Heteroskedastic BART and time-to-event outcomes

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September 17, 2025

This research funded, in part, by the US Office of Naval Research

Heteroskedastic BART (HBART)

Pratola, Chipman, George & McCulloch 2020 JCGS

$$y_{i} = f(x_{i}) + s(x_{i})\epsilon_{i} \qquad \epsilon_{i} \stackrel{\text{iid}}{\sim} N(0, \sigma^{2})$$

$$f \stackrel{\text{prior}}{\sim} BART (H, \mu, \kappa, \tau, \alpha, \beta)$$

$$s^{2} \stackrel{\text{prior}}{\sim} HBART (\widetilde{H}, \widetilde{\lambda}, \widetilde{\nu}, \widetilde{\alpha}, \widetilde{\beta})$$

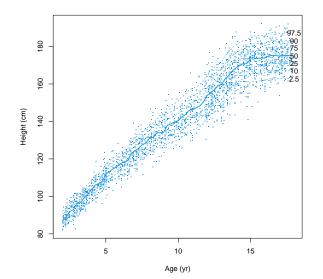
$$s^{2}(x_{i}) \equiv \prod_{h=1}^{\widetilde{H}} g(x_{i}; \widetilde{T}_{h}, \widetilde{M}_{h}) \qquad \widetilde{H} \approx H/5$$

$$\sigma_{hl}^{2} |\widetilde{T}_{h}| \stackrel{\text{prior}}{\sim} \lambda \nu \chi^{-2} (\nu) \text{ leaves of } \widetilde{T}_{h} \qquad \lambda = \widetilde{\lambda}^{1/\widetilde{H}}$$

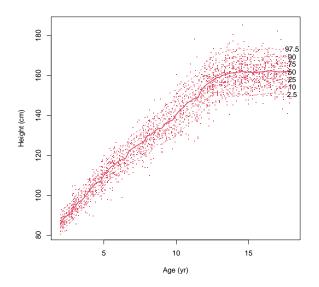
$$\stackrel{\text{prior}}{\sim} Gamma^{-1} (\nu/2, \lambda \nu/2) \qquad E\left[\sigma_{hl}^{2}\right] = \lambda \nu/(\nu - 2)$$

$$\in \widetilde{M}_{h} \qquad \nu = 2\left[1 - \left(1 - \frac{2}{\widetilde{\nu}}\right)^{1/\widetilde{H}}\right]^{-1}$$

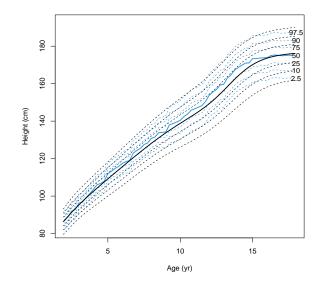
Marginal effect of age: HBART predictions for M $H=300, \widetilde{H}=60, \mathrm{numcut}=200$



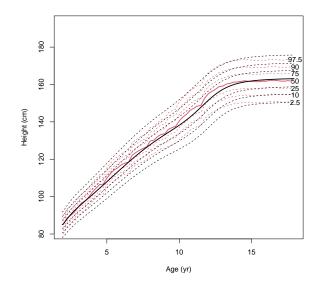
Marginal effect of age: HBART predictions for F



Marginal effect of age: HBART vs. CDC for M



Marginal effect of age: HBART vs. CDC for F



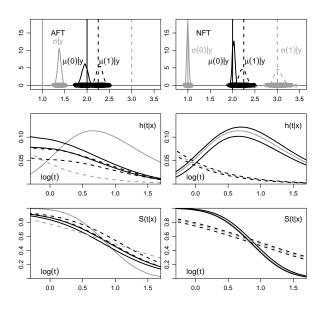
Personalized Hematopoietic Stem Cell Transplant (HSCT)

- HSCT is a treatment for white blood/bone marrow cancers
- Here we are concerned with unrelated donors that are human leukocyte antigen (HLA) 8/8 matched to the recipients transplanted from 2016:2019
- Goal: optimal donor matching for better recipient outcomes
- The outcome here is time to an event, i.e., event-free survival with both right and left censoring
- Events include death, relapse, graft failure/rejection or moderate/severe chronic graft vs. host disease (GVHD): whichever comes first
- There are P = 45 covariates that may have an impact
- 5 are donor-related characteristics: age, sex/childbearing, HLA DPB1 match, HLA DQB1 match and CMV match
- We wanted to *learn* the (likely complex) functional relationship between these covariates and the outcome with BART
- The cohort has 10016 for training and 1802 for validation
- A bit too large for our Discrete Time BART approach
- For this application, we developed NFT BART methodology

Methodological/Computational Pros and Cons

	Comparison of BART survival analysis methods				
	Hier-	Discrete	AFT	Mod-	NFT
Property	archical	Time		ulated	
Flexible	Con	Pro	Con	Pro	Pro
assumptions					
Non-	Con	Pro	Pro	Pro	Pro
parametric					
Left-	Con	Con	Pro	Con	Pro
censoring					
Time-dep.	Con	Pro	Con	Pro	Con
covariates					
Friendly to	Pro	Con	Pro	Con	Pro
compute					
First-author	Bonato	Sparapani	Henderson	Linero	Sparapani
Year	2011	2016	2018	2021	2023

Two groups: AFT BART vs. NFT BART



Bayesian Additive Regression Trees (BART) NFT notation

Sparapani, Logan, Laud & McCulloch 2023 Biometrics

$$\mu \stackrel{\text{prior}}{\sim} \text{BART} \ (a = 0.95, b = 2, H = 200, \kappa = 2, \tilde{\mu} = \bar{y})$$

$$y_i = \mu(x_i) + \epsilon_i \text{ where } \epsilon_i \stackrel{\text{iid}}{\sim} \text{N}(0, \sigma^2)$$

$$\mu(x_i) \equiv \tilde{\mu} + \sum_h g(x_i; \mathcal{T}_h, \mathcal{M}_h)$$

the **BART** prior implies the following priors (among others)

$$\mu_{hl} | \mathcal{T}_h \overset{\text{prior}}{\sim} N \left(0, \frac{0.25 \operatorname{range}(y)^2}{H \kappa^2} \right) \text{ leaves of } \mathcal{T}_h$$

$$\in \mathcal{M}_h$$

$$\sigma^2 \overset{\text{prior}}{\sim} \lambda \nu \chi^{-2} (\nu)$$

Heteroskedastic BART (HBART) NFT notation

Pratola, Chipman, George & McCulloch 2019 JCGS

$$\mu \overset{\text{prior}}{\sim} \text{BART} \ (a, b, H = 200, \kappa = 5, \tilde{\mu})$$

$$\sigma^{2} \overset{\text{prior}}{\sim} \text{HBART} \ (\tilde{a} = 0.95, \tilde{b} = 2, \tilde{H} = 40, \tilde{\lambda}, \tilde{v})$$

$$y_{i} = \mu(x_{i}) + \epsilon_{i} \text{ where } \epsilon_{i} \overset{\text{iid}}{\sim} \text{N}(0, \sigma^{2}(x_{i}))$$

$$\sigma^{2}(x_{i}) \equiv \prod_{h=1}^{\tilde{H}} g(x_{i}; \tilde{T}_{h}, \tilde{M}_{h}) \text{ where } \tilde{H} \approx H/5$$

the **HBART** prior implies the following priors (among others)

$$\sigma_{hl}^{2} | \widetilde{\mathcal{T}}_{h} \stackrel{\text{prior}}{\sim} \lambda \nu \chi^{-2} (\nu) \text{ leaves of } \widetilde{\mathcal{T}}_{h}$$

$$\in \widetilde{\mathcal{M}}_{h}$$

The Accelerated Failure Time (AFT) model: part 1

- Time-to-event data notation: (t_i, δ_i) i = 1, ..., N subjects if $\delta_i = 0$, then t_i is a right censoring time else if $\delta_i = 1$, then a failure time else if $\delta_i = 2$, then left censoring
- How is failure time explained by a vector of covariates x_i ?
- take logarithms $y_i = \log t_i$ and use a linear model (Con) $y_i = [1, x_i']\beta + \sigma \epsilon_i = \beta_0 + x_i'\beta_x + \sigma \epsilon_i$ where β and σ are unknown coefficients to be estimated with $\epsilon_i \stackrel{\text{iid}}{\sim} F_\epsilon(\mu_\epsilon = 0, \sigma_\epsilon^2 = 1)$ which is typically parametric (Con)

The Accelerated Failure Time (AFT) model: part 2

- Consider a *baseline* survival function for a *standard* subject where the covariates are all zero, i.e., $S_0(t) = S(t|x=0)$.
- We can define the survival function for any given subject with a standard subject by accelerating, or decelerating, failure time

$$S(t|x_i) = P[s_i > t|x_i] = P[y_i > \log t|x_i]$$

$$= P[\beta_0 + x_i'\beta_x + \sigma\epsilon_i > \log t|x_i]$$

$$= P[\beta_0 + \sigma\epsilon_i > \log t - x_i'\beta_x|x_i]$$

$$= S_0(t \exp\{-x_i'\beta_x\})$$

• however, AFT is a precarious restrictive assumption (Con) $S(t|x) = P[\log s > \log t] = 1 - F_{\epsilon} (\log t; x'\beta, \sigma^2)$ the covariates can only explain a log-linear location shift

Survival analysis with AFT BART NFT notation

Henderson, Louis et al. 2018 Biostatistics

- $y_i = \mu(x_i) + \epsilon_i$ where $\epsilon_i | \mu_i \sim N(\mu_i, \sigma^2)$: Pro $\mu \stackrel{\text{prior}}{\sim} BART$
- To ensure identifiability, constrain $\frac{1}{N} \sum_{i} \mu_{i} = 0$
- $\mu_i | G \sim G$ $G | \alpha \stackrel{\text{prior}}{\sim} \text{DP} (\alpha, F_0)$
- $S(t,x) = 1 \frac{1}{N} \sum_i \Phi\left(\frac{\log t \mu_i \mu(x)}{\sigma}\right)$ Con: the covariates still only explain a log-linear location shift

Survival analysis with NFT BART

Sparapani et al. 2023 Biometrics

- $y_i = \mu(x_i) + \epsilon_i$ where $\epsilon_i | (\mu_i, \sigma_i) \sim N(\mu_i, \sigma_i^2 \sigma^2(x_i))$: Pro $\mu \stackrel{\text{prior}}{\sim} \text{BART}$ $\sigma^2 \stackrel{\text{prior}}{\sim} \text{HBART}$
- To ensure identifiability: $\frac{1}{N}\sum_i \mu_i = 0$ and $\frac{1}{N}\sum_i \sigma_i^2 = 1$
- if $\delta_i = 1$, then $y_i = \log t_i$ else draw

$$y_i \sim N(\mu_i + \mu(x_i), \ \sigma_i^2 \sigma^2(x_i)) \begin{cases} I(\log t_i, \infty) & \text{if } \delta_i = 0 \\ I(-\infty, \log t_i) & \text{if } \delta_i = 2 \end{cases}$$

- $(\mu_i, \sigma_i)|G \sim G$ $G|\alpha \stackrel{\text{prior}}{\sim} \text{DP}(\alpha, F_0)$
- $S(t,x) = 1 \frac{1}{N} \sum_{i} \Phi\left(\frac{\log t \mu_{i} \mu(x)}{\sigma_{i}\sigma(x)}\right)$ Pro: the covariates can explain a location shift and rescaling!

Dirichlet Process Mixtures (DPM): infinite mixtures

Ferguson 1973 & Antoniak 1974 Annals of Statistics; Escobar & West 1995 JASA; Neal 2000 JCGS DPM-like finite mixture clustering: Miller & Harrison 2017 JASA

$$\begin{aligned} y_i|\theta_i &\sim F(\theta_i) & \text{usual notation} \\ & \text{where } i=1,\dots,N \\ y_i|\theta_{c_i}^* &\sim F(\theta_{c_i}^*) & \text{ephemeral clusters} \\ & \text{where } c_i \in \{1,\dots,k\} & k \text{ is random} \\ \theta_i|G &\sim G & \text{nonparametric (Pro)} \\ G|\alpha \overset{\text{prior}}{\sim} \mathrm{DP}\left(\alpha,\,F_0\right) & G \text{ "centered" on } F_0 \\ & \alpha \overset{\text{prior}}{\sim} \mathrm{Gamma}\left(a,\,b\right) & \text{concentration parameter} \\ & \propto k \\ & \theta_1 &\sim F_0 & \text{integrating over } G \\ & \theta_2|\theta_1 &\sim \frac{1}{1+\alpha}\delta_K(\theta_1) + \frac{\alpha}{1+\alpha}F_0 & \text{mixture} \end{aligned}$$

Constrained DPM

Yang, Dunson & Baird 2010

Computational Statistics & Data Analysis

- How do we constrain $\frac{1}{N} \sum_{i} \mu_{i} = 0$?
- Simply sample $(\tilde{\mu}_i, \tilde{\sigma}_i)|G \sim G$ as usual Let $\tilde{\mu}_0 = \frac{1}{N} \sum_i \tilde{\mu}_i$ And $\mu_i = \tilde{\mu}_i - \tilde{\mu}_0$
- Similarly, if we need to constrain $\frac{1}{N}\sum_i \sigma_i^2 = 1$ Let $\tilde{\sigma}_0 = \sqrt{\frac{1}{N}\sum_i \tilde{\sigma}_i^2}$ And $\sigma_i = \tilde{\sigma}_i/\tilde{\sigma}_0$

Low Information Omnibus (LIO) Dirichlet Process Mixtures prior hierarchy

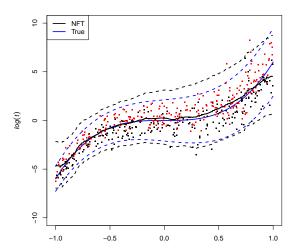
Shi, Martens, Banerjee, Laud 2018 *Bayesian Analysis* Sparapani et al. 2023 *Biometrics*

- With either DPM or Constrained DPM
- For convenience, re-parameterize in terms of $\tau_i = \sigma_i^{-2}$ $F_0(\mu_0, k_0, a_0, b_0)$ is a Normal-Gamma prior $[\mu_i, \tau_i | k_0, b_0] = [\tau_i | b_0] [\mu_i | \tau_i, k_0]$ with $\mu_i | \tau_i, k_0$ $\stackrel{\text{prior}}{\sim} \text{N}(\mu_0, (\tau_i k_0)^{-1})$ and $\tau_i | b_0 \stackrel{\text{prior}}{\sim} \text{Gamma}(a_0, b_0)$
- NFT LIO prior parameter settings $\mu_0 = 0$, $k_0 \stackrel{\text{prior}}{\sim} \text{Gamma} (1.5, 7.5)$ $a_0 = 3$, $b_0 \stackrel{\text{prior}}{\sim} \text{Gamma} (2, 1)$

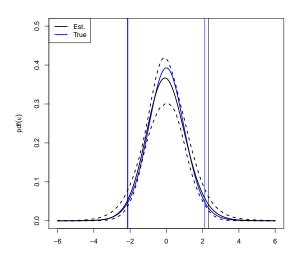
NFT model: prediction intervals

- $\log t_i = y_i = \mu(x_i) + \epsilon_i$ where $\epsilon_i \sim \mathrm{N}\left(\mu_i, \ \sigma_i^2 \sigma^2(x_i)\right)$ To ensure identifiability: $\frac{1}{N} \sum_i \mu_i = 0$ and $\frac{1}{N} \sum_i \sigma_i^2 = 1$
- $F_{\epsilon} = \frac{1}{N} \sum_{i} N(\mu_{i}, \sigma_{i}^{2})$: nonparametric mixture of Normals
- $(1-\alpha) \times 100\%$ Prediction Interval $(\mu(x) + \frac{c_{\alpha/2}\sigma(x)}{\sigma(x)}, \ \mu(x) + \frac{c_{1-\alpha/2}\sigma(x)}{\sigma(x)})$ where $\frac{c_{\pi}}{\sigma(x)} = \frac{c_{\pi}}{\epsilon}$

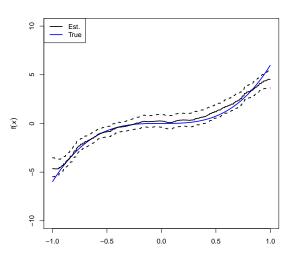
$$\begin{split} f(x) &= 6x^3, \ s(x) = \exp 0.5x, \\ \log t &= f(x) + s(x)\epsilon \text{ where } \epsilon \sim t(16) \\ \text{and } x \sim \text{U}(-1,1): \ R^2 = 84.8\% \text{ uncensored, } R^2 = 85.1\% \text{ censored} \end{split}$$



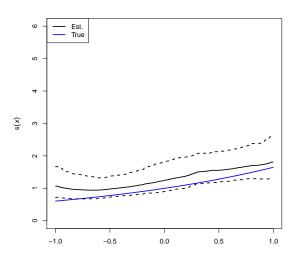
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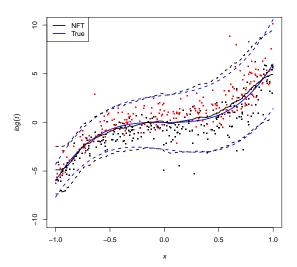


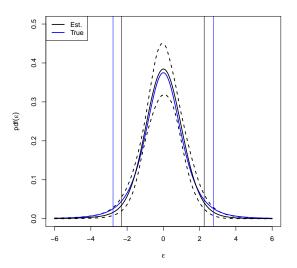
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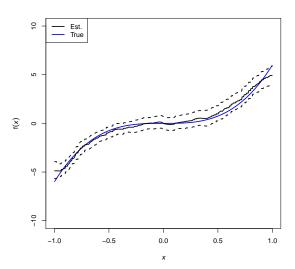


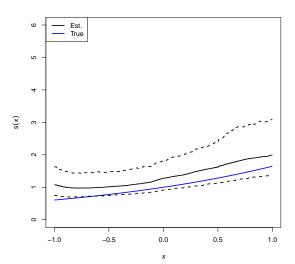
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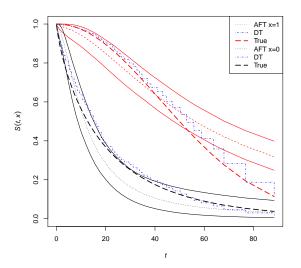






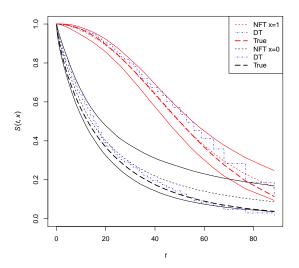
Neither AFT nor NFT scenario: AFT failure!

N = 500 with 50% censoring Wei (0.8 + 1.2x, 20 + 40x) where $x \sim B(0.5)$



Neither AFT nor NFT scenario: NFT success!

N = 500 with 50% censoring Wei (0.8 + 1.2x, 20 + 40x) where $x \sim B(0.5)$



NFT BART posterior inference: the survival and distribution functions

$$\begin{split} S_m(t|x) &= 1 - F_m(t|x) \\ F_m(t|x) &= \int \mathbf{\Phi} \left\{ \frac{\log t - \mu_* - \mu_m(x)}{\sigma_* \sigma_m(x)} \right\} G_m(\mathrm{d}\mu_*, \mathrm{d}\sigma_*) \\ &= \sum_{j=1}^\infty \omega_j \mathbf{\Phi} \left\{ \frac{\log t - \mu_j^* - \mu_m(x)}{\sigma_j^* \sigma_m(x)} \right\} \\ &\approx \sum_{j=1}^{K_m} \omega_{jm} \mathbf{\Phi} \left\{ \frac{\log t - \mu_{jm}^* - \mu_m(x)}{\sigma_{jm}^* \sigma_m(x)} \right\} \\ &\text{where } (\mu_{jm}^*, \sigma_{jm}^*) \text{ are from the training set} \end{split}$$

NFT BART posterior inference: the survival function

$$\widehat{S}(t|x) = M^{-1} \sum_m S_m(t|x)$$

 $1-2\pi$ level credible intervals from π and $1-\pi$ quantiles $(\widehat{S}_{\pi}(t|x),\widehat{S}_{1-\pi}(t|x))$ such that $\widehat{S}_{p}(t|x)=S_{m_{p}}(t|x)$ where m_{p} corresponds to the $p=\pi$ or $p=1-\pi$

NFT BART posterior inference: the hazard and density functions

$$\begin{split} h_m(t|x) &= f_m(t|x)/S_m(t|x) \\ f_m(t|x) &= \int \frac{\phi\left\{\frac{\log t - \mu_* - \mu_m(x)}{\sigma_*\sigma_m(x)}\right\}}{t\sigma_*\sigma_m(x)} G_m(\mathrm{d}\mu_*, \mathrm{d}\sigma_*) \\ &= \sum_{j=1}^{\infty} \frac{\omega_j \phi\left\{\frac{\log t - \mu_j^* - \mu_m(x)}{\sigma_j^*\sigma_m(x)}\right\}}{t\sigma_j^*\sigma_m(x)} \\ &\approx \sum_{j=1}^{K_m} \frac{\omega_{jm} \phi\left\{\frac{\log t - \mu_{jm}^* - \mu_m(x)}{\sigma_{jm}^*\sigma_m(x)}\right\}}{t\sigma_{jm}^*\sigma_m(x)} \\ &\approx \sum_{j=1}^{K_m} \frac{\omega_{jm} \phi\left\{\frac{\log t - \mu_j^* - \mu_m(x)}{\sigma_{jm}^*\sigma_m(x)}\right\}}{t\sigma_{jm}^*\sigma_m(x)} \\ &\text{where } (\mu_{jm}^*, \sigma_{jm}^*) \text{ are from the training set} \end{split}$$

NFT BART posterior inference: marginal effects by Friedman's partial dependence function

Friedman 2001 Annals of Statistics

- ullet The covariates of interest are fixed at settings of interest: a single setting denoted x_A
- The complement take on the observed values found in the training data set denoted x_{iB} for subject i
- So the setting for all covariates denoted as (x_A, x_{iB})

$$F_{Am}(t|x_A) = N^{-1} \sum_i \Phi\left(\frac{\log t - \mu_{im} - \mu_m(x_A, x_{iB})}{\sigma_{im}\sigma_m(x_A, x_{iB})}\right)$$

where (μ_{im}, σ_{im}) are from the training set

$$\widehat{S}_A(t|x_A) = 1 - M^{-1} \sum_m F_{Am}(t|x_A)$$

- Nonparametric estimates of RMST are an alternative measure that may be more interpretable than survival probabilities Royston & Parmar 2013 BMC Medical Research Methodology
- The mean survival time is an infinite integral: $\int_0^\infty S(t|x) dt$
- This is impractical, i.e., the observation period cannot possibly be lengthened until every participant passes away
- Rather, let's limit the observation period to, τ , a clinically meaningful follow-up period: $\text{RMST}(\tau) = \int_0^{\tau} S(t|x) dt$
- Consider a log-Normal time-to-event, e^y , where $y \sim N(\mu, \sigma^2)$

$$\mathbb{E}\left[\mathrm{e}^{y} \middle| y < \log(\tau)\right] = \mathrm{e}^{\mu + \sigma^2/2} \Phi\left(\frac{\log(\tau) - (\mu + \sigma^2)}{\sigma}\right)$$

- To extend this concept to NFT BART, we develop RMST for a mixture of log-Normals: $\log t = y^* \sim \sum_i \omega_i \phi(\mu_i, \sigma_i^2)$
- The probability that $\log(t)$ falls within the observation period

Derive the RMST as an expectation of random variable $\min(t, \tau)$

$$\begin{aligned} \text{RMST}(\tau) &= \text{E}\left[\min(t,\tau)\right] \\ &= \text{E}\left[\text{e}^{y^*}|y^* < \log(\tau)\right] + q\tau \\ &\quad \text{where } q = 1 - p \end{aligned}$$

This result can be decomposed into its atoms: $y_j \sim N(\mu_j, \sigma_j^2)$

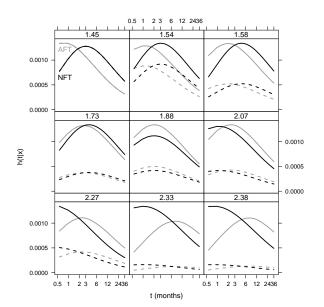
$$\mathrm{E}\left[\mathrm{e}^{y^*}|y^*<\log(\tau)\right]=\sum_j\omega_j\mathrm{E}\left[\mathrm{e}^{y_j}|y_j<\log(\tau)\right]$$

$$E\left[e^{y_j}|y_j < \log(\tau)\right] = \pi_j e^{\mu_j + \sigma_j^2/2} \text{ where } \pi_j = \Phi\left(\frac{\log(\tau) - (\mu_j + \sigma_j^2)}{\sigma_j}\right)$$

$$\mathbb{E}\left[\mathrm{e}^{y^*}|y^* < \log(\tau)\right] = \sum_j \omega_j \pi_j \mathrm{e}^{\mu_j + \sigma_j^2/2}$$

- So, finally: RMST(au) = $q au + \sum_j \omega_j \pi_j \mathrm{e}^{\mu_j + \sigma_j^2/2}$
- It is a simple extension to NFT BART like so $E[RMST(\tau|x_i,y)] \approx M^{-1} \sum_m RMST_m(\tau|x_i,y).$
- And we can quantify uncertainty with posterior quantiles

Real data example: AFT BART vs. NFT BART %-iles of $\widehat{\sigma}(x_i)$: 1, 5, 10, 30, 50, 70, 90, 95, 99



Thompson Sampling Variable Selection (TSVS)

Liu & Rockova 2023 JASA

Set *H small*: 10, 20 or 40; smaller numbers engender more sparsity

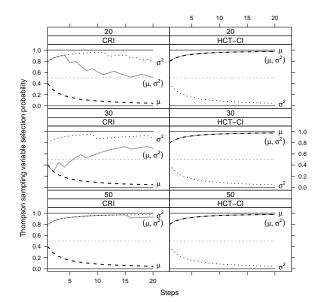
$$(\widetilde{H} \approx H/5)$$
. TSVS is an iterative process: $k = 1, ..., K$

Pseudo-Bayesian prior parameter defaults: a_{j0} = 1 and b_{j0} = 0.5

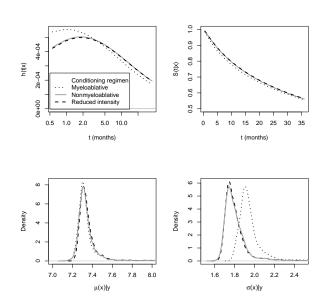
- a. For $j = 1, \ldots, P$: draw $\eta_{jk} \sim \text{Beta}(a_{j,k-1}, b_{j,k-1})$
- b. Set $B_k = \{j : \eta_{jk} \ge 0.5\}$: covariate subset selected at step k
- c. Fit an NFT BART model with covariates x_{ij} where $j \in B_k$
- d. For j = 1, ..., P: do each sub-step
 - (i) Reward: if $j \notin B_k$, then $\gamma_{jk} = 0$, else $\gamma_{jk} = I(u_{jkM} + v_{jkM} > 0)$ where u_{jkM} and v_{jkM} are the number of branches for variable $x_{.j}$ in step k from μ and σ^2 , respectively, at posterior draw M
 - (ii) Update via the reward: $a_{jk} = a_{j,k-1} + \gamma_{jk}$ and $b_{jk} = b_{j,k-1} + 1 \gamma_{jk}$
 - (iii) Calculate inclusion probabilities: $\pi_{jk} = \frac{a_{jk}}{a_{jk} + b_{jk}}$
- e. If k < K, then return to a. and increment k

Important variables have trajectories of π_{ik} exceeding 0.5 by K

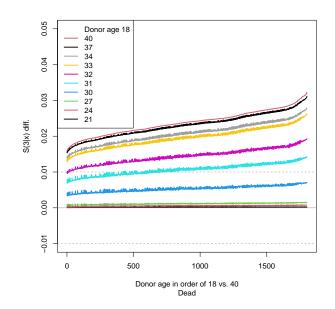
Real data example: TSVS with H=20,30,50Conditioning regimen (CRI) and Comorbidity (HCT-CI)



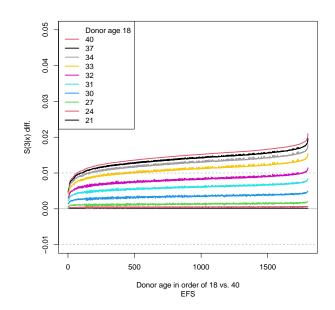
Real data example: Heteroskedasticity of the Conditioning Regimen Intensity (CRI)



Real data example: Death and donor age



Real data example: EFS and donor age



Conclusions: part 1

- We constructed our new Nonparametric Failure Time (NFT) approach from robust Bayesian Nonparametric building blocks
 - Bayesian Additive Regression Trees (BART) and Heteroskedastic BART (HBART)
 - Constrained Dirichlet Process Mixtures (DPM)
 with the Low Information Omnibus (LIO) prior hierarchy
- along with the **nftbart** v2.1 R package available on the Comprehensive R Archive Network (CRAN)

Conclusions: part 2

- NFT has desirable properties
 - computationally friendly via MCMC
 - very flexible model which does not resort to precarious restrictive assumptions
 - default prior parameter settings that work well without computationally expensive cross-validation
 - natural extensions to variable selection via Thompson Sampling and marginal effects by Friedman's partial dependence function
- Personalized Hematopoietic Stem Cell Transplant (HSCT)
 - For Event-free Survival of HSCT recipients younger male donors likely result in better outcomes