

Shrinkage 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 different forms of average treatment effect estimations under regular assignment mechanisms ?. In this work, we focus on methods to discover heterogeneous effects in the presence of imperfect compliance leading to an irregular assignment mechanism.

- 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 use 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 π_{G_i} , i.e. the proportion of compliers reads π_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.

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

The ITT effect refers to the instrument's average effect. Based on the subgroups in Definition 2.2 and their proportions π_{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) can be identified.

Definition 2.4. Complier Average Causal Effect (CACE).

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

The CACE can be estimated from observational data where 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 (LATE, 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

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

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 τ_{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 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.

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

Intuitively, Definition 2.6 implies to use TSLS subgroup-wise for every \mathbb{X}_j under Assumptions 2.4. The system of two simultaneous equations from above can be conditionalized by

$$\begin{aligned} Y_{i,\mathbb{X}_j}^{\text{obs}} &= \alpha_{\mathbb{X}_j} + \tau_{\mathbb{X}_j}^{\text{CACE}} W_{i,\mathbb{X}_j} + \epsilon_{i,\mathbb{X}_j}, \\ W_{i,\mathbb{X}_j} &= \pi_{0,\mathbb{X}_j} + \pi_{C,\mathbb{X}_j} Z_{i,\mathbb{X}_j} + \eta_{i,\mathbb{X}_j}, \end{aligned}$$

such that the reduced form reads

$$\begin{aligned} Y_{i,\mathbb{X}_j}^{\text{obs}} &= \left(\alpha_{\mathbb{X}_j} + \tau_{\text{CACE},\mathbb{X}_j} \pi_{0,\mathbb{X}_j} \right) + \\ &\quad \left(\tau_{\text{CACE},\mathbb{X}_j} \pi_{C,\mathbb{X}_j} \right) Z_{i,\mathbb{X}_j} + \\ &\quad \left(\epsilon_{i,\mathbb{X}_j} + \tau_{\mathbb{X}_j}^{\text{CACE}} \eta_{i,\mathbb{X}_j} \right). \end{aligned}$$

The intercept $\left(\alpha_{\mathbb{X}_j} + \tau_{\text{CACE},\mathbb{X}_j} \pi_{0,\mathbb{X}_j} \right)$ and slope parameter $\left(\tau_{\text{CACE},\mathbb{X}_j} \pi_{C,\mathbb{X}_j} \right)$ can be estimated by ordinary least squares, given a sufficient number of *i.i.d* observations in each subgroup \mathcal{X}_j . More information regarding theoretical properties of ... can be found in Appendix A of Bargagli-Stoffi et al. (2022). In Definition 2.6, the estimator $\hat{\tau}_{\text{CACE}}(x)$ is defined by relying on the existence of accurately pre-specified

subgroups. The main contribution of BCF-IV in Bargagli-Stoffi et al. (2022) revolves around providing a full algorithm that (1) honestly splits the data into two disjunct subsamples $\mathcal{I}_{disc}, \mathcal{I}_{inf}$, (2) discovers heterogeneity in cCACE in an interpretable way using \mathcal{I}_{disc} and (3) infers precise estimates of cCACE on \mathcal{I}_{inf} . The next chapter explains BCF-IV in detail and describes the extension to a sparsity-inducing version.

3 Bayesian Causal Forests and Instrumental Variables

This paper proposes an algorithm for the estimation of cCACE for sparse data scenarios. More precisely, we propose an extension of the BCF-IV algorithm in Bargagli-Stoffi et al. (2022) to handle scenarios with many irrelevant covariates in the dataset. Section 3.1 describes the original BCF-IV algorithm while section 3.2 explains the proposed extension based on the Shrinkage Bayesian Causal Forest. As pointed out in the literature review of this paper, current ensemble methods that operate under an irregular assignment mechanism with imperfect compliance face some difficulties. Algorithms like Deep IV ? and the Generalized Random Forest ? provide precise cCACE estimates but are rather uninformative about relevant covariates, or subsets of possibly many covariates, that drive heterogeneity in cCACE. Tree-based methods like the Causal Tree with IV Bargagli Stoffi & Gnecco (2020) propose to estimate treatment effects under imperfect compliance and the existence of a suitable IV while retaining interpretability. However, although the single tree structure enables interpretability it also lacks of stability and replicability. Bargagli-Stoffi et al. (2022) argue to overcome those shortcomings using the BCF-IV algorithm as outlined in the following Section 3.1.

3.1 BCF-IV

The main steps of the BCF-IV algorithm are outlined in Algorithm 1. Details of these three steps of honest sample splitting, discovery of treatment effect heterogeneity and inference of treatment effects are discussed in Sections 3.1.1, 3.1.2 and 3.1.3.

3.1.1 Honest sample splitting

The first step concerns honest sample splitting. This step enables a data-driven discovery of heterogeneous subgroups such that there is no need to specify those subgroups beforehand. Defining subgroups before estimating treatment effects based on relevant data of the studied population is a challenging task. It requires deep knowledge about the intricacies of the treatment effect at hand and may be prone to

overlook relevant subgroups. Honest sample splitting as proposed in ? is a remedy for those issues by making distinctions between model selection and treatment effect inference.

Algorithm 1: Bayesian Causal Forest with Instrumental Variable (BCF-IV)

Input : N units i (X_i, Z_i, W_i, Y_i), with feature vector X_i , treatment assignment (instrumental variable) Z_i , treatment receipt W_i , observed response Y_i

Output : A tree structure discovering the heterogeneity in the causal effects and estimates of the Complier Average Causal Effects (CACE) within its leaves.

1. The Honest Splitting Step:

- Randomly split the total sample into a discovery subsample (I_{dis}) and an inference subsample (I_{inf}).

2. The Discovery Step (performed on I_{dis}):

Estimation of the Conditional CACE:

- (a) Estimate the conditional Intention-To-Treat: $\widehat{\text{ITT}}(x)$.
- (b) Estimate the conditional proportion of compliers: $\widehat{\pi}_C(x)$.
- (c) Estimate the conditional CACE, $\widehat{\tau}_{\text{CACE}}(x)$, using the estimated values from (a) and (b).

Heterogeneous subpopulations discovery:

- (d) Discover the heterogeneous effects by fitting a decision tree using the data $(\widehat{\tau}_{\text{CACE}}(x), X_i)$.

3. The Inference Step (performed on I_{inf}):

- (a) Estimate the $\widehat{\tau}_{\text{CACE}}(x)$ for all discovered subpopulations (i.e., nodes and leaves) in the tree discovered in Step 3(d).
 - (b) Perform multiple hypothesis tests and adjust p-values to control for the familywise error rate or, less stringently, the false discovery rate.
 - (c) Run weak-instrument tests within every node and discard nodes where weak-instrument issues are detected.
-

3.1.2 Discovery of heterogeneous subgroups

The Bayesian Causal Forest (BCF) algorithm is proposed in Hahn et al. (2020) to use the Bayesian Additive Regression Trees (BART) algorithm ? to estimate CATE in a regular assignment mechanism. BART is related to the CART algorithm of ? which constructs binary trees by recursively partitioning the covariate space to produce accurate predictions. BART rests on a complete Bayesian probability model by using different regularizing prior distributions such that the overall model fit dominates fits of single trees. Distinct prior distributions are used for the complexity of the tree structure, data shrinkage within the nodes and the variance of the error term.

3.1.3 Inference of conditional CACE

3.2 Shrinkage 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 Π_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_{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

Moreover, ? provide theorems for consistency and asymptotic normality for the unconditional TSLS estimator for the true population parameter τ_{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 6.1 (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) $\hat{\tau}_{X_j}^{2SLS} - \tau_{X_j} \xrightarrow{p} 0$ 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:*

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

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

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