T_m, r_m, \sigma^2,$$

where $r_m$ is the vector of residual responses. The distribution of $T_m \mid r_m, \sigma^2$ has a closed form up to a normalizing constant and therefore can be sampled by a Metropolis-Hastings algorithm. Chipman, Edward I. George, and Robert E. McCulloch (1998) develop a Metropolis-Hastings algorithm that proposes a new
tree based on the current tree using one of the four moves: BIRTH, DEATH, CHANGE and SWAP. The BIRTH and DEATH proposals are the essential moves for sufficient mixing of the Gibbs sampler, so both the CRAN R package BART (Sparapani, Spanbauer, and R. McCulloch (2021)) and our package BartMixVs (Luo and Daniels (2021)) implement these two proposals, each with equal probability. A BIRTH proposal turns a terminal node into a splitting node and a DEATH proposal replaces a splitting node leading to two terminal nodes by a terminal node. Thus, the proposed tree $T^*$ is identical to the current tree $T_m$ except growing/pruning one splitting node.

We consider using the Metropolis ratio for accepting a BIRTH proposal to construct a variable importance measure. For convenience, we suppress the subscript $m$ in the following. The Metropolis ratio for accepting a BIRTH proposal at a terminal node $\eta$ of the current tree $T$ can be written as

$$\pi_{\text{BIRTH}}(\eta) = \min \{1, r(\eta)\},$$

where

$$r(\eta) = \frac{P(T \mid T^*) P(T^* \mid r, \sigma^2)}{P(T^* \mid T) P(T \mid r, \sigma^2)}.$$  

The BART prior splits a node of depth $d$ into two child nodes of $d+1$ with probability $\gamma(1 + d)^{-\beta}$ for some $\gamma \in (0, 1)$ and $\beta \in [0, \infty)$. Given that, the untruncated Metropolis ratio $r(\eta)$ can be explicitly expressed as the product of three ratios:

- **Nodes Ratio** = $\frac{2b}{b + 2}$,
- **Depth Ratio** = $\frac{\gamma [1 - \gamma/(2 + d_\eta)^\beta]^2}{(1 + d_\eta)^\beta - \gamma}$,
- **Likelihood Ratio** = $\frac{P(r \mid T^*, \sigma^2)}{P(r \mid T, \sigma^2)}$,

where $b$ is the number of terminal nodes in the current tree $T$ and $d_\eta$ is the depth of the node $\eta$ in the current tree $T$. The derivation can be found in Section S.2 of the Supplementary Material.

Figure S.5 of the Supplementary Material shows the nodes ratios for different numbers of terminal nodes and the depth ratios for different depths when the hyper-parameters $\gamma$ and $\beta$ are set as default, i.e., $\gamma = 0.95$ and $\beta = 2$. From the figure, we can see that the product of nodes ratio and depth ratio is mostly affected by the depth ratio, which decreases as the proposed depth $d_\eta$ increases, implying that $r(\eta)$ assigns a greater value to a shallower node which typically contains more samples. Since the likelihood ratio indicates the
conditional improvement to fitting brought by the new split, the untruncated Metropolis ratio \( r(\eta) \) considers both the proportion of samples affected at the node \( \eta \) and the conditional improvement to fitting brought by the new split at the node \( \eta \). However, it is not appropriate to directly use \( r(\eta) \) to construct a variable importance measure, due to the occurrence of extremely large \( r(\eta) \) which dominates the others. Instead, we use the Metropolis ratio in (8) to construct the following BART Metropolis importance.

**Definition 3.4** (BART Metropolis Importance). Let \( K \) be the number of posterior samples obtained from a BART model. For every \( k = 1, \cdots, K \) and \( j = 1, \cdots, p \), define the average Metropolis acceptance ratio per splitting rule using the predictor \( x_j \) at the \( k \)th posterior sample as follows:

\[
\tilde{u}_{jk} = \frac{\sum_{m=1}^{M} \sum_{\eta \in \phi_{mk}} \mathbb{I}(j_{\eta} = j) \pi_{\text{BIRTH}}(\eta)}{\sum_{m=1}^{M} \sum_{\eta \in \phi_{mk}} \mathbb{I}(j_{\eta} = j)},
\]

where \( \phi_{mk} \) is the set of splitting nodes in the \( k \)th posterior sample of the \( m \)th tree and \( j_{\eta} \) is the indicator of the split variable at the node \( \eta \). The BART Metropolis Importance (MI) for the predictor \( x_j \) is defined as the normalized \( \tilde{u}_{jk} \), averaged across \( K \) posterior samples:

\[
v_{\text{MI}}^j = \frac{1}{K} \sum_{k=1}^{K} \frac{\tilde{u}_{jk}}{\sum_{j=1}^{p} \tilde{u}_{jk}}.
\]  

(10)

The intuition of BART MI is that a relevant predictor is expected to be consistently accepted with a high Metropolis ratio. Figure 3 shows that the Metropolis ratios of the splits using relevant predictors \( (x_1, x_2, x_{11}, x_{12} \text{ and } x_{13}) \) as the split variable have a higher median and smaller standard error than those using irrelevant predictors, implying that relevant predictors are consistently accepted with a higher Metropolis ratio. BART MI and BART VIP have similar forms. The key difference is the “kernel” they use. While BART VIP uses the number of splits \( c_{j} \) which tends to be biased against binary predictors, BART MI uses the average Metropolis acceptance ratio \( \tilde{u}_{jk} \) which is similar between the relevant binary predictors and relevant continuous predictors, as shown in Figure 3. Hence, the average Metropolis acceptance ratio \( \tilde{u}_{jk} \) not only helps BART MI distinguish relevant and irrelevant predictors, but also helps BART MI not be biased against predictors of a certain type.

The vector of average Metropolis acceptance ratios \( (\tilde{u}_{1k}, \cdots, \tilde{u}_{pk}) \) does not sum to 1 and each of them varies from 0 to 1. We normalize the vector \( (\tilde{u}_{1k}, \cdots, \tilde{u}_{pk}) \) in (10) based on the idea that \( \tilde{u}_{jk} \)’s are correlated.
in the sense that once some predictors that explain the response more are accepted with higher Metropolis ratios, the rest of predictors will be accepted with lower Metropolis ratios or not be used. In addition, we take the average over $K$ posterior samples in (10) because averaging further helps identify relevant predictors. In fact, an irrelevant predictor can be accepted with a high Metropolis ratio at some MCMC iterations, but it can be quickly removed from the model by the DEATH proposal. As a result, the irrelevant predictor can have a few large $\tilde{u}_{jk}$’s and many small $\tilde{u}_{jk}$’s, thereby resulting in a small BART MI $v_{jMI}$, as shown in Figure 3.

Figure 3: Each barplot (w.r.t. the left y-axis) depicts $c_j$, the number of splits using a predictor as the split variable over all the posterior samples. Each boxplot (w.r.t. the right y-axis) depicts the Metropolis ratios $\pi_{BIRTH}(\eta)$ of the splits using a predictor as the split variable, over all the posterior samples. Each red triangle (w.r.t. the right y-axis) displays the BART MI $v_{jMI}$ for a predictor. Posterior samples are obtained from a BART model for Example 2.

We further explore BART MI under null settings. We create a null dataset of Example 2 and fit a BART model on it. Figure S.6 of the Supplementary Material shows that not all the MIs, $v_{jMI}$’s, converge to $1/p = 0.05$, implying that $1/p$ may not be a good selection threshold for $v_{jMI}$’s. We repeat the experiment of Bleich et al. (2014) for BART MI under null settings to explore the variation among $v_{jMI}$’s. Specifically, we create 100 null datasets of the data generated from Example 2, and for each null dataset, we run BART 50 times with different initial values of the hyper-parameters. Let $v_{ijk}$ be the BART MI for the predictor $x_j$ from the $k^{th}$ BART model on the $i^{th}$ null dataset. We investigate three nested variances listed in Table 1.

Results of the experiment are shown in Figure S.7 of the Supplementary Material. The non-zero $s_{ij}$’s imply that there is variation in $v_{jMI}$’s among the repetitions of BART with different initial values, so it is
necessary to average MIs over a certain number of repetitions of BART to get stable MIs. In practice, we find that among the repetitions of BART, irrelevant predictors occasionally get outliers of MI. Thus, instead of averaging MIs over BART repetitions, we take the median of them. Similar to Bleich et al. (2014), we also find that 10 repetitions of BART is sufficient to get stable MIs (see Figure S.8 of the Supplementary Material). Figure S.7 also shows that the second type of standard deviation $s_j$ is significantly greater than the median of $s_{ij}$'s for each predictor, which suggests that BART tends to overfit noise. Since the overall MI $\bar{v}^\text{MI}$ is always $1/p$, the relatively large $s$ indicates that not all the $\bar{v}^\text{MI}_{j \cdot}$ are approximately $1/p$, suggesting that it is not possible to determine a single selection threshold for all the MIs. Therefore, we employ the permutation-based approach (Algorithm 1) to select thresholds for each MI. A slight modification is applied to line 4 of Algorithm 1: we take the median, rather than the average, of BART MIs, over the repetitions of BART on the original dataset. The variable selection result of this approach for Example 2 is shown in Figure 4.

### 3.3 Backward Selection with Two Filters

In this section, we propose an approach to select a subset of predictors with which the BART model gives the best prediction. In general, to select the best subset of predictors from the model space consisting of $2^p$ possible models, one needs a search strategy over the model space and decision-making rules to compare models. Here we use the backward elimination approach to search the model space, mainly because it is a deterministic approach and is efficient with a moderate number of predictors. Typically, backward selection starts with the full model with all the predictors, followed by comparing the deletion of each predictor using a chosen model fit criterion and then deleting the predictor whose loss gives the most statistically insignificant deterioration of the model fit. This process is repeated until no further predictors can be deleted without a statistically insignificant loss of fit. Some popular model fit criterions such as AIC and BIC are not available for BART, because the maximum likelihood estimates are unavailable and the number of parameters in the

| Variance | Description |
|----------|-------------|
| $s_{ij}^2 = \frac{1}{50} \sum_{k=1}^{50} (v_{ijk}^\text{MI} - \bar{v}_{ij}^\text{MI})^2$ | The variability of BART MI for the predictor $x_j$ in the $i$th dataset; $\bar{v}_{ij}^\text{MI} = (\sum_{k=1}^{50} v_{ijk}^\text{MI})/50$. |
| $s_j^2 = \frac{1}{50} \sum_{i=1}^{100} (\bar{v}_{ij}^\text{MI} - \bar{v}_{\cdot j}^\text{MI})^2$ | The variability due to chance capitalization, i.e., fitting noise, of BART for the predictor $x_j$ across datasets; $\bar{v}_{ij}^\text{MI} = (\sum_{i,k=1}^{100,50} v_{ijk}^\text{MI})/(100 \times 50)$. |
| $s^2 = \frac{1}{19} \sum_{j=1}^{20} (\bar{v}_{\cdot j}^\text{MI} - \bar{v}_{\cdot \cdot}^\text{MI})^2$ | The variability of BART MI across predictors; $\bar{v}_{\cdot j}^\text{MI} = (\sum_{i,j,k=1}^{100,20,50} v_{ijk}^\text{MI})/(100 \times 20 \times 50)$. |
Figure 4: Variable selection results of the permutation-based approach using BART MI as the variable importance measure for Example 2. The same setting and BART posterior samples as Figure S.1 of the Supplementary Material and Figure 2 are used. With BART MI, all the relevant predictors ($x_1$, $x_2$, $x_{11}$, $x_{12}$, and $x_{13}$) are identified.

model is hard to determine. To overcome this issue, we propose a backward selection approach with two easy-to-compute selection criterions as the decision-making rules.

We first split the dataset $\{y_i, x_i\}_{i=1}^n$ into a training set and a test set before starting the backward procedure. To measure the model fit, we make use of the mean squared errors (MSE) of the test set

$$MSE_{test} = \frac{1}{n_{test}} \sum_{i \in \text{test set}} \left[ y_i - \hat{f}(x_i) \right]^2,$$

where $\hat{f}$ is the estimated sum-of-trees function. Figure 5 shows that $MSE_{test}$ can distinguish between acceptable models and unacceptable models, where acceptable models are defined as those models including all the relevant predictors and unacceptable models are defined as those missing some relevant predictors. At each backward selection step, we run BART models on the training set and compute the MSE of the test set. The model with the smallest $MSE_{test}$ is chosen as the “winner” at that step. However, due to the lack of stopping rules under such nonparametric setting, the backward selection has to continue until there is only one predictor in the model, and ultimately returns $p$ “winner” models with different model sizes ranging from 1 to $p$. 

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Figure 5: MSE test’s of all the models evaluated in the backward selection approach for Example 2. Each green (or red) boxplot depicts the MSE test’s of all the acceptable (or unacceptable) models evaluated at a backward selection step. The MSE test’s for acceptable models are close to 0 and have tiny standard error, so green boxplots are very narrow and near 0.

Given the $p$ “winner” models, we compare them using the expected log pointwise predictive density based on leave-one-out (LOO) cross validation:

$$\text{elpd}_{\text{loo}} = \sum_{i=1}^{n} \log \left[ f \left( y_i \mid y_{-i} \right) \right] = \sum_{i=1}^{n} \log \left[ \int f \left( y_i \mid \theta \right) f \left( \theta \mid y_{-i} \right) d\theta \right],$$

(11)

where $y_{-i} = \{y_j\}_{j \neq i}$, $\theta = \{\{T_m, \mu_m\}_{m=1}^M, \sigma^2\}$ represents the set of BART parameters, $f \left( y_i \mid y_{-i} \right)$ is the predictive density of $y_i$ given $y_{-i}$, $f(y_i \mid \theta)$ is the likelihood of $y_i$, and $f(\theta \mid y_{-i})$ is the posterior density of BART given the observations $y_{-i}$. The quantity elpd$_{\text{loo}}$ not only measures the predictive capability of a model, but also penalizes the complexity of the model, i.e., the number of predictors used in the model. Hence, we choose the model with the largest elpd$_{\text{loo}}$ as the best model.

Direct computing (11) involves fitting BART $n$ times. To avoid this, we use the approach of Vehtari, Gelman, and Gabry (2017) that estimates each $f(y_i \mid y_{-i})$ using importance sampling with the full posterior distribution $f(\theta \mid y)$ as the sampling distribution and the smoothed ratios $\{f(\theta^k \mid y_{-i})/f(\theta^k \mid y) \propto 1/f(y_i \mid \theta^k)\}_{k=1}^{K}$ as the importance ratios, where $\{\theta^k\}_{k=1}^{K}$ are the $K$ posterior samples from the full posterior distribution $f(\theta \mid y)$. The smoothness is achieved by fitting a generalized Pareto distribution to the upper tail of each set of the importance ratios $1/f(y_i \mid \theta^k)_{k=1}^{K}$, $i = 1, \ldots, n$. Thus, elpd$_{\text{loo}}$ in (11) can be estimated by using the likelihoods $\{f(y_i \mid \theta^k) = \phi(y_i \mid \hat{f}^k(x_i), \sigma^k)\}_{i,k=1}^{n,K}$ based on $K$ posterior samples $\{\hat{f}^k\}_{k=1}^{K}$ from
the BART model fit on the dataset \( \{ y_i, x_i \}_{i=1}^n \), where \( \hat{f}^k \) is the \( k \)th posterior sample of the sum-of-trees function (2) and \( \phi(\cdot | \mu, \sigma) \) is the normal density with mean \( \mu \) and standard error \( \sigma \).

The approach above can also be extended to the probit BART model (3) by changing the MSE\(_{test} \) to the mean log loss (MLL) of the test set

\[
\text{MLL}_{test} = -\frac{1}{n_{test}} \sum_{i \in \text{test set}} [y_i \log (\hat{p}_i) + (1 - y_i) \log (1 - \hat{p}_i)]
\]  

(12)

and replacing the normal likelihoods with the Bernoulli density \( \{ f(y_i | \theta^k) = \hat{p}^k_i y_i + (1 - \hat{p}^k_i)(1 - y_i) \}_{i,k=1}^{n,K} \), where \( \hat{p}^k_i = \Phi(\hat{f}^k(x_i)) \) is the estimated probability based on the \( k \)th posterior sample of probit BART for the \( i \)th observation and \( \hat{p}_i = \Phi(\sum_{k=1}^K \hat{f}^k(x_i)/K) \). We summarize this algorithm in Algorithm 2. Although this algorithm requires fitting BART \( p(p-1)/2 \) times, models at the same backward selection step can be fitted in parallel, which implies that the time complexity \( O(p(p-1)/2) \) can be reduced to \( O(p) \) if there are sufficient computing resources.

**Algorithm 2** Backward selection with two filters

**Input:** \( X \): predictors; \( y \): response; \( s \): split ratio  
**Output:** A subset of predictors.

1. Randomly split the data \((y, X)\) into \((y_{train}, X_{train})\) and \((y_{test}, X_{test})\) according to the split ratio \( s \)
2. Run BART, say Model\(_1\), on \((y_{train}, X_{train})\) with all the predictors and compute the LOO score: elpd\(_{loo}^1\)
3. for \( l = 1, \cdots, p-1 \) do
4. \hspace{1em} for \( t = 1, \cdots, p-l+1 \) do
5. \hspace{2em} Remove the \( t \)th predictor from the predictors used in Model\(_l\)
6. \hspace{2em} Run BART, say Model\(_{l+1,t}\), with the remaining predictors on \((y_{train}, X_{train})\)
7. \hspace{2em} Compute the MSE of the test set: MSE\(_{test}^{l+1,t}\) (or MLL\(_{test}^{l+1,t}\) if \( y \) is binary)
8. \hspace{2em} Compute the LOO score of the training set: elpd\(_{loo}^{l+1,t}\)
9. end for
10. Find \( t^* \) that minimizes \{MSE\(_{test}^{l+1,t} \}_{t=1}^{p-l+1}\) (or \{MLL\(_{test}^{l+1,t} \}_{t=1}^{p-l+1}\) if \( y \) is binary)
11. Denote Model\(_{l+1,t^*}\) by Model\(_{l+1}\) and elpd\(_{loo}^{l+1,t^*}\) by elpd\(_{loo}^{l+1}\)
12. end for
13. Find \( l^* \) that maximizes \{elpd\(_{loo}^l \}_{l=1}^{p}\)
14. Return Model\(_{l^*}\).

4 Simulations

In this section, we compare the proposed variable selection approaches: (1) permutation-based approach using within-type BART VIP, (2) permutation-based approach using BART MI, and (3) backward selection with two filters, with the existing BART-based variable selection approaches: (4) median probability model from DART, (5) permutation-based approach using BART VIP, and (6) ABC Bayesian forest. For the
permutation-based approaches (1), (2) and (5), we set $L_{\text{rep}} = 10$, $L = 100$ and $\alpha = 0.05$ (see Algorithm 1), and use $M = 20$ trees for BART to encourage competition among the predictors. The three permutation-based approaches are based on the same posterior samples and the one using within-type BART VIP is only applied to scenarios with mixed-type predictors. For the backward selection procedure (3), we set $s = 80\%$ (see Algorithm 2) and use $M = 50$ trees for BART to ensure its prediction power. For DART (4), we consider $M = 20$ and $M = 200$ trees, respectively. For ABC Bayesian forest, as Liu, Ročková, and Y. Wang (2021) suggest, we assume the prior $\pi(S)$ on the model space to be the beta-binomial prior with $\theta \sim \text{Beta}(1,1)$, set the split ratio as 50%, and use $M = 10$ and $M = 20$ trees for BART respectively; we generate 1000 ABC samples, rank the samples by MSE in ascending order if the response variable is continuous (or by MLL if the response variable is binary), and keep the top 10% of samples for selection; we report selection results for two selection thresholds 0.25 and 0.5. All the methods above, except ABC Bayesian forest, burn in the first 1000 and keep 1000 posterior samples in each BART run. ABC Bayesian forest burns in 200 posterior samples and saves the 201st posterior sample, as Liu, Ročková, and Y. Wang (2021) suggest. Other hyper-parameters of BART are the same as the default recommended by Chipman, Edward I. George, and Robert E. McCulloch (2010). The simulation results were obtained using the R package BartMixVs (Luo and Daniels (2021)) which is briefly introduced in Section S.3 of the Supplementary Material.

To evaluate variable selection results, we consider precision ($\text{prec}$), recall ($\text{rec}$), $F_1$ score, and the proportion of the replications that miss at least one relevant predictor ($r_{\text{miss}}$), given by

$$\text{prec} = \frac{\text{TP}}{\text{TP} + \text{FP}}, \quad \text{rec} = \frac{\text{TP}}{\text{TP} + \text{FN}}, \quad F_1 = \frac{2 \cdot \text{prec} \cdot \text{rec}}{\text{prec} + \text{rec}},$$

$$r_{\text{miss}} = \frac{\# \text{ of replications missing at least one relevant predictor}}{\# \text{ of total replications}},$$

where TP is the number of relevant predictors correctly selected, FP is the number of predictors incorrectly selected and FN is the number of relevant predictors not selected. High precision indicates good ability of excluding irrelevant predictors and high recall indicates good ability of including relevant predictors. The $F_1$ score is a balanced score between precision and recall. The lowest $r_{\text{miss}}$ score is 0, implying that the method does not miss any relevant predictors over all the replications.

We evaluate the aforementioned variable selection approaches under four possible combination scenarios of \{continuous response $y$, binary response $y$\} \times \{continuous predictors $x$, mixed-type predictors $x$\}. Each scenario is replicated 100 times. The simulation results for the scenario of binary response and continuous predictors can be found in Section S.4.2 of the Supplementary Material.
4.1 Continuous Response and Continuous Predictors

In this setting, we consider two scenarios. Scenario C.C.1 is an example from Friedman (1991); Scenario C.C.2, which includes correlation between predictors, is borrowed from Zhu, Zeng, and Kosorok (2015). For both of them, we consider \( n = 500 \), \( p \in \{50, 200\} \) and \( \sigma^2 = 1 \).

**Scenario C.C.1.** Sample the predictors \( x_1, \cdots, x_p \) from Uniform(0, 1) independently and the response \( y \) from Normal\( (f_0(x), \sigma^2) \), where

\[
f_0(x) = 10 \sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5.
\]  

(13)

**Scenario C.C.2.** Sample the predictors \( x_1, \cdots, x_p \) from Normal(0, \( \Sigma \)) with \( \Sigma_{jk} = 0.3^{|j-k|} \), \( j, k = 1, \cdots, p \), and the response \( y \) from Normal\( (f_0(x), \sigma^2) \), where

\[
f_0(x) = 2x_1 x_4 + 2x_7 x_{10}.
\]  

(14)

Results are given in Table 2. When the predictors are independent (Scenario C.C.1) and \( p = 50 \), none of the methods miss any relevant predictors, i.e., \( r_{\text{miss}} = 0 \) and \( \text{rec} \equiv 1 \). The permutation-based approach using BART VIP and the ABC Bayesian forest methods, except the one using \( M = 20 \) trees and selection threshold 0.25 (i.e., ABC-20-0.25), are the best in terms of precision and the \( F_1 \) scores, followed by the permutation-based approach using BART MI and DART with \( M = 20 \) trees. When \( p = 200 \), only the ABC Bayesian forest with \( M = 10 \) trees and selection threshold 0.5 (i.e., ABC-10-0.50) fails to include all the relevant predictors. As discussed in Section 2.2.4, ABC Bayesian forest using a small number of trees and keeping a small number of posterior samples makes it easy to miss relevant predictors, especially when the number of predictors is large and the selection threshold is high. As shown in Table 2, increasing the number of trees to \( M = 20 \) or decreasing the selection threshold to 0.25 can improve the result. The other three ABC Bayesian forest methods achieve the best precision and \( F_1 \) scores, followed by the two permutation-based approaches. The backward selection procedure is not a top choice in terms of precision, but its precision (0.75 for \( p = 50 \) and 0.74 for \( p = 200 \)) is acceptable in the sense that it only includes about 1.7 irrelevant predictors on average. In fact, we find that the LOO score used in the backward selection, though penalizing the model complexity, appears to have difficulty in distinguishing between the true model and an acceptable model with a similar number of predictors, thereby resulting in a relatively low precision score.

When the predictors are correlated (Scenario C.C.2) and \( p = 50 \), the two permutation-based approaches,
Table 2: Simulation results for the scenarios using continuous $y$ and continuous $x$. Scenario C.C.1 is Friedman’s example; Scenario C.C.2 includes correlation between predictors. Each score is the average across 100 replications and Monte Carlo standard error is given inside the parentheses.

### Scenario C.C.1

|          | $n = 500$, $p = 50$, $\sigma^2 = 1$ | $n = 500$, $p = 200$, $\sigma^2 = 1$ |
|----------|--------------------------------------|--------------------------------------|
|          | $r_{\text{miss}}$ $|rec$ | $prec$ | $F_1$ | $r_{\text{miss}}$ $|rec$ | $prec$ | $F_1$ |
| DART-20  | 0  | 1(0) | 0.87(0.01) | 0.93(0.01) | 0  | 1(0) | 0.86(0.01) | 0.92(0.01) |
| DART-200 | 0  | 1(0) | 0.7(0.02) | 0.81(0.01) | 0  | 1(0) | 0.63(0.02) | 0.76(0.01) |
| ABC-10-0.25 | 0  | 1(0) | 1(0) | 1(0) | 0  | 1(0) | 1(0) | 1(0) |
| ABC-10-0.50 | 0  | 1(0) | 1(0) | 1(0) | 0.33 | 0.93(0.01) | 1(0) | 0.96(0.01) |
| ABC-20-0.25 | 0  | 1(0) | 0.5(0.01) | 0.66(0.01) | 0  | 1(0) | 1(0) | 1(0) |
| ABC-20-0.50 | 0  | 1(0) | 1(0) | 1(0) | 0  | 1(0) | 1(0) | 1(0) |
| Permute (VIP) | 0  | 1(0) | 1(0) | 1(0) | 0  | 1(0) | 0.95(0.01) | 0.97(0) |
| Permute (MI) | 0  | 1(0) | 0.98(0.01) | 0.99(0) | 0  | 1(0) | 0.94(0.01) | 0.97(0.01) |
| Backward | 0  | 1(0) | 0.75(0.02) | 0.83(0.02) | 0  | 1(0) | 0.74(0.02) | 0.83(0.02) |

### Scenario C.C.2

|          | $n = 500$, $p = 50$, $\sigma^2 = 1$ | $n = 500$, $p = 200$, $\sigma^2 = 1$ |
|----------|--------------------------------------|--------------------------------------|
|          | $r_{\text{miss}}$ $|rec$ | $prec$ | $F_1$ | $r_{\text{miss}}$ $|rec$ | $prec$ | $F_1$ |
| DART-20  | 0.43 | 0.8(0.03) | 0.86(0.02) | 0.8(0.02) | 0.97 | 0.37(0.03) | 0.47(0.04) | 0.39(0.03) |
| DART-200 | 0  | 1(0) | 0.83(0.02) | 0.9(0.01) | 0.64 | 0.65(0.03) | 0.49(0.03) | 0.53(0.03) |
| ABC-10-0.25 | 0.02 | 1(0) | 0.69(0.02) | 0.8(0.01) | 1  | 0.08(0.01) | 0.28(0.04) | 0.13(0.02) |
| ABC-10-0.50 | 0.82 | 0.61(0.02) | 0.98(0.01) | 0.73(0.02) | 1  | 0(0) | 0.02(0.01) | 0.01(0.01) |
| ABC-20-0.25 | 0  | 1(0) | 0.12(0) | 0.22(0) | 0.99 | 0.28(0.02) | 0.45(0.04) | 0.33(0.03) |
| ABC-20-0.50 | 0.1 | 0.97(0.01) | 0.97(0.01) | 0.97(0.01) | 1  | 0.01(0) | 0.04(0.02) | 0.02(0.01) |
| Permute (VIP) | 0  | 1(0) | 0.98(0.01) | 0.99(0) | 0.71 | 0.68(0.03) | 0.26(0.01) | 0.37(0.01) |
| Permute (MI) | 0  | 1(0) | 0.89(0.01) | 0.93(0.01) | 0.93 | 0.43(0.03) | 0.27(0.02) | 0.32(0.02) |
| Backward | 0  | 1(0) | 0.86(0.02) | 0.92(0.01) | 0.02 | 0.99(0.01) | 0.79(0.03) | 0.84(0.03) |

the backward selection approach, DART with $M = 200$ trees, and the ABC-20-0.25 approach successfully identify all the relevant predictors for all the replications; the first four of them have competitive precision and $F_1$ scores. When more correlated and irrelevant predictors are included ($p = 200$), the backward selection procedure has superior performance in all metrics. It identifies all the relevant predictors for 98% of the times and achieves the highest precision (0.79) and $F_1$ scores (0.84). Compared with the independent setting (Scenario C.C.1), ABC Bayesian forest suffers the most from the multicollinearity as we found that this approach often does not select out any predictors.

With the first three examples in Table 2 being considered, the two proposed approaches along with the approach of Bleich et al. (2014) and DART with $M = 200$ trees consistently perform well in identifying all the relevant predictors. For Scenario C.C.2 with $p = 200$ predictors, the backward selection approach significantly outperforms other methods.
4.2 Continuous Response and Mixed-Type Predictors

In this setting, we consider Scenario C.M.1, a modified Friedman’s example, and Scenario C.M.2, an example including correlation between predictors. We consider $n \in \{500,1000\}$, $p \in \{50,200\}$ and $\sigma^2 \in \{1,10\}$ for Scenario C.M.1, and $n \in \{500,1000\}$ and $\sigma^2 \in \{1,10\}$ for Scenario C.M.2.

**Scenario C.M.1.** Sample the predictors $x_1,\cdots,x_{\lfloor p/2 \rfloor}$ from Bernoulli(0.5) independently, $x_{\lfloor p/2 \rfloor + 1},\cdots,x_p$ from Uniform$(0,1)$ independently, and the response $y$ from Normal$(f_0(x),\sigma^2)$, where

$$f_0(x) = 10 \sin (\pi x_{\lfloor p/2 \rfloor + 1} x_{\lfloor p/2 \rfloor + 2}) + 20 \left( x_{\lfloor p/2 \rfloor + 3} - 0.5 \right)^2 + 10x_1 + 5x_2. \quad (15)$$

**Scenario C.M.2.** Sample the predictors $x_1,\cdots,x_{20}$ from Bernoulli(0.2) independently, $x_{21},\cdots,x_{40}$ from Bernoulli(0.5) independently, $x_{41},\cdots,x_{84}$ from a multivariate normal distribution with mean 0, variance 1 and correlation 0.3, and the response $y$ from Normal$(f_0(x),\sigma^2)$, where

$$f_0(x) = -4 + x_1 + \sin (\pi x_{41} x_{44}) - x_{21} + 0.6x_{41} x_{42} - \exp \left[ -2 \left( x_{42} + 1 \right)^2 \right] - x_{33}^2 + 0.5x_{44}. \quad (16)$$

We report the simulation results for Scenario C.M.1 with the settings, $n = 500$, $p \in \{50,200\}$ and $\sigma^2 = 1$, and Scenario C.M.2 with the settings, $n \in \{500,1000\}$ and $\sigma^2 = 1$, in Table 3. Simulation results for other settings are reported in Table S.1 of the Supplementary Material.

When the predictors are independent (Scenario C.M.1) and $p = 50$, all the methods, except the permutation-based approach using BART VIP, are able to identify all the relevant predictors. The two proposed permutation-based approaches, DART with $M = 20$ trees, and the ABC Bayesian forest approaches except ABC-20-0.25 have comparable best precision and $F_1$ scores, followed by the backward selection procedure. When the dimension is increased to $p = 200$, the ABC-10-0.50 method again fails to include all the relevant predictors, like Scenario C.C.1. The permutation-based approach using BART VIP does not perform poorly in this case, because as $p$ gets larger, $\bar{c}_{L_{rep,j}}$ stays in a similar magnitude and $c_{l,j}^*$ gets smaller (see the left subfigure of Figure S.4 of the Supplementary Material). As such, the offset effect discussed in Section 3.1 disappears. The three proposed approaches are still able to identify all the relevant predictors, but their precision scores are slightly worse than other methods.

When the mixed-type predictors are correlated (Scenario C.M.2), variable selection becomes more challenging. When $\sigma^2 = 1$, the permutation-based approach using BART MI and the backward selection procedure are the best in terms of the $r_{miss}$ and recall scores. Furthermore, only these two methods successfully
Table 3: A part of simulation results for Scenario C.M.1 where predictors are of mixed type and independent and Scenario C.M.2 where predictors are of mixed type and correlated. The rest of simulation results can be found in Table S.1 of the Supplementary Material.

| Scenario C.M.1 | $n = 500, p = 50, \sigma^2 = 1$ | $n = 500, p = 200, \sigma^2 = 1$ |
|----------------|---------------------------------|---------------------------------|
| $r_{\text{miss}}$ | rec | prec | $F_1$ | $r_{\text{miss}}$ | rec | prec | $F_1$ |
| DART-20 | 0 | 0.96(0.01) | 0.98(0) | 0 | 0.95(0.01) | 0.97(0) |
| DART-200 | 0 | 0.65(0.02) | 0.78(0.01) | 0 | 0.63(0.02) | 0.76(0.01) |
| ABC-10-0.25 | 0 | 0.99(0) | 0.99(0) | 0 | 1(0) | 0(0) |
| ABC-10-0.50 | 0 | 1(0) | 1(0) | 0.56 | 0.89(0.01) | 0.94(0.01) |
| ABC-20-0.25 | 0 | 0.62(0.01) | 0.76(0.01) | 0 | 0(0) | 0(0) |
| ABC-20-0.50 | 0 | 1(0) | 1(0) | 0.63 | 0.64(0.01) | 0.75(0.01) |
| Permute (VIP) | 0.29 | 0.94(0.01) | 0.97(0.01) | 0 | 0(0) | 0.85(0.01) |
| Permute (Within-Type VIP) | 0 | 0.99(0.01) | 0.99(0) | 0 | 0(0) | 0.73(0.02) |
| Permute (MI) | 0 | 0.97(0.01) | 0.98(0) | 0 | 0(0) | 0.82(0.01) |
| Backward | 0 | 0.76(0.02) | 0.84(0.02) | 0 | 0(0) | 0.82(0.02) |

| Scenario C.M.2 | $n = 500, p = 84, \sigma^2 = 1$ | $n = 1000, p = 84, \sigma^2 = 1$ |
|----------------|---------------------------------|---------------------------------|
| $r_{\text{miss}}$ | rec | prec | $F_1$ | $r_{\text{miss}}$ | rec | prec | $F_1$ |
| DART-20 | 0.37 | 0.91(0.01) | 0.92(0.01) | 0.09 | 0.94(0.01) | 0.94(0.01) |
| DART-200 | 0.17 | 0.94(0.01) | 0.94(0.01) | 0.01 | 1(0) | 0.78(0.01) |
| ABC-10-0.25 | 0.95 | 0.91(0.01) | 0.92(0.01) | 0.54 | 0.91(0.01) | 0.94(0.01) |
| ABC-10-0.50 | 1 | 0.89(0.01) | 0.90(0.01) | 0.96 | 0.82(0.01) | 0.90(0.01) |
| ABC-20-0.25 | 0.57 | 0.9(0.01) | 0.9(0.01) | 0.05 | 0.99(0) | 0.8(0.01) |
| ABC-20-0.50 | 1 | 0.78(0.01) | 0.87(0.01) | 0.7 | 0.88(0.01) | 0.93(0) |
| Permute (VIP) | 0.18 | 0.97(0.01) | 0.97(0.01) | 0.51 | 0.99(0.01) | 0.93(0.01) |
| Permute (Within-Type VIP) | 0.44 | 0.93(0.01) | 0.93(0.01) | 0.06 | 0.99(0.01) | 0.95(0.01) |
| Permute (MI) | 0.07 | 0.99(0) | 0.91(0.01) | 0 | 0(0) | 0.89(0.01) |
| Backward | 0.11 | 0.76(0.01) | 0.84(0.02) | 0 | 0(0) | 0.82(0.02) |

identify all the relevant predictors over all the replications when $n = 1000$. When high noise ($\sigma^2 = 10$) is included, all the methods have difficulty identifying all the true predictors.

In terms of the recall and $r_{\text{miss}}$ scores, the permutation-based approach using BART MI and the backward selection approach are always the top choices for all the examples in Table 3 and Table S.1, except Scenario C.M.2 with $\sigma^2 = 10$. Compared to the other two proposed approaches, the permutation-based approach using BART within-type VIP suffers from multicollinearity, though it does improve the approach of Bleich et al. (2014) in presence of a small number of mixed-type predictors.

4.3 Binary Response and Mixed-Type Predictors

In this setting, we consider two scenarios, Scenario B.M.1 and Scenario B.M.2. For Scenario B.M.1, we consider $n \in \{500, 1000\}$ and $p \in \{50, 200\}$; for Scenario B.M.2, we consider $n \in \{500, 1000\}$.

**Scenario B.M.1.** Sample the predictors $x_1, \cdots, x_{\lceil p/2 \rceil}$ from Bernoulli(0.5) independently, $x_{\lceil p/2 \rceil+1}, \cdots, x_p$ from Uniform(0, 1) independently, and the response $y$ from Bernoulli($\Phi(f_0(\mathbf{x}))$, where $f_0(\mathbf{x})$ is defined in (15).
Scenario B.M.2. Sample the predictors $x_1, \ldots, x_{20}$ from Bernoulli($0.2$) independently, $x_{21}, \ldots, x_{40}$ from Bernoulli($0.5$) independently, $x_{41}, \ldots, x_{84}$ from a multivariate normal distribution with mean 0, variance 1 and correlation 0.3, and the response $y$ from Bernoulli($\Phi(f_0(x))$, where $f_0(x)$ is defined in (16).

Table 4: Simulation results for the scenarios using binary response and mixed-type predictors. Predictors in Scenario B.M.1 are independent and predictors in Scenario B.M.2 are correlated.

| Scenario B.M.1 | $n = 500, p = 50$ | $n = 500, p = 200$ | Scenario B.M.2 | $n = 1000, p = 50$ | $n = 1000, p = 200$ |
|----------------|------------------|------------------|----------------|------------------|------------------|
|                | $r_{\text{miss}}$ | $\text{rec}$ | $\text{prec}$ | $F_1$ | $r_{\text{miss}}$ | $\text{rec}$ | $\text{prec}$ | $F_1$ | $r_{\text{miss}}$ | $\text{rec}$ | $\text{prec}$ | $F_1$ |
| DART-20        | 0.26             | 0.95(0.01)   | 0.99(0.01)   | 0.96(0.01) | 0.65             | 0.87(0.01)   | 0.99(0)      | 0.92(0.01) |
| DART-200       | 0.13             | 0.97(0.01)   | 0.75(0.02)   | 0.83(0.01) | 0.53             | 0.89(0.01)   | 0.79(0.02)   | 0.83(0.01) |
| ABC-10-0.25    | 0.55             | 0.89(0.01)   | 0.87(0.01)   | 0.87(0.01) | 1                | 0.8(0)       | 0.98(0.01)   | 0.88(0)    |
| ABC-10-0.50    | 0.97             | 0.81(0)      | 1(0)         | 0.89(0)   | 1                | 0.69(0.01)   | 1(0)         | 0.81(0.01) |
| ABC-20-0.25    | 0.03             | 0.99(0)      | 0.18(0)      | 0.31(0)   | 0.92             | 0.82(0.01)   | 0.85(0.01)   | 0.83(0.01) |
| ABC-20-0.50    | 0.85             | 0.83(0.01)   | 0.98(0.01)   | 0.9(0)    | 1                | 0.78(0.01)   | 0.99(0)      | 0.87(0)    |
| Permute (VIP)  | 0.1              | 0.98(0.01)   | 0.99(0)      | 0.9(0)    | 0.16             | 0.97(0.01)   | 0.81(0.01)   | 0.88(0.01) |
| Permute (Within-Type VIP) | 0.08           | 0.98(0.01)   | 1(0)         | 0.99(0)   | 0.22             | 0.96(0.01)   | 0.5(0.02)    | 0.87(0.01) |
| Permute (MI)   | 0.1              | 0.98(0.01)   | 0.96(0.01)   | 0.97(0.01)| 0.25             | 0.95(0.01)   | 0.79(0.01)   | 0.86(0.01) |
| Backward       | 0.09             | 0.98(0.01)   | 0.93(0.02)   | 0.94(0.01)| 0.37             | 0.93(0.01)   | 0.87(0.02)   | 0.88(0.01) |

Simulation results are shown in Table 4. In presence of binary responses and mixed-type predictors, the variable selection results are clearly improved by increasing the sample size from $n = 500$ to $n = 1000$. Under the independent setting (Scenario B.M.1), the three proposed approaches along with the approach of Bleich et al. (2014) achieve $r_{\text{miss}} = 0$ and $\text{rec} = 1$ for both $p = 50$ and $p = 200$, with $n = 1000$ samples. DART with $M = 200$ trees gets slightly worse $r_{\text{miss}}$ and recall scores under these two settings. However, when correlation is introduced, none of the methods work very well in identifying all the relevant predictors,
though the backward selection procedure still gets the best recall and $r_{\text{miss}}$ scores. In fact, we find that the result of the backward selection procedure can be greatly improved by thinning the MCMC chain of BART. For the Scenario B.M.2 with $n = 1000$, we get $r_{\text{miss}} = 0.06$, rec = 0.99(0.01), prec = 0.67(0.05) and $F_1 = 0.73(0.05)$ by keeping every 10th posterior sample in each BART run.

4.4 Conclusion of Simulation Results

We summarize the simulation results above and in Section S.4 of the Supplementary Material in Table 5. We call a variable selection approach with $r_{\text{miss}}$ no greater than 0.1 and precision no less than 0.6, i.e., an approach with excellent capability of including all the relevant predictors and acceptable capability of excluding irrelevant predictors, a successful approach, and check it in Table 5. From the table, we can see that the backward selection approach achieves the highest success rate, followed by the two new permutation-based approaches, meaning that the three proposed approaches consistently perform well in identifying all the relevant predictors and excluding irrelevant predictors. A drawback of the three proposed approaches is that, like existing BART-based variable selection approaches, they also suffer from multicollinearity (Scenario C.M.2, Scenario B.C.2 and Scenario B.M.2), especially when the noise is high or the response is binary. Another shortcoming of the backward selection approach is the computational cost of running BART multiple times, but it should be noted that at each step of the backward selection, BART models can be fitted in parallel on multiple cores.

Table 5: Summary of the simulation studies based on Table 2–4 and Table S.1–S.2 of the Supplementary Material. Variable selection approaches with $r_{\text{miss}}$ no greater than 0.1 and precision no less than 0.6 are checked.
5 Discussion and Future Work

This paper reviews and explores existing BART-based variable selection methods and introduces three new variable selection approaches. These new approaches are designed for adapting to data with mixed-type predictors, and more importantly, for better allowing all the relevant predictors into the model.

We outline some interesting areas for future work. First, the distribution of the null importance scores in the permutation-based approach is unknown. If the distribution can be approximated appropriately, then a better threshold can be used. Second, from the simulation studies for the backward selection approach, we note that there is only a slight difference in MSE_{test} between the winner models from two consecutive steps, when both of them include all the relevant predictors. However, if one of the winner models drops a relevant predictor, the difference can become very large. In light of this, it would be advantageous to develop a formal stopping rule, which would also improve the precision score and the efficiency of the backward selection approach. Finally, a potential direction of conducting variable selection based on BART is to take further advantage of the model selection property of BART itself. As discussed in Section 2.1, BART can be regarded as a Bayesian model selection approach, but it does not perform well due to a large number of noise predictors. We may alleviate this issue by muting noise predictors adaptively and externally (Zhu, Zeng, and Kosorok (2015)).

Acknowledgements

Luo and Daniels were partially supported by NIH R01CA 183854.

References

Albert, James H. and Siddhartha Chib (1993). “Bayesian analysis of binary and polychotomous response data”. In: J. Amer. Statist. Assoc. 88.422, pp. 669–679. issn: 0162-1459. url: http://links.jstor.org/sici?sici=0162-1459(199306)88:422%3C669:BAOBAP%3E2.0.CO;2-T&origin=MSN.

Altmann, André et al. (Apr. 2010). “Permutation importance: a corrected feature importance measure”. In: Bioinformatics 26.10, pp. 1340–1347. issn: 1367-4803. doi: 10.1093/bioinformatics/btq134. url: https://doi.org/10.1093/bioinformatics/btq134.
Barbieri, Maria Maddalena and James O. Berger (2004). “Optimal predictive model selection”. In: *Ann. Statist.* 32.3, pp. 870–897. issn: 0090-5364. doi: 10.1214/009053604000000238. url: https://doi.org/10.1214/009053604000000238.

Bhattacharya, Anirban et al. (2015). “Dirichlet-Laplace priors for optimal shrinkage”. In: *J. Amer. Statist. Assoc.* 110.512, pp. 1479–1490. issn: 0162-1459. doi: 10.1080/01621459.2014.960967. url: https://doi.org/10.1080/01621459.2014.960967.

Bleich, Justin et al. (2014). “Variable selection for BART: an application to gene regulation”. In: *Ann. Appl. Stat.* 8.3, pp. 1750–1781. issn: 1932-6157. doi: 10.1214/14-AOAS755. url: https://doi.org/10.1214/14-AOAS755.

Breiman, Leo (2001). “Random forests”. In: *Machine learning* 45.1, pp. 5–32.

Carvalho, Carlos M., Nicholas G. Polson, and James G. Scott (2010). “The horseshoe estimator for sparse signals”. In: *Biometrika* 97.2, pp. 465–480. issn: 0006-3444. doi: 10.1093/biomet/asq017. url: https://doi.org/10.1093/biomet/asq017.

Chipman, Hugh A., Edward I. George, and Robert E. McCulloch (1998). “Bayesian CART Model Search”. In: *J. Amer. Statist. Assoc.* 93.443, pp. 935–948. doi: 10.1080/01621459.1998.10473750. url: https://doi.org/10.1080/01621459.1998.10473750.

— (2010). “BART: Bayesian additive regression trees”. In: *Ann. Appl. Stat.* 4.1, pp. 266–298. issn: 1932-6157. doi: 10.1214/09-AOAS285. url: https://doi.org/10.1214/09-AOAS285.

Efroymson, M. A. (1960). “Multiple regression analysis”. In: *Mathematical methods for digital computers.* Wiley, New York, pp. 191–203.

Friedman, Jerome H. (1991). “Multivariate adaptive regression splines”. In: *Ann. Statist.* 19.1. With discussion and a rejoinder by the author, pp. 1–141. issn: 0090-5364. doi: 10.1214/aos/1176347963. url: https://doi.org/10.1214/aos/1176347963.

— (2001). “Greedy function approximation: a gradient boosting machine”. In: *Ann. Statist.* 29.5, pp. 1189–1232. issn: 0090-5364. doi: 10.1214/aos/1013203451. url: https://doi.org/10.1214/aos/1013203451.

— (2002). “Stochastic gradient boosting”. In: *Comput. Statist. Data Anal.* 38.4, pp. 367–378. issn: 0167-9473. doi: 10.1016/S0167-9473(01)00065-2. url: https://doi.org/10.1016/S0167-9473(01)00065-2.

Geman, Stuart and Donald Geman (1984). “Stochastic Relaxation, Gibbs Distributions, and the Bayesian Restoration of Images”. In: *IEEE PAMI* PAMI-6.6, pp. 721–741. doi: 10.1109/TPAMI.1984.4767596.
George, Edward I and Robert E McCulloch (1993). “Variable Selection via Gibbs Sampling”. In: J. Amer. Statist. Assoc. 88.423, pp. 881–889. doi: 10.1080/01621459.1993.10476353. url: https://www.tandfonline.com/doi/abs/10.1080/01621459.1993.10476353.

Hastie, Trevor and Robert Tibshirani (2000). “Bayesian backfitting (with comments and a rejoinder by the authors”. In: Statist. Sci. 15.3, pp. 196–223. doi: 10.1214/ss/1009212815. url: https://doi.org/10.1214/ss/1009212815.

Hastings, W. K. (1970). “Monte Carlo sampling methods using Markov chains and their applications”. In: Biometrika 57.1, pp. 97–109. issn: 0006-3444. doi: 10.1093/biomet/57.1.97. url: https://doi.org/10.1093/biomet/57.1.97.

Kapelner, Adam and Justin Bleich (2016). “bartMachine: Machine Learning with Bayesian Additive Regression Trees”. In: J. Stat. Softw. 70.4, pp. 1–40. doi: 10.18637/jss.v070.i04. url: https://www.jstatsoft.org/index.php/jss/article/view/v070i04.

Linero, Antonio R. (2018). “Bayesian regression trees for high-dimensional prediction and variable selection”. In: J. Amer. Statist. Assoc. 113.522, pp. 626–636. issn: 0162-1459. doi: 10.1080/01621459.2016.1264957. url: https://doi.org/10.1080/01621459.2016.1264957.

Liu, Yi, Veronika Ročková, and Yuexi Wang (2021). “Variable selection with ABC Bayesian forests”. In: J. R. Stat. Soc. Ser. B. Stat. Methodol. 83.3, pp. 453–481. issn: 1369-7412. doi: 10.1111/rssb.12423. url: https://doi.org/10.1111/rssb.12423.

Louppe, Gilles (2014). “Understanding random forests”. In: Cornell University Library.

Luo, Chuji and Michael J. Daniels (2021). “The BartMixVs R package”. In: url: https://github.com/chujiluo/BartMixVs.

Ročková, Veronika and Stéphanie van der Pas (2020). “Posterior concentration for Bayesian regression trees and forests”. In: Ann. Statist. 48.4, pp. 2108–2131. issn: 0090-5364. doi: 10.1214/19-AOS1879. url: https://doi.org/10.1214/19-AOS1879.

Sparapani, Rodney, Charles Spanbauer, and Robert McCulloch (2021). “Nonparametric machine learning and efficient computation with bayesian additive regression trees: the BART R package”. In: J. Stat. Softw. 97.1, pp. 1–66.

Strobl, Carolin et al. (2007). “Bias in random forest variable importance measures: Illustrations, sources and a solution”. In: BMC bioinformatics 8.1, p. 25. doi: 10.1186/1471-2105-8-25. url: https://doi.org/10.1186/1471-2105-8-25.
Tibshirani, Robert (1996). “Regression shrinkage and selection via the lasso”. In: *J. Roy. Statist. Soc. Ser. B* 58.1, pp. 267–288. ISSN: 0035-9246. URL: http://links.jstor.org/sici?sici=0035-9246(1996)58:1%3C267:RSASVT%3E2.0.CO;2-G&origin=MSN.

Vehtari, Aki, Andrew Gelman, and Jonah Gabry (2017). “Erratum to: Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC [MR3647105]”. In: *Stat. Comput.* 27.5, p. 1433. ISSN: 0960-3174. DOI: 10.1007/s11222-016-9709-3. URL: https://doi.org/10.1007/s11222-016-9709-3.

Wang, Chi, Giovanni Parmigiani, and Francesca Dominici (2012). “Bayesian effect estimation accounting for adjustment uncertainty”. In: *Biometrics* 68.3, pp. 680–686. ISSN: 0006-341X. DOI: 10.1111/j.1541-0420.2011.01735.x. URL: https://doi.org/10.1111/j.1541-0420.2011.01735.x.

Zhu, Ruoqing, Donglin Zeng, and Michael R. Kosorok (2015). “Reinforcement learning trees”. In: *J. Amer. Statist. Assoc.* 110.512, pp. 1770–1784. ISSN: 0162-1459. DOI: 10.1080/01621459.2015.1036994. URL: https://doi.org/10.1080/01621459.2015.1036994.

Zou, Hui and Trevor Hastie (2005). “Regularization and variable selection via the elastic net”. In: *J. R. Stat. Soc. Ser. B Stat. Methodol.* 67.5, p. 768. ISSN: 1369-7412. DOI: 10.1111/j.1467-9868.2005.00527.x. URL: https://doi.org/10.1111/j.1467-9868.2005.00527.x.
Supplement to "Variable Selection Using Bayesian Additive Regression Trees"

S.1 Proof of Lemma 3.2

Proof. From Cauchy-Schwarz inequality, Definition 2.1 and Definition 3.1 of the main paper, it is clear that

\[ |\tilde{v}_j - v_j| = \left| \sum_{k=1}^{K} \left( \frac{c_{jk} c_{k}}{K \tilde{c}_K c_{k}} \right) \cdot \sum_{k=1}^{K} \left( \frac{1}{K} c_{jk} |c_{k} - \tilde{c}_K| \right) \right| \]

\[ \leq \left[ \frac{1}{K} \sum_{k=1}^{K} \left( \frac{c_{jk} c_{k}}{c_{k}} \right)^2 \right]^{1/2} \cdot \left[ \frac{K}{\tilde{c}_K} \right] \cdot \left[ \sum_{k=1}^{K} \left( \frac{(c_{k} - \tilde{c}_K)^2}{K} \right) \right]^{1/2} \]

\[ \leq \delta_1^{1/2} \delta_2. \]

S.2 Decomposition of Untruncated Metropolis Ratio

The untruncated Metropolis ratio in Equation (9) of the main paper can be explicitly expressed as

\[ r(\eta) = \frac{P(T \mid T^*) \cdot P(T^*) \cdot P(r \mid T^*, \sigma^2)}{P(T^* \mid T) \cdot P(T) \cdot P(r \mid T, \sigma^2)} \]

\[ = \frac{P(\text{DEATH})}{P(\text{BIRTH})} \cdot \frac{P(\text{r} \mid T^*, \sigma^2)}{P(\text{r} \mid T, \sigma^2)} \cdot \frac{\gamma \cdot \left[ 1 - \gamma/(2 + d_{\eta}) \right]^{\beta}}{(1 + d_{\eta})^{\beta} - \gamma} \cdot \frac{1}{\gamma \cdot \left[ 1 - \gamma/(2 + d_{\eta}) \right]^{\beta}} \cdot \frac{P(\text{r} \mid T^*, \sigma^2)}{P(\text{r} \mid T, \sigma^2)} \]

\[ = \frac{b}{w_2^*} \cdot \frac{\gamma \cdot \left[ 1 - \gamma/(2 + d_{\eta}) \right]^{\beta} \gamma^{1/2}}{(1 + d_{\eta})^{\beta} - \gamma} \cdot \frac{P(\text{r} \mid T^*, \sigma^2)}{P(\text{r} \mid T, \sigma^2)}, \]

where \( w_2^* \) is the number of second generation internal nodes (i.e., nodes with two terminal child nodes) in the proposed tree \( T^* \), \( b \) is the number of terminal nodes in the current tree \( T \), \( p_{\text{adj}}(\eta) \) is the number of predictors available to split on at the node \( \eta \) in the current tree \( T \), \( n_{\text{adj}}(\eta) \) is the number of available values to choose for the selected predictor \( x_j \) at the node \( \eta \) in the current tree \( T \), and \( d_{\eta} \) is the depth of node \( \eta \) in the current tree \( T \).

The second equality is because the proposed tree \( T^* \) is identical to the current tree \( T \) except for the new
split node. The third equality is from that $P(\text{BIRTH}) = P(\text{DEATH}) = 0.5$. The last equality is due to the properties of a binary tree, $b = 2w_2$ and $w_2^* = w_2 + 1$, where $w_2$ is the number of second generation internal nodes in the current tree $T$.

### S.3 Brief Introduction to BartMixVs

Built upon the CRAN R package BART (Sparapani, Spanbauer, and R. McCulloch (2021)), the R package BartMixVs (Luo and Daniels (2021)) is developed to implement the three proposed variable selection approaches of the main paper and three existing BART-based variable selection approaches: the permutation-based variable selection approach using BART VIP (Bleich et al. (2014)), DART (Linero (2018)) and ABC Bayesian forest (Liu, Ročková, and Y. Wang (2021)). The simulation results of this work were obtained using this package which is available at [https://github.com/chujiluo/BartMixVs](https://github.com/chujiluo/BartMixVs).

### S.4 More Simulations

#### S.4.1 Additional Simulations for Continuous Response and Mixed-Type Predictors

In this section, we provide additional simulation results for Scenario C.M.1 and Scenario C.M.2 of the main paper, as shown in Table S.1.

#### S.4.2 Simulations for Binary Response and Continuous Predictors

In this setting, we consider the following two scenarios with $n = 500$ and $p \in \{50, 200\}$.

**Scenario B.C.1.** Sample the predictors $x_1, \cdots, x_p$ from Uniform$(0, 1)$ independently and the response $y$ from Bernoulli$(\Phi(f_0(x)))$, where $f_0(x)$ is defined in (12) of the main paper.

**Scenario B.C.2.** Sample the predictors $x_1, \cdots, x_p$ from Normal$(0, \Sigma)$ with $\Sigma_{jk} = 0.3^{\lvert j - k \rvert}$, $j, k = 1, \cdots, p$, and the response $y$ from Bernoulli$(\Phi(f_0(x)))$, where $f_0(x)$ is defined in (13) of the main paper.

Table S.2 shows the simulation results. When the predictors are independent (Scenario B.C.1) and $p = 50$, all the methods except ABC-10-0.50 show similar performance. As the dimension increases, the two permutation-based approaches and the backward selection approach significantly outperform other methods in terms of the $r_{\text{miss}}$ and recall scores. When correlation is introduced (Scenario B.C.2), the backward
selection approach is the best in all metrics. Moreover, it is the only method that identifies all the relevant predictors over all the replications when $p = 50$.

Table S.1: Additional simulation results for Scenario C.M.1 where predictors are of mixed type and independent, and Scenario C.M.2 where predictors are of mixed type and correlated.

| Scenario C.M.1 | $n = 1000, p = 50, \sigma^2 = 1$ | $n = 1000, p = 200, \sigma^2 = 1$ |
|----------------|----------------------------------|----------------------------------|
|                | $r_{\text{miss}}$  | $\text{rec}$  | $\text{prec}$  | $F_1$                   | $r_{\text{miss}}$  | $\text{rec}$  | $\text{prec}$  | $F_1$                   |
| DART-20        | 0                    | 1.00            | 0.95(0.01)  | 0.96(0.01)  | 0                    | 1.00            | 0.91(0.01)  | 0.95(0.01)  |
| DART-200       | 0                    | 1.00            | 0.65(0.02)  | 0.78(0.01)  | 0                    | 1.00            | 0.65(0.02)  | 0.78(0.01)  |
| ABC-10-0.25    | 0                    | 1.00            | 1.00        | 1.00        | 0                    | 1.00            | 1.00        | 1.00        |
| ABC-10-0.50    | 0                    | 1.00            | 1.00        | 1.00        | 0                    | 1.00            | 1.00        | 1.00        |
| ABC-20-0.25    | 0                    | 1.00            | 0.79(0.01)  | 0.88(0.01)  | 0                    | 1.00            | 0.98(0.01)  | 0.99(0.00)  |
| ABC-20-0.50    | 0                    | 1.00            | 1.00        | 1.00        | 0                    | 1.00            | 1.00        | 1.00        |
| Permute (VIP)  | 1                    | 0.76(0.01)      | 1.00        | 0.86(0.01)  | 0                    | 1.00            | 0.94(0.01)  | 0.97(0.01)  |
| Permute (Within-Type VIP) | 0 | 1.00 | 0.99(0.01) | 0.99(0.01) | 0 | 1.00 | 0.69(0.02) | 0.81(0.01) |
| Permute (MI)   | 0                    | 1.00            | 0.98(0.01)  | 0.99(0.00)  | 0                    | 1.00            | 0.89(0.01)  | 0.94(0.01)  |
| Backward       | 0                    | 1.00            | 0.80(0.02)  | 0.87(0.01)  | 0                    | 1.00            | 0.80(0.02)  | 0.87(0.01)  |

| Scenario C.M.2 | $n = 500, p = 84, \sigma^2 = 10$ | $n = 1000, p = 84, \sigma^2 = 10$ |
|----------------|----------------------------------|----------------------------------|
|                | $r_{\text{miss}}$  | $\text{rec}$  | $\text{prec}$  | $F_1$                   | $r_{\text{miss}}$  | $\text{rec}$  | $\text{prec}$  | $F_1$                   |
| DART-20        | 1                    | 0.50(0.02)      | 0.75(0.02)  | 0.58(0.01)  | 0.95                  | 0.68(0.01)      | 0.85(0.02)  | 0.75(0.01)  |
| DART-200       | 1                    | 0.61(0.01)      | 0.26(0.01)  | 0.36(0.01)  | 0.91                  | 0.77(0.01)      | 0.36(0.01)  | 0.48(0.01)  |
| ABC-10-0.25    | 1                    | 0.72(0.01)      | 0.72(0.02)  | 0.58(0.01)  | 0.91                  | 0.64(0.01)      | 0.84(0.02)  | 0.72(0.01)  |
| ABC-10-0.50    | 1                    | 0.28(0.01)      | 0.98(0.01)  | 0.43(0.01)  | 1                    | 0.43(0.01)      | 0.99(0.00)  | 0.59(0.01)  |
| ABC-20-0.25    | 0.99                 | 0.70(0.01)      | 0.18(0.01)  | 0.29(0.01)  | 0.93                  | 0.79(0.01)      | 0.31(0.01)  | 0.45(0.01)  |
| ABC-20-0.50    | 0.99                 | 0.39(0.01)      | 0.89(0.02)  | 0.53(0.01)  | 1                    | 0.55(0.01)      | 0.97(0.01)  | 0.70(0.01)  |
| Permute (VIP)  | 0.99                 | 0.62(0.02)      | 0.67(0.02)  | 0.64(0.01)  | 0.91                  | 0.79(0.01)      | 0.77(0.02)  | 0.77(0.01)  |
| Permute (Within-Type VIP) | 1 | 0.61(0.02) | 0.69(0.03) | 0.64(0.02) | 0.98 | 0.75(0.02) | 0.79(0.02) | 0.76(0.01) |
| Permute (MI)   | 0.99                 | 0.62(0.02)      | 0.65(0.02)  | 0.63(0.01)  | 0.91                  | 0.8(0.01)       | 0.73(0.02)  | 0.75(0.01)  |
| Backward       | 0.75                 | 0.65(0.03)      | 0.36(0.03)  | 0.36(0.02)  | 0.67                  | 0.81(0.02)      | 0.31(0.03)  | 0.37(0.02)  |
Table S.2: Simulation results for the scenarios using binary responses and continuous predictors. Predictors in Scenario B.C.1 are independent and predictors in Scenario B.C.2 are correlated.

| Scenario B.C.1 | \( n = 500, p = 50 \) | \( n = 500, p = 200 \) |
|----------------|--------------------------|--------------------------|
| \( r_{\text{miss}} \) | \( r_{\text{rec}} \) | \( \text{prec} \) | \( F_1 \) | \( r_{\text{miss}} \) | \( r_{\text{rec}} \) | \( \text{prec} \) | \( F_1 \) |
| DART-20 | 0 | 1(0) | 0.98(0.01) | 0.99(0) | 0.28 | 0.94(0.01) | 0.98(0.01) | 0.96(0.01) |
| DART-200 | 0 | 1(0) | 0.97(0.01) | 0.98(0) | 0.11 | 0.98(0.01) | 0.96(0.01) | 0.97(0.01) |
| ABC-10-0.25 | 0.33 | 0.93(0.01) | 1(0) | 0.96(0.01) | 0.67 | 0.86(0.01) | 1(0) | 0.92(0.01) |
| ABC-10-0.50 | 0.33 | 0.95(0.01) | 0.97(0) | 0.99(0.01) | 0.99 | 0.74(0.01) | 1(0) | 0.84(0.01) |
| ABC-20-0.25 | 0 | 1(0) | 0.17(0) | 0.29(0) | 0.15 | 0.97(0.01) | 0.98(0.01) | 0.97(0.01) |
| ABC-20-0.50 | 0.03 | 0.99(0) | 1(0) | 0.99(0) | 0.91 | 0.8(0.01) | 1(0) | 0.88(0.01) |
| Permute (VIP) | 0 | 1(0) | 1(0) | 1(0) | 0 | 1(0) | 0.88(0.01) | 0.94(0.01) |
| Permute (MI) | 0 | 1(0) | 0.96(0.01) | 0.98(0) | 0 | 1(0) | 0.91(0.01) | 0.95(0.01) |
| Backward | 0.03 | 0.99(0) | 0.92(0.02) | 0.94(0.02) | 0.05 | 0.99(0) | 0.94(0.02) | 0.95(0.01) |

| Scenario B.C.2 | \( n = 500, p = 50 \) | \( n = 500, p = 200 \) |
|----------------|--------------------------|--------------------------|
| \( r_{\text{miss}} \) | \( r_{\text{rec}} \) | \( \text{prec} \) | \( F_1 \) | \( r_{\text{miss}} \) | \( r_{\text{rec}} \) | \( \text{prec} \) | \( F_1 \) |
| DART-20 | 0.87 | 0.49(0.03) | 0.71(0.04) | 0.57(0.03) | 1 | 0.06(0.02) | 0.09(0.02) | 0.07(0.02) |
| DART-200 | 0.42 | 0.78(0.03) | 0.67(0.03) | 0.69(0.02) | 0.92 | 0.35(0.03) | 0.09(0.01) | 0.11(0.02) |
| ABC-10-0.25 | 0.46 | 0.82(0.02) | 0.54(0.02) | 0.64(0.02) | 1 | 0(0) | 0.01(0.01) | 0(0) |
| ABC-10-0.50 | 1 | 0.05(0.01) | 0.14(0.04) | 0.07(0.02) | 1 | 0(0) | 0(0) | 0(0) |
| ABC-20-0.25 | 0 | 1(0) | 0.1(0) | 0.18(0) | 1 | 0.01(0) | 0.02(0.01) | 0.01(0.01) |
| ABC-20-0.50 | 0.95 | 0.43(0.03) | 0.77(0.04) | 0.53(0.03) | 1 | 0(0) | 0(0) | 0(0) |
| Permute (VIP) | 0.32 | 0.9(0.02) | 0.85(0.02) | 0.86(0.01) | 0.99 | 0.16(0.02) | 0.07(0.01) | 0.1(0.01) |
| Permute (MI) | 0.7 | 0.65(0.03) | 0.74(0.02) | 0.67(0.02) | 1 | 0.03(0.01) | 0.04(0.01) | 0.03(0.01) |
| Backward | 0 | 1(0) | 0.9(0.02) | 0.94(0.01) | 0.29 | 0.86(0.02) | 0.62(0.04) | 0.61(0.04) |

S.5 More Figures

In this section, we list Figure S.1, Figure S.2, Figure S.3, Figure S.4, Figure S.5, Figure S.6, Figure S.7 and Figure S.8, which are discussed in the main paper.

Figure S.4 is based on the following example, a generalized example of Example 2 of the main paper.

**Example S.1.** For each \( i = 1, \ldots, 500 \), sample \( x_{i,1}, \ldots, x_{i,\lceil p/2 \rceil} \) from Bernoulli(0.5) independently, \( x_{i,\lceil p/2 \rceil+1}, \ldots, x_{i,p} \) from Uniform(0,1) independently and \( y_i \) from Normal(\( f_0(x_i) \), 1) independently, where

\[
f_0(x) = 10 \sin(\pi x_{\lceil p/2 \rceil+1} x_{\lceil p/2 \rceil+2}) + 20(x_{\lceil p/2 \rceil+3} - 0.5)^2 + 10x_1 + 5x_2.
\]

We consider Example S.1 with \( p \in \{20, 50, 100\} \) in Figure S.4, where \( p = 20 \) corresponds to Example 2 of the main paper.
Figure S.1: Variable selection results of Bleich et al. (2014) with the setting, $L = 100$, $L_{\text{rep}} = 10$, $\alpha = 0.05$ and $M = 20$, for Example 2 of the main paper. Red (or green) dots are for continuous (or binary) predictors. Solid (or open) dots are for selected (or not selected) predictors. Each vertical grey line is the local threshold for the corresponding predictor. Relative binary predictors $x_1$ and $x_2$ are not identified by this method.

Figure S.2: The top two subfigures depict the error bars of $\{c_{\cdot k}\}_{k=1}^K$, the number of splitting nodes in a posterior sample, for different BART models. The bottom two subfigures depict $\left[\sum_{k=1}^K (c_{jk}/c_{\cdot k})^2 / K\right]^{1/2}$, the squared root of the second moment of the proportion of the usage $c_{jk}/c_{\cdot k}$, for different predictors. Each line is for a BART model. The posterior samples are obtained from the BART models fitted in the approach of Bleich et al. (2014) applied to Example 2 of the main paper. The left two subfigures are based on the 10 repeated BART models (with different initial values) on the original dataset. The right two subfigures are based on the 100 BART models on the null datasets.
Figure S.3: The two subfigures depict the overall counts ratios $\bar{c}_{L_{\text{rep}}}/c_{L_{\text{rep}}}$ (black dots) and the counts ratios $\bar{c}_{L_{\text{rep}},j}/c_{L_{\text{rep}},j}$ of a predictor (non-black dots) for $L = 100$ permutations. The counts ratio of the binary predictor $x_1$ not satisfying $\bar{c}_{L_{\text{rep}},1}/c_{L_{\text{rep}},1} > \bar{c}_{L_{\text{rep}},\cdot}/c_{L_{\text{rep}},\cdot}$ are marked as red. The posterior samples are obtained from the BART models fitted in the approach of Bleich et al. (2014) applied to Example 2 of the main paper.

Figure S.4: The left subfigure depicts $\bar{c}_{L_{\text{rep}},j}$ (bar) and $\{c_{L_{\text{rep}},j}\}_{j=1}^L$ (boxplot) for each relevant predictor; the right subfigure depicts $\bar{c}_{L_{\text{rep}},\cdot} = \sum_{j=1}^L \sum_{r \in S_{\text{cts}}} c_{r,j} / L_{\text{rep}}$, $\bar{c}_{L_{\text{rep}},\cdot} = \sum_{r=1}^L \sum_{j \in S_{\text{bin}}} c_{r,j} / L_{\text{rep}}$, and $\bar{c}_{L_{\text{rep}},\cdot} = \sum_{j \in S_{\text{bin}}} c_{L_{\text{rep}},j} / L_{\text{rep}}$, and $\{c_{L_{\text{rep}},\cdot}\}_{j=1}^L$ (boxplots). The posterior samples are obtained from the BART models fitted in the approach of Bleich et al. (2014) applied to Example S.1 with different $p \in \{20, 50, 100\}$. 

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Figure S.5: The left subfigure depicts nodes ratios for different $b$'s, the number of terminal nodes; the right subfigure depicts depth ratios for different depths $d_\eta$ when $\gamma = 0.95$ and $\beta = 2$.

Figure S.6: Each line depicts the BART MIs of a predictor for different numbers of posterior samples (after burning in 1000 samples) obtained from a BART model built on a null dataset of Example 2 of the main paper.
Figure S.7: Each boxplot depicts \(\{s_{ij}\}_{i=1}^{100}\) for the predictor \(x_j\). Each blue dot represents \(s_j\) for the predictor \(x_j\). The black dashed line represents \(s\). The red dashed line represents the \(s\) within continuous predictors and the green dashed line represents the \(s\) within binary predictors.

Figure S.8: Each line depicts the median of BART MIs for a predictor over different numbers of repetitions of BART built on the data generated from Example 2 of the main paper.