Causal Inference with the Instrumental Variable Approach and Bayesian Nonparametric Machine Learning

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Abstract

We provide a new flexible framework for inference with the instrumental variable model. Rather than using linear specifications, functions characterizing the effects of instruments and other explanatory variables are estimated using machine learning via Bayesian Additive Regression Trees (BART). Error terms and their distribution are inferred using Dirichlet Process mixtures. Simulated and real examples show that when the true functions are linear, little is lost. But when nonlinearities are present, dramatic improvements are obtained with virtually no manual tuning.

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1 Introduction

The instrumental variable (IV) approach has long been a cornerstone of causal inference from both the theoretical and applied perspectives. For example, the distribution-free method of two-stage least squares (TSLS) goes back to Theil (1953) and it is based on earlier IV work that goes back decades further such as Wright (1928). The focus on distribution-free methods is paramount since the reliance on parametric assumptions has been roundly criticized (LaLonde, 1986). Therefore, there has been a movement towards nonparametric methods that do not rely on precarious restrictive assumptions such as functional forms and/or convenient choices of distributions (Angrist and Imbens, 1995). Conversely, unrestricted nonparametric approaches may have theoretical challenges such as the lack of causal identification (Pearl, 2009). While in practical performance, distribution-free methods such as TSLS have come under attack as more biased and less powerful than Ordinary Least Squares (OLS) with standard errors generated by either bootstrapping or jack-knifing (Young, 2019).

We take a Bayesian approach to IV as many others have before us (Imbens and Rubin, 1997; Rossi et al., 2005; Conley et al., 2008; Rossi, 2014). For example, Rossi et al. (2005) take a Bayesian parametric approach that we will refer to as *linear-normal* or *lin-nor* (for linear IV with normal errors) based upon the linear structural equations of TSLS. Conley et al. (2008) expand on this previous work via a semi-parametric method that relaxes the parametric error distribution with Dirichlet Process Mixtures (DPM) (Escobar and West, 1995) while retaining the linear model structural equations of TSLS: we will refer to this method as *linear-DPM* or *lin-DPM*. For a comprehensive exposition of the IV framework from the Bayesian perspective, along with Bayesian nonparametric priors, see Rossi (2014).

Herein, we propose a new nonparametric method based on Bayesian Additive Regression Trees (BART) (Chipman et al., 2010) and DPM capable of handling structural equations that may be non-linear and/or may have non-normal errors. We will refer to our new method as *IVBART* which we describe in Section 2. In Section 3, we explore our new method with simulated data sets and compare with lin-nor and lin-DPM. Section 4 is where we delve into a real data set that demonstrates our new method to estimate the monetary returns of post-secondary education (as have others (Card, 1993; Conley et al., 2008)). In Sections 5 and 6, we provide the details for implementing our new method via Markov chain Monte Carlo (MCMC) sampling of the posterior. Section 7 concludes the article with a brief discussion of the merits of our new method and some potential future directions for extensions. In the Appendix, we provide a brief introduction to the **ivbart R** package that implements our new method and a proof of the causal identification of our new method.

2 Flexible IV Modeling

In this section we present our model and basic computational approach.

The classic TSLS linear approach to IV modeling is expressed by the following two equations:

$$T_i = \mu_T + \gamma' z_i + \alpha' x_i + \epsilon_{Ti} \quad (1)$$

$$Y_i = \mu_Y + \beta\, T_i + \delta' x_i + \epsilon_{Yi}\ . \quad (2)$$

Equation 1 is the *treatment* or *first stage* equation where z are the instruments and x are the confounders. Equation 2 is the *outcome* or *second stage* equation. We do not want to assume that the errors ϵ_{Ti} and ϵ_{Yi} are independent since unmeasured variables may be affecting both T and Y. The idea of the model is that the instrumental variable z provides a *source of variation* in T, such as a *natural experiment*, that is analogous to the variation induced by an experimenter who controls the value of T assigned.

Our goal is to eliminate the need to assume that the relationships are linear and to make minimal assumptions about the nature of the errors. We simply replace the linear functions in Equations 1 and 2 above with general functions. To facilitate the modeling of the errors, we combine the error terms with the means as follows:

$$T_i = f(z_i, x_i) + \epsilon_{Ti} \quad (3)$$

$$Y_i = \beta T_i + h(x_i) + \epsilon_{Yi} \ . \quad (4)$$

We model each of the functions f and h using the BART methodology and we model the errors using Bayesian nonparametrics as in Conley et al. (2008). Our hope is that the model given by Equations 3 and 4 will be tremendously appealing to applied investigators. Our belief is that the relaxation of the linearity assumption is a much more powerful elaboration of the model than the relaxation of the normal error assumption. In practice, applied investigations typically struggle to deal with potential nonlinearity by transformations of z and/or x in the model. This leads to an unappealing model specification since z and/or x have been transformed from their natural representation. A basic goal of Machine Learning is to learn the functions f and h fairly automatically from the data. In practice, Machine Learning can involve a complex model training phase and extensive use of cross-validation to select the tuning parameters. Our choice of BART as the method for learning has some fundamental advantages.

- BART is able to learn high-dimensional, complex, non-linear relationships
- BART is a fully Bayesian procedure with an effective MCMC algorithm that inherently provides an assessment of uncertainty.
- BART often obtains an adequate fit with minimal tuning.
- Multiple additive BART models can be embedded in a larger model
  (as in Equations 3 and 4 above).

To model the error terms we use the Dirichlet process mixture (DPM) approach of Escobar and West (1995). A simple way to think about the DPM model is to let

$$\epsilon_i = (\epsilon_{Ti}, \epsilon_{Yi})' \sim N(\mu_i, \Sigma_i)$$

so that each error ϵ_i has its own mean μ_i and variance matrix Σ_i. Of course, this model is too flexible without further structure. Let $\theta_i = (\mu_i, \Sigma_i)$. The DPM method adds a hierarchical model for the set of θ_i so that there is a random number of unique values. Each observation can have its own θ, but observations share θ values so that the number of unique values is far less than the sample size. This reduces the effective complexity of the parameter space.

The DPM hierarchical model draws a discrete distribution using the Dirichlet process (DP) and then draws the θ_i from the discrete distribution. Because the distribution is discrete, with positive probability, some of the θ_i values will be repeats. To simplify notation, let $\{x_i\}$ represent $\{x_i\}_{i=1}^n$ in (5). Letting G denote the random discrete distribution, our hierarchical model is:

$$\{\epsilon_i\} \,|\, \{\theta_i\}, \;\; \{\theta_i\} \,|\, G, \;\; G \,|\, G_0, \alpha \tag{5}$$

where

$$\epsilon_i \sim N(\mu_i, \Sigma_i), \;\; \theta_i = (\mu_i, \Sigma_i) \sim G, \;\; G \sim DP(G_0, \alpha).$$

DP denotes the Dirichlet process distribution over discrete distributions given parameters G_0 and α. We refer the reader to Conley et al. (2008) for the complete details. Briefly, to motivate our prior choices, we need some basic intuition about how the choices for G_0 and α affect the inference. G_0 is the *central* distribution over the space of $\theta = (\mu, \Sigma)$. The atoms of G are independent and identically distributed, or *iid*, draws from G_0. The *concentration* parameter α determines the distribution of the weights given to each atom of the discrete G. A larger α tends to give you a discrete G with more atoms receiving non-negligible weight. A smaller α means only of few of the weights are likely to be large so that G tends to have most of its mass concentrated on just a few atoms. In terms of the *mixture of normals* interpretation, G_0 tells us what normal distributions are likely (what $\theta = (\mu, \Sigma)$ are likely); and α tells us how many normals there are and with what weight.

Thus, our parameter space can be thought as:

$$f, \; h, \; \beta, \; \{\theta_i\}.$$

Our computational algorithm is the obvious Gibbs sampler (Gelfand and Smith, 1990):

$$f \,|\, h, \beta, \{\theta_i\}, D \tag{6}$$
$$h \,|\, f, \beta, \{\theta_i\}, D \tag{7}$$
$$\beta \,|\, f, h, \{\theta_i\}, D \tag{8}$$
$$\{\theta_i\} \,|\, f, h, \beta, D \tag{9}$$
$$\tag{10}$$

where D denotes the observed data $\{T_i, Y_i, x_i, z_i\}_{i=1}^n$. Most of these draws are straightforward and follow Conley et al. (2008). The exception is the draw of f where the nonlinearity calls for special treatment. Details of the draws are given in Section 5.

3 Simulated Examples

In this section we illustrate our methodology on simulated data. The parameters of our model we must choose in order to simulate data are the value of β, the (f, h) pair of functions, and the error distribution. We must also choose distributions to draw x and z from and the sample size. We will always use $\beta = 1$.

We will consider a nonlinear pair of (f, h):

$$f(x,z) = x_1 + .5\,x_1x_2 + .5x_2^2 + z_1 + z_2x_1 + .5z_2^2 \quad (11)$$
$$h(x) = x_1 - .25x_1x_2^3 + x_3 \quad (12)$$

and a linear pair of (f, h):

$$f(x,z) = x_1 + x_2 + x_3 + z_1 + z_2 \quad (13)$$
$$h(x) = x_1 - x_2 + .5x_4\ . \quad (14)$$

The nonlinear functions are chosen to be simple polynomials. This is not too different from what a practitioner might try but a practitioner may have difficulty finding the exact right polynomial terms in practice. The linear functions are chose to be a simple as possible while having h not too similar to the x part of f.

For the error distribution we use:

$$\epsilon_T = \sigma_T\, Z_T \quad (15)$$
$$\epsilon_Y = \gamma Z_T + \sigma_Y Z_Y \quad (16)$$

where (Z_T, Z_Y) are indepenent t_ν random variables with $\nu = 5$. We let $\sigma_T = 1$ and $(\gamma, \sigma_Y) = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$. Note that a linear combination of independent t random variables is not a t random variable so that the error ϵ_Y has a non-standard distribution. Clearly γ controls the degree of dependence between ϵ_T and ϵ_Y. With these choices, both errors have the same variance as the Z's and the correlation is $1/\sqrt{2} \approx .707$. The pair of errors $(\epsilon_{Ti}, \epsilon_{Yi})$ are iid over observations.

Each coordinate of both x and z are iid uniform on the interval $(-2, 2)$. For x, we simulate $x_j, j = 1, 2, \ldots, 10$ and for z we simulated $z_j, j = 1, 2, \ldots 5$. So, there are 10 x variables and 5 potential z instruments. Notice that in the nonlinear case (Equations 11 and 12), f uses only (x_1, x_2, z_1, z_2) while h uses only (x_1, x_2, x_3). The method is given all 10 x and all 5 z and the two BART models in IVBART have to learn which variables matter. In the linear case (Equations 13 and 14), f and h use $(x_1, x_2, x_3, z_1, z_2)$ and (x_1, x_2, x_4) respectively.

We consider four different simulation scenarios by letting the sample size n be 2,000 or 500 and letting the functions be nonlinear or linear. We draw 90 samples and run MCMC estimation of each of the three models IVBART, linear-normal, and linear-DPM on each of the 90 samples.

All IVBART results are obtained using a default prior specification explained in Section 3.2 and, in more detail, in Section 6. Results for the linear-normal and linear-DPM models are obtained using the default prior specifications provided by the functions `rivGibbs` and `rivDP` in the `R` package `bayesm` (Rossi, 2019).

3.1 Inference for β

Figure 1 displays the MCMC draws of β from the three models IVBART, linear-normal, and linear-DPM. The four plots in the figure correspond to our four simulation scenarios.

	IVBART	linear-normal	linear-DPM
n=2,000, nonlinear	(0.022, 1.000)	(0.040, 1.858)	(0.038, 1.769)
n=2000, linear	(0.029, 1.275)	(0.024, 1.059)	(0.023, 1.000)
n=500, nonlinear	(0.060, 1.000)	(0.085, 1.417)	(0.080, 1.348)
n=500, linear	(0.062, 1.220)	(0.051, 1.000)	(0.051, 1.002)

Table 1: RMSE and relative RMSE. Rows are for our four simulation scenarios and columns are for our three models. Each table entry reports (RMSE, relative RMSE). The relative RMSE for each simulation scenario is obtained by dividing the RMSE for each of the three models by the minimum over the three models.

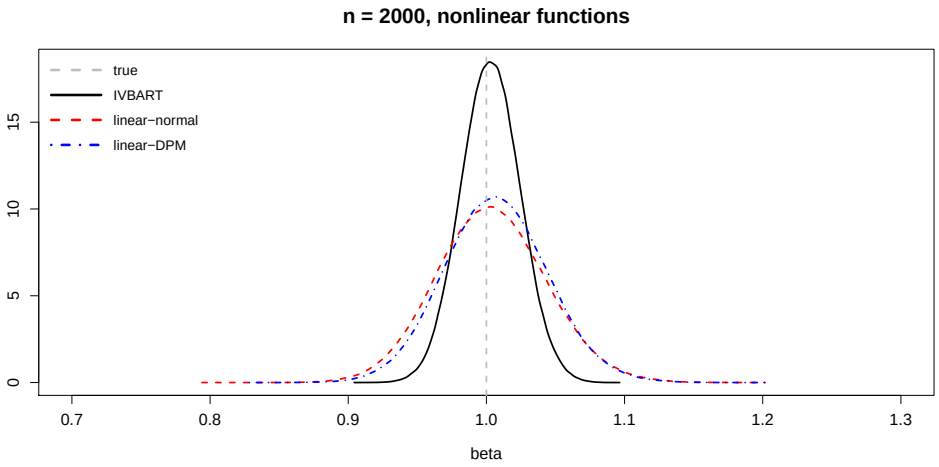
The top-left plot of Figure 1 corresponds to the scenario where we have simulated 2,000 observations (90 times) using the nonlinear specifications of f and h. From each simulated data set we obtain a set of MCMC draws of β and we combine all the draws into one large set of draws and then use a density estimate to represent the draws. The point of the paper is clearly illustrated by the fact that the distribution of draws from the IVBART model (solid density curve) is much tigher around the true value of $\beta = 1$ than the densities for the linear-normal model (dashed) or the linear-DPM model (dot-dash). By figuring out the functions f and h from the data, with no user input, IVBART is able to get a more precise inference for β than is obtained by simply assuming the functions are linear.

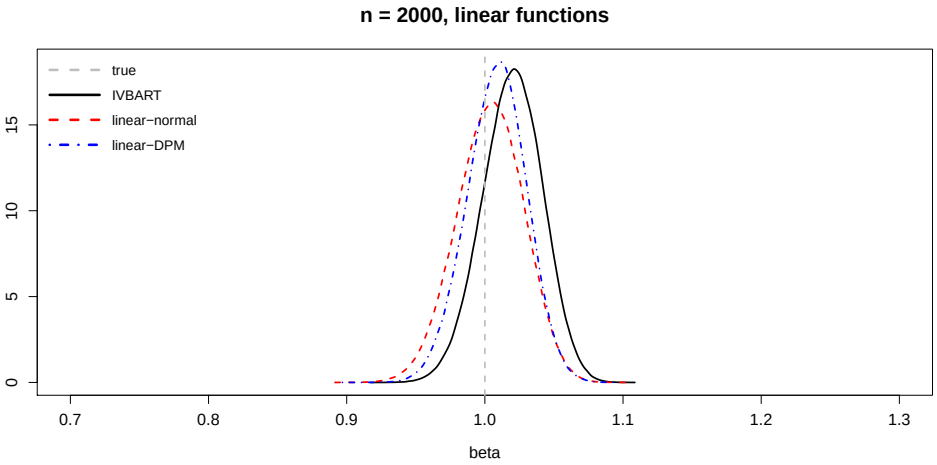
From the top-right plot in Figure 1 we see that with $n = 2,000$ and linear functions, the inference from the IVBART model is very similar to that obtained from the two linear models linear-normal and linear-DPM. The IVBART model is slightly more upward biased.

The two bottom plots of Figure 1 show that when the sample size is smaller, as we expect, things are tougher for the flexible model. IVBART still produces draws closer to β in the nonlinear case but there is some downward bias. In the linear case, the IVBART draws are again slightly upwardly biased but still quite similar to the linear methods.

Table 1 summarizes the results by reporting the root mean squared error (RMSE) of the β draws, again averaged over all MCMC draws and all simulations. We also report the relative RMSE for each simulation scenario by dividing the RMSE of each model by the minimum over the three models. With $n = 2,000$ and nonlinear functions, IVBART has the smallest RMSE and the RMSE for the linear-normal model is 86% larger while the RMSE for the linear-DPM model is 77% larger. With $n = 500$, and nonlinear functions, IVBART is again the best with the linear-normal and linear-DPM models being 42% and 35% worse. In the linear cases, the linear models win, but the IVBART model is at most 28% worse. The numbers in Table 1 reinforce the message of Figure 1. When there is strong nonlinearity, IVBART is much better and not too much worse in the linear case.

Figure 2 displays 95% posterior intervals for each simulation and each model. The four plots again correspond to our four simulation scenarios. Within each plot, each short vertical line segment represents a 95% interval obtained from the .025 and .975 quantiles of the MCMC β draws. The first 90 line segments display the posterior intervals for the IVBART method while the second and thirds sets of 90 display the intervals for the linear-normal and linear-DPM models. In each plot the final three (thicker) vertical line-seqments display the .025 and .975 quantiles for all draws combined for each method (as in Figure 1 and Table 1). In the top plot we clearly see the good performance of the IVBART model as the intervals are shorter and located near


n = 2000, nonlinear functions
true
IVBART
linear−normal
linear−DPM
0
5
10
15
0.7
0.8
0.9
1.0
1.1
1.2
1.3
beta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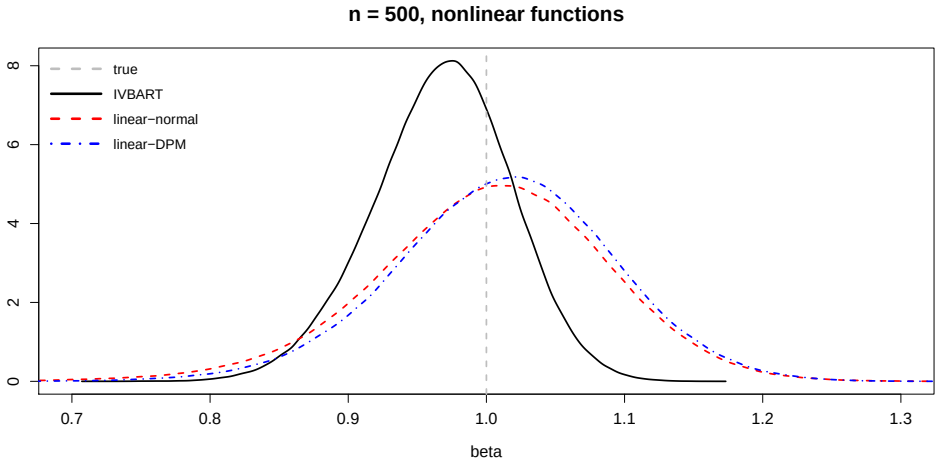
true
IVBART
linear−normal
linear−DPM
0
5
10
15
0.7
0.8
0.9
1.0
1.1
1.2
1.3
beta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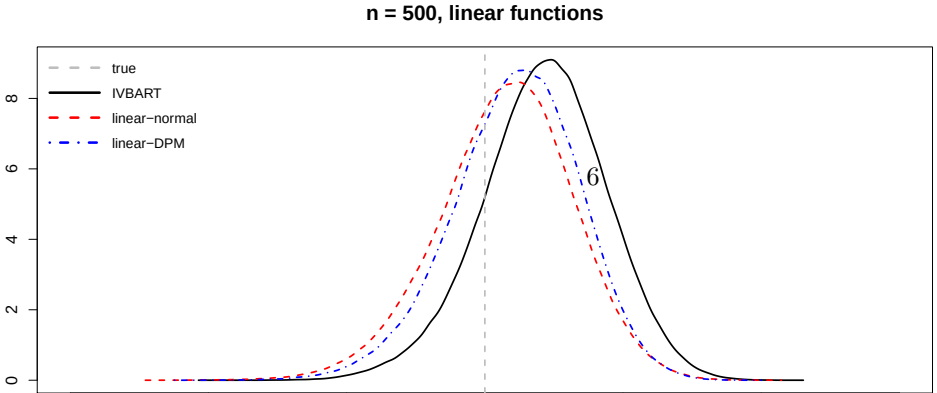
true
IVBART
linear−normal
linear−DPM
0
2
4
6
8
0.7
0.8
0.9
1.0
1.1
1.2
1.3
beta


n = 500, linear functions
true
IVBART
linear−normal
linear−DPM
0
2
4
6
8

the true value of β. In the linear cases (second and fourth plot) we see that IVBART is not too different from the linear models but somewhat biased upward. In the nonlinear case with $n = 500$, the IVBART intervals are smaller than the linear ones but slightly downard biased. We discuss the bias further in Section 3.2.

3.2 Prior Sensitivity

In the bottom-left plot if Figure 1 we see a bias in the inference for β. We also see this in the third plot in Figure 2. Two basic features of our model may be contributing to this bias. First, even when f and h are linear, our model is intrinsically nonlinear in inferring β. This is made clear in the Gibbs conditional for β given in Section 5.1. Secondly, the extreme flexibility of our model makes our inference sensitive to the prior. In Equations 3 and 4, both the nonlinear functions (f or h) and the error terms (ϵ_T or ϵ_Y) are capable of adaptively capturing the variation on T and Y. Of course, the degree to which the variation in T and Y is captured by the functions as opposed to the errors, will affect our inference for β. When the data are sufficiently informative (top-left of Figure 1) the prior is less influential. But for smaller sample sizes (bottom-left of Figure 1) the prior may affect our inference.

In (Chipman et al., 2010) great care is taken to develop a data dependent prior for the error term and nonlinear function for the simple single equation predictive model. In (George et al., 2019), the approach is extended to a single equation with nonparametric error estimation. While we are working to extend these approaches to our IV model, we first take the alternative approach of studying the prior sensitivity. In our current model, emphasis is on the estimation of the causal parameter β as opposed the predictive goal emphasized in (Chipman et al., 2010). In this case, we find the prior sensitivity approach helpful. See also (Hahn et al., 2020) for an important contribution to the problem of model and prior specification when using BART type models for causal inference.

The key prior choices involve the BART priors for f and h and the priors for the DPM estimation of the joint error distribution of (ϵ_T, ϵ_Y). Details for these prior choices are given in Section 6. In this section we give an overview of the prior choices and examine the sensitivity of our inference to a key aspect of the prior.

The prior for the error term estimation follows (Conley et al., 2008; Rossi, 2014). We first rescale both T and Y by subtracting off the sample mean and then dividing by the sample standard deviation. Draws of β are then rescaled to return to the original units. The error DPM prior is then designed to be informative, but flexible enough to cover the full range of the data. Of course the scaling based on the sample mean and standard deviation is sensitive to the error distribution but (Conley et al., 2008) report good results for severly non-normal errors. We also note that the results reported in Section 3.1 provide further evidence for the excellent performance of the (Conley et al., 2008) approach. Note that for a single equation, this is a much more spread out prior for the errors than used in (Chipman et al., 2010) or (George et al., 2019).

For the priors on f and h we start with the very simple BART prior specification:

$$f(x, z) \sim N(0, \sigma_f^2), \quad h(x) \sim N(0, \sigma_h^2), \tag{17}$$

where σ_f and σ_h are prior parameters that must be chosen. This remarkably simple prior specification is key the success of BART. Given we have standardize both T and Y simple prior choices could be $\sigma_f \approx 1.0$ and $\sigma_h \approx 1$. The default used for all results in Section 3.1 are $\sigma_f = 1.2$ and $\sigma_h = 1.2$.

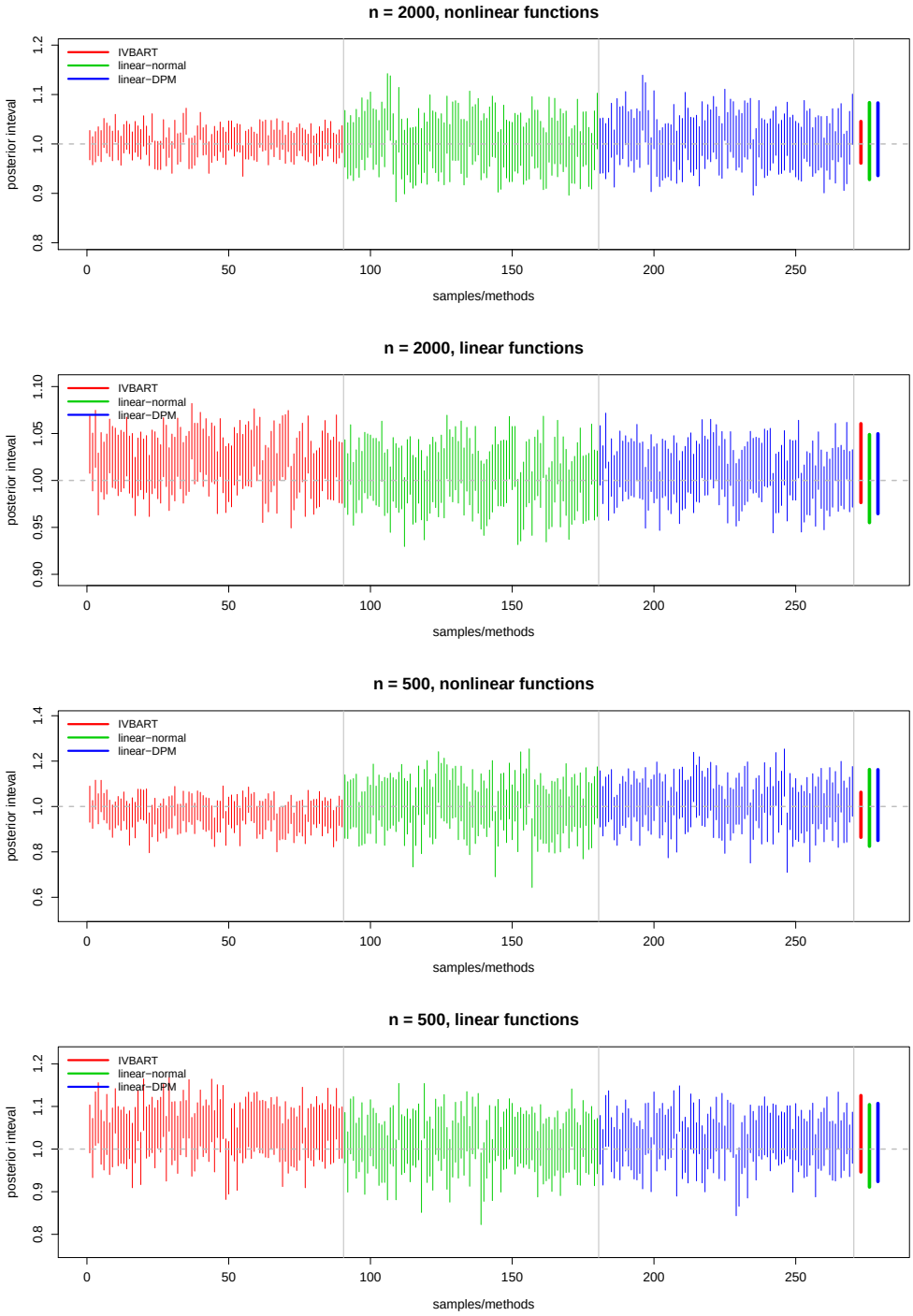


Figure 2: 95% Posterior intervals for β. Each vertical segment represents a 95% posterior interval. Top two plots are for simlulation data sample size $n = 2,000$ and the bottom two are for $n = 500$. Within each pair, the first is for the nonlinear functions and the second is for the linear functions. Within each plot, the first 90 intervals are from IVBART while the second is from linear-normal and the third set of 90 is from linear-DPM. The final three (thicker) intervals display .025 and.975 quantiles where all draw from all simulations are combined (as in Figure 1).

While these choices are simple and motived by the data standardization, they may be too spread out in that both the error and the functions are allowed to capture all of the variation. In (Chipman et al., 2010) and (George et al., 2019) the priors on the error process are tuned to guide the model towards exploring inferences where the error is smaller. We now explore the sensitivity of our results to the choices of σ_f and σ_h.

Figures 3 and 4 present inference for β based on a single simulated data set. Density estimates from MCMC draws of β are presented where the prior choice is varied. In Figure 3, $n = 500$ while in Figure 4, $n = 2,000$. In the top plot of each Figure, σ_f and σ_h are equal and varied in the set of values $S_\sigma = \{.8, 1, 1.2, 1.4\}$. In the bottom plot of each figure all 16 possible combinations $\{(\sigma_f, \sigma_h) : \sigma_f \in S_\sigma, \sigma_h \in S_\sigma\}$ are tried. The thicker density corresponds to the choice $(\sigma_f, \sigma_h) = (1.2, 1.2)$ used throughout Section 3.1.

Clearly when is n large (Figure 4) the results are fairly insensitive to the choice of prior and indicative of a larger value for β than suggested by the linear models. When n is smaller, (Figure 3) the results are more sensitive to the prior, but we still have the correct suggestion that β may be smaller than the values suggested by the linear models.

In practice we view the above sensitivity to be key part of the analysis as in Section 4 where we analyze the famous Card data. We are currenlty researching effective data based default prior choices, but feel than in this model analysis of prior sensitivity will continue to be an essential part of the investigation. Note that this is still much simpler than attempting to explore the sensitivity of two-stage least squares to the inclusion of possible transformed x and z. As currently engineered, our approach is not targeted towards a "big p" scenario where we entertain verly large x or z vectors of variables. However, we feel the case we have investigated in our simulations with ten x and five z instruments is representative of many applied problems. We explore the "big p" problem in future research.

3.3 Markov Chain Monte Carlo Performance

In Figure 5 we take a quick look at the time series characteristics of our MCMC draws of β. Figure 5 displays time series plots of the β draws for a single drawn sample of $n = 2,000$ observations and the nonlinear choices of f and h.

The top left plot displays all draws and the top right displays the corresponding ACF. The bottom left plot displays draws thinned to keep every tenth and the bottom right displays the corresponding ACF.

While the dependence is strong, we can obtain an effective inference in this case by simply taking every thenth draw.

4 Card Example

In a famous work (Card, 1993), instrumental variables are used to estimate the returns to education. A standard specification of the first stage regression relates the treatment variable years-of-schooling by 1976 (`ed76` $= T$) to two instruments that measure how close a subject lives to a two- or a four-year college ((`nearc2`, `nearc4`) $= z$) and the confounders (x): years of experience by 1976 (`exp76`), years of experience

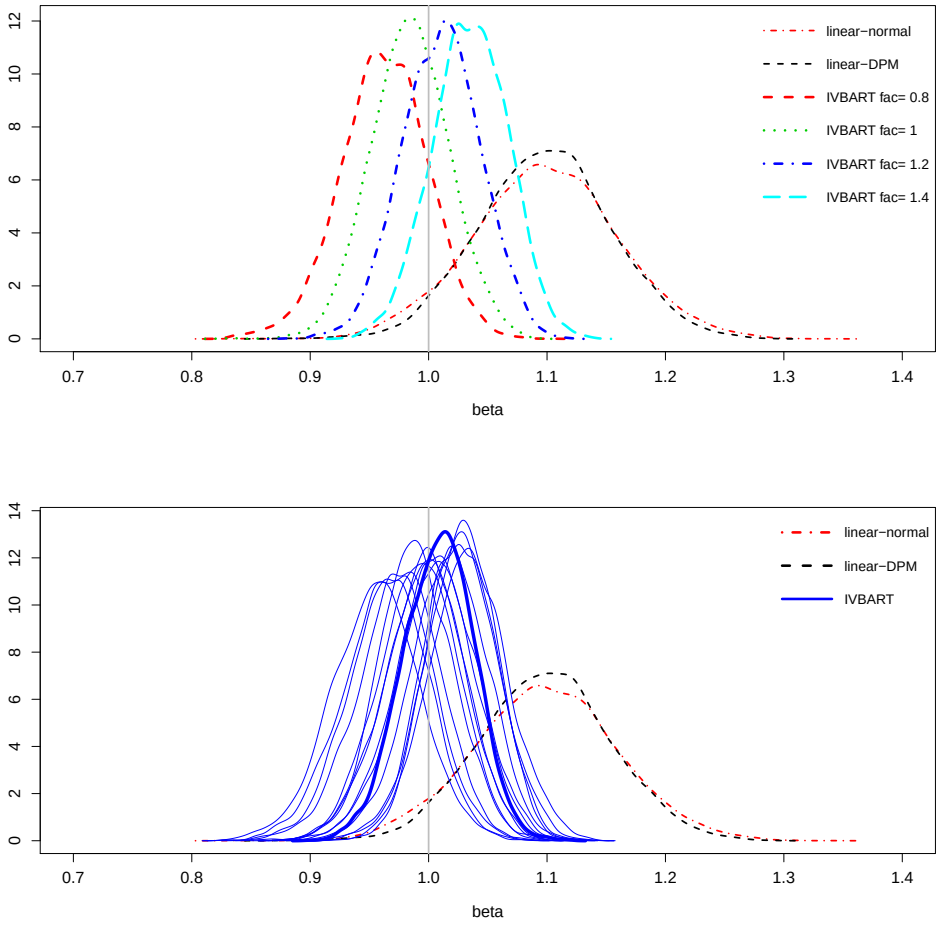


Figure 3: Prior sensitivity with $n = 500$. In the top plot $\sigma_f = \sigma_h$ and these values are varied in $S_\sigma = \{.8, 1, 1.2, 1.4\}$. In the bottom plot, all 16 density estimates obtained using $\sigma_f \in S_\sigma$ and $\sigma_h \in S_\sigma$ are shown. The thicker density corresponds to $(\sigma_f, \sigma_h) = (1.2, 1.2)$. Densities for draws from the linear-normal (dot-dash line) and linear-DPM (dashed line) models are also shown in each plot.

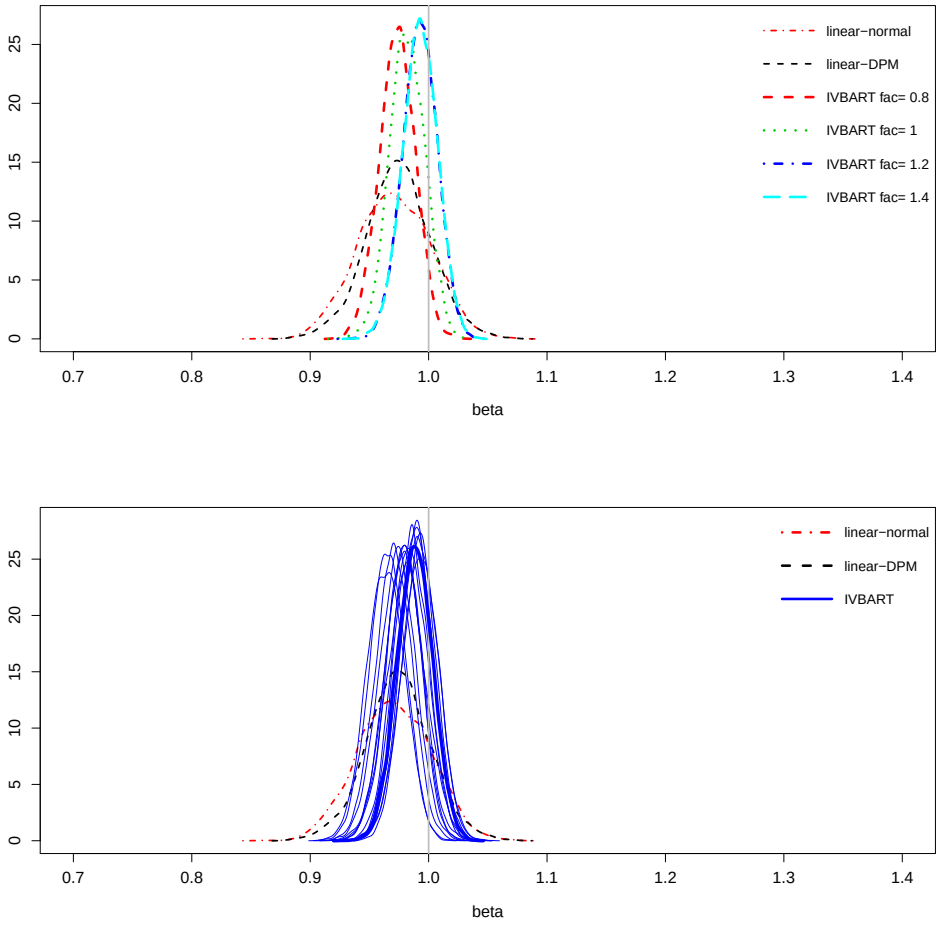


Figure 4: Prior sensitivity with $n = 2,000$. In the top plot $\sigma_f = \sigma_h$ and these values are varied in $S_\sigma = \{.8, 1, 1.2, 1.4\}$. In the bottom plot, all 16 density estimates obtained using $\sigma_f \in S_\sigma$ and $\sigma_h \in S_\sigma$ are shown. The thicker density corresponds to $(\sigma_f, \sigma_h) = (1.2, 1.2)$. Densities for draws from the linear-normal (dot-dash line) and linear-DPM (dashed line) models are also shown in each plot.

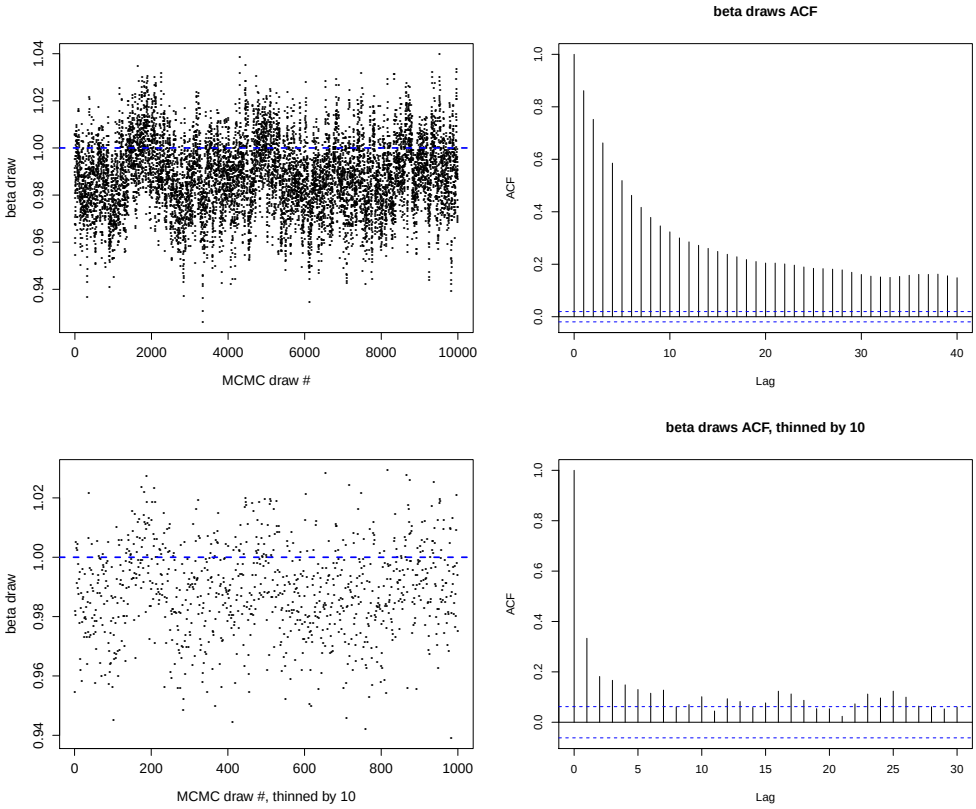


Figure 5: Time series behaviour of the β MCMC draws.

squared (`exp762`), an African-American race indicator (`black`), an indicator for whether the subject lives in a standard metropolitan statistical area in 1976 (`smsa76r`), and an indicator for whether the subject lives in the south (`reg76r`). The measures of proximity to college are the instruments in that they plausibly induce exogenous variation in the cost of education and hence the amount of education. The second stage equation relates wages to the years of schooling and x.

Note that when running IVBART, we do not include `exp762` since the whole point of the model is that the BART models for f and h are supposed to be able to uncover such nonlinearities without user input. When running linear-normal and linear-DPM we do include `exp762`.

Figures 6 and 7 display the inference for β using our three models IVBART, normal-linear, and normal-DPM. The format of Figure 6 is the same as that of the bottom plot in Figures 3 and 4 in which 16 IVBART inferences are displayed to capture the prior sensitivity to varying both σ_f and σ_h in (.8,1.0,1.2,1.4). For each of the 16 IVBART runs the posterior density of β is displayed using a solid curve. The linear-model inference is displayed using a dash-dot curve and the linear-DPM inference is displayed using a dashed curve.

The inference for β from the linear-DPM (posterior mean .08) model suggests a value dramatically less than that suggested by the linear-normal model (posterior mean .16). As expected, the posterior mean from the linear-normal model is close to the estimate obtained from standard two-stage least-squares (vertical dash-dot line). Clearly, the IVBART inference suggests that, for reasonable priors, the value of β may be less than than suggested by the linear-DPM model. However, the IVBART analysis still strongly supports the belief that β is far from zero as a practical matter with values around .05 being strongly favored.

Figure 7 has the same information as Figure 6 but the density estimates of the posterior distribution of β obtained from the 16 prior choices are laid out in 16 separate plots. There is one prior choice ($\sigma_f = 1.4$, $\sigma_h = 1.2$) such that the IVBART inference is very similar to the linear-DPM inference. However, for most choices that inference suggests a smaller value. All IVBART posteriors suggest a value of β much larger than zero.

Using IVBART we have obtained very strong inferences about the returns to schooling without having to make any judgements about the fundamental functions f and h. This is much easier then searching through some catalogue of possible transformations however this is done. Of course we still have the assumption of an additive linear treatment effect and relaxing this investigation is a subject of our current research. The sensitivity of the inference to the choice of the prior is an issue, but this is a natural consequence of the flexibility of the model and the level of information in the data.

To quickly get a rough sense of the practical difference in the inferences show in Figure 6, we can say that according to the linear-normal, linear-DPM, and IVBART models, β could be about .15, .08, or .05. A change of 4 more years of schooling would then change y=log wage by .6, .32, and .2. If we exponentiate these amounts, we get 1.8, 1.38, and 1.22 for the ratio of the wage level with and without the four years schooling. All of these amounts are quite different from one as a practical matter and a 38% increase in wages is quite a bit more than a 22% increase.

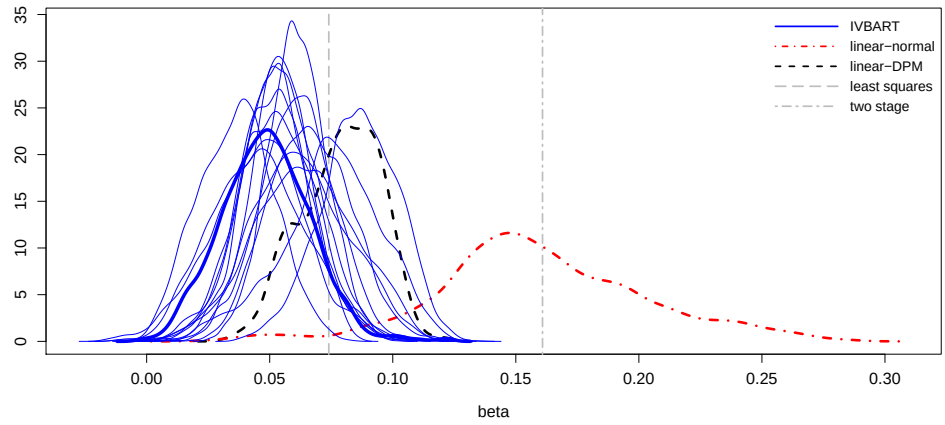


Figure 6: Inference for β for the Card data. To assess prior sensitivity, we vary both σ_f and σ_g in (.8,1.0,1.2,1.4) giving 16 possible choices for the pair. All 16 IVBART posteriors are drawn with a solid curve. The thicker IVBART line is for the setting $(\sigma_f, \sigma_h) = (1.2, 1.2)$. Densities for draws from the linear-normal (dot-dash line) and linear-DPM (dashed line) models are also shown.

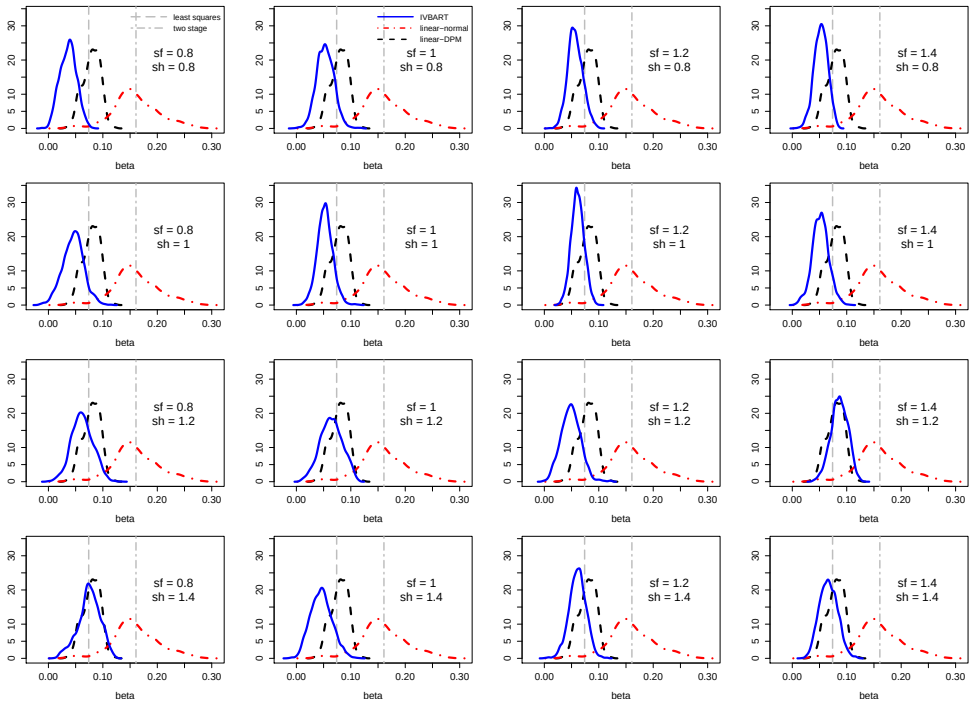


Figure 7: Inference for β from the Card data. To assess prior sensitivity, we vary both σ_f and σ_g in (.8,1.0,1.2,1.4) giving 16 possible choices for the pair. Each plot in the figure corresponds to a different choice of (σ_f, σ_h). Densities for draws from the linear-normal (dot-dash line) and linear-DPM (dashed line) models are also shown in each plot.

5 Details for the Gibbs Sampler

In this section we provide some details for the Gibbs sampler.

For some of the development it will be useful to work in terms of the Cholesky root of Σ_i.

Let,

$$L_i = \begin{bmatrix} \sigma_{Ti} & 0 \\ \gamma_i & \sigma_{Yi} \end{bmatrix}$$

so, that

$$\Sigma_i = L_i \, L_i'.$$

We can then write our model as:

$$\begin{aligned} T_i &= \mu_{Ti} + f(z_i, x_i) + \sigma_{Ti} \, Z_{Ti} && (18) \\ Y_i &= \mu_{Yi} + \beta \, T_i + h(x_i) + \gamma_i Z_{Ti} + \sigma_{Yi} \, Z_{Yi} && (19) \end{aligned}$$

where we recall that Σ_i and the corresponding $(\sigma_{Ti}, \gamma_i, \sigma_{Yi})$ along with (μ_{Ti}, μ_{Yi}), comprise the θ_i of Section 2.

We now detail the four conditionals in the Gibbs sampler of Section 2. We present them in an order which we believe corresponds to increasing difficulty. The first three are quite easy, while the last one, the draw of f, takes a little work.

Note also that for the model

$$Y_i = f(x_i) + \epsilon_i, \ \epsilon_i \sim N(0, w_i^2), \tag{20}$$

with known w_i, the BART prior and MCMC algorithm allows us to iterate a Markov Chain whose stationary distribution the posterior of f. We will have BART draws for both f and h conditional on the other parameters. In each case we will see that we can write the information in the data in the form of Equation 20 where the Y_i and the w_i depend on the data and the values of the known parameters.

5.1 The β Conditional

Given all of the parameters except β we can compute

$$Z_{Ti} = (T_i - \mu_{Ti} + f(z_i, x_i))/\sigma_{Ti} \tag{21}$$

from Equation 18.

We let

$$V_i = (Y_i - \mu_{Yi} - h(x_i) - \gamma_i Z_{Ti})/\sigma_{Yi} \ \text{ and } \ W_i = T_i/\sigma_{Yi},$$

from Equation 19.

This gives,

$$V_i = \beta\, W_i + Z_{Yi}, \;\; Z_{Yi} \overset{iid}{\sim} N(0,1)\ .$$

Given the normal prior for β we have standard normal draw for the conditional.

5.2 The h Conditional

This is similar to the β conditional.

We then let

$$V_i = (Y_i - \mu_{Yi} - \beta\, T_i - \gamma_i Z_{Ti}),$$

from Equations 21 and 19.

This gives,

$$V_i = h(x_i) + \sigma_{Yi} Z_{Yi},$$

which allows for a BART draw of h using 20.

5.3 The $\{\theta_i\}$ Conditional

Let,

$$\tilde{Y} = (\tilde{Y}_{i1}, \tilde{Y}_{i2})' = (T_i - f(z_i, x), (Y_i - \beta\, T_i - h(x_i))'. \tag{22}$$

Then,

$$\tilde{Y}_i \sim N(\mu_i, \Sigma_i).$$

Then, given $\{\tilde{Y}_i\}$, we can draw $\{\theta_i\} = \{(\mu_i, \Sigma_i)\}$ using the standard DPM methodology as described in Rossi (2014), Conley et al. (2008), and originally in Escobar and West (1995).

5.4 The f Conditional

Finally, we draw f.

From Equations 18 and 19,

$$\begin{aligned} Y_i - \mu_{Yi} - h(x_i) &= \beta\, T_i + \gamma_i\, Z_{Ti} + \sigma_{Yi} Z_{Yi} \\ &= \beta(\mu_{Ti} + f(z_i, x_i) + \sigma_{Ti} Z_{Ti}) + \gamma_i\, Z_{Ti} + \sigma_{Yi} Z_{Yi}. \end{aligned}$$

So,

$$Y_i - \mu_{Yi} - h(x_i) - \beta\mu_{Ti} = \beta f(z_i, x_i) + Z_{Ti}(\beta\sigma_{Ti} + \gamma_i) + \sigma_{Yi} Z_{Yi}.$$

We then let,

$$\begin{aligned} R_i &= (\beta\sigma_{Ti} + \gamma_i)(T_i - \mu_{Ti}) - \sigma_{Ti}(Y_i - \mu_{Yi} - h(x_i) - \beta\mu_{Ti}) \\ &= \gamma_i f(z_i, x_i) - \sigma_{Ti}\sigma_{Yi} Z_{Yi}. \end{aligned}$$

Thus, for each $i = 1, 2, \ldots, n$ we have the pair of independent observations,

$$T_i - \mu_{Ti} = f(z_i, x_i) + \sigma_{Zi} Z_{Ti}, \quad \frac{R_i}{\gamma_i} = f(z_i, x_i) - \frac{\sigma_{Ti}\sigma_{Yi}}{\gamma_i} Z_{Yi}.$$

This gives us $2n$ observations which may be put in the form of Equation 20.

Note that if $|\gamma_i|$ is small, then we automatically throw out the information in the $\frac{R_i}{\gamma_i}$ observation since the resulting large error variance will downweight the observation. This makes intuitive sense since if $|\gamma_i|$ is small the errors in the two equations are independent so that our information about f comes soley from the first equation.

6 Prior Details

In this section we provide details on the choice of prior. As illustrated in sections 3 and 4, the choice of prior is influential. This is inevitable in a flexible Bayesian model. In our basic model (equations 3 and 4) the nature of (T, Y) can be captured by nonparametrically modeling the error (ϵ_T, ϵ_Y) or the functions f and h and we are doing both.

Priors must be chosen for β, the functions f and h, and the Dirichlet process mixture for ϵ. We discuss each of these in turn.

As in many Bayesian analyses, we want to be able to inject prior information when available and we want reasonable defaults that enable users to get sensible results with minimal input. In order to have sensible default choices we typically start by standardizing the data. In all of the examples run in Sections 3 and 4 we started by stardizing the data to have zero mean and standard deviation one:

$$T \to \frac{T - \bar{T}}{s_T}, \quad Y \to \frac{Y - \bar{Y}}{s_Y} \tag{23}$$

where $\bar{x}$ and s_x are the sample mean and standard deviation of the data in x.

6.1 Prior on β

While the simple linear specification for the treatment effect is a limitation, it facilitates the very simple prior specification

$$\beta \sim N(\bar{\beta}, A_\beta^{-1}). \tag{24}$$

Important prior information about β may well be available in application. As often the information in the data is not overwhelmingly strong, inclusion of sensible prior information may be an essential part of the analysis.

Note that if we standardize the data as in (23), then

$$\beta_s = \beta \frac{s_T}{s_Y},$$

where β_s is the coefficient on the standardized scale and β is the coefficient on the original scale.

In all the examples, the prior in (24) is applied to β_s. The posterior draws of β_s are then transformed back to the original β scale.

6.2 Priors for f and h

A major strength of the BART approach is the remarkably simple specification for the prior on an unknown function. We have:

$$f(z,x) \sim N(0,\sigma_f^2), \;\; h(x) \sim N(0,\sigma_h^2). \tag{25}$$

We need only choose the two standard deviations σ_f and σ_h. Note that the marginal prior for $f(z,x)$ does not depend on (z,x). Similarly, the prior for $h(x)$ does not depend on x.

There are additional details to the full BART specification. For example, there are prior choices that describe beliefs about the trees underlying the functions f and h. All such choices are done as discussed in (Chipman et al., 2010) and implemented in the package (Sparapani et al., 2021) in (R Core Team, 2018).

Given the data has been standardized, a diffuse but hopefully not too spread out prior is obtained by letting σ_f and σ_h be in the neighborhood of one. In our examples, our exploration of prior sensitivity consists of varying σ_f and σ_f about one with the choice $\sigma_f = \sigma_h = 1.2$ being highlighted (Figures 3, 4, 6, and 7). The motivation for the choice 1.2 is that it gives a prior which allows for more variation than the more obvious choice of 1, while hopefully not being too spread out. More spread out priors (that is, larger σ_f and σ_h) give f and h more freedom to fit the data. Of course, we live in constant fear of over-fitting. As is standard practice in applied Machine Learning we could reasonably use some kind of out-of-sample test to guide our choices.

This approach to choosing σ_f and σ_h is roughly in accordance with the standard choice in (Chipman et al., 2010) and (Sparapani et al., 2021). There, the default is chosen so that twice the standard deviation of f covers the range of Y in the simpler model $Y = f(x) + \epsilon$. However, even our simple two equation IV model is highly nonlinear and the consequences of prior choices may be hard to anticipate. These considerations motivate the prior sensitivity approach taken in Sections 3 and 4. We explore values of σ_f and σ_h in neighborhoods of one.

6.3 Dirichlet process mixture Prior

In this section we describe the choice of G_0 and prior on α. Recall (Section 2) that the atoms of the discrete distribution from which we draw $\theta_i = (\mu_i, \Sigma_i)$ are draws form G_0 and α determines the distribution of the number of unique θ_i.

Our choices follow (Conley et al., 2008) exactly. In particular we review the basic rational and argue that the same choices are reasonable in our more flexible model. As previously noted, (Rossi, 2014) is also an excellent reference, giving a less terse textbook style presentation.

The basic idea is to calibrate these fundamental prior choices by considering the scenario where β, f, and h are all zero. In this case, $(\epsilon_{Ti}, \epsilon_{Yi})' = (T_i, Y_i)'$ and our DPM model should nonparametically estimate the bivariate joint distribution of the standardized (T, Y). These choices are "noninformative" but not so spread out as to limit the effectiveness of the DPM. The examples in Conley et al. (2008) and Section 3 suggest that these choices are quite generally effective in the linear case.

Note however that this approach deviates from the approach motivating the prior choices made in (Chipman et al., 2010). In (Chipman et al., 2010), we have the single equation $Y = f(x) + \epsilon$ with $\epsilon \sim N(0, \sigma^2)$. The data on Y are demeaned, f is shrunk to zero, and the prior on σ is chosen to suggest that f will fit Y better than a linear function would. That is, the prior on the single parameter σ is designed to suggest that it is smaller than that obtained from a linear fit. Here the prior is calibrated be even more spread out that needed to completely fit the data. The Conley et al. (2008) DPM prior is less informative about the errors so that our prior sensitivity approach is useful in uncovering the range of plausible inferences. Note that in (George et al., 2019), a single equation $Y = f(x) + \epsilon$ was considered and the DPM modeling approach was used to univariate distribution of ϵ. In that paper, the DPM choices were motivated by a desire to mimic the kind of prior information used in (Chipman et al., 2010) rather than the relatively noninformative specification used here for the joint distribution of $(\epsilon_T, \epsilon_Y)'$.

6.4 Specification of G_0

The base prior G_0 is a prior on $\theta = (\mu, \Sigma)$. We start from the standard conjugate setup:

$$\Sigma^{-1} \sim \text{Wishart}_\nu(V^{-1}), \;\; \mu \,|\, \Sigma \sim N(\bar{\mu}, \frac{\Sigma}{a}).$$

The parametrization of the Wishart distribution is such that $E(\Sigma^{-1}) = \nu\, V^{-1}$.

Given our standardization of T and Y, $\bar{\mu}$ is set to zero. We also let $V = v\, I$ where I is the 2×2 identity matrix.

With these simplifications we only have to choose the three numbers (a, ν, v). Using $\sigma_1 = \sqrt{\sigma_{11}}$, we first choose c_1, c_2, c_3, κ and then find (a, ν, v) such that

$$P(-c_3 < \mu_1 < c_3) = 1 - \kappa, \;\; P(\sigma_1 < c_1) = \kappa/2, \; P(\sigma_1 > c_2) = \kappa/2,$$

so that $P(c_1 < \sigma_1 < c_2) = 1 - \kappa$. The defaults used throughout this paper are $c_3 = 10$, $c_1 = .25$, $c_2 = 3.25$, and $\kappa = .2$, giving $a = .016$, $\nu = 2.004$ and $v = .17$. Again, this is exactly as in (Conley et al., 2008).

The value of c_3 is very large and the value of ν is very small. These priors are chosen to be very diffuse but not so diffuse as to derail our basic DPM MCMC algorithm.

Note that the marginals from the conjugate prior are analytically available with,

$$\sigma_{11} \sim \frac{v}{\chi^2_{\nu-1}}, \text{ and } \mu_1 \sim \sqrt{\frac{v}{a(\nu-1)}}\, t_{\nu-1}.$$

6.5 Prior on α

The idea of the prior is to relate α to the number of unique θ_i. Let I denote the number of unique θ_i. The user chooses a minimum and maximum number of components I_{min} and I_{max}. We then solve for α_{min} so that the mode of the consequent distribution for I is I_{min}. Similarly, we obtain α_{max} from I_{max}. We then let

$$p(\alpha) \propto (1 - \frac{\alpha - \alpha_{min}}{\alpha_{max} - \alpha_{min}})^{\psi}.$$

The default values for I_{min}, I_{max}, and ψ are 2, $[.1n] + 1$, and .5, where [] denotes the integer part and n is the sample size. A nice thing about this prior is it automatically scales sensibly with n.

7 Conclusion

The linear instrumental variables model has long been fundamental in causal analysis. It simply and elegantly captures the fundamental intuition that an instrumental variable z, may provide a source of variation in a treatment T, comparable to that of an experiment in which variation is induced by an investigator who controls the value of T.

However the assumption of linearity is rarely one that we can comfortably impose. In practice, this usually leads to a search for a set of transformations of the instruments z and the additional variables x which are then used in the linear setting. Even with modern methods for finding transformations this process is tedious and depends on choices for the set of transformations considered.

Our use of Bayesian Additive Regression trees (BART) allows us to capture a wide range of possible functions with no user input and still do a full Bayesian analysis including nonparametric modeling of the error terms.

For our nonparametric error term analysis we have followed Conley et al. (2008) closely given its success. This as led to a prior-sensitivity approach in which we vary the prior beliefs about the nonlinear functions f and h. Also, our goal here is inferential in that we seek to learn β while in BART, the prior development has been more focused on the goal of out of sample prediction. The BART models for these two functions allow for a relatively simple scheme for varying our prior beliefs. We hope that the top-left plot of Figure 1 and the analysis of the Card data in Figure 6 will suggest to practictioners that IVBART provides a relatively simple alternative to the difficult challenges presented by the general sensitivity of inference for the treatment effect β to the model specification.

In future work we will consider the use of more informative data based priors for the error distribution as in (Chipman et al., 2010) and (George et al., 2019). In addition, future work will seek to relax the additive linear assumption for the treatment effect. While are current analysis is very flexible and allows for simple interpretation of the causal effect through the parameter β, we wish to consider the possibility of hetergeneous treatment effects. We note that our current model is already very flexible and powerful and extentions to a still more flexible model will entail careful prior choices as in (Hahn et al., 2020).

We note that the simlulation study presented in this paper provides further support for the efficacy of the linear approaches provided by the `R` package `bayesm` (Rossi, 2019) in the functions `rivGibbs` for the linear model with correlated normal errors and `rivDP` for the linear model with nonparametrically modeled errors.

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A The ivbart R package

All of the calculations in this article with respect to the IVBART model were performed with the **ivbart R** package. **ivbart** is free open-source software that is publicly available at `https://github.com/rsparapa/bnptools`. The following snippet of **R** code installs **ivbart** with the `install_github` function from the **remotes R** package (available on the Comprehensive R Archive Network at `https://cran.r-project.org/package=remotes`).

```
R> library("remotes")
R> install_github("rsparapa/bnptools/ivbart")
```

The `nlsym` object is a data frame providing the Card example data of Section 4. With `system.file("demo/nlsym.R", package="ivbart")`, you can find the installed **R** program that analyzes the Card data with IVBART that is provided as a demonstration. You can run this program with the following snippet.

```
R> source(system.file("demo/nlsym.R", package="ivbart"), echo=TRUE)
```

See the documentation of the `ivbart` function for more details.

B Causal Identification

In this section, we prove that the estimation of β is causally identified. First, let's return to the structural equations in the classic IV framework. Here, we ignore the confounders for simplicity since they are not needed, i.e., we can simply assume that they are unobserved. Furthermore, let the constant intercept terms be zero for convenience, i.e., $\mu_T = \mu_Y = 0$. And, finally, we substitute the first stage into the second stage.

$$T_i = \gamma' Z_i + \epsilon_{Ti} \tag{26}$$

$$Y_i = \beta\, T_i + \epsilon_{Yi}$$

$$Y_i = \beta(\gamma' Z_i + \epsilon_{Ti}) + \epsilon_{Yi} \tag{27}$$

We will show that β is identifiable by resorting to the so-called instrumental variable formula (Bowden and Turkington, 1990).

$$\begin{aligned} \beta &\triangleq \frac{\partial}{\partial T}\left[\mathrm{E}\left[Y|T\right]\right] \\ &\triangleq \frac{\mathrm{E}\left[Y|Z\right]}{\mathrm{E}\left[T|Z\right]} \\ &\triangleq \frac{r_{YZ}}{r_{TZ}} \end{aligned} \tag{28}$$

The middle formula (28), a ratio of expectations, is the key to our proof of causal identification; rather than the last line which is the most cited form of this result. To apply the middle formula, we plug the first

stage into the denominator (26) and the re-written second stage into the numerator (27) to show that β is identifiable.

$$\begin{aligned}\beta &\triangleq \frac{\mathrm{E}\left[Y|Z\right]}{\mathrm{E}\left[T|Z\right]} \\ &= \frac{\beta\gamma' Z_i}{\gamma' Z_i} = \beta\end{aligned}$$

This is a well-known result with respect to linear structural equations.

Now, let's investigate our BART IV framework while, once again, ignoring confounders and letting the intercepts be zero.

$$T_i = f(Z_i) + \epsilon_{Ti} \tag{29}$$

$$\begin{aligned}Y_i &= \beta\, T_i + \epsilon_{Yi} \\ &= \beta(f(Z_i) + \epsilon_{Ti}) + \epsilon_{Yi}\end{aligned} \tag{30}$$

And, we apply the instrumental variable formula (28) as before to show that β is identifiable, i.e., plug the first stage into the denominator (29) and the re-written second stage into the numerator (30).

$$\begin{aligned}\beta &\triangleq \frac{\mathrm{E}\left[Y|Z\right]}{\mathrm{E}\left[T|Z\right]} \\ &= \frac{\beta f(Z_i)}{f(Z_i)} = \beta\end{aligned}$$

This is a more surprising result. Generally, it is well-known that nonparametric methods are not identifiable without strong assumptions (Imbens and Angrist, 1994; Pearl, 2009). We illustrate the typical non-idenfiability of β by a more general model as follows.

$$T_i = f(Z_i) + \epsilon_{Ti} \tag{31}$$

$$\begin{aligned}Y_i &= g(T_i) + \epsilon_{Yi} \\ &= g(f(Z_i) + \epsilon_{Ti}) + \epsilon_{Yi}\end{aligned} \tag{32}$$

Now, apply the instrumental variable formula (28), i.e., plug the first stage into the denominator (31) and the re-written second stage into the numerator (32).

$$\frac{\mathrm{E}\left[Y|Z\right]}{\mathrm{E}\left[T|Z\right]} = \frac{\mathrm{E}\left[g(f(Z_i) + \epsilon_{Ti})\right]}{f(Z_i)} \neq \beta$$

The denominator is unchanged. However, the numerator does not have a simple form; therefore, the true value β is not identifiable without further assumptions about $g(.)$. For example, if we assume that $g(T_i) = \beta\, T_i$ (as we have above), then β is identifiable as we have shown.

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