Horseshoe processes in partial linear models

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Motivation

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Biomedical data sometimes exhibit jumps or sharp changes:

- PSA data monitored over prostate cancer course[1]
- Women's basal body temperature monitored over time[2]
- U.S. prostate cancer incidence over time[3]

How should we fit these data?

A good statistical method would be able to fit the sharp jump without introducing excess noise into the smooth portions.

Horseshoe Prior

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Suppose we wish to fit the classic linear regression model:

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + ... + \beta_p x_{pi} + \epsilon_i, \ \epsilon_i \overset{iid}{\sim} N(0, \sigma^2) \quad (1)$$

for $i = 1, ..., n$ subjects, each of whom have a vector of p predictors.

If p is large, we might want to impose some shrinkage on the coefficients $\beta_1, ..., \beta_p$.

Horseshoe Prior

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Within a Bayesian framework, the horseshoe prior is one popular way to do so. It takes the form:

$$\begin{aligned} \beta_j|\tau,\lambda_j &\sim N(0,\tau^2\lambda_j^2) \\ \tau &\sim C^+(0,1) \\ \lambda_j &\overset{iid}{\sim} C^+(0,1) \end{aligned} \tag{2}$$

for $j = 1, ..., p$.[4]

For each β_j in turn, the horseshoe favors either total shrinkage ($\beta_j = 0$) or minimal shrinkage (leaving β_j close to its MLE).

Gaussian Processes

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Suppose we have some outcome y observed over time t. In its simplest form, a Gaussian process can be defined as:

$$y(t) - y(t-s) \sim N(0, s\tau_g^2) \tag{3}$$

A Gaussian process assumes that motion over time is normally-distributed, and it relies on a single parameter, τ_g^2.

If τ_g^2 is large, $y(t)$ will vary a lot; if τ_g^2 is small, $y(t)$ will be fairly constant.

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What if motion over time were horseshoe-distributed rather than normally-distributed?

A Horseshoe Process

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Using a discrete definition, for discretely observed timepoints t_k, $k = 1, ..., m$, we can define a horseshoe process:

$$\begin{aligned} y_{t_k} - y_{t_{k-1}} | \tau_h, \lambda_k &\sim N(0, \tau_h^2 \lambda_k^2 (t_k - t_{k-1})), \ \ k = 2, ..., m \\ y_{t_1} &= 0 \\ \tau_h &\sim C^+(0, c) \\ \lambda_k &\overset{iid}{\sim} C^+(0, 1), k = 2, ..., m \end{aligned} \tag{4}$$

Each increment is horseshoe distributed; each increment has its own local shrinkage parameter λ_k. Variance continues to scale with elapsed time.

A Horseshoe Process

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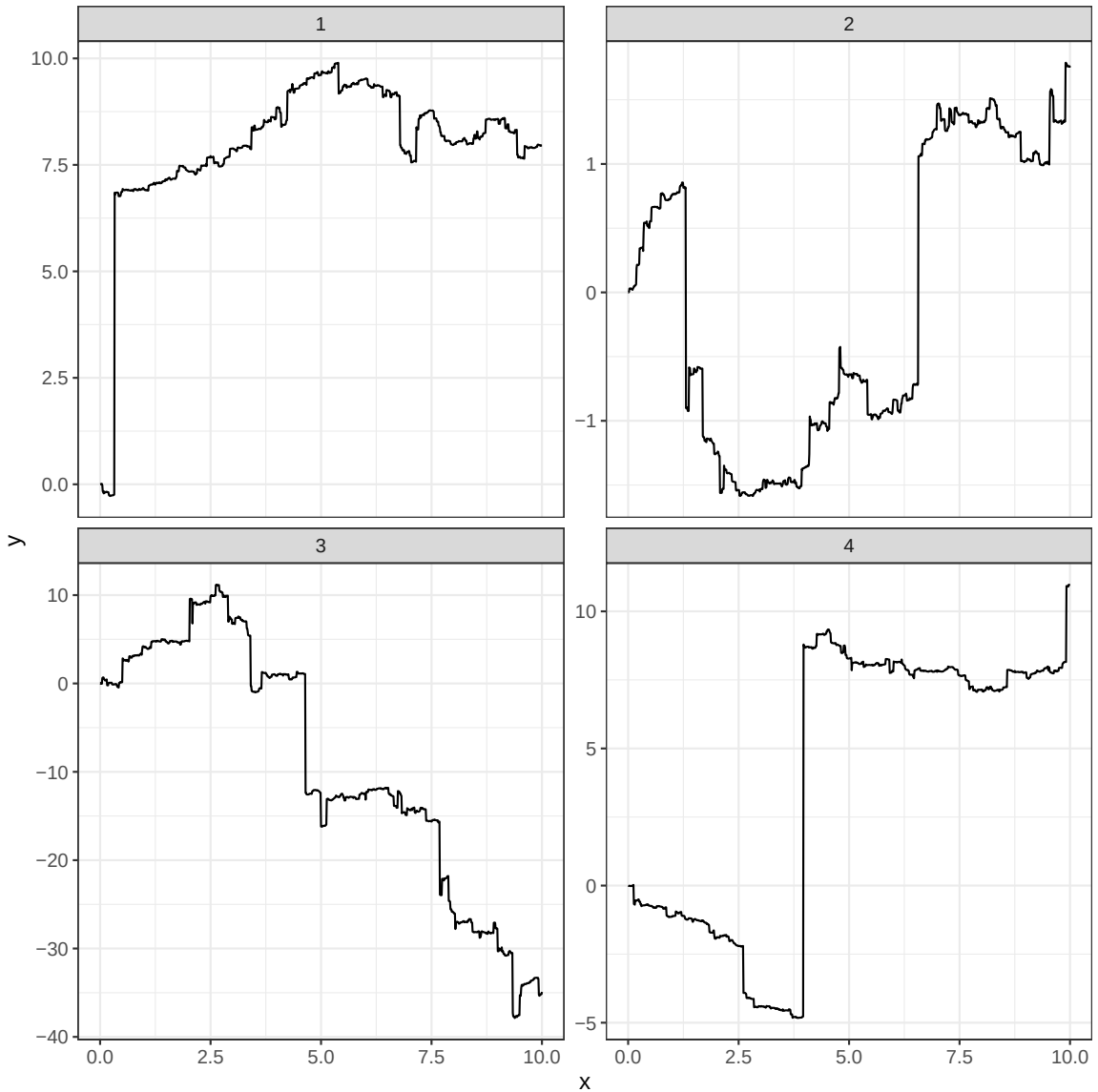

Basic Model

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Let y_i be some outcome observed for subjects $i = 1, ..., n$ at continuous predictor value x_i. Define $\boldsymbol{t}$ as a length m vector containing the unique, ordered values of $\boldsymbol{x}$. Suppose that $x_i = t_j$.

$$g(E(y_i)) = f_j = \alpha + \sum_{k=1}^{j} h_k \tag{5}$$

$$h_k|\tau, \lambda_k \sim N(0, \tau_h^2 \lambda_k^2 (t_k - t_{k-1})), \ \ k = 2, ..., m$$

$$h_1 = 0$$

$$\tau_h \sim C^+(0, c)$$

$$\lambda_k \overset{iid}{\sim} C^+(0, 1), k = 2, ..., m$$

$$\alpha \sim N(a, b^2)$$

Extension: Monotonicity Constraints

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We may want to constrain our horseshoe process to be monotonic increasing or decreasing. This is easily accommodated in our model through the use of a transformation m:

$$g(E(y_i)) = f_j = \alpha + \sum_{k=1}^{j} m(h_k) \tag{6}$$

m could be exponentiation or the absolute value function. We found that the absolute value function yields better performance.

Extension: Partial Linear Models

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Additional covariates are easy to include. Suppose we have an additional length p vector of covariates $\boldsymbol{z}_i$ for each subject, yielding an n x p matrix $\boldsymbol{Z}$ of covariates. Then we can model:

$$g(E(y_i)) = f_i = \alpha + \beta \boldsymbol{z}_i + \sum_{k=1}^{j} h_k \tag{7}$$

$$\beta \sim N(\mathbf{0}, \boldsymbol{d}^2)$$

In theory, we could also include multiple horseshoe terms through an additive framework, although the number of parameters would grow rapidly.

Extension: Data Interpolation

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There may be values of x at which we wish to obtain predictions, or to obtain a more finely-spaced grid of increments h_k with which to approximate the horseshoe process.[5]

We perform Bayesian imputation to obtain estimates of $\boldsymbol{f}$ at these augmentation points, placing the same prior on $\boldsymbol{f}_{aug}$ as is already on $\boldsymbol{f}_{obs}$.

Computation

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All models are implemented using Hamiltonian Monte Carlo via Stan and the cmdstanr package in R.[6,7]

For sampling, we use 4 chains, each with a warm-up phase of 1000 samples and a sampling phase of 2000 samples, without thinning, yielding 8000 posterior samples total.

All of the methods described above are implemented in the R package HPR, available on GitHub.

Sample Fits

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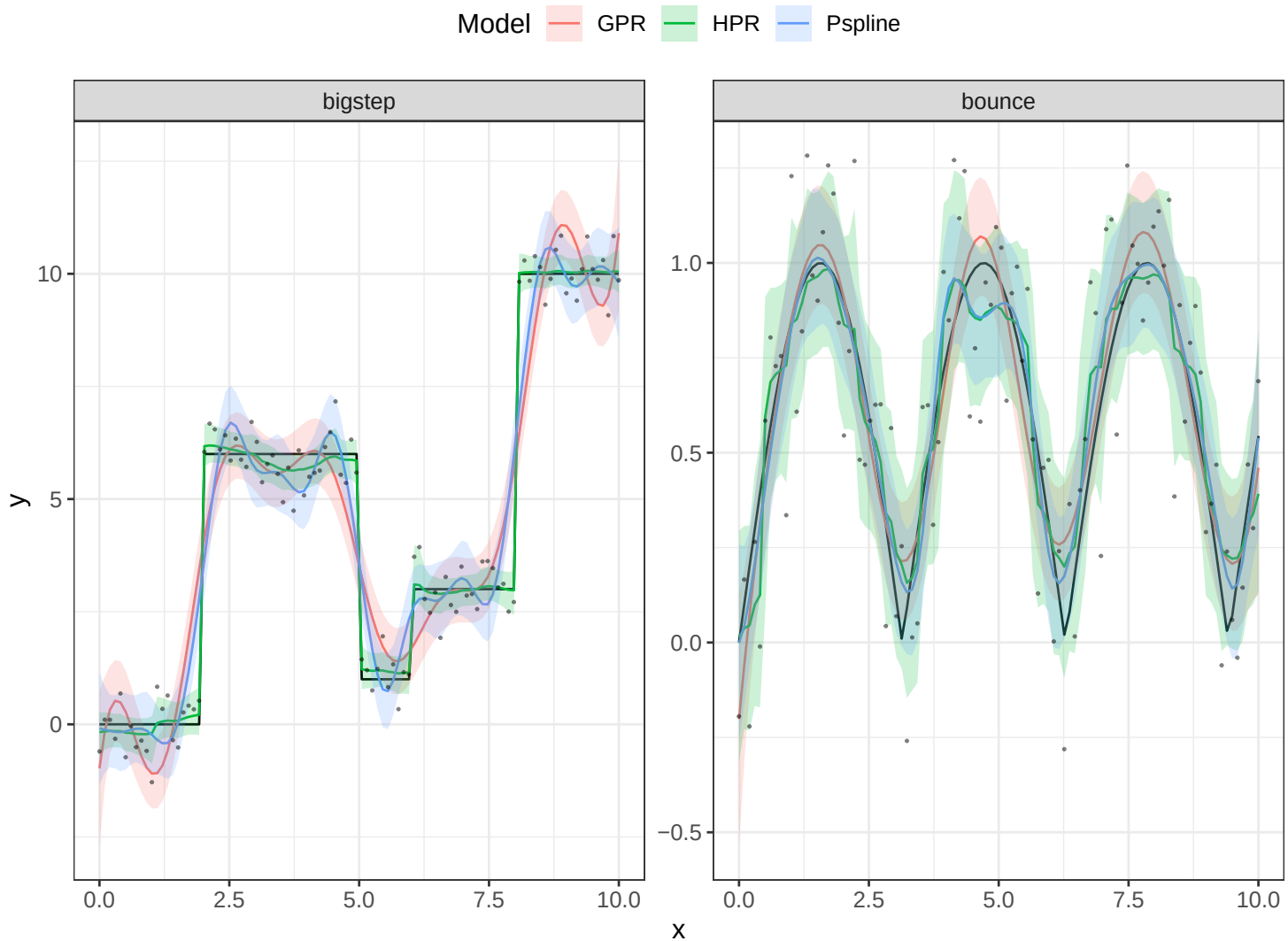

Performance Overview

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- We find that HPR performs well for step functions and piecewise linear functions, and outperforms the comparison methods at fitting step functions.
- Its performance for functions with constant variability is adequate, but not as good as methods like Gaussian process regression or penalized splines.
- We find that our data interpolation scheme returns sensible results across varying numbers of augmentation points.
- We find that our HPR partial linear model performs well at estimating the coefficients of the linear predictors in all settings, and outperforms other methods when fitting step function nonlinear components.

Full Results

Motivating Data

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We use HPR to model women's basal body temperature (BBT) over the course of the menstrual cycle.

In healthy women, BBT usually starts low at the beginning of the menstrual cycle, jumping sharply immediately after ovulation, and then returning to pre-ovulation temperatures with the start of the next period.

Tracking this pattern over several months may give insight into reproductive health challenges or assist with family planning.

Here, we use example BBT charts abstracted from Weschler (2015).[8]

Motivating Data

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We fit a horseshoe process regression (HPR), Gaussian process regression (GPR),[9,10,11] and zero-degree penalized spline model (Pspline)[12] separately for each woman's chart.

Results

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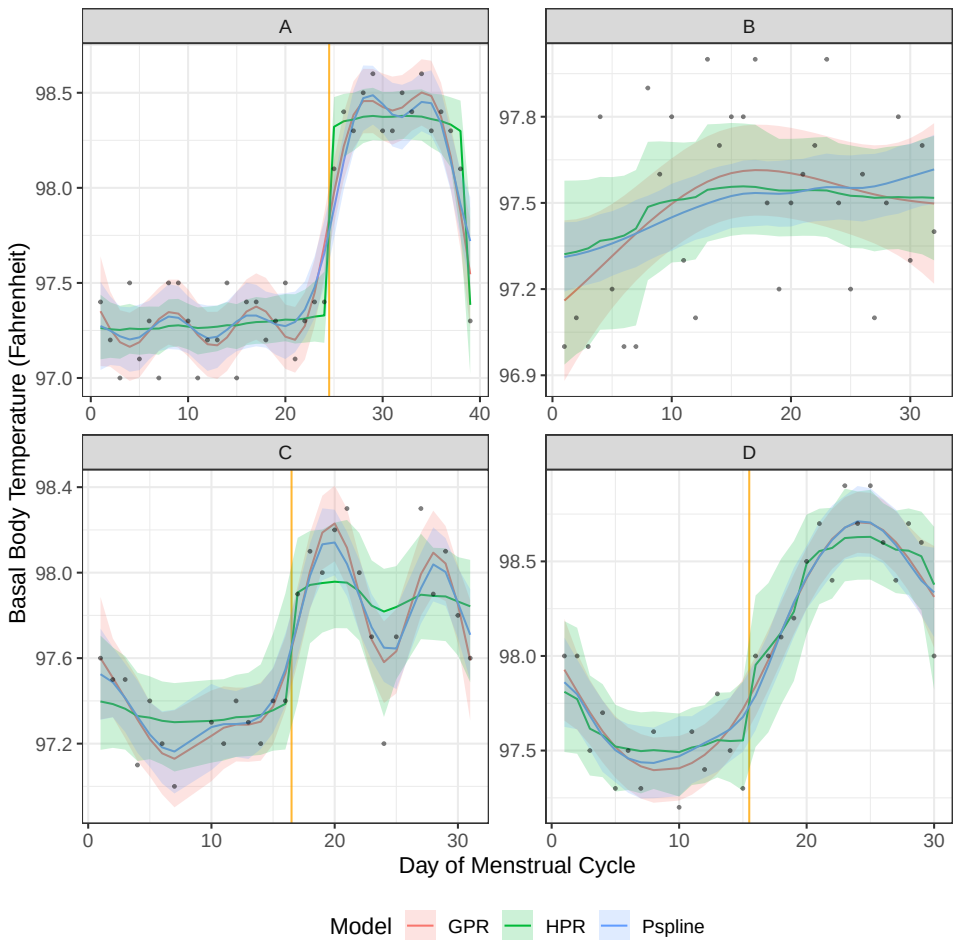
Figure: Fitted basal body temperature trajectory and 95% credible/confidence intervals for four women.



Results

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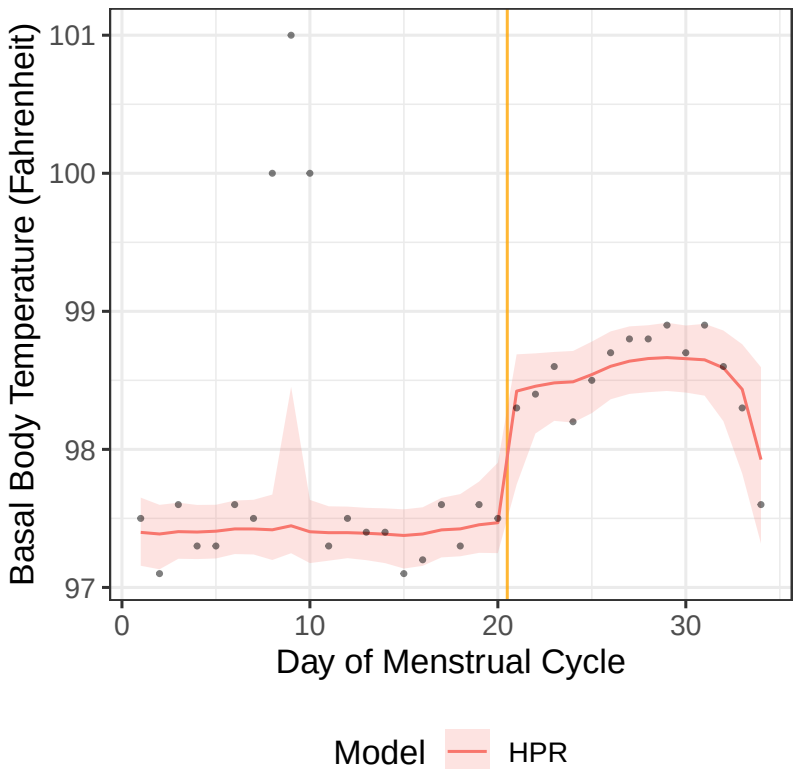
Figure: Fitted basal body temperature trajectory and 95% credible/confidence intervals from a horseshoe process regression (HPR) adjusted for the presence of fever for a woman who was ill during days 8-10 of her menstrual cycle.



Unanswered Questions

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- Alternative approaches for computation (variational inference?)
- Regularized horseshoe?
- Alternative approaches for data interpolation
- Other non-Gaussian outcomes (negative binomial, ordinal)

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References II

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[7] J Gabry and R Cesnovar. CmdStanR: the R interface to CmdStan. `https://mc-stan.org/cmdstanr/reference/cmdstanr-package.html`, 2021.

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[9] SN Wood. mgcv: GAMs and generalized ridge regression for R. *R News*, 1/2:20–25, 2001.

[10] SN Wood, N Pya, and B Safken. Smoothing parameter and model selection for general smooth models (with discussion). *JASA*, 111:1548–1575, 2016.

References III

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[12] PHC Eilers, BD Marx, and M Durbán. Twenty years of p-splines. *Statistics and Operations Research Transactions*, 39 (2):149–186, 2015.

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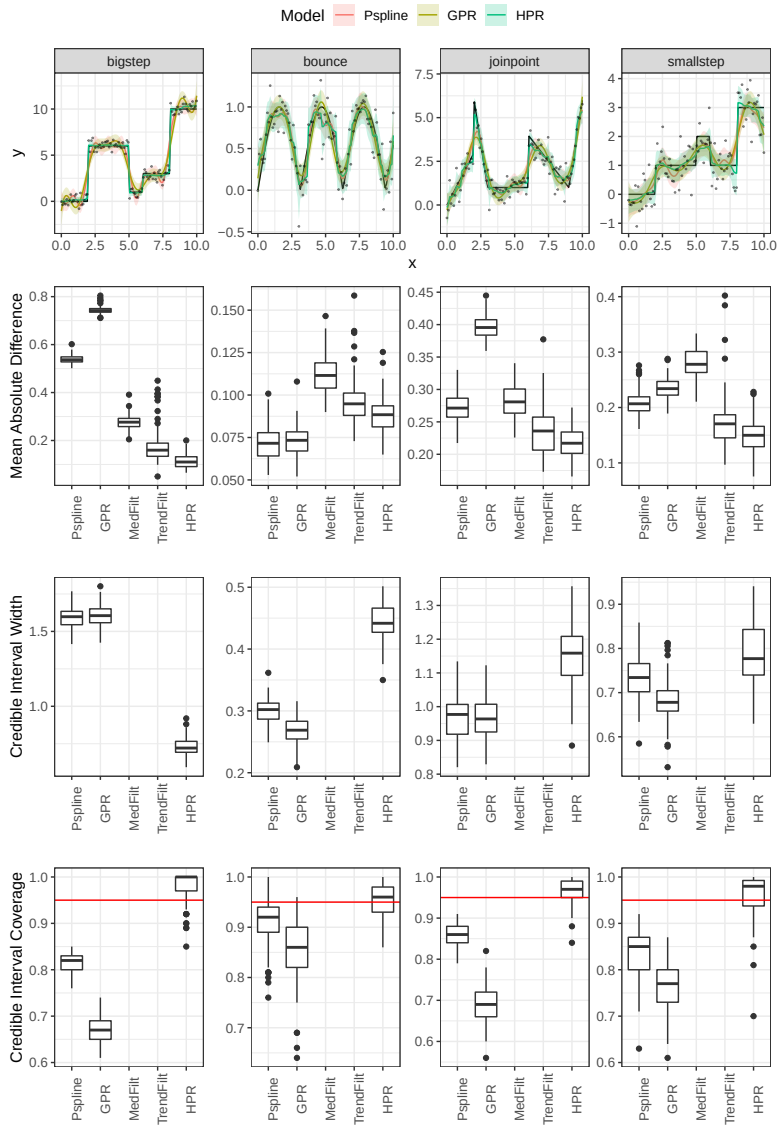
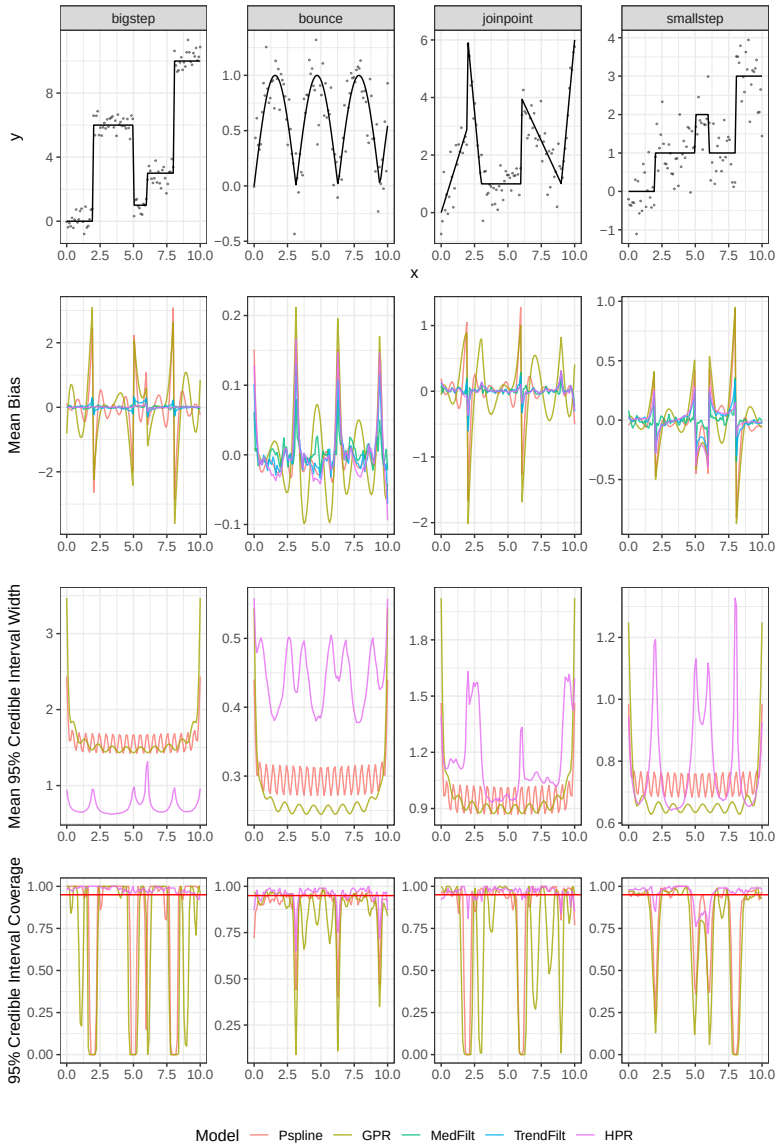
Thank you! Any questions?

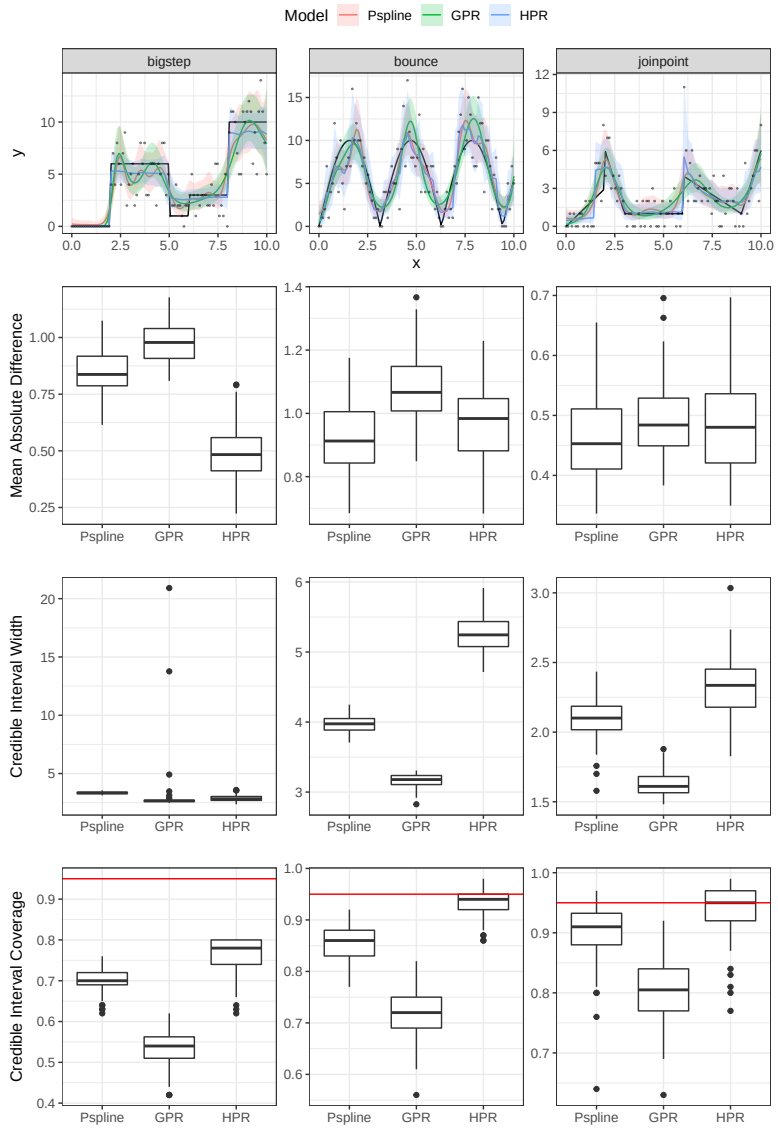
Gaussian Results



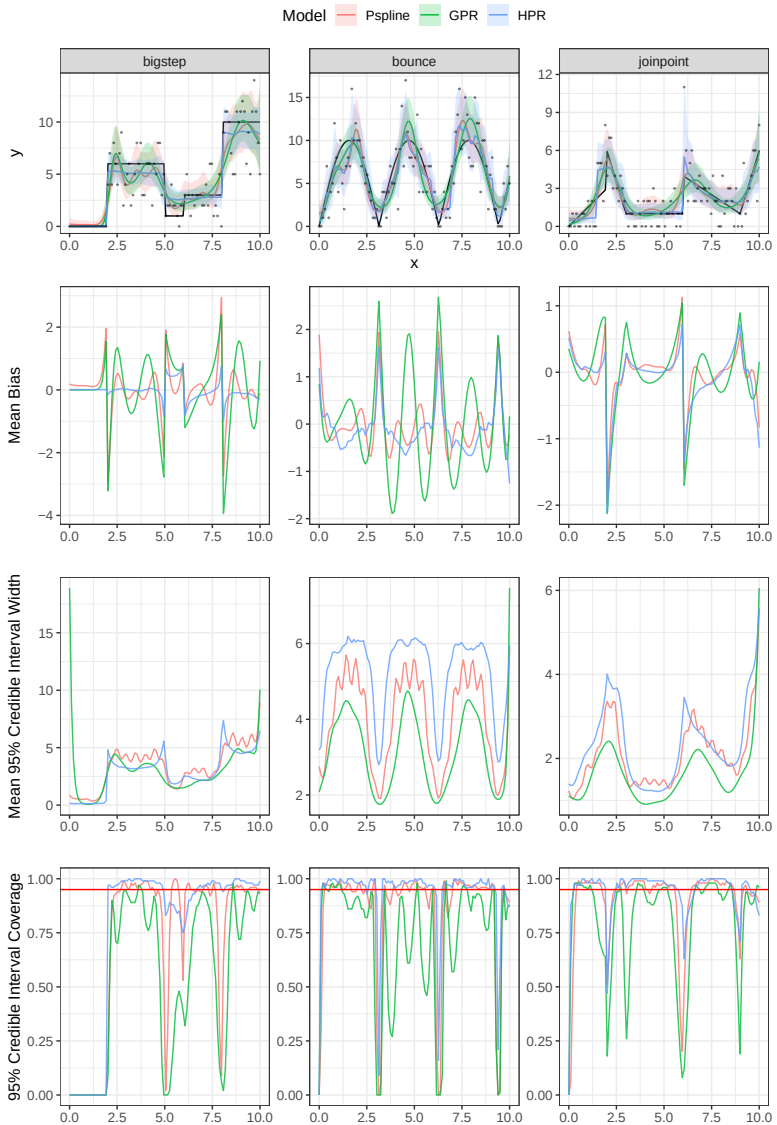
Gaussian Results



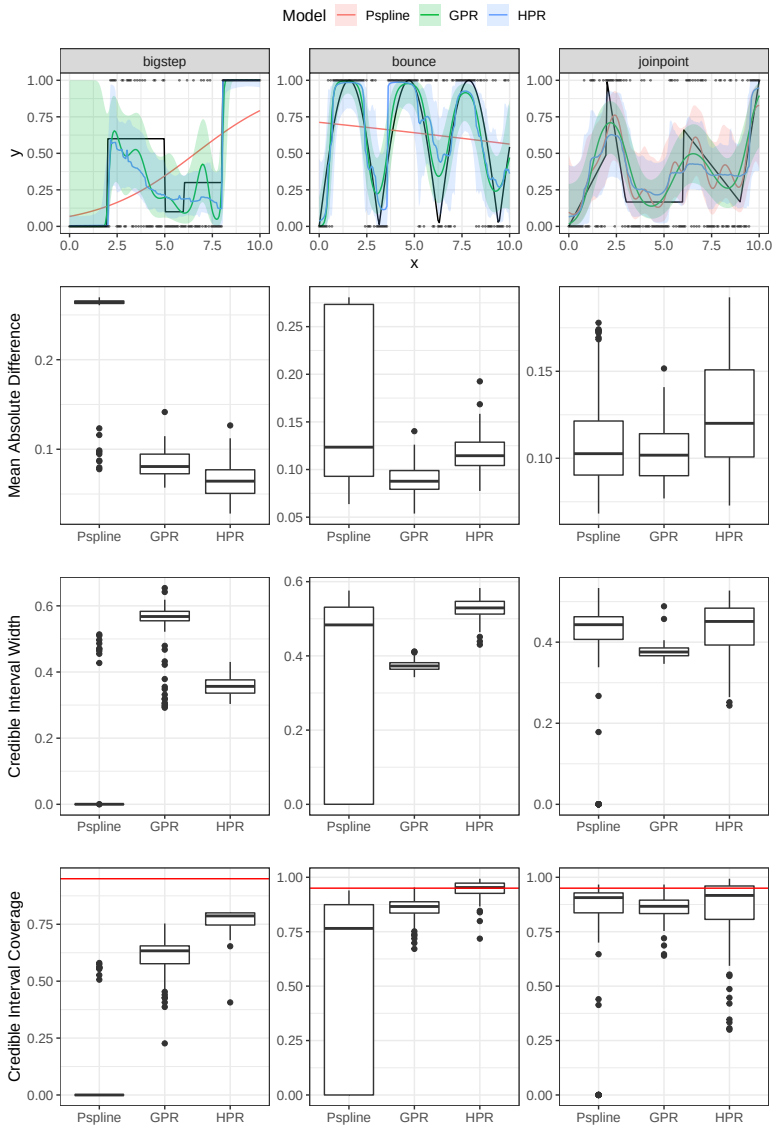
Poisson Results



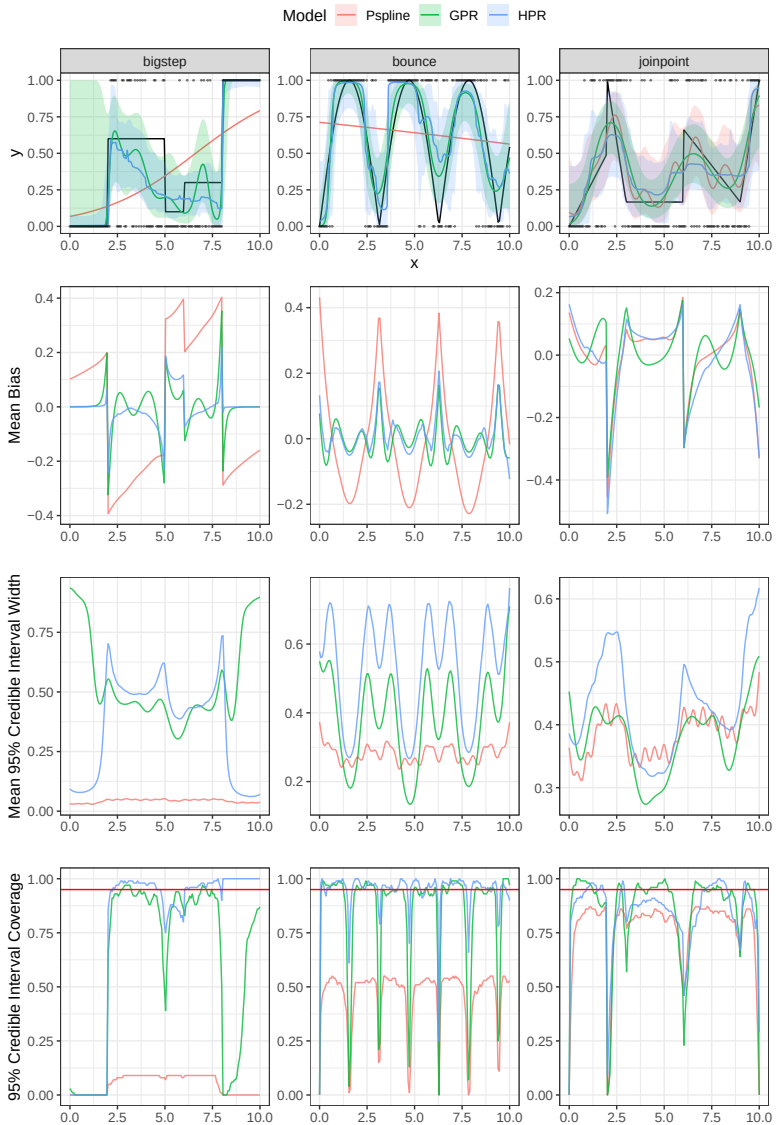
Poisson Results



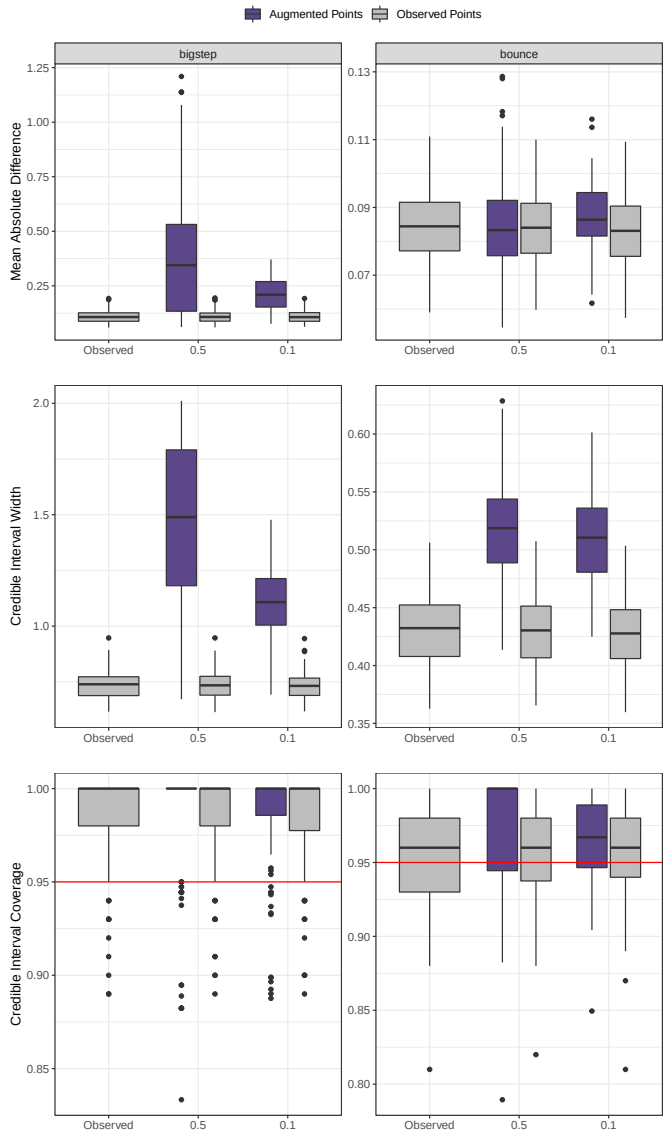
Binomial Results



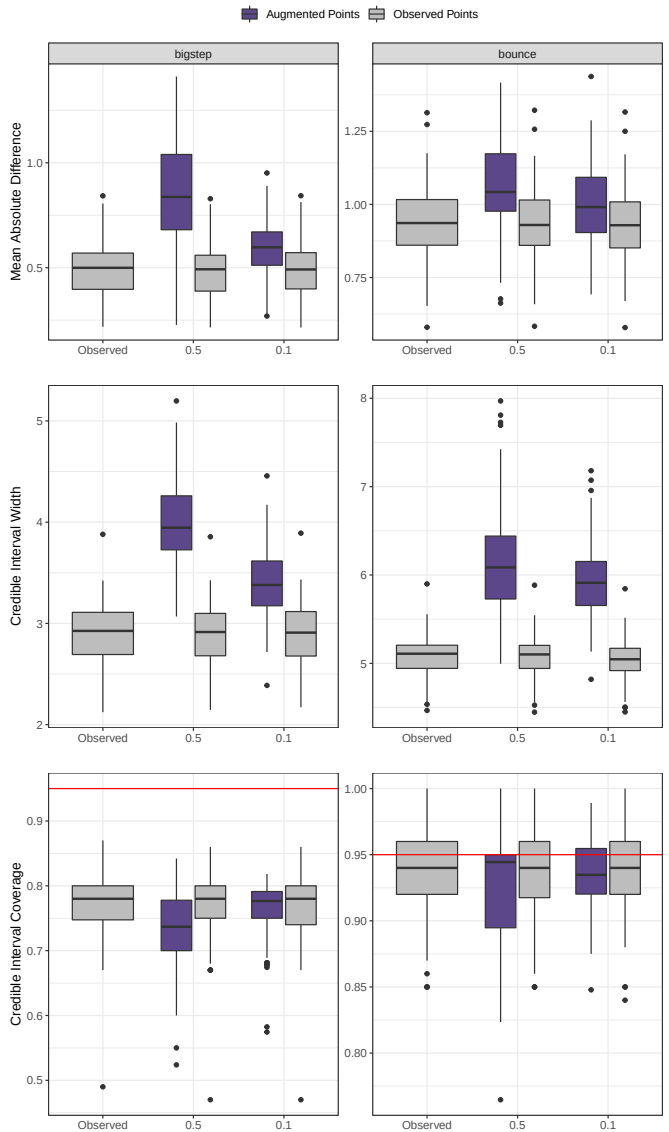
Binomial Results



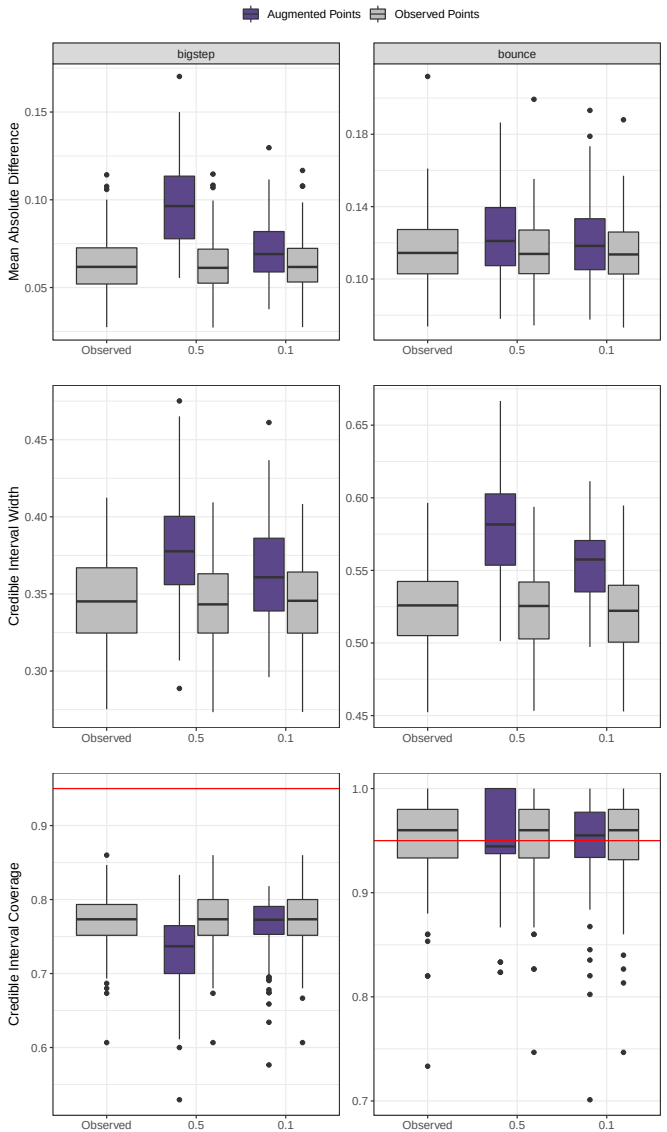
Gaussian Interpolation



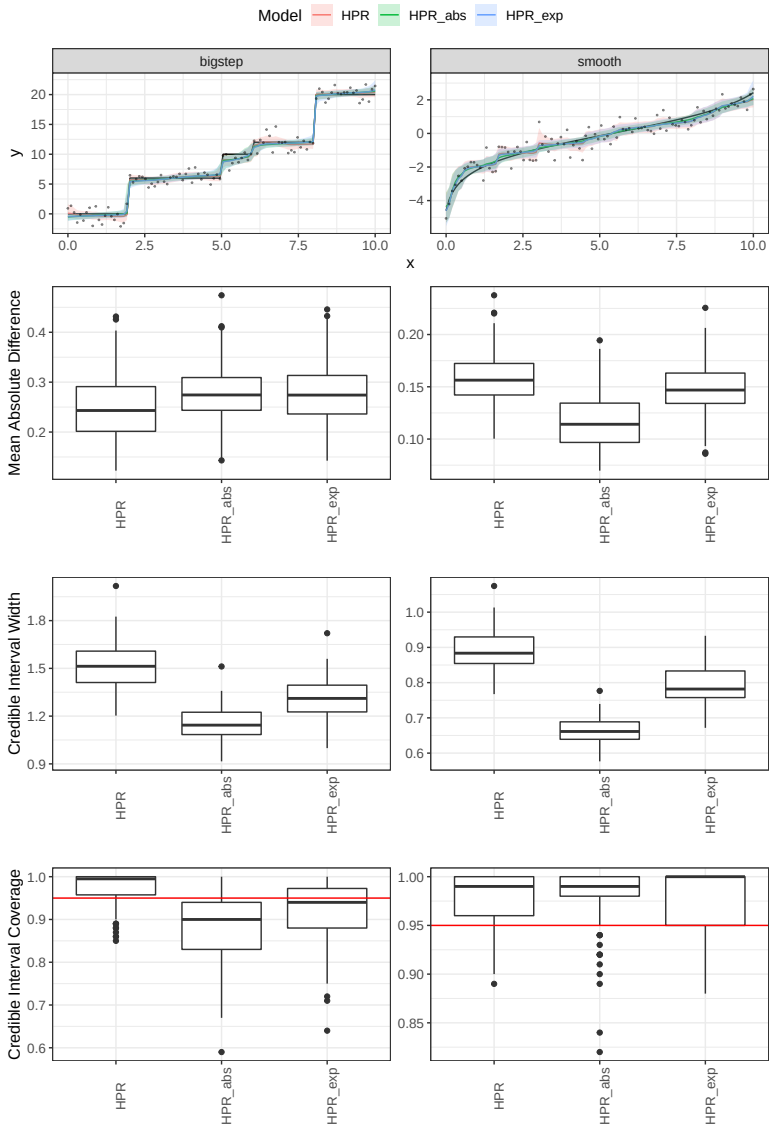
Poisson Interpolation



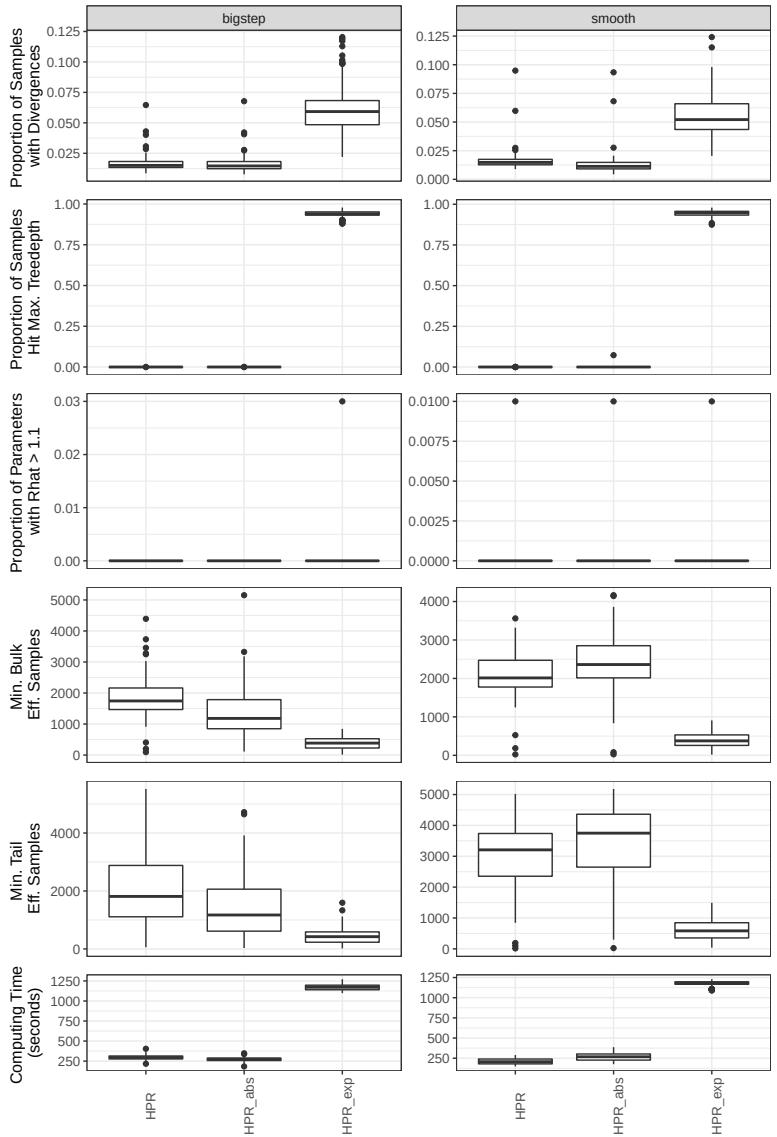
Binomial Interpolation



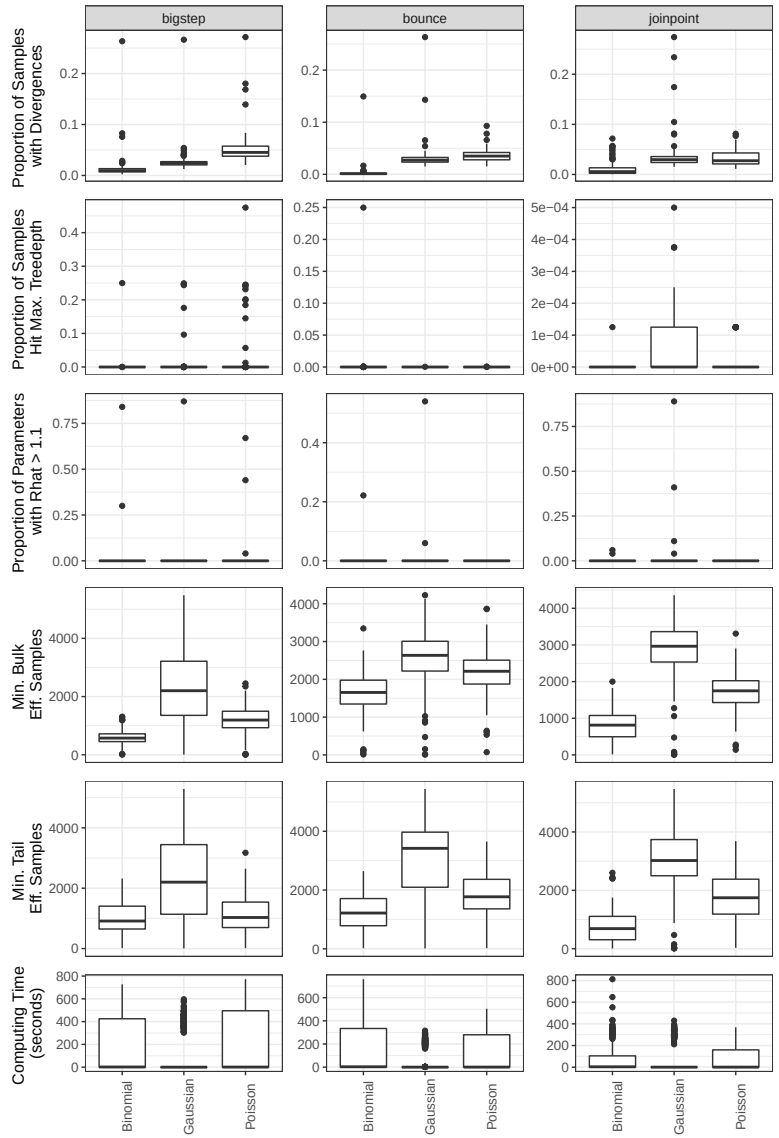
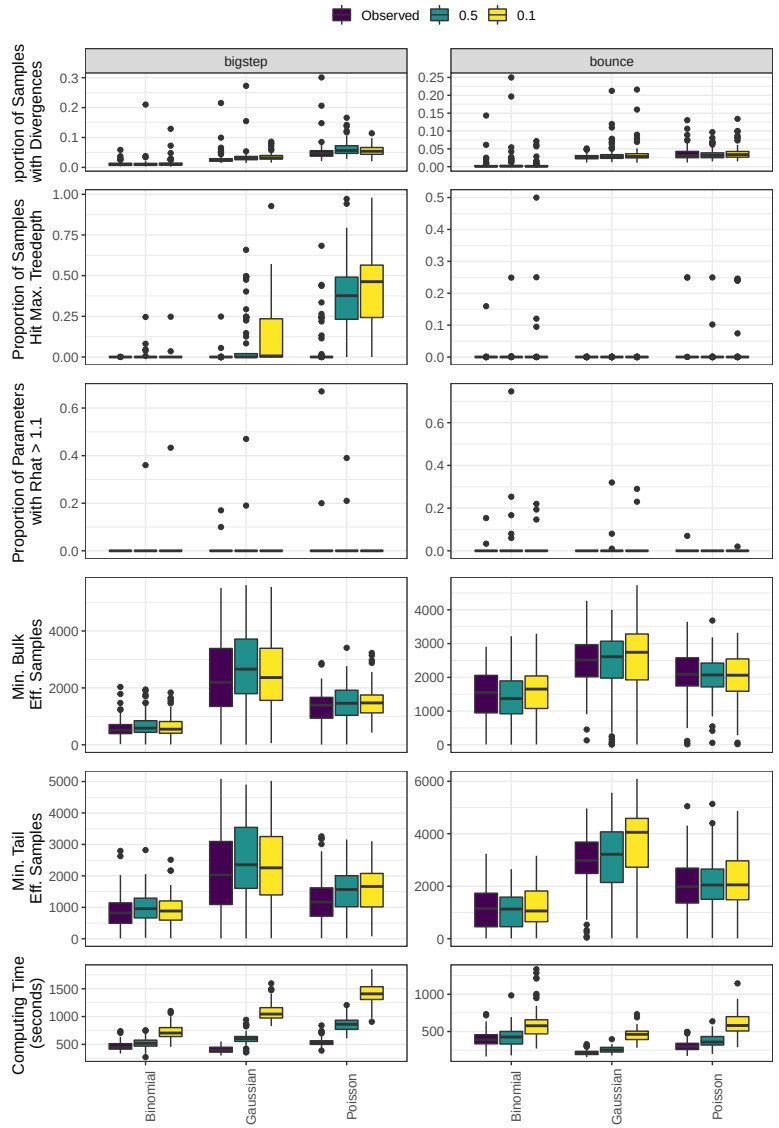
Monotonic Results



Monotonic Results



Computational Assessment



Computational Assessment - Interpolation