Heteroskedastic BART and time-to-event outcomes

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Heteroskedastic BART (HBART)

Pratola, Chipman, George & McCulloch 2020 *JCGS*

$$y_i = f(x_i) + s(x_i)\epsilon_i \qquad \epsilon_i \overset{\text{iid}}{\sim} \mathrm{N}(0,\ \sigma^2)$$

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

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

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

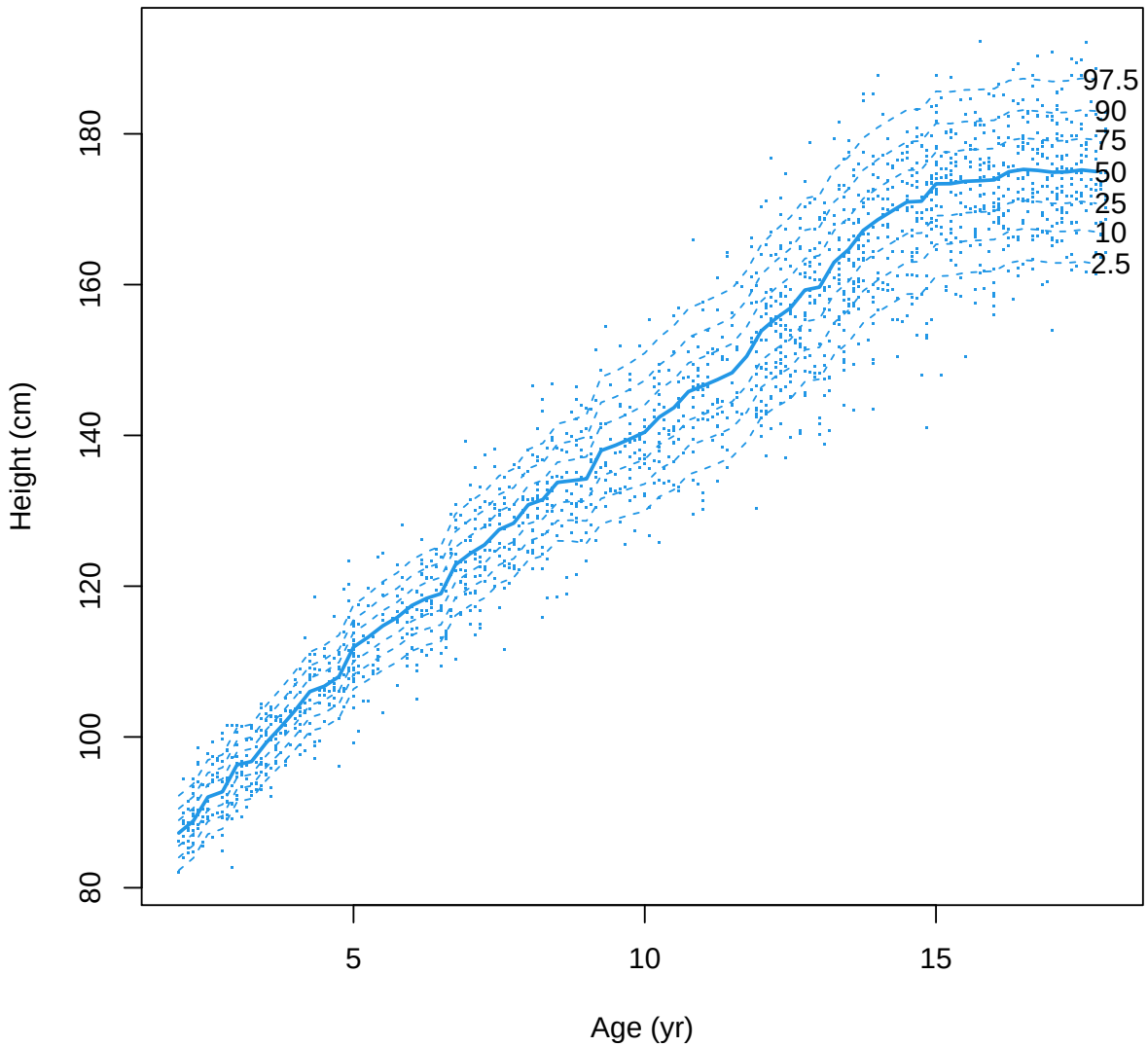
$$\sigma^2_{hl} | \widetilde{\mathcal{T}}_h \overset{\text{prior}}{\sim} \lambda\nu\chi^{-2}(\nu) \text{ leaves of } \widetilde{\mathcal{T}}_h \qquad \lambda = \tilde{\lambda}^{1/\widetilde{H}}$$

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

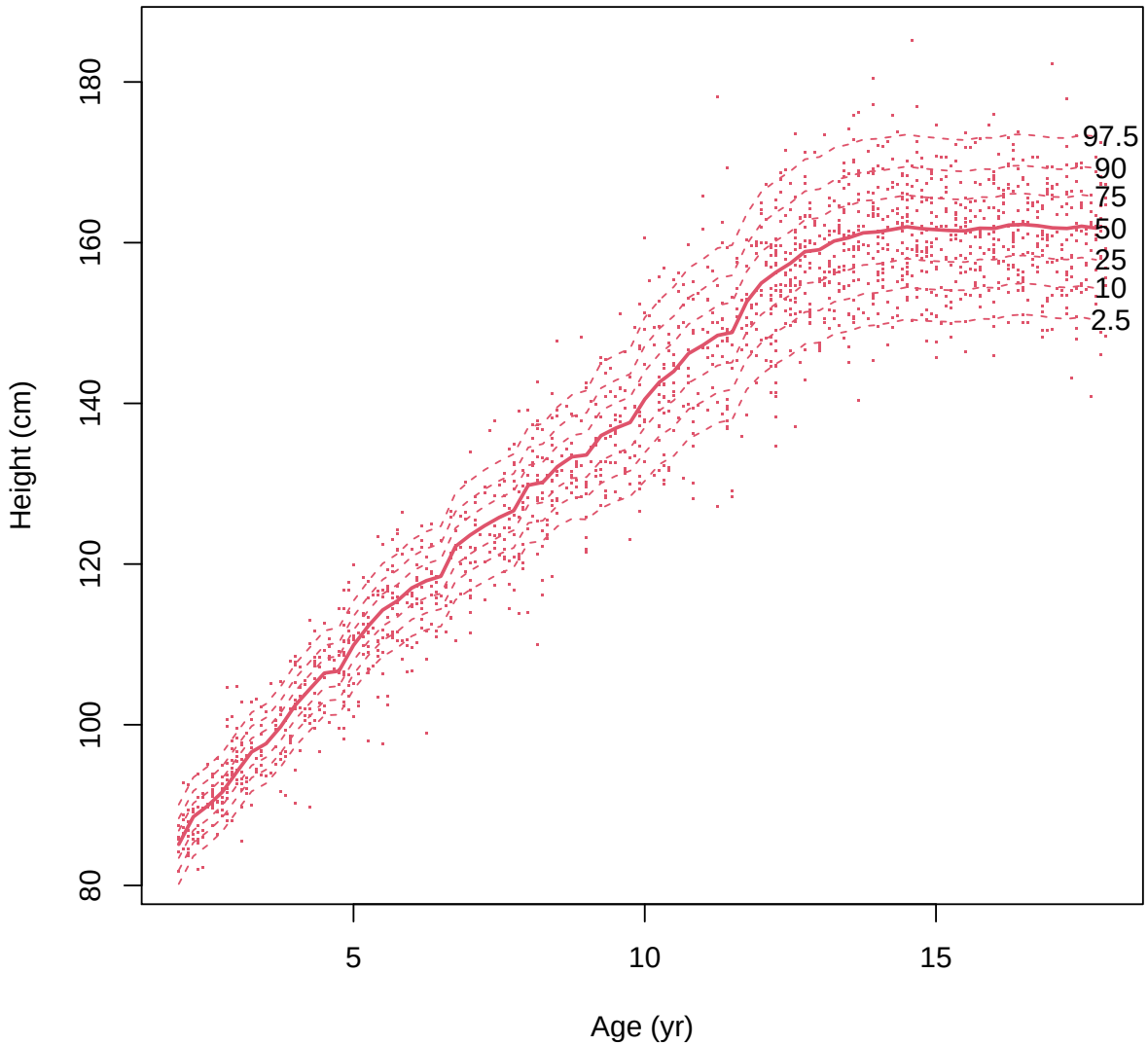
$$\in \widetilde{\mathcal{M}}_h \qquad \nu = 2\left[1 - \left(1 - \frac{2}{\tilde{\nu}}\right)^{1/\widetilde{H}}\right]^{-1}$$

Marginal effect of age: HBART predictions for M

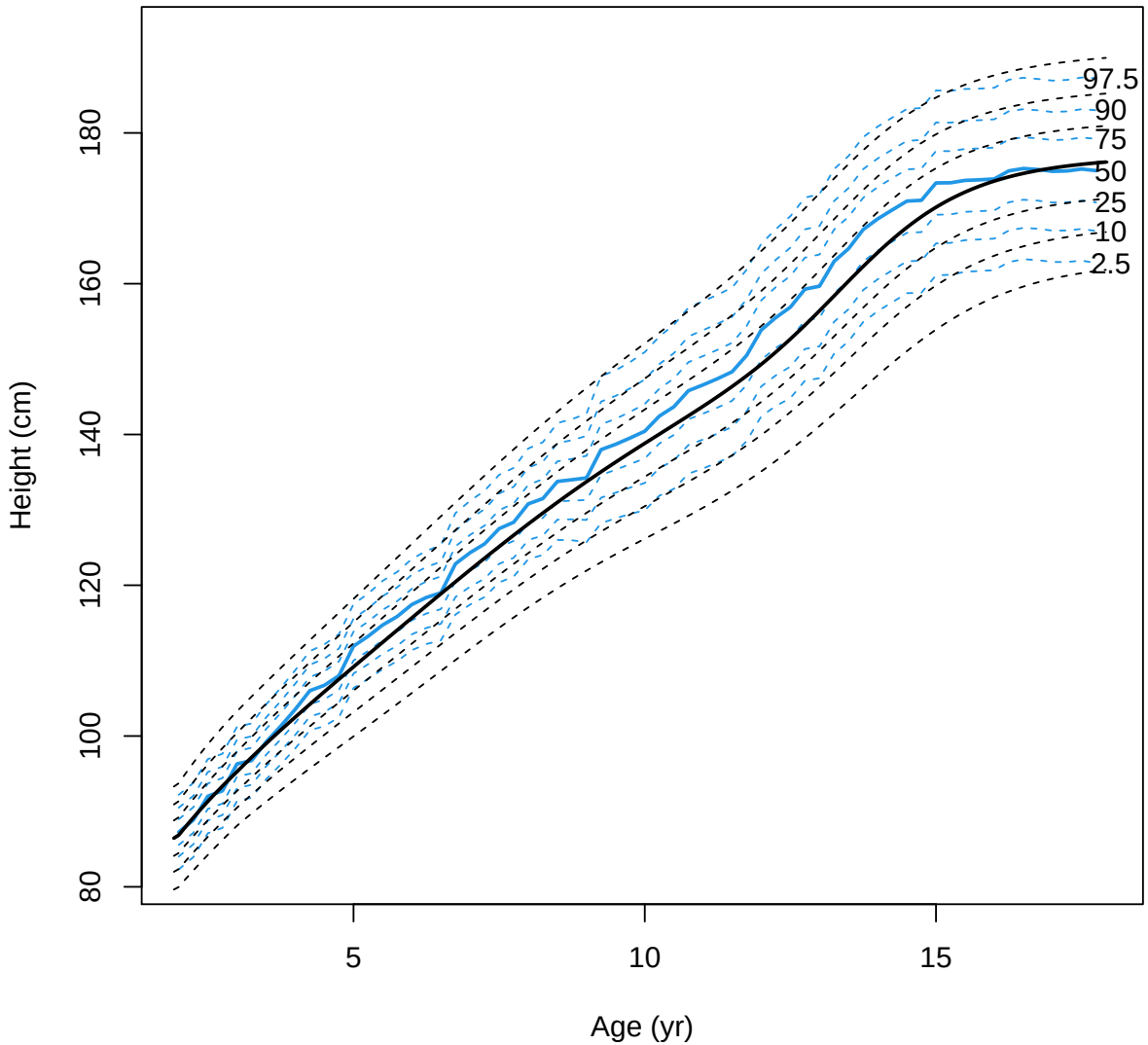
$$H = 300, \widetilde{H} = 60, \texttt{numcut} = 200$$



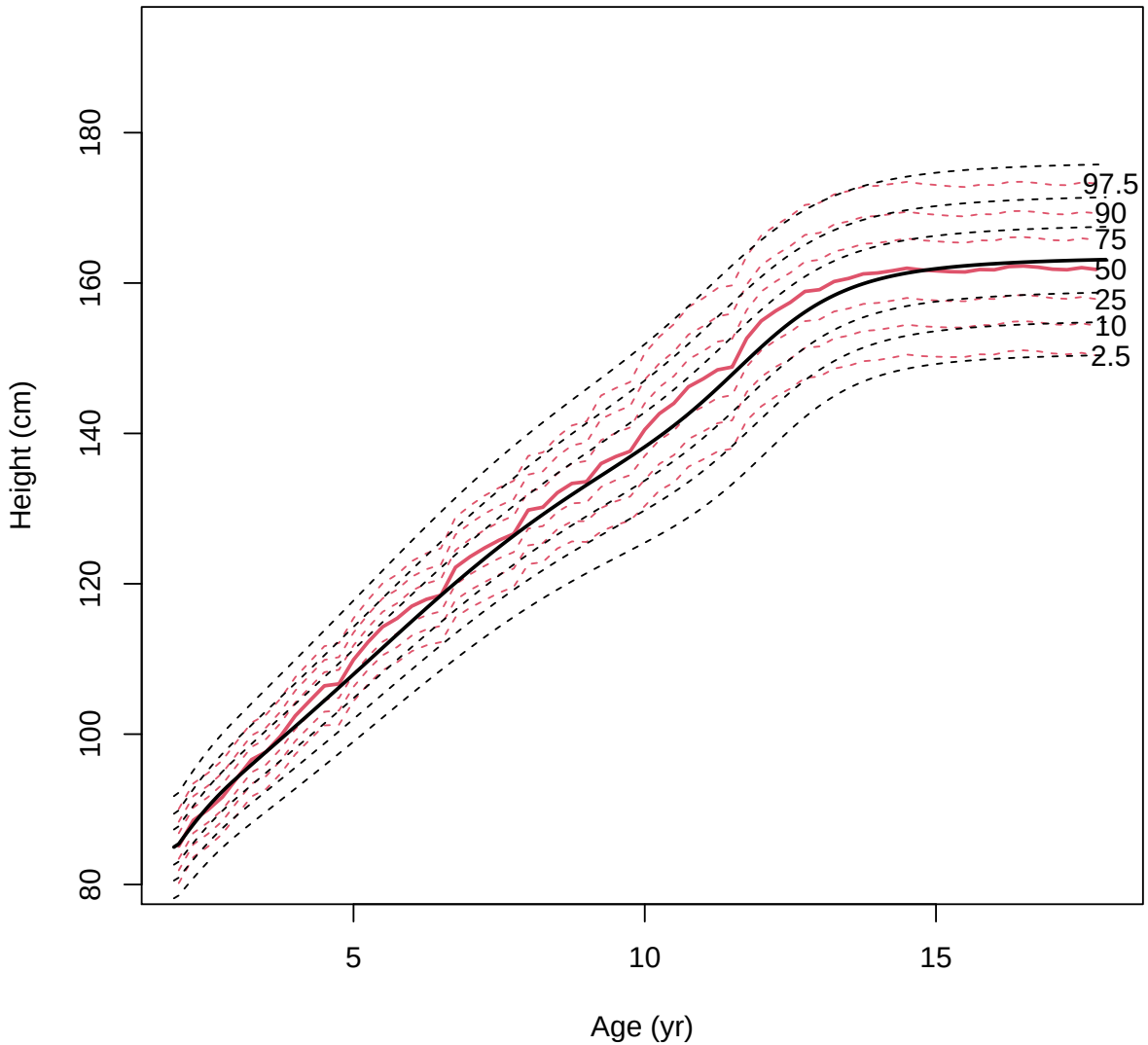
Marginal effect of age: HBART predictions for F



Marginal effect of age: HBART vs. CDC for M



Marginal effect of age: HBART vs. CDC for F



Outline

- Motivation: a clinical application in Personalized Hematopoietic Stem Cell Transplant (HSCT) requires a new time-to-event BART methodology that scales better
- Pros and Cons of BART survival analysis methods
- BART and Heteroskedastic BART (HBART)
- Accelerated Failure Time (AFT) and AFT BART
- Nonparametric Failure Time (NFT) BART
- Dirichlet Process Mixtures (DPM), Constrained DPM and the Low Information Omnibus (LIO) DPM prior hierarchy
- Simulated data sets and methodology comparisons
- **nftbart** v2.1 R package on CRAN

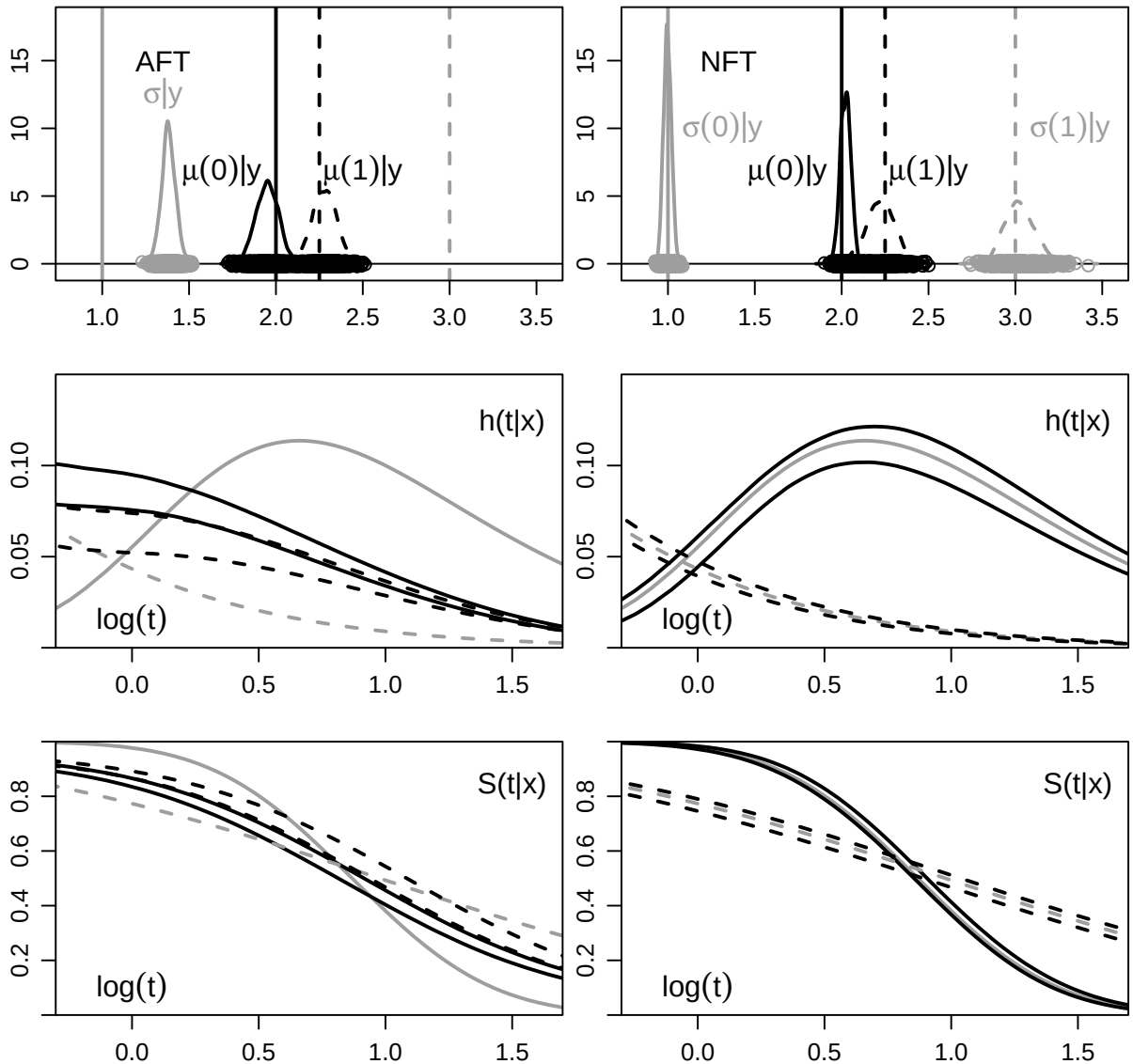
Personalized Hematopoietic Stem Cell Transplant (HSCT)

- 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 $\boldsymbol{P = 45}$ covariates that may have an impact
- $\mathbf{5}$ 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 $\mathbf{10016}$ for training and $\mathbf{1802}$ 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				
Property	Hier-archical	Discrete Time	AFT	Mod-ulated	NFT
Flexible assumptions	Con	Pro	Con	Pro	Pro
Non-parametric	Con	Pro	Pro	Pro	Pro
Left-censoring	Con	Con	Pro	Con	Pro
Time-dep. covariates	Con	Pro	Con	Pro	Con
Friendly to compute	Pro	Con	Pro	Con	Pro
First-author Year	Bonato 2011	Sparapani 2016	Henderson 2018	Linero 2021	Sparapani 2023

Two groups: AFT BART vs. NFT BART



Bayesian Additive Regression Trees (BART)
NFT notation

Sparapani, Logan, Laud & McCulloch 2023 *Biometrics*

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

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

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

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

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

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

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

Heteroskedastic BART (HBART)
NFT notation

Pratola, Chipman, George & McCulloch 2019 *JCGS*

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

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

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

$$\sigma^2(x_i) \equiv \prod_{h=1}^{\widetilde{H}} g(x_i; \widetilde{\mathcal{T}}_h, \widetilde{\mathcal{M}}_h) \text{ where } \widetilde{H} \approx H/5$$

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

$$\sigma^2_{hl} | \widetilde{\mathcal{T}}_h \overset{\text{prior}}{\sim} \lambda\nu\chi^{-2}(\nu) \text{ leaves of } \widetilde{\mathcal{T}}_h$$

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

The Accelerated Failure Time (AFT) model: part 1

- Time-to-event data notation: (t_i, δ_i) $i = 1, \ldots, N$ 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 $\epsilon_i \overset{\text{iid}}{\sim} F_\epsilon(\mu_\epsilon = 0, \sigma_\epsilon^2 = 1)$
  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

$$\begin{aligned} S(t|x_i) =& \mathrm{P}[s_i > t|x_i] = \mathrm{P}[y_i > \log t|x_i] \\ =& \mathrm{P}\left[\beta_0 + x_i'\beta_x + \sigma\epsilon_i > \log t|x_i\right] \\ =& \mathrm{P}\left[\beta_0 + \sigma\epsilon_i > \log t - x_i'\beta_x|x_i\right] \\ =& S_0(t\exp\{-x_i'\beta_x\}) \end{aligned}$$

- however, AFT is a precarious restrictive assumption (Con)
  $S(t|x) = \mathrm{P}[\log s > \log t] = 1 - F_\epsilon\left(\log t; x'\beta, \sigma^2\right)$
  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 $\epsilon_i | \mu_i \sim \mathrm{N}\left(\mu_i,\ \sigma^2\right)$: Pro
  $\mu \overset{\text{prior}}{\sim}$ **BART**
- To ensure identifiability, constrain $\frac{1}{N}\sum_i \mu_i = 0$
- $\mu_i | G \sim G$
  $G | \alpha \overset{\text{prior}}{\sim} \mathrm{DP}\left(\alpha,\ F_0\right)$
- $S(t,x) = 1 - \frac{1}{N}\sum_i \Phi\left(\frac{\log t - \mu_i - \mu(x)}{\sigma}\right)$
  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 $\epsilon_i | (\mu_i, \sigma_i) \sim \mathrm{N}\left(\mu_i,\ \sigma_i^2 \sigma^2(x_i)\right)$: Pro
  $\mu \overset{\text{prior}}{\sim} \mathbf{BART}$
  $\sigma^2 \overset{\text{prior}}{\sim} \mathbf{HBART}$
- 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

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

- $(\mu_i, \sigma_i) | G \sim G$
  $G | \alpha \overset{\text{prior}}{\sim} \mathrm{DP}\left(\alpha,\ F_0\right)$
- $S(t, x) = 1 - \frac{1}{N}\sum_i \Phi\left(\frac{\log t - \mu_i - \mu(x)}{\sigma_i \sigma(x)}\right)$
  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*

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

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 $\mu_i | \tau_i, k_0 \overset{\text{prior}}{\sim} \mathrm{N}\left(\mu_0,\ (\tau_i k_0)^{-1}\right)$
  and $\tau_i | b_0 \overset{\text{prior}}{\sim} \mathbf{Gamma}\,(a_0,\ b_0)$
- NFT LIO prior parameter settings
  $\mu_0 = 0,\ k_0 \overset{\text{prior}}{\sim} \mathbf{Gamma}\,(1.5,\ 7.5)$
  $a_0 = 3,\ b_0 \overset{\text{prior}}{\sim} \mathbf{Gamma}\,(2,\ 1)$

NFT model: prediction intervals

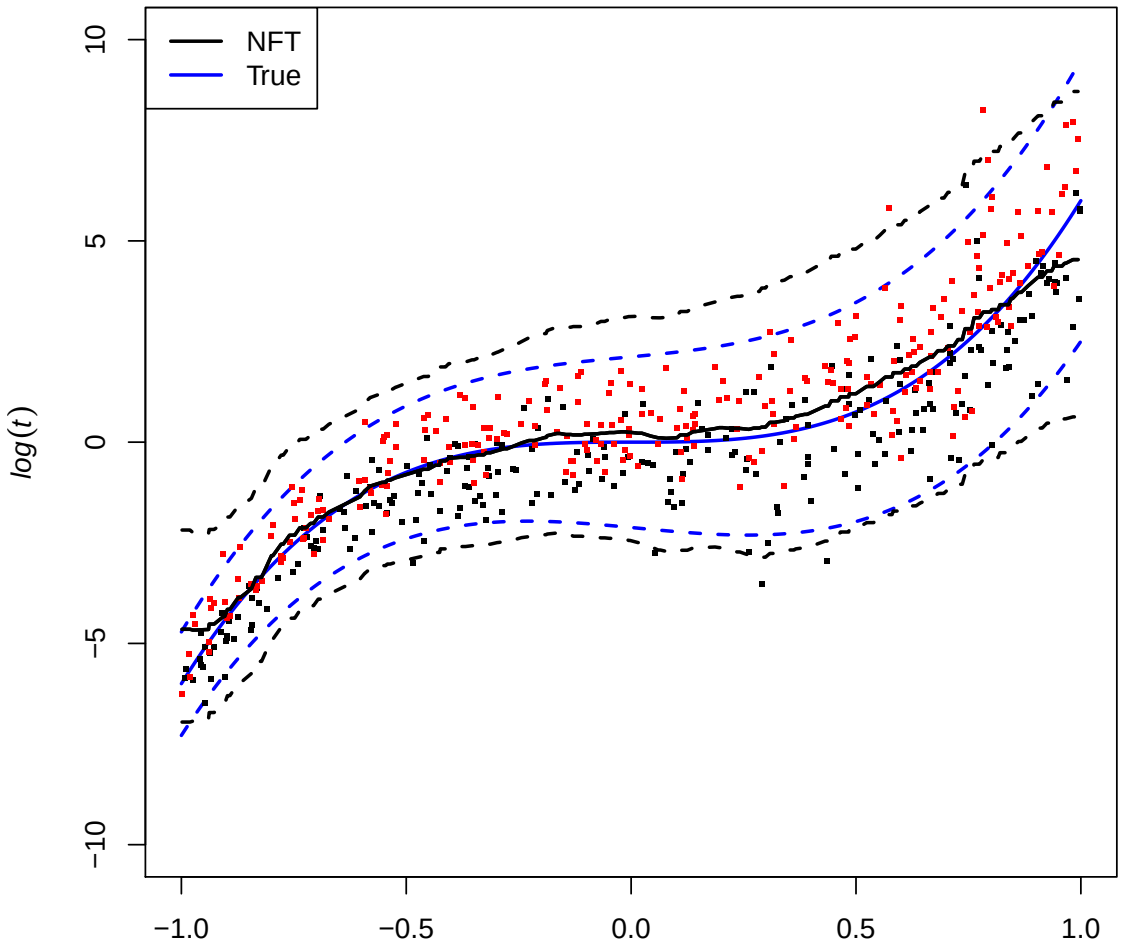
- $\log t_i = y_i = \mu(x_i) + \epsilon_i$ where $\epsilon_i \sim \mathrm{N}\left(\mu_i,\ \sigma_i^2\sigma^2(x_i)\right)$
  To ensure identifiability: $\frac{1}{N}\sum_i \mu_i = 0$ and $\frac{1}{N}\sum_i \sigma_i^2 = 1$
- $F_\epsilon = \frac{1}{N}\sum_i \mathrm{N}\left(\mu_i,\ \sigma_i^2\right)$: nonparametric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

NFT scenario $t(16)$: $N = 500$ with 50% censoring

$f(x) = 6x^3$, $s(x) = \exp 0.5x$,

$\log t = f(x) + s(x)\epsilon$ where $\epsilon \sim t(16)$

and $x \sim \mathrm{U}(-1, 1)$: $R^2 = 84.8\%$ uncensored, $R^2 = 85.1\%$ censored



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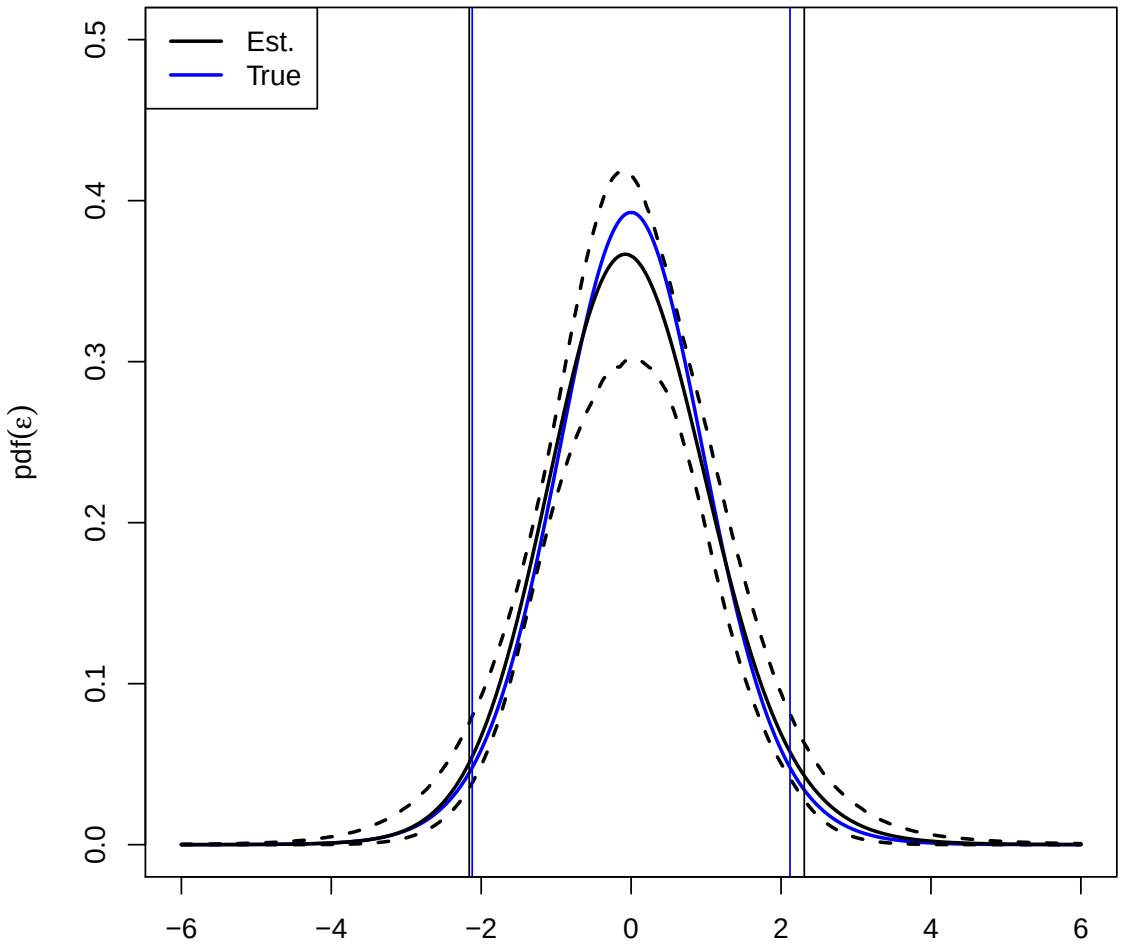

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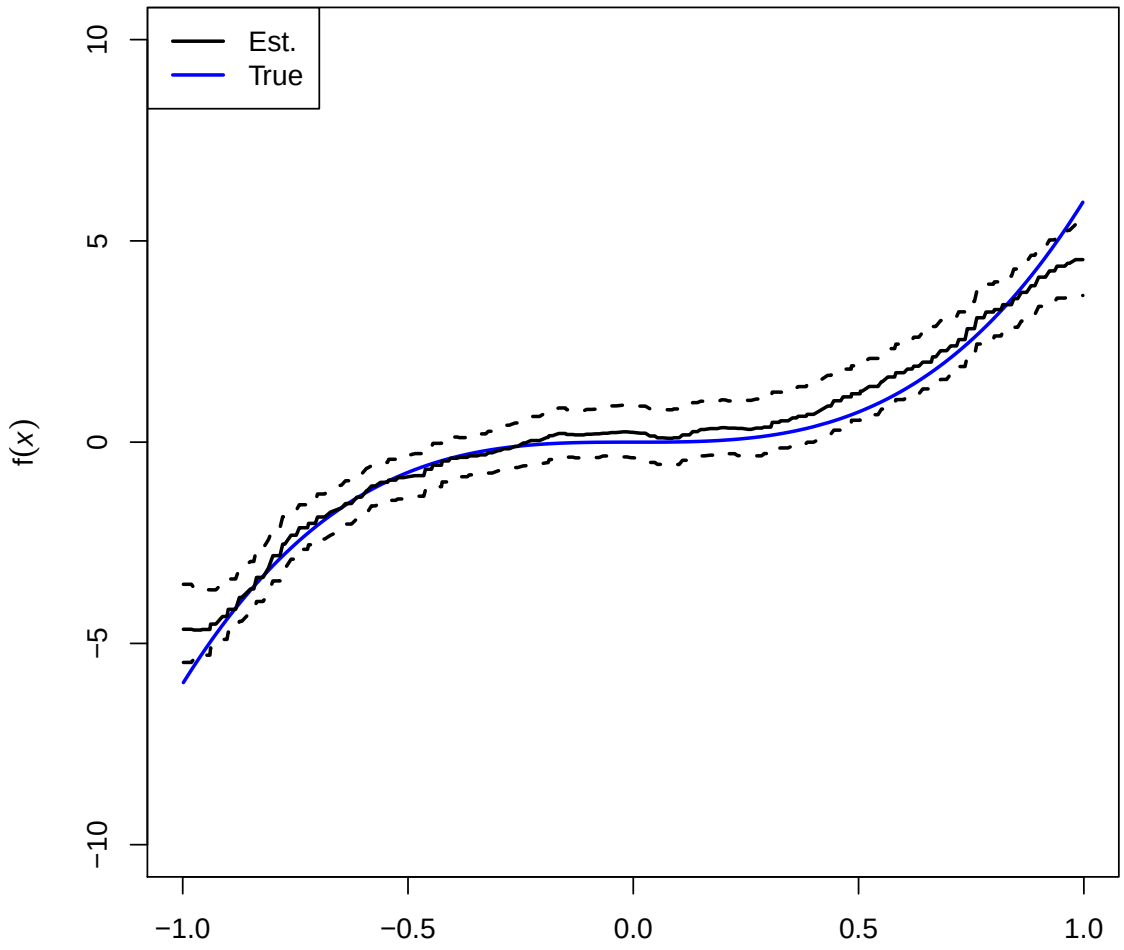

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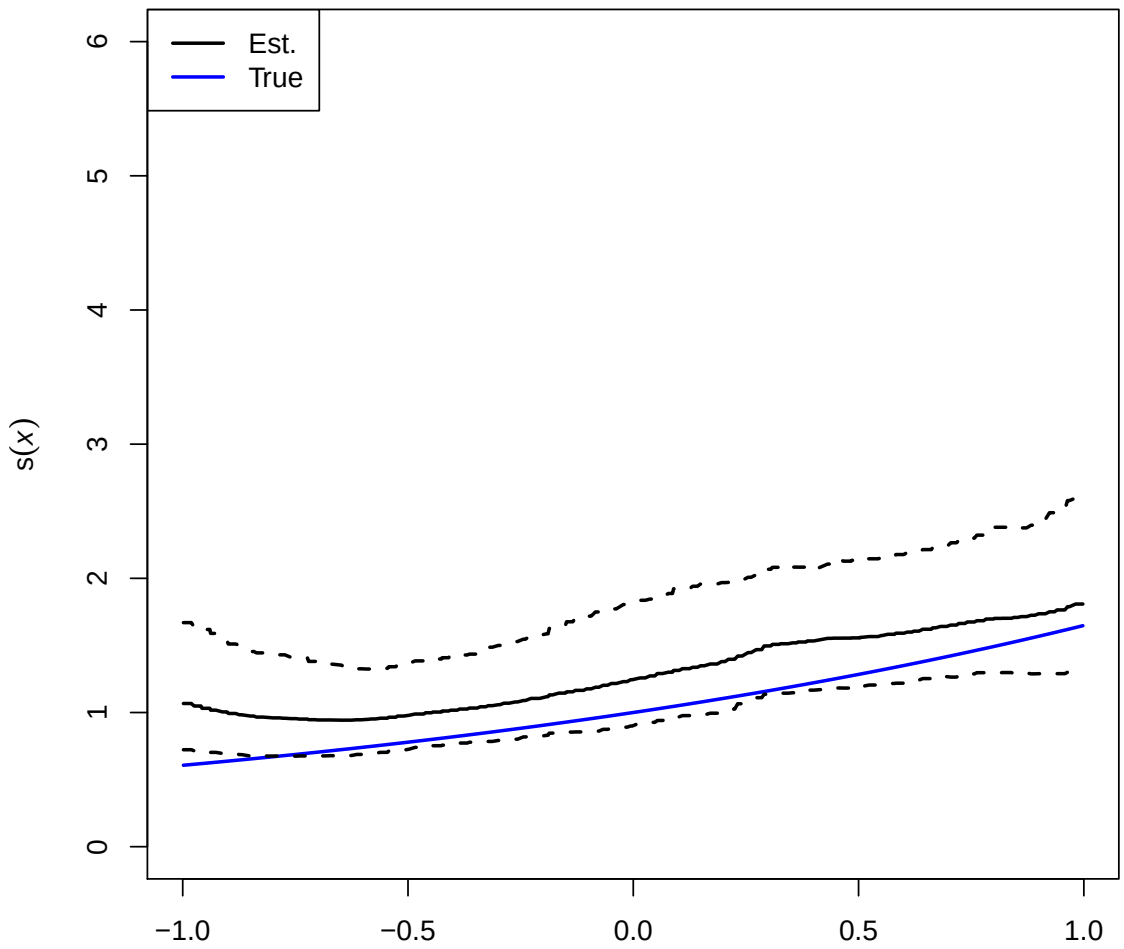
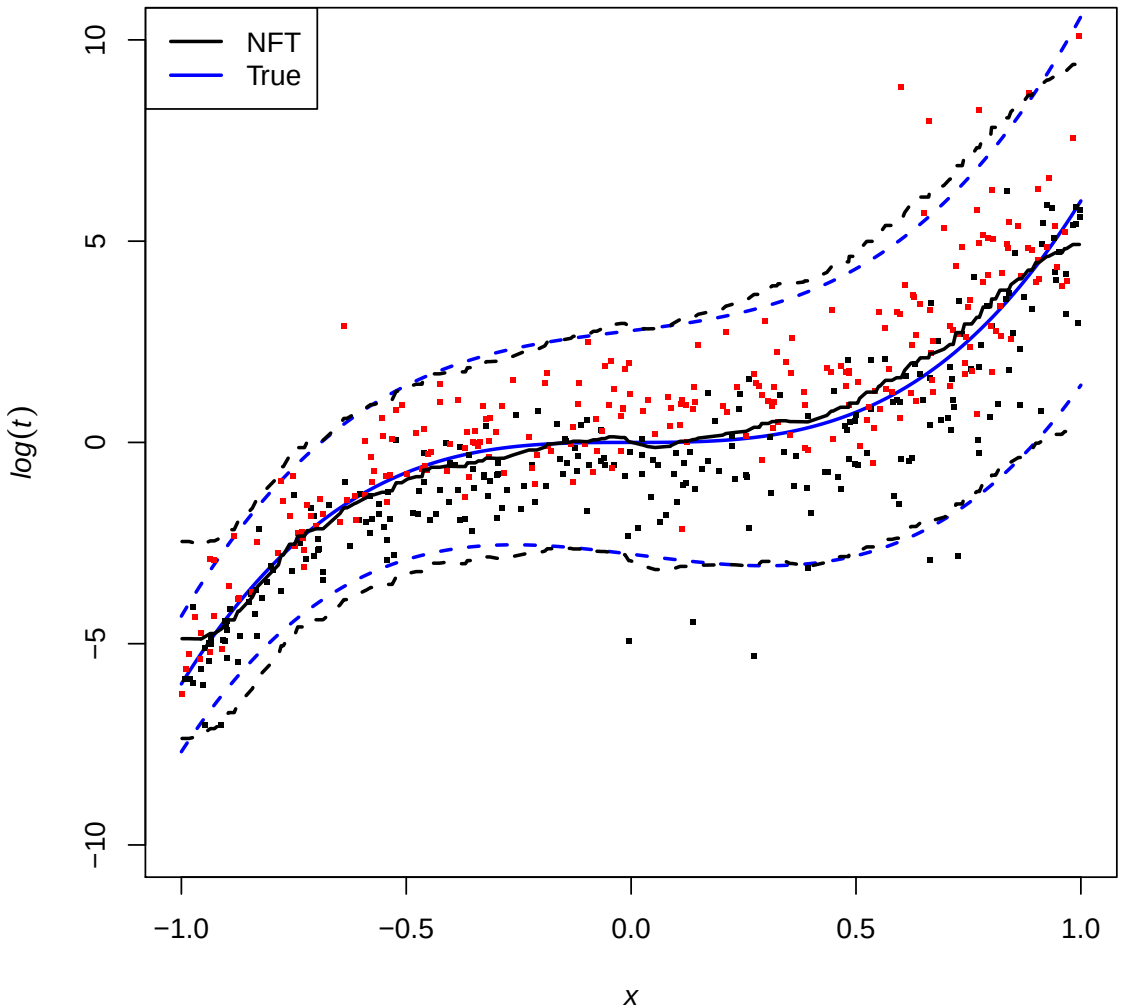


NFT scenario $t(4)$: $N = 500$ with 50% censoring

$f(x) = 6x^3$, $s(x) = \exp 0.5x$, $\log t = f(x) + s(x)\epsilon$ where $\epsilon \sim t(4)$ and $x \sim \mathrm{U}(-1, 1)$: $R^2 = 80.7\%$ uncensored, $R^2 = 78.3\%$ censored



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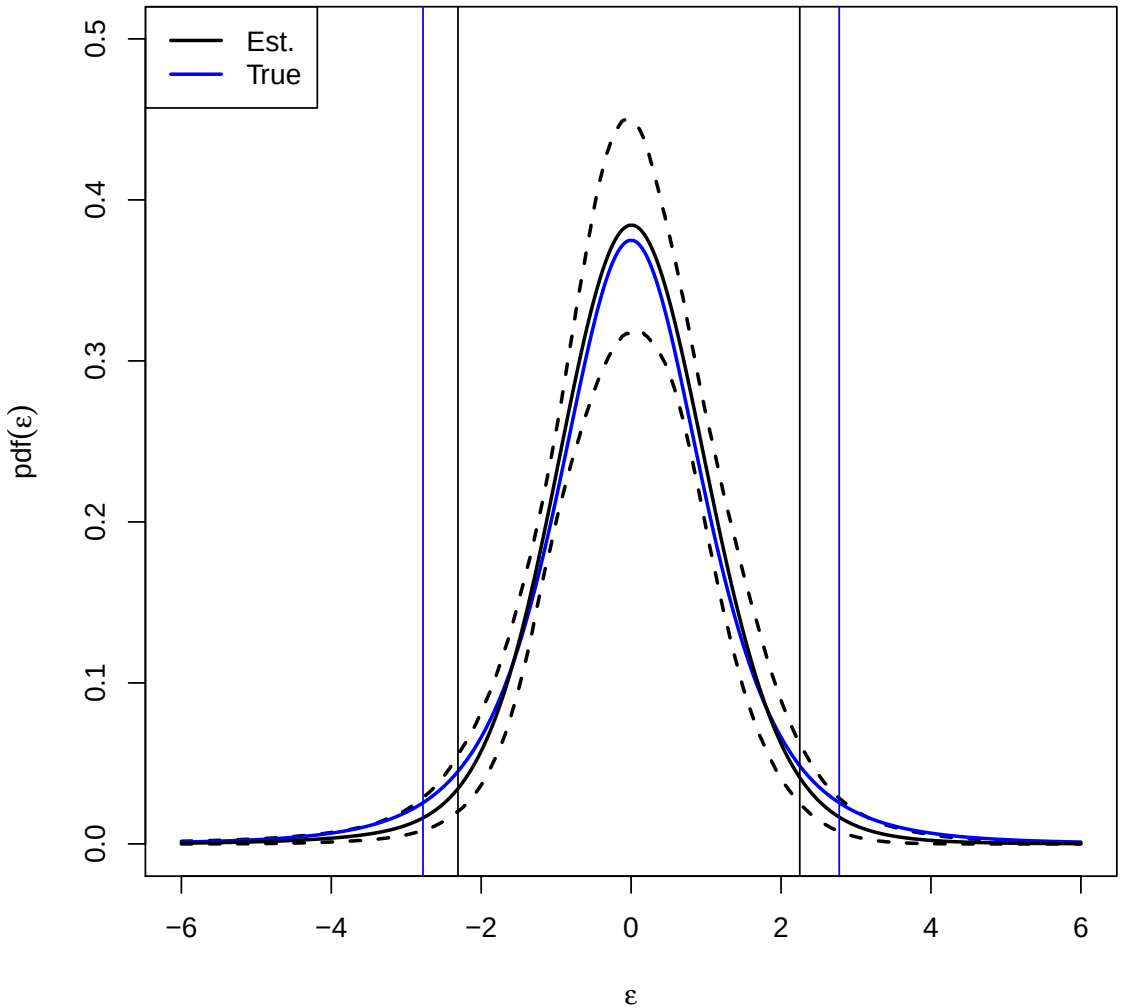

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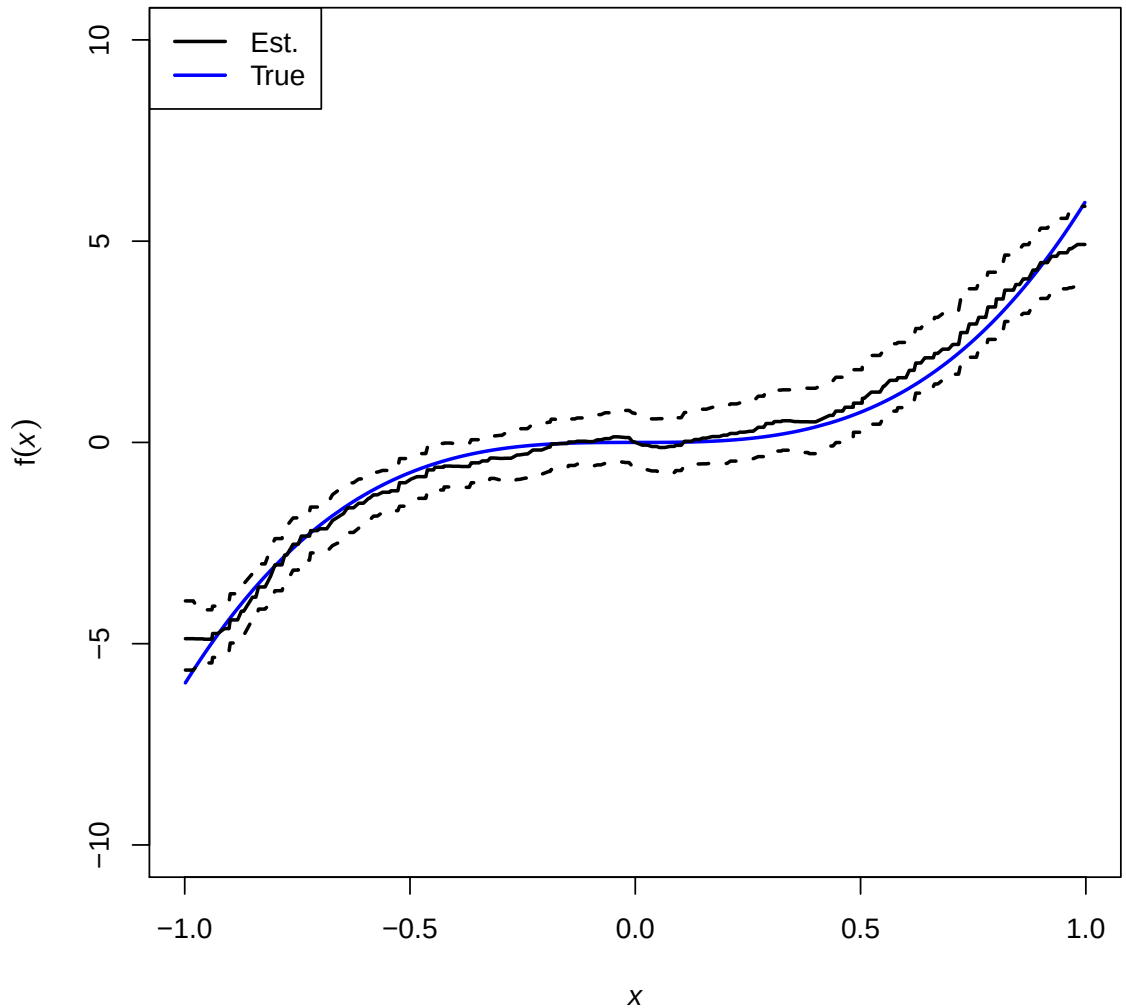

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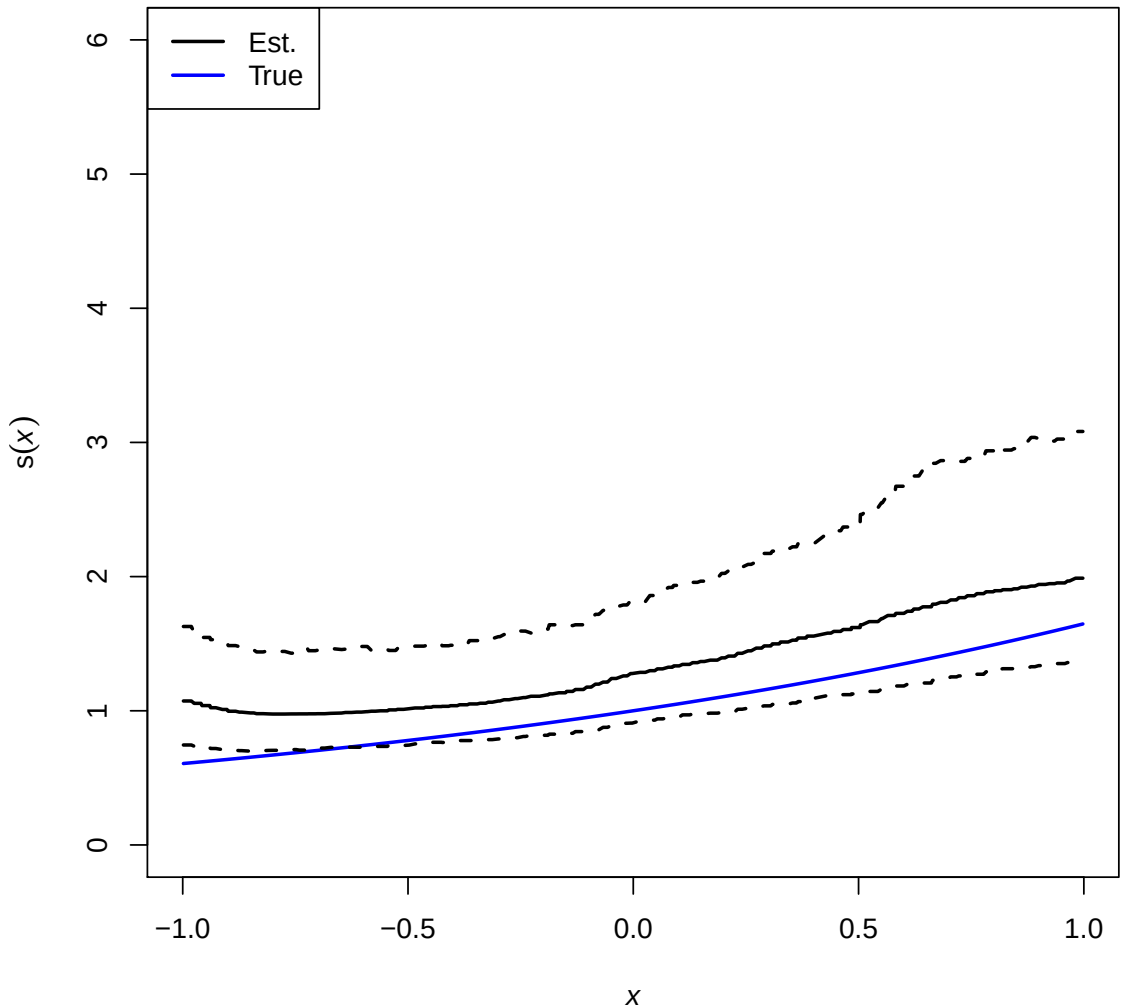
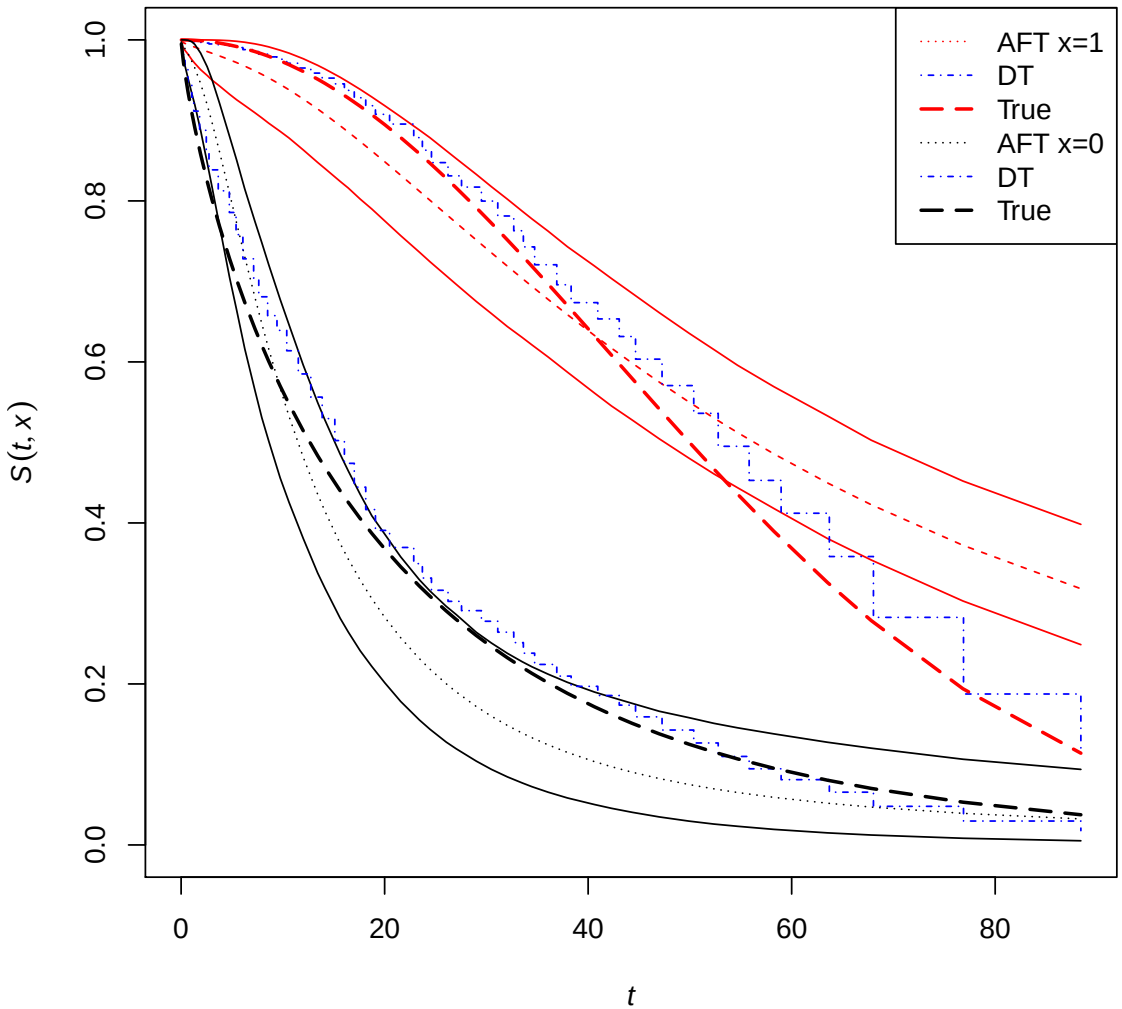


Neither AFT nor NFT scenario: AFT failure!

$N = 500$ with 50% censoring

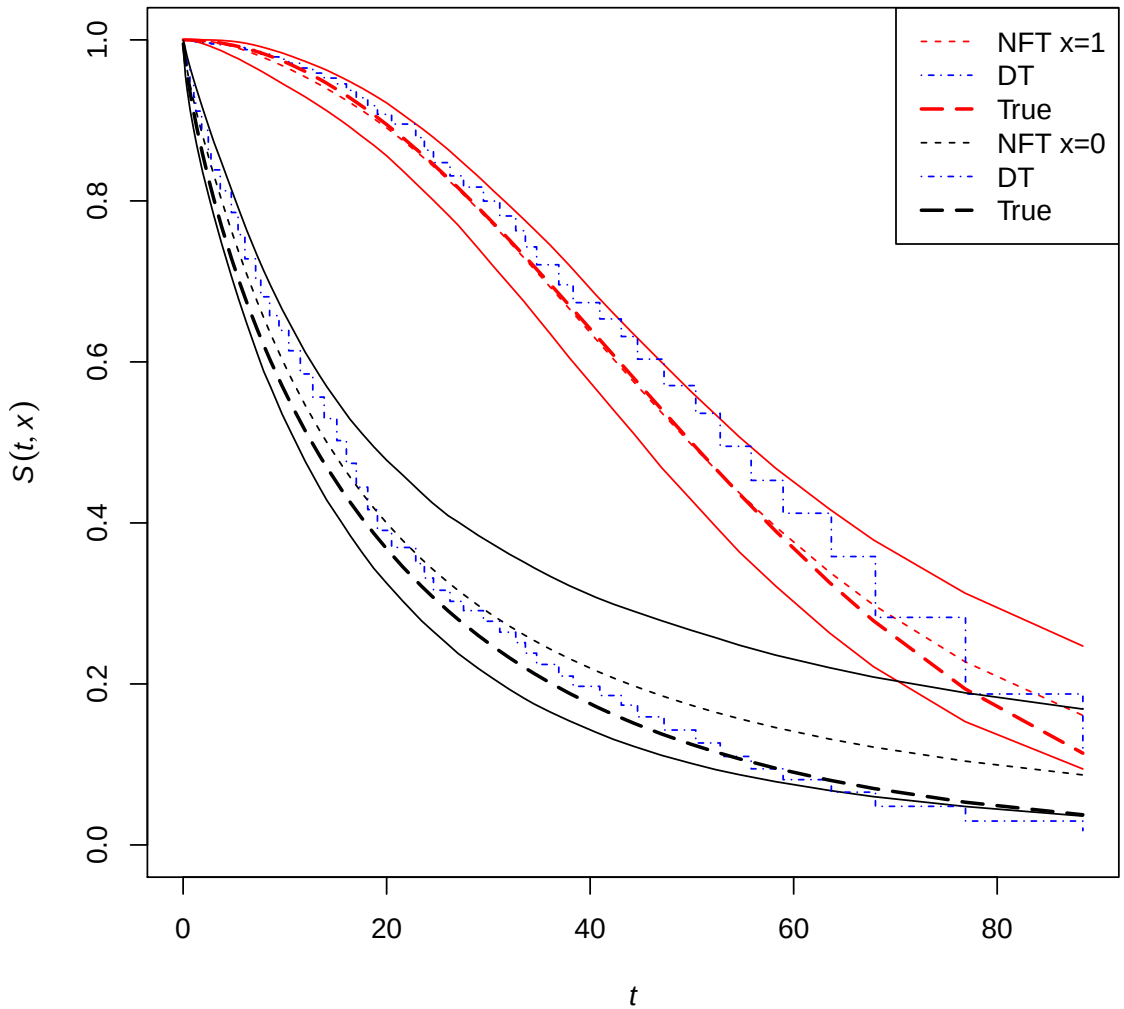
$\mathrm{Wei}\,(0.8 + 1.2x, 20 + 40x)$ where $x \sim \mathrm{B}(0.5)$



Neither AFT nor NFT scenario: NFT success!

$N = 500$ with 50% censoring

$\mathrm{Wei}\,(0.8 + 1.2x, 20 + 40x)$ where $x \sim \mathrm{B}(0.5)$



NFT BART posterior inference: the survival and distribution functions

$$S_m(t|x) = 1 - F_m(t|x)$$

$$F_m(t|x) = \int \Phi\left\{\frac{\log t - \mu_* - \mu_m(x)}{\sigma_* \sigma_m(x)}\right\} G_m(\mathrm{d}\mu_*, \mathrm{d}\sigma_*)$$

$$= \sum_{j=1}^{\infty} \omega_j \Phi\left\{\frac{\log t - \mu_j^* - \mu_m(x)}{\sigma_j^* \sigma_m(x)}\right\}$$

$$\approx \sum_{j=1}^{K_m} \omega_{jm} \Phi\left\{\frac{\log t - \mu_{jm}^* - \mu_m(x)}{\sigma_{jm}^* \sigma_m(x)}\right\}$$

where $(\mu_{jm}^*, \sigma_{jm}^*)$ are from the training set

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

$$h_m(t|x) = f_m(t|x)/S_m(t|x)$$

$$f_m(t|x) = \int \frac{\phi\left\{\frac{\log t - \mu_* - \mu_m(x)}{\sigma_* \sigma_m(x)}\right\}}{t\sigma_*\sigma_m(x)} G_m(\mathrm{d}\mu_*, \mathrm{d}\sigma_*)$$

$$= \sum_{j=1}^{\infty} \frac{\omega_j \phi\left\{\frac{\log t - \mu_j^* - \mu_m(x)}{\sigma_j^* \sigma_m(x)}\right\}}{t\sigma_j^*\sigma_m(x)}$$

$$\approx \sum_{j=1}^{K_m} \frac{\omega_{jm} \phi\left\{\frac{\log t - \mu_{jm}^* - \mu_m(x)}{\sigma_{jm}^* \sigma_m(x)}\right\}}{t\sigma_{jm}^*\sigma_m(x)}$$

where $(\mu_{jm}^*, \sigma_{jm}^*)$ are from the training set

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

Friedman 2001 *Annals of Statistics*

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

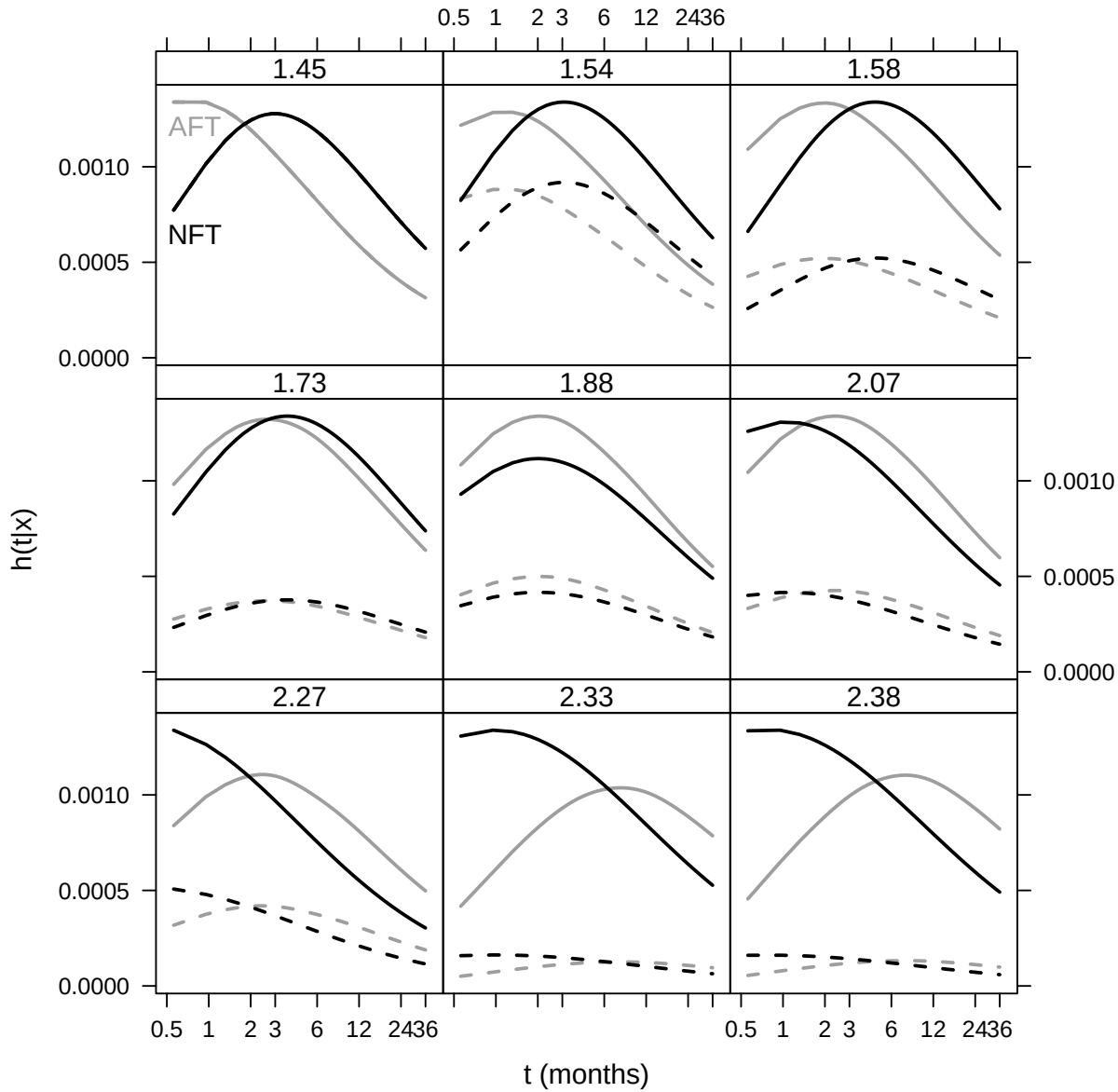
$$F_{Am}(t|x_A) = N^{-1} \sum_i \Phi\left(\frac{\log t - \mu_{im} - \mu_m(x_A, x_{iB})}{\sigma_{im}\sigma_m(x_A, x_{iB})}\right)$$

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

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

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*

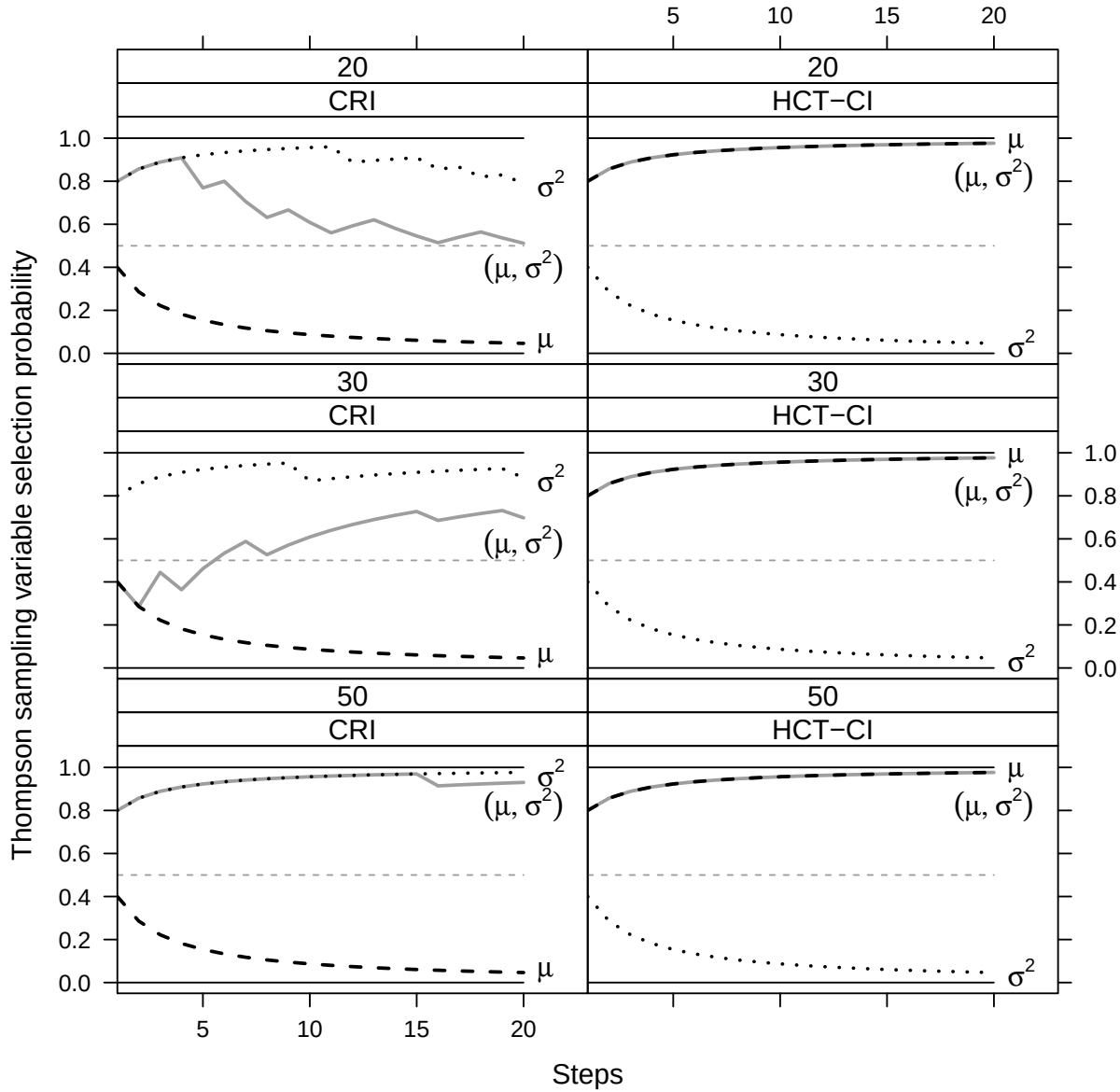
Set $\boldsymbol{H}$ *small*: 10, 20 or 40; smaller numbers engender more sparsity ($\widetilde{\boldsymbol{H}} \approx \boldsymbol{H}/\mathbf{5}$). TSVS is an iterative process: $\boldsymbol{k = 1, \ldots, K}$

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

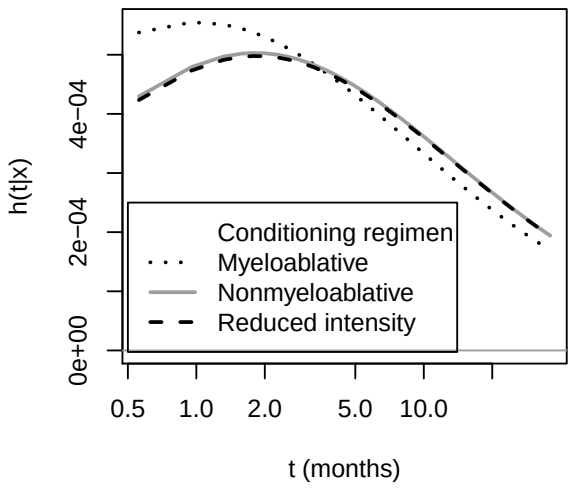
a. For $\boldsymbol{j = 1, \ldots, P}$: draw $\boldsymbol{\eta_{jk} \sim \mathbf{Beta}\left(a_{j,k-1},\ b_{j,k-1}\right)}$
b. Set $\boldsymbol{B_k = \{j : \eta_{jk} \geq 0.5\}}$: covariate subset selected at step $\boldsymbol{k}$
c. Fit an NFT BART model with covariates $\boldsymbol{x_{ij}}$ $\mathbf{where}$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

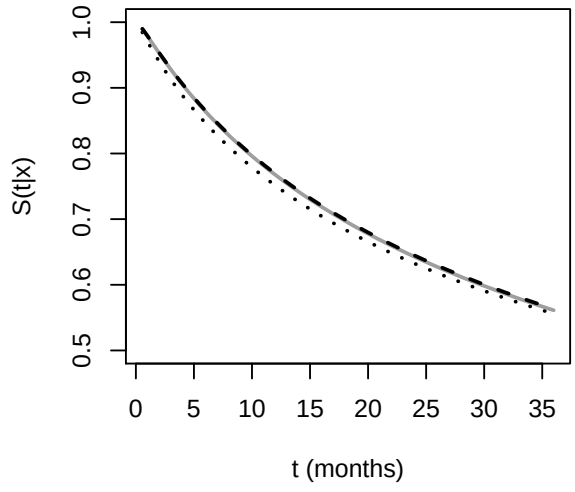
Important variables have trajectories of $\boldsymbol{\pi_{jk}}$ exceeding $\mathbf{0.5}$ by $\boldsymbol{K}$

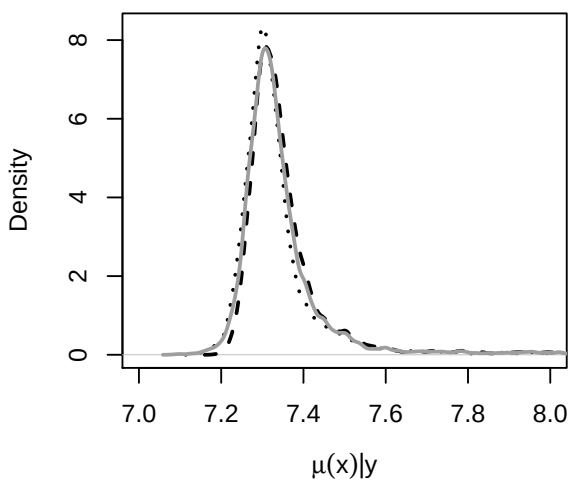
Real data example: TSVS with $\boldsymbol{H = 20, 30, 50}$ Conditioning regimen (CRI) and Comorbidity (HCT-CI)

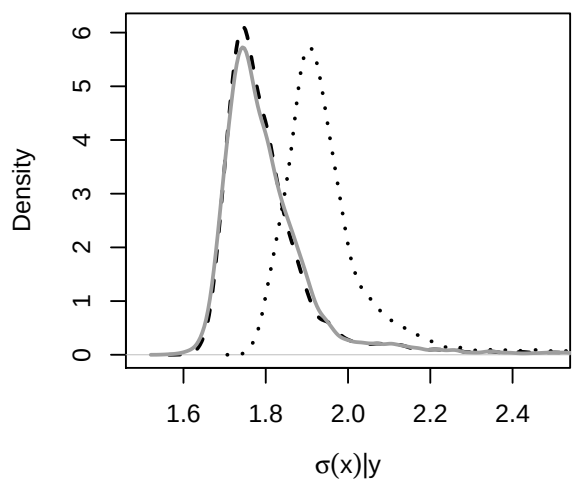


Real data example: Heteroskedasticity of the Conditioning Regimen Intensity (CRI)

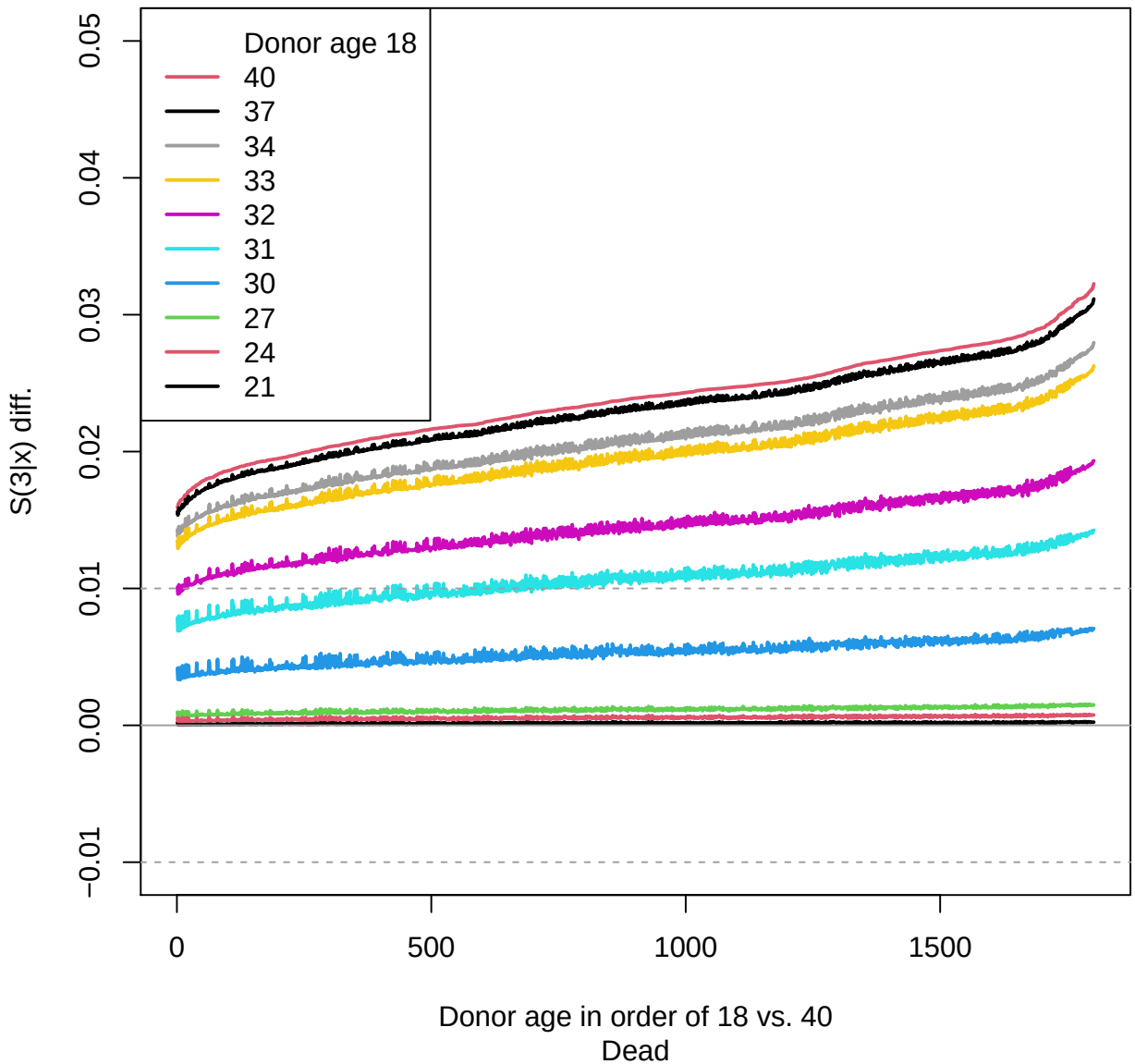




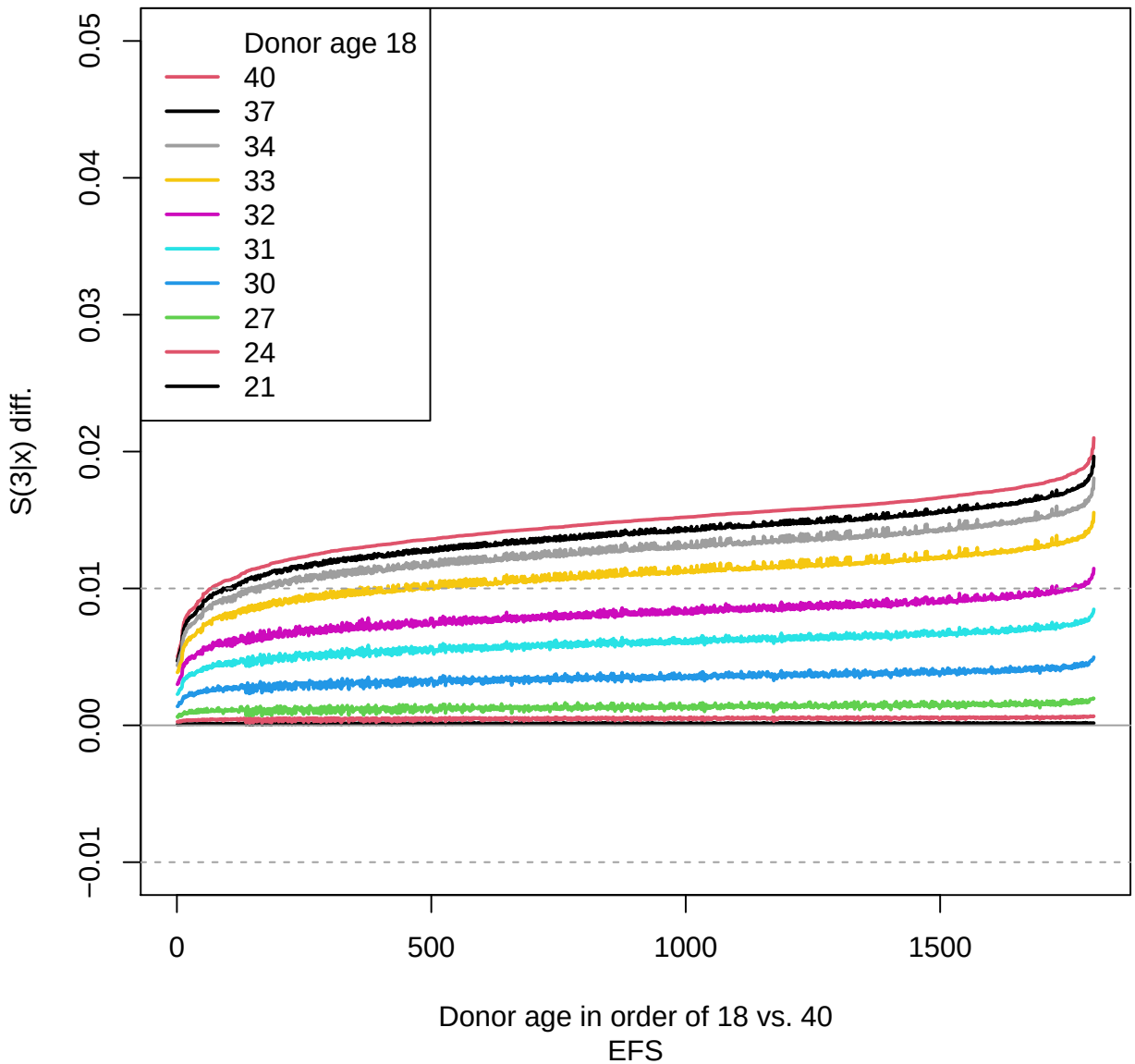




Real data example: Death and donor age



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