Bayesian nonparametric models for treatment effect heterogeneity: model parameterization, prior choice, and posterior summarization

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#### Motivation

Bayesian nonparametric modeling is an effective tool for inferring heterogenous causal effects.

Bayes estimates from these models can have excellent frequentist properties – no need to drink the Kool-Aid.

Some insights about model and prior specification apply to flexible estimation of effect heterogeneity more generally

### Putting BNP to work for inference about effect heterogeneity

#### Three considerations:

- Model parameterization: When you can, isolate your estimand as a parameter
- **Prior specification:** Priors are important for encoding beliefs but also for applying regularization. Regularization that ignores selection can be disasterous.
- Posterior summarization: "Solving" the Bayesian analogue of the post-selection inference problem, focusing on stable estimands, and giving actionable insights from complex models.

# Some generic identifying assumptions

Strong ignorability:

$$Y_i(0), Y_i(1) \perp Z_i \mid X_i = x_i,$$

Positivity:

$$0 < \Pr(Z_i = 1 \mid X_i = x_i) < 1$$

for all *i*. Then

$$P(Y(z) \mid \mathbf{x}) = P(Y \mid Z = z, \mathbf{x})$$

,

and the conditional average treatment effect (CATE) is

$$\begin{split} \tau(\mathbf{x}_i) &:= \mathrm{E}(Y_i(1) - Y_i(0) \mid \mathbf{x}_i) \\ &= \mathrm{E}(Y_i \mid \mathbf{x}_i, Z_i = 1) - \mathrm{E}(Y_i \mid \mathbf{x}_i, Z_i = 0). \end{split}$$

**Model Parameterization** 

Forget confounding and covariates and consider estimating average treatment effect for a binary treatment in a randomized trial.

A simple model:

$$(Y_i \mid Z_i = 0) \stackrel{iid}{\sim} N(\mu_0, \sigma^2)$$
$$(Y_i \mid Z_i = 1) \stackrel{iid}{\sim} N(\mu_1, \sigma^2)$$

where the estimand of interest is  $\tau \equiv \mu_1 - \mu_0$ .

If 
$$\mu_0, \mu_1 \sim N(\phi_j, \delta_j)$$
 independently then  $\tau \sim N(\phi_1 - \phi_0, \delta_0 + \delta_1)$ 

Often we have stronger prior information about  $\tau$  than  $\mu_1$  or  $\mu_0$  – in particular, we expect it to be small.

A more natural parameterization:

$$(Y_i \mid Z_i = 0) \stackrel{iid}{\sim} N(\mu, \sigma^2)$$
$$(Y_i \mid Z_i = 1) \stackrel{iid}{\sim} N(\mu + \tau, \sigma^2)$$

where the estimand of interest is still  $\tau$ .

Now we can express prior beliefs on  $\tau$  directly and independent of nuisance parameters.

How does this relate to models for heterogeneous treatment effects? Consider (mostly) separate models for treatment arms:

$$y_i = f_{z_i}(\mathbf{x}_i) + \epsilon_i \quad \epsilon_i \sim N(0, \sigma^2)$$

$$(Y_i \mid Z_i = 0, \mathbf{x}_i) \stackrel{iid}{\sim} N(f_0(\mathbf{x}), \sigma^2)$$

$$(Y_i \mid Z_i = 1, \mathbf{x}_i) \stackrel{iid}{\sim} N(f_1(\mathbf{x}), \sigma^2)$$

Independent priors on  $f_0, f_1 \to \text{prior}$  on  $\tau(\mathbf{x}) \equiv f_1(\mathbf{x}) - f_0(\mathbf{x})$  has larger variance than prior on  $f_0$  or  $f_1$ 

No direct prior control  $\rightarrow$  simple  $f_0, f_1$  can compose to complex  $\tau$  (e.g. Künzel et al (2019)).

In addition, every variable in x is a potential effect modifier.

What about the "just another covariate" parameterization?

$$y_i = f(\mathbf{x}_i, z_i) + \epsilon_i \quad \epsilon_i \sim N(0, \sigma^2)$$
  
$$(Y_i \mid Z_i = z_i, \mathbf{x}_i) \stackrel{iid}{\sim} N(f(\mathbf{x}_i, z_i), \sigma^2)$$

Then the heterogeneous treatment effects are given by

$$\tau(\mathbf{x}) \equiv f(\mathbf{x}, 1) - f(\mathbf{x}, 0)$$

and we still (generally) have no direct prior control!

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For binary treatments, set  $f(\mathbf{x}_i, z_i) = \mu(\mathbf{x}_i) + \tau(\mathbf{w}_i)z_i$ , where **w** is (possibly) a subset of **x**:

$$y_i = \mu(\mathbf{x}_i) + \tau(\mathbf{w}_i)z_i + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2)$$

$$(Y_i \mid Z_i = z_i) \stackrel{iid}{\sim} N(\mu(\mathbf{x}_i) + \tau(\mathbf{w}_i)z_i, \sigma^2)$$

The heterogeneous treatment effects are given by  $\tau(\mathbf{w})$  so we have direct prior control!

In Hahn et. al. (2020), we use independent BART priors on  $\mu$  and  $\tau$  ("Bayesian causal forests").

# Prior Selection

### Tweaking priors on au

Several adjustments to the BART prior on  $\tau$  in BCF:

- $\cdot$  Higher probability on smaller au trees (than BART defaults)
- Higher probability on "stumps" (all stumps = homogeneous effects)
- $\cdot$  N<sup>+</sup>(0, v) Hyperprior on the scale of leaf parameters in au

Other nonparametric priors for  $\tau$  have similar "knobs" (scale, smoothness, sparsity, etc.)

For observational data, we need to adjust the prior on  $\mu(\mathbf{x})$  as well, to avoid regularization induced confounding (Hahn et al (2016, 2020))

## Regularization can induce confounding (bias)

Let's return to a linear model with homogeneous effects:

$$y_i = f(\mathbf{x}_i, z_i) + \varepsilon_i$$
  
=  $\tau z_i + \beta^t \mathbf{x}_i + \varepsilon_i$ 

and suppose  $x_i$  is high dimensional.

Assume  $\beta \sim N(0, \lambda^{-1}I)$  (ridge prior) and  $p(\tau) \propto 1$ 

What effect does the prior (regularization) have on estimating  $\tau$  using the posterior mean?

# Regularization can induce confounding (bias)

The bias of  $\tilde{\tau} = E(\tau \mid Y, z, \mathbf{x})$  is

$$bias(\tilde{\tau}) = \lambda \hat{\delta}^t [\lambda \mathbf{I} + \mathbf{X}^t (\mathbf{I} - \mathbf{P}_z) \mathbf{X}]^{-1} \beta$$
 (1)

where  $\hat{\delta}_j$  = the OLS estimate of  $x_{ij} = \delta_j z_i + \epsilon_{ij}$ . Alternatively:

$$bias(\tilde{\tau}) = \lambda [z^{t}(z - \tilde{z}_{\lambda})]^{-1} \tilde{\gamma}_{\lambda}^{t} \beta$$
 (2)

where  $\tilde{\gamma}_{\lambda} = [\lambda \mathbf{I} + \mathbf{X}^t \mathbf{X}]^{-1} \mathbf{X}^t \mathbf{z}$  and  $\tilde{\mathbf{z}}_{\lambda} = \mathbf{X} \tilde{\gamma}_{\lambda}$ 

In general, if z and x are correlated the bias is nonzero and depends on the nuisance parameter!

### Solution: Don't penalize variation in f(x, z) along $E(Z \mid x)$

Expand the model to include  $\hat{z}_i$  (a function of z and X) that estimates  $E(Z \mid \mathbf{x})$ :

$$y_i = f(\mathbf{x}_i, z_i) + \varepsilon_i$$
  
=  $\tau z_i + \phi \hat{z}_i + \beta^t \mathbf{x}_i + \varepsilon_i$ 

Keep  $\beta \sim N(0, \lambda^{-1}I)$  (ridge prior) with  $p(\tau, \phi) \propto 1$ , so that variation in the direction of  $\hat{z}_i$  is unregularized

$$bias(\tilde{\tau}) = \lambda \hat{\delta}^{t} [\lambda \mathbf{I} + \mathbf{X}^{t} (\mathbf{I} - \mathbf{P}_{z}) \mathbf{X}]^{-1} \beta$$
 (3)

where  $\hat{\delta}_i$  = the OLS estimate of  $x_{ij} = \alpha_i \hat{z} + \delta_i z_i + \epsilon_{ij}$  ( $\approx 0$ ).

### Solution: Don't penalize variation in f(x, z) along $E(Z \mid x)$

Expand the model to include  $\hat{z}_i$  (a function of z and X) that estimates  $E(Z \mid \mathbf{x})$ :

$$y_i = f(\mathbf{x}_i, z_i) + \varepsilon_i$$
  
=  $\tau z_i + \phi \hat{z}_i + \beta^t \mathbf{x}_i + \varepsilon_i$ 

Keep  $\beta \sim N(0, \lambda^{-1}I)$  (ridge prior) with  $p(\tau, \phi) \propto 1$ , so that variation in the direction of  $\hat{z}_i$  is unregularized

$$bias(\tilde{\tau}) = \lambda \hat{\delta}^{t} [\lambda \mathbf{I} + \mathbf{X}^{t} (\mathbf{I} - \mathbf{P}_{z}) \mathbf{X}]^{-1} \beta$$
 (4)

where  $\hat{\delta}_i$  = the OLS estimate of  $x_{ij} = \alpha_i \hat{z}_i + \delta_i z_i + \epsilon_{ij} \ (\approx 0)$ .

#### Regularization induced confounding is a general phenomenon

There is nothing special about the ridge prior or the linear model – RIC is easy to produce with nonlinear models and nonlinear data generating processes. (Hahn et al (2020))

In essence: Since Z is a proxy for  $E(Z \mid \mathbf{x})$ , if the prior on  $f(\mathbf{x}, \mathbf{z})$  strongly penalizes variation in the "direction" of  $E(Z \mid \mathbf{x})$  (and not Z) the prior encourages misattributing that variation in f to Z.

This is not a Bayes problem; it's a generic regularization problem.

#### How to avoid penalizing variation in f(x, z) along $E(Z \mid x)$

Including  $\hat{z}_i$  as an extra coordinate/feature/covariate is often enough to mitigate regularization induced confounding.

Depending on the model, there may be easier/more efficient ways to accomplish this (e.g. residualization).

In Hahn et al (2020) we evaluate BART priors on  $f(\mathbf{x}, z)$  with and without  $\hat{z}$  and BCF:

$$y_i = \mu(\mathbf{x}_i, \hat{\mathbf{z}}_i) + \tau(\mathbf{w}_i)\mathbf{z}_i + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2)$$

The latter two are often *much* better and rarely worse, especially when selection into treatment is based on expected outcomes under control ("targeted selection").

**Posterior Summarization** 

#### Posterior summaries, or: I fit this model, now what?

Examine the "best" (in a user-defined sense) simple approximation to a "true" g(x) (Woody et al (2020))

Given samples of a function g(x),

- 1. Consider a class of simple/interpretable approximations  $\Gamma$  to g
- 2. Make inference on

$$\gamma = \mathop{\arg\min}_{\tilde{\gamma} \in \Gamma} d(g, \tilde{\gamma}, \tilde{\mathbf{X}}) + p(\tilde{\gamma})$$

for an appropriate distance function d and (optional) complexity penalty  $p(\gamma)$ 

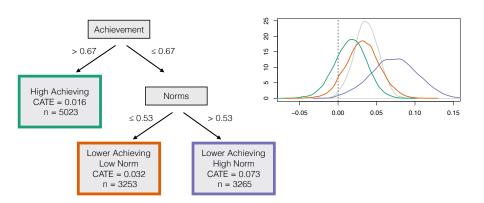
Get draws of  $\gamma$  by solving the optimization for each draw of g. Get point estimates by solving

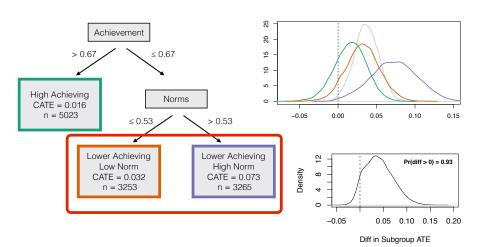
$$\hat{\gamma} = \mathop{\arg\min}_{\tilde{\gamma} \in \Gamma} \textit{E}_{\textit{g}}[\textit{d}(\textit{g}, \tilde{\gamma}, \tilde{\mathbf{X}}) + \textit{p}(\tilde{\gamma}) \mid \mathbf{Y}, \mathbf{x}]$$

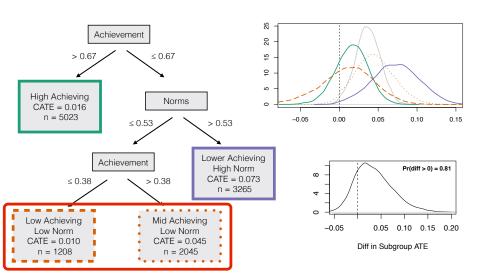
#### Posterior summaries, or: I fit this model, now what?

#### Posterior summaries:

- Are more interpretable (subgroup analysis, linear/additive/sparse approximations) and can be targeted to scientific questions
- Obviate the "need" to fit multiple models for different questions (Bayesians need to think about post-selection issues too) – multiple summaries use the data once to go prior → posterior
- 3. Are often more stable (coarse subgroup effects vs. individualized estimates)
- 4. Come with (Bayes) valid estimates of uncertainty







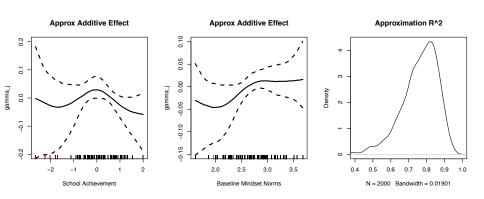
#### Additive summaries

We can get pproximate partial effect curves via additive summaries:

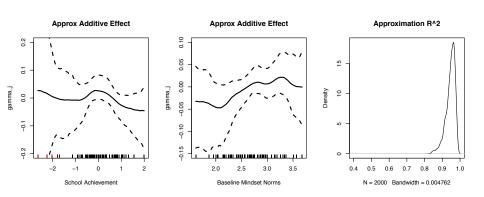
$$\tau(\mathbf{w}) \approx \gamma_0 + \sum_{j=1}^p \gamma_j(\mathbf{w}_j)$$

with appropriate forms for  $\gamma_i$  plus smoothing penalties.

We can also get posterior on discrepancy metrics, like pseudo- $R^2$ :  $Cor^2(\gamma(\mathbf{w}_i), \tau(\mathbf{w}_i))$ 



(Partial effect of minority composition not shown)



(Partial effect of minority composition not shown)

## Other applications of posterior summarization

- Interaction detection (Woody et al (2020)): If an additive summary is poor how do we search for missing interactions?
- Sensitivity to control function specification (Woody et al (2020b)): How do I expect removing confounders (or nonlinear/interaction terms) to change my effect estimate?
- "Explanations": Linear summaries in neighborhoods of  $\mathbf{x}_i$  = LIME with uncertainty

# Thank you!

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