

# Sparsity-inducing Bayesian Causal Forest with Instrumental Variable

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## Abstract

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# 1 Introduction

Hahn et al. (2020)

## 1.1 Literature

- Using machine learning to infer heterogeneous effects in observational studies often focuses on CATE estimation under regular assignment mechanisms
- Focus in this work: Methods to discover heterogeneous effects in the presence of imperfect compliance
- Methods
  - tree-based
  - ensemble-of-trees
  - deep-learning-based methods
- BCF-IV: Discovers and estimates HTE in an interpretable way
  - BCF: BART-based semi-parametric Bayesian regression model, able to estimate HTE in regular assignment mechanisms, even with strong confounding
  - Use BCF to estimate  $\hat{\tau}_C(x)$  and  $\widehat{ITT}_Y(x)$  such that the conditional Complier Average Causal Effect  $\hat{\tau}^{cace}(x) = \frac{\widehat{ITT}_Y(x)}{\hat{\tau}_C(x)}$
- - BART benefits in general
  - good performance in high-noise settings
  - shrinkage to/emphasize on low-order interactions
  - established software implementations ('BayesTree', 'bartMachine', 'dbarts')
- BART shortcomings
  - non-smooth predictions as BART prior produces stepwise-continuous functions
  - BART prior is overconfident in regions with weak common support

- Research proposal: Rewrite the BCF-IV model with SoftBART instead of BART prior to account for sparsity

## 1.2 Contribution

We contribute to the literature on machine learning techniques designed to uncover heterogeneous effects while addressing imperfect compliance by developing adaptations of tree-based algorithms. Most of the recent scientific contributions in this area revolve around estimating the Conditional Average Treatment Effect (CATE) by combining machine learning algorithms with the potential outcome framework under a regular assignment mechanism (literature overview here). In this work, we focus on the estimation of the conditional Complier Average Causal Effect (cCACE) which is the treatment effect on the subgroup of compliers under the usual four assumptions within an IV framework. Specifically, we generalize Bayesian Instrumental Variable Causal Forest (BCF-IV) from (Bargagli-Stoffi et al. 2022) to estimate cCACE precisely when there are many covariates. BCF-IV is a semi-parametric Bayesian regression model that builds directly on the Bayesian Additive Regression Trees (BART) algorithm (Chipman et al., 2010). Instead of using BART for pure predictions of outcomes, BCF-IV is designed to identify and estimate heterogeneous effects within the subpopulation of units that comply with the treatment assignment, known as compliers. Consequently, the estimated effects can be considered doubly local, representing subgroup effects within the compliers subpopulation. BCF-IV identifies heterogeneity through an interpretable tree structure, with each node representing a distinct subgroup. For each leaf node of the generated tree, BCF-IV supports multiple hypothesis test adjustments to control the Type I error rate (familywise error rate) or the false discovery rate.

In our work, we extend BCF-IV in several ways. First, we use the shrinkage prior adaptation of BART (SoftBART) as proposed in (Linero & Yang 2018, Linero 2018). More precisely, by dividing the conditional Intention-To-Treat (cITT) effects with the corresponding conditional Proportion of Compliers (cPC), one can show to arrive at the conditional Complier Average Causal Effect (cCACE). In the discovery step the original BCF-IV algorithm of (Bargagli-Stoffi et al. 2022) uses the Bayesian Causal Forest (BCF) (Hahn et al. 2020) to estimate the cITT effects. BCF is a nonlinear regression model that builds upon BART and is proposed for estimating heterogeneous treatment effects. It is specifically designed for scenarios characterized by small effect sizes, heterogeneous effects, and significant confounding by observables. First, BCF addresses the issue of highly biased treatment effect estimates in the presence of strong confounding by incorporating an estimate of the propensity function directly into the response model. Thereby, it induces a covariate-dependent prior on the

regression function. Second, BCF allows for the separate regularization of treatment effect heterogeneity from the prognostic effect of control variables. Conventional response surface modeling approaches often fail to adequately model regularization over effect heterogeneity. Instead, BCF enables an informative shrinkage towards homogeneity such that one is able to control the degree of regularization over effect heterogeneity. In our work, we generalize the cITT effect estimation by replacing BCF with the Shrinkage Bayesian Causal Forest (SBCF) proposed by (Caron et al. 2022). SBCF extends BCF by using additional priors proposed in SoftBART that enable to adjust the influence of each covariate based on the number of corresponding splits in the tree ensemble. These priors enhance the model’s adaptability to sparse data-generating processes and facilitate fully Bayesian feature shrinkage within the framework for estimating treatment effects. Consequently, it improves to uncover the moderating factors that drive heterogeneity when there is sparsity in the data. Moreover, this method allows the incorporation of prior knowledge regarding relevant confounding covariates and the relative magnitude of their impact on the outcome.

Second, BCF-IV uses a single binary tree based on the CART model of (Breiman1984) to analyse possible heterogeneity patterns within cCACE. In our work, we use posterior splitting probabilities retrieved from SBCF as a measure of variable importance within the `cost`-argument of `rpart`. These are scalings to be applied when considering splits, so the improvement on splitting on a variable is divided by its cost in deciding which split to choose in `rpart`.

Open questions for further contributions. Use Random Forests (Causal Rule Ensemble) instead of single CART for subgroup discovery? More rigorous Bayesian estimation by replacing `ivreg` with `brms` (implementation of credible intervals, estimation error, counterparts to something like weak instrument tests, bayesian model averaging)?

## 2 Potential outcomes and irregular assignment

We follow the setup of Bargagli-Stoffi & Gnecco (2020) and Bargagli-Stoffi et al. (2022) who follow the usual notation of the Rubin’s causal model. Given a set of  $N$  individuals, indexed by  $i = 1, \dots, N$ , we denote with  $Y_i$  a generic outcome variable, with  $W_i$  a binary treatment indicator, with  $X$  an  $N \times P$  matrix of  $P$  control variables, and with  $X_i$  the  $i$ -th  $P$ -dimensional row vector of covariates. Let us define the pair of potential outcomes  $Y_i(W_i)$  by using the Stable Unit Treatment Value Assumption (SUTVA).

**Assumption 2.1.** Stable unit treatment value assumption (SUTVA).

$$\text{If } W_i = w, \text{ then } Y_i(w) = Y_i^{obs}, \forall w \in \{0, 1\}, \forall i \in \{1, \dots, N\}.$$

Therefore, it holds that  $Y_i(W_i = 1) = Y_i(1)$  for an individual  $i$  under assignment to the treatment group and  $Y_i(W_i = 0) = Y_i(0)$  under assignment to control group. Despite one is unable to observe both potential outcomes at the same time for each individual one is able to observe the potential outcome that aligns with the assigned treatment status such that

$$Y_i^{obs} = Y_i(1)W_i + Y_i(0)(1 - W_i).$$

Under the following strong ignorability assumptions of Assumption 2.2 and Assumption 2.3 we operate under the regular assignment mechanism which, through Assumption 2.2, prevents the existence of unmeasured confounding and, by Assumption 2.3, allows for unbiased treatment effect estimation in support of the covariate space.

**Assumption 2.2.** Unconfoundedness.

$$W_i \perp\!\!\!\perp (Y_i(1), Y_i(0)) \mid X_i, \text{ or equivalently,}$$

$$Pr(W_i | (Y_i(1), Y_i(0), X_i)) = Pr(W_i | X_i).$$

**Assumption 2.3.** Positivity.

$$\epsilon < p(X_i = x) < 1 - \epsilon \text{ with probability } 1, \forall \epsilon > 0, \forall x \text{ in support of } X_i.$$

Using strong ignorability, one can define, for instance, the CATE to analyze heterogeneous treatment effects by

**Definition 2.1.** Conditional Average Treatment Effect (CATE).

$$\tau(x) = \mathbb{E}[Y_i^{\text{obs}} | W_i = 1, X_i = x] - \mathbb{E}[Y_i^{\text{obs}} | W_i = 0, X_i = x].$$

In this work, we deviate from this regular assignment mechanism that is implied by Assumptions 2.2 and 2.3 and operate under the scenario of an irregular assignment mechanism. This irregular assignment mechanism allows for a violation of compliance between (quasi-)randomized treatment assignment,  $Z_i$ , and treatment receipt,  $W_i$ , such that just the assignment to treatment is assumed to be unconfounded through a valid choice of  $Z_i$  but the treatment receipt might be confounded. A remedy to the issue of confoundedness in treatment receipt is the Instrumental Variable (IV) approach. A proper instrumental variable,  $Z_i$ , affects treatment receipt,  $W_i$ , while not being allowed to affect  $Y_i$  directly such that treatment receipt depends on the treatment assignment by  $W_i(Z_i)$ . Based on the functional relation between  $W_i$  and  $Z_i$  and in case of a binary treatment variable, one can define four subgroups of individuals,  $G_i$ , such that

**Definition 2.2.** Subgroups  $G_i$ .

$$G_i = \begin{cases} C, & \text{if } W_i(Z_i = 0) = 0, W_i(Z_i = 1) = 1 \\ D, & \text{if } W_i(Z_i = 0) = 1, W_i(Z_i = 1) = 0 \\ AT, & \text{if } W_i(Z_i = 0) = 1, W_i(Z_i = 1) = 1 \\ NT, & \text{if } W_i(Z_i = 0) = 0, W_i(Z_i = 1) = 0 \end{cases}.$$

where  $C$ ,  $D$ ,  $AT$  and  $NT$  are abbreviations for Compliers, Defiers, Always-Takers, Never-Takers. The proportion of individuals that belong to each subgroup is defined as  $\pi_{G_i}$ , i.e. the proportion of compliers reads  $\pi_C$ . Considering the distinction between  $Z_i$  and  $W_i$ , the Intention-To-Treat (ITT) effect is defined as



**Definition 2.3.** Intention-To-Treat (ITT) effect.

$$ITT_Y = \mathbb{E}[Y_i | Z_i = 1] - \mathbb{E}[Y_i | Z_i = 0],$$

which refers to the instrument's average effect. Based on the subgroups in Definition 2.2 and their proportions  $\pi_{G_i}$ , an IV setting can be formalized by the usual four IV assumptions following ?.

**Assumption 2.4.** Classical IV assumptions with a binary treatment.

$$\begin{aligned} \text{Exclusion restriction:} & \quad Y_i(0) = Y_i(1), \text{ for } G_i \in \{AT, NT\}. \\ \text{Monotonicity:} & \quad W_i(1) \geq W_i(0) \rightarrow \pi_D = 0. \\ \text{Existence of compliers:} & \quad P(W_i(0) < W_i(1)) > 0 \rightarrow \pi_C \neq 0. \\ \text{Unconfoundedness of IV:} & \quad Z_i \perp (Y_i(0, 0), Y_i(0, 1), Y_i(1, 0), Y_i(1, 1), W_i(0), W_i(1)). \end{aligned}$$

If Assumptions 2.4 hold, the Complier Average Causal Effect (CACE) is identified.

**Definition 2.4.** Complier Average Causal Effect (CACE).

$$\tau_{\text{CACE}} = \frac{ITT_Y}{\pi_C} = \frac{\mathbb{E}[Y_i | Z_i = 1] - \mathbb{E}[Y_i | Z_i = 0]}{\mathbb{E}[W_i | Z_i = 1] - \mathbb{E}[W_i | Z_i = 0]},$$

and can be estimated from observational data. The numerator represents the average effect of the instrument, also referred to as the Intention-To-Treat (ITT) effect. The denominator represents the overall proportion of individuals that comply with the treatment assignment, also referred to as the proportion of compliers ?. CACE is also sometimes referred to as Local Average Treatment Effects (see ?) and represents the estimate of the causal effect of the assignment to treatment on the principal outcome,  $Y_i$ , for the subpopulation of compliers ?. Consider the system of two simultaneous equations

$$\begin{aligned} Y_i^{obs} &= \alpha + \tau_{\text{CACE}} W_i + \epsilon_i, \\ W_i &= \pi_0 + \pi_C Z_i + \eta_i, \end{aligned}$$

with  $\mathbb{E}(\epsilon_i) = \mathbb{E}(\eta_i) = 0$  and we assume by the first equation a linear projection of  $W_i$  onto  $Z_i$  with  $\mathbb{E}(Z_i \eta_i) = 0$ . Then, ? and ? show that  $\tau_{\text{CACE}}$  can be estimated by a Two Stage Least Square (TSLS) estimator which is consistent and asymptotic normal as displayed in ?.

In this work, we follow Bargagli-Stoffi et al. (2022) and consider the conditional version of the CACE,

**Definition 2.5.** Conditional CACE (cCACE).

$$\tau_{\text{CACE}}(x) = \frac{\text{ITT}_Y(x)}{\pi_C(x)} = \frac{\mathbb{E}[Y_i \mid Z_i = 1, X_i = x] - \mathbb{E}[Y_i \mid Z_i = 0, X_i = x]}{\mathbb{E}[W_i \mid Z_i = 1, X_i = x] - \mathbb{E}[W_i \mid Z_i = 0, X_i = x]}.$$

The cCACE is a straightforward extension of the CACE in Definition 2.4 presented in with Bargagli-Stoffi et al. (2022). A natural, subgroup-related estimator  $\tau_{\text{CACE}}(x)$  can be defined by acknowledging  $\mathbf{X}_i \in \mathbb{X}_j$  with  $\mathbb{X}_j$  being a pre-specified subgroup.

**Definition 2.6.** Estimator of cCACE.

$$\begin{aligned} \hat{\tau}_{\text{CACE}}(x) &= \frac{\text{ITT}_Y(x)}{\pi_C(x)} \\ &= \frac{\frac{1}{N_{1,j}} \sum_{l: X_l \in \mathbb{X}_j} Y_l^{\text{obs}} Z_l - \frac{1}{N_{0,j}} \sum_{l: X_l \in \mathbb{X}_j} Y_l^{\text{obs}} (1 - Z_l)}{\frac{1}{N_{1,j}} \sum_{l: X_l \in \mathbb{X}_j} W_l Z_l - \frac{1}{N_{0,j}} \sum_{l: X_l \in \mathbb{X}_j} W_l (1 - Z_l)} \end{aligned}$$

Intuitively, Definition 2.6 proposes to use TSLS subgroup-wise for every  $\mathbb{X}_j$  under Assumptions 2.4. Moreover, ? provide theorems for consistency and asymptotic normality for the unconditional TSLS estimator for  $\tau_{\text{CACE}}$ . Bargagli-Stoffi et al. (2022) show that those theorems can be transferred to the conditional TSLS estimator if there are sufficient number of observations for every subgroup in which the cCACE is estimated.

**Theorem 2.1** (Consistency and Asymptotic Normality of the Conditional 2SLS Estimator). *Let Assumptions 1, 2, and 3 hold, i.e.,  $E(Z_{i,X_j}^2) \neq 0$  (Assumption 1),  $E(Z_{i,X_j} \varepsilon_{i,X_j}) = 0$  (Assumption 2), and  $\pi_{C,X_j} \neq 0$  (Assumption 3). Then:*

1. (Consistency)  $\hat{\tau}_{X_j}^{2\text{SLS}} - \tau_{X_j} \xrightarrow{p} 0$  as  $N_{X_j} \rightarrow \infty$ , where  $\xrightarrow{p}$  denotes convergence in probability, and  $N_{X_j}$  is the number of observations within the node  $X_j$ .
2. (Asymptotic Normality) If, in addition,  $E(Z_{i,X_j}^2 \varepsilon_{i,X_j}^2)$  is finite (Assumption 4), then:

$$\sqrt{N_{X_j}}(\hat{\tau}_{X_j}^{2\text{SLS}} - \tau_{X_j}) \xrightarrow{d} \mathcal{N}(0, N_{X_j} \cdot \text{avar}(\hat{\tau}_{X_j}^{2\text{SLS}}))$$

as  $N_{X_j} \rightarrow \infty$ , where  $\xrightarrow{d}$  denotes convergence in distribution,  $\mathcal{N}(0, N_{X_j} \cdot \text{avar}(\hat{\tau}_{X_j}^{2\text{SLS}}))$  stands for the normal distribution, and  $\text{avar}(\hat{\tau}_{X_j}^{2\text{SLS}})$  is the asymptotic variance of the 2SLS estimator that can be approximated as in Chapter 15 of Wooldridge (2015).

## **3 Sparsity-inducing Bayesian Causal Forest with Instrumental Variable**

### **3.1 Sparse Bayesian Causal Forest**

### **3.2 Sparse BCF-IV**

## 4 Simulation study

Performance criteria according to bargagli-stoffi:

1. Average number of truly discovered heterogeneous subgroups corresponding to the nodes of the generated CART (proportion of correctly discovered subgroups);
2. Monte Carlo estimated bias for the heterogeneous subgroups:

$$\text{Bias}_m(I_{\text{inf}}) = \frac{1}{N_{\text{inf}}} \sum_{i=1}^{N_{\text{inf}}} \sum_{l=1}^L (\tau_{\text{cace},i}(\ell) - \hat{\tau}_{\text{cace},i}(\ell, \Pi_m, I_{\text{inf}})), \quad (4.0.1)$$

$$\text{Bias}(I_{\text{inf}}) = \frac{1}{M} \sum_{m=1}^M \text{Bias}_m(I_{\text{inf}}), \quad (4.0.2)$$

where  $\Pi_m$  is the partition selected in simulation  $m$ ,  $L$  is the number of subgroups with heterogeneous effects (i.e., two for the case of strong heterogeneity and four for the case of slight heterogeneity), and  $N_{\text{inf}}$  is the number of observations in the inference sample.

3. Monte Carlo estimated MSE for the heterogeneous subgroups:

$$\text{MSE}_m(I_{\text{inf}}) = \frac{1}{N_{\text{inf}}} \sum_{i=1}^{N_{\text{inf}}} \sum_{l=1}^L (\tau_{\text{cace},i}(\ell) - \hat{\tau}_{\text{cace},i}(\ell, \Pi_m, I_{\text{inf}}))^2, \quad (4.0.3)$$

$$\text{MSE}(I_{\text{inf}}) = \frac{1}{M} \sum_{m=1}^M \text{MSE}_m(I_{\text{inf}}); \quad (4.0.4)$$

4. Monte Carlo coverage, computed as the average proportion of units for which the estimated 95% confidence interval of the causal effect in the assigned leaf includes the true value, for the heterogeneous subgroups:

$$C_m(I_{\text{inf}}) = \frac{1}{N_{\text{inf}}} \sum_{i=1}^{N_{\text{inf}}} \sum_{l=1}^L \left( \tau_{\text{cace},i}(\ell) \in \hat{\text{CI}}_{95}(\hat{\tau}_{\text{cace},i}(\ell, \Pi_m, I_{\text{inf}})) \right), \quad (4.0.5)$$

$$C(I_{\text{inf}}) = \frac{1}{M} \sum_{m=1}^M C_m(I_{\text{inf}}). \quad (4.0.6)$$

## **5 Empirical application**

## **6 Discussion**

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