Introduction to BART with binary outcomes

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Outline

- Motivation: chronic spine pain and obesity
- Probit regression with BART
- Logistic regression with BART
- Geweke convergence diagnostics for binary BART

Motivation: chronic spine pain and obesity

- We believe that obesity is a risk factor for chronic lower back/buttock pain
- Conversely, obesity is not a risk factor for chronic neck pain
- Data available from the National Health and Nutrition Examination Survey (NHANES) 2009-2010 Arthritis Questionnaire
- 5106 subjects were surveyed
- Demographics: age and gender
- Anthropometrics available: weight (kg), height (cm), body mass index (kg/m^2), waist circumference (cm)
- Sampling weights to estimate for the US as a whole

Probit BART for binary outcomes

Probit regression with latent variables: Albert & Chib 1993 *JASA*

$$y_i|p_i \overset{\text{ind}}{\sim} \mathrm{B}(p_i)$$

$$p_i|f = \Phi(\mu + f(x_i)) \text{ where } f \overset{\text{prior}}{\sim} \text{BART}$$

$$z_i|y_i, f \sim \mathrm{N}(f(x_i),\ 1) \begin{cases} \mathrm{I}(-\infty, 0) & \text{if } y_i = 0 \\ \mathrm{I}(0, \infty) & \text{if } y_i = 1 \end{cases}$$

$$f|z_i, y_i \overset{d}{=} f|z_i$$

$$[y|f] = \prod_{i=1}^{N} p_i^{y_i}(1-p_i)^{1-y_i} \qquad \text{Likelihood}$$

Continuous BART with unit variance, $\sigma^2 = 1$, and z_i are the data

Friedman's partial dependence function

Friedman 2001 *AnnStat*

$$f(x) = f(x_S, x_C) \qquad \text{BART function where } x = [x_S, x_C]$$

$$f(x_S) = \mathbf{E}_{x_C}\left[f(x_S, x_C)|x_S\right]$$

$$\approx N^{-1}\sum_i f(x_S, x_{iC})$$

$$f_m(x_S) \equiv N^{-1}\sum_i f_m(x_S, x_{iC})$$

$$\hat{f}(x_S) \equiv M^{-1}\sum_m f_m(x_S)$$

`pbart` and `mc.pbart` input and output

```
post <- pbart(x.train, y.train, ...,
        ndpost=M, keepevery=1) or
post <- mc.pbart(x.train, y.train, ...,
        ndpost=M, keepevery=1, mc.cores=2, seed=99)
```

Input matrices: `x.train` and, optionally, `x.test`: x_i

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

Output object, `post`, of type `pbart` which is essentially a list

Matrices: `post$yhat.train` and `post$yhat.test`: $\hat{y}_{im} = f_m(x_i)$

$$\begin{bmatrix} \hat{y}_{11} & \cdots & \hat{y}_{N1} \\ \vdots & \vdots & \vdots \\ \hat{y}_{1M} & \cdots & \hat{y}_{NM} \end{bmatrix}$$

`predict.pbart` input and output

```
pred <- predict(post, x.test, mc.cores=1, ...)
```

Input matrices: `x.test`: x_i

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_Q \end{bmatrix}$$

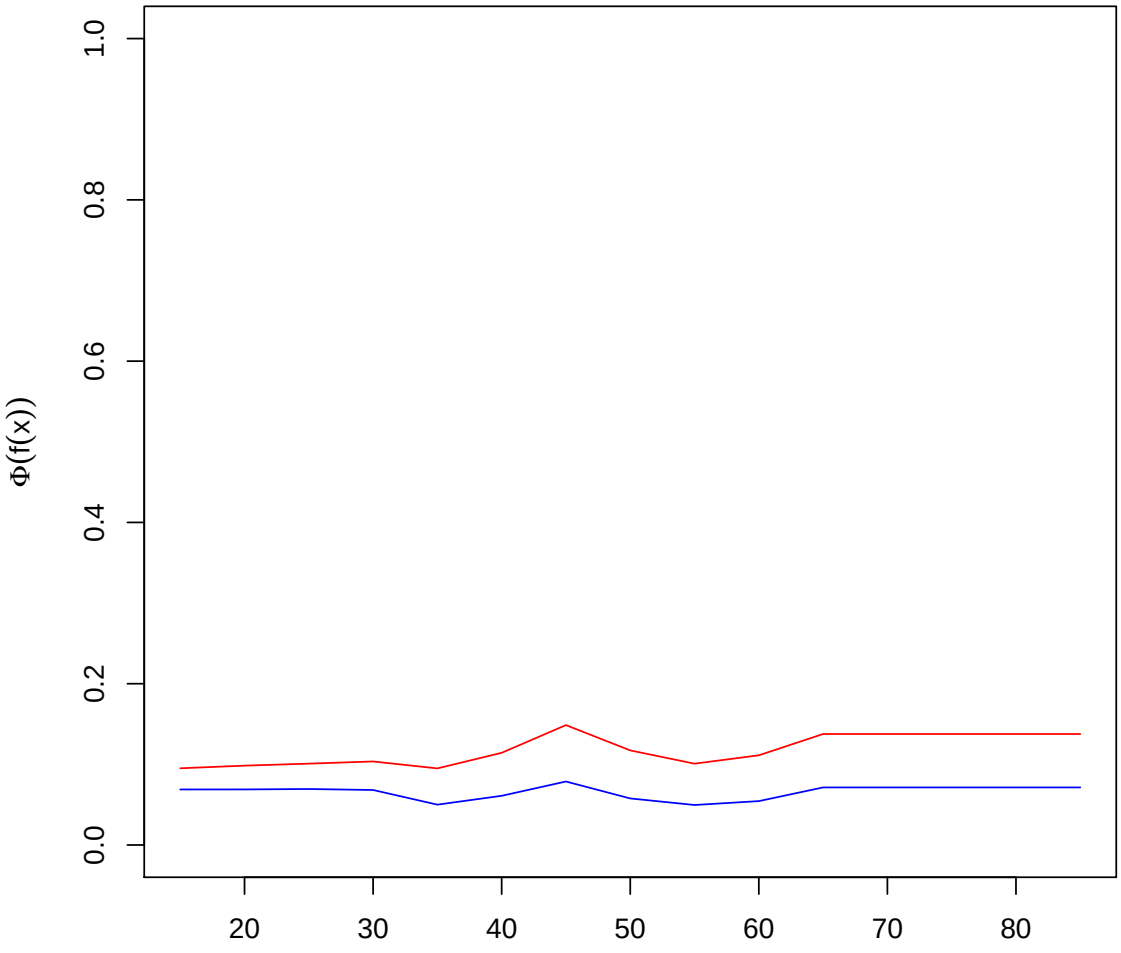
Output matrix `pred`: $\hat{y}_{im} = f_m(x_i)$

$$\begin{bmatrix} \hat{y}_{11} & \cdots & \hat{y}_{Q1} \\ \vdots & \vdots & \vdots \\ \hat{y}_{1M} & \cdots & \hat{y}_{QM} \end{bmatrix}$$

Live demo: chronic spine pain and obesity

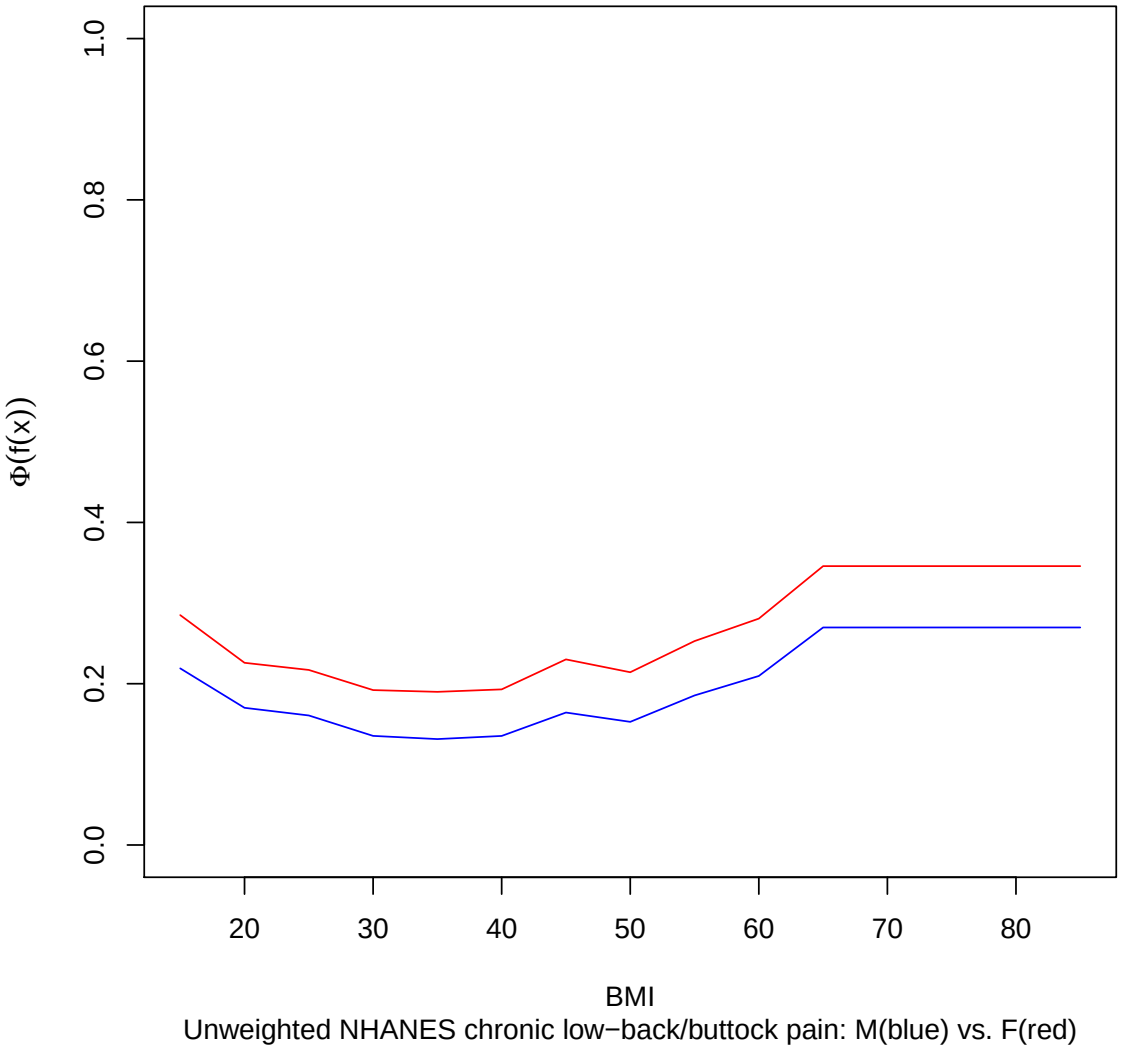
- `system.file('demo/nhanes.pbart1.R', package='BART')`
- `system.file('demo/nhanes.pbart2.R', package='BART')`

Friedman's partial dependence function: Probability of chronic neck pain vs. BMI



Unweighted NHANES chronic neck pain: M(blue) vs. F(red)

Friedman's partial dependence function:
Probability of chronic lower back/buttock pain vs. BMI



Logistic BART for binary outcomes

Logistic regression: Holmes & Held 1993 *Bayesian Analysis*
Devroye 1986 *Non-uniform random variate generation*

$$y_i|p_i \overset{\text{ind}}{\sim} \mathbf{B}(p_i)$$

$$p_i|f = \Phi(f(x_i)) \text{ where } f \overset{\text{prior}}{\sim} \text{BART}$$

$$z_i|y_i,f \sim \mathbf{N}\big(f(x_i),\ \sigma_i^2\big) \begin{cases} \mathbf{I}(-\infty,0) & \text{if } y_i = 0 \\ \mathbf{I}(0,\infty) & \text{if } y_i = 1 \end{cases}$$

$$\sigma_i^2 = 4\psi_i^2 \text{ where } \psi_i \sim \text{Kolmogorov-Smirnov (see Devroye)}$$

Continuous BART with heteroskedastic variance and z_i is the data

Geweke convergence diagnostics for binary BART

Hastings 1970 *Biometrika*, Silverman 1986 *Chapman and Hall*

$$\hat{\theta}_M = M^{-1} \sum_{m=1}^{M} \theta_m$$ Bayesian estimator

$$\sigma^2_{\hat{\theta}} = \lim_{M \to \infty} \mathbf{V}\left[\hat{\theta}_M\right]$$ Asymptotic variance

Suppose θ_m is an **ARMA** (p, q)

$$\gamma(w) = (2\pi)^{-1} \sum_{m=-\infty}^{\infty} \mathbf{V}\left[\theta_0, \theta_m\right] \mathbf{e}^{imw}$$ Spectral density

$$\hat{\sigma}^2_{\hat{\theta}} = \hat{\gamma}^2(0)$$ Variance estimator

Geweke convergence diagnostics for binary BART

Geweke 1992 *Bayesian Statistics*

- Divide your chain into two segments: A and B
- $m \in A = \{1, \ldots, M_A\}$ where $M_A = aM$
- $m \in B = \{M - M_B + 1, \ldots, M\}$ where $M_B = bM$
- $a + b < 1$, Geweke suggests $a = 0.1$ and $b = 0.5$

$$\hat{\theta}_A = M_A^{-1} \sum_{m \in A} \theta_m \qquad \hat{\theta}_B = M_B^{-1} \sum_{m \in B} \theta_m$$

$$\hat{\sigma}^2_{\hat{\theta}_A} = \hat{\gamma}^2_{m \in A}(0) \qquad \hat{\sigma}^2_{\hat{\theta}_B} = \hat{\gamma}^2_{m \in B}(0)$$

$$z = \frac{\sqrt{M}(\hat{\theta}_A - \hat{\theta}_B)}{\sqrt{a^{-1}\hat{\sigma}^2_{\hat{\theta}_A} + b^{-1}\hat{\sigma}^2_{\hat{\theta}_B}}} \qquad \sim \mathrm{N}(0,\ 1)$$

Geweke convergence diagnostics for binary BART

- We have a z_i corresponding to each $\theta_i = h(f(x_i))$
- In the **BART** R package, we created the `gewekediag` function which was adapted from the **coda** R package
  Plummer, Best et al. 2006

```
system.file('demo/geweke.pbart2.R', package='BART') &
system.file('demo/geweke.pbart3.R', package='BART')
```

Geweke convergence diagnostics for binary BART: simulated data scenario

```
system.file('demo/geweke.pbart2.R', package='BART') &
system.file('demo/geweke.pbart3.R', package='BART')
```

$$N = 100, 1000, 10000$$

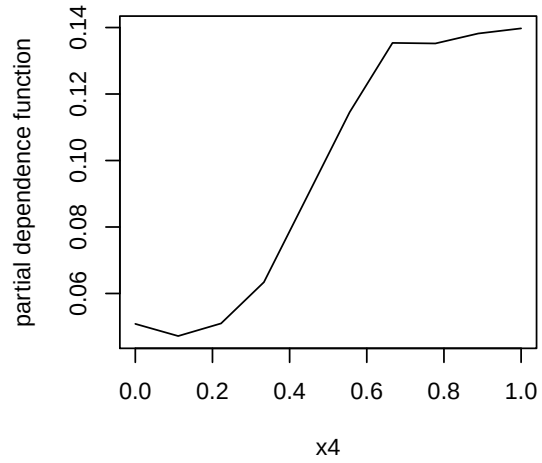
$$K = 50$$

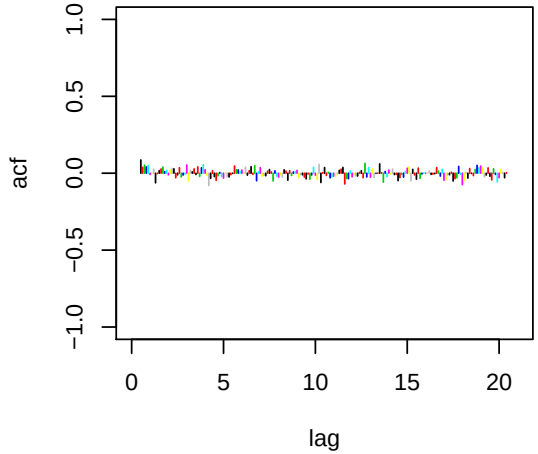
$$f(x_i) = -1.5 + \sin(\pi x_{1i} x_{2i}) + 2(x_{3i} - 0.5)^2 + x_4 + 0.5x_5$$

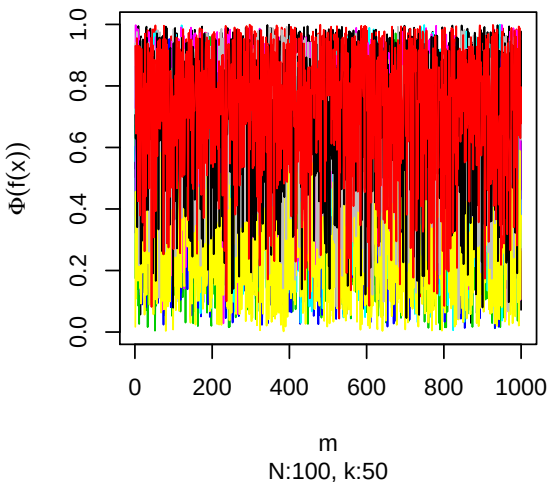
$$z_i \sim \mathrm{N}(f(x_i),\ 1)$$

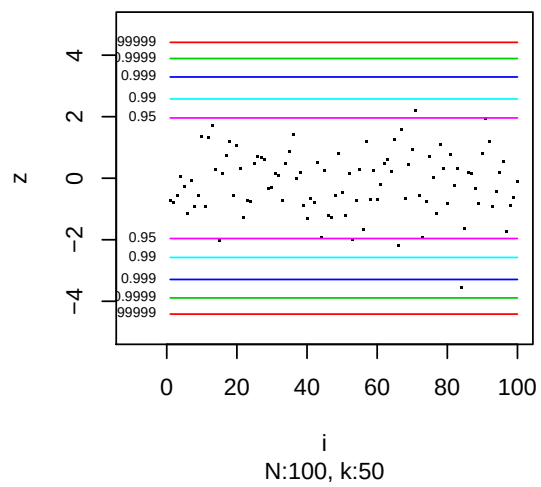
$$y_i = \mathrm{I}(z_i > 0)$$

Geweke convergence diagnostics for binary BART: $N = 100$

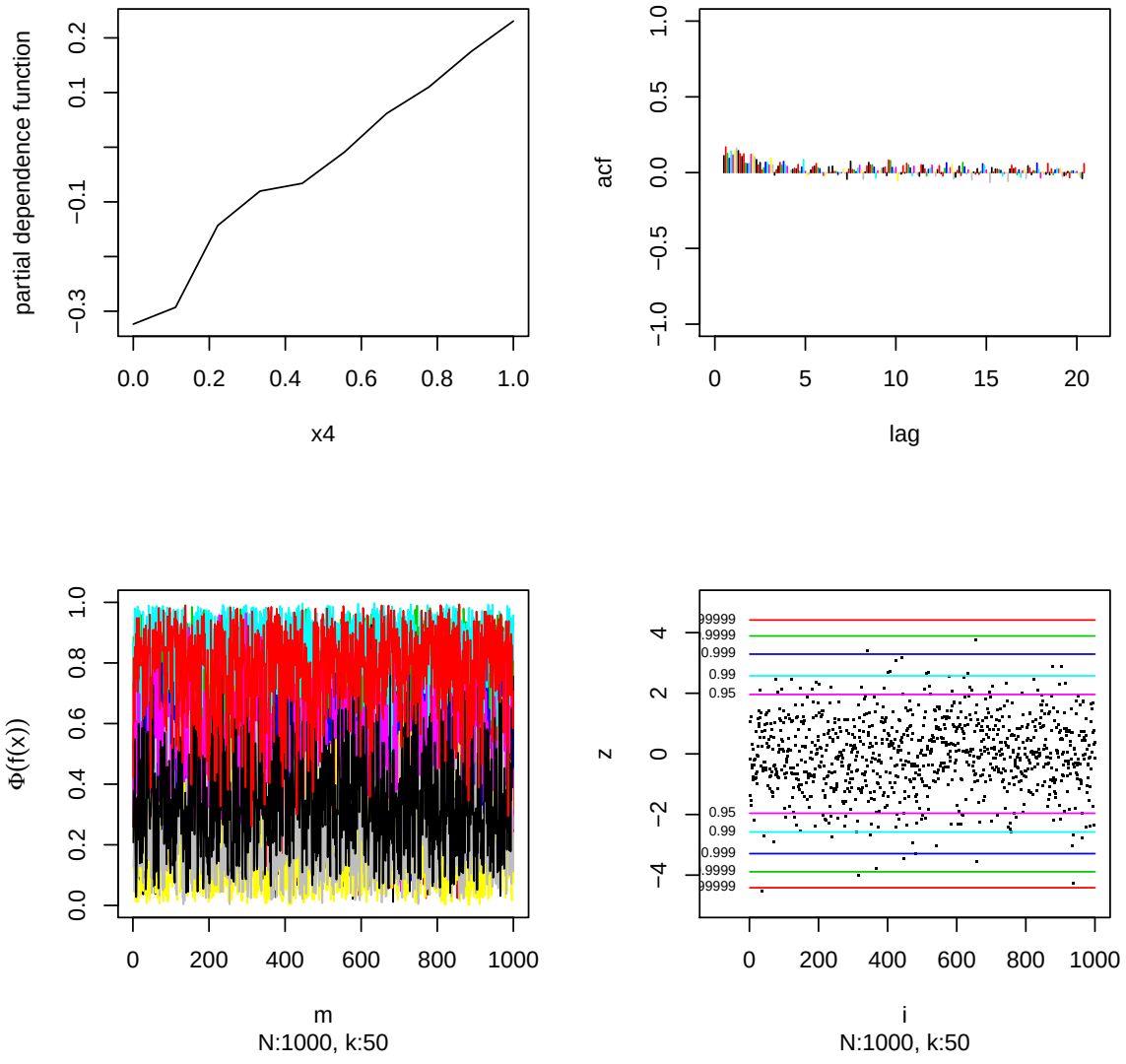




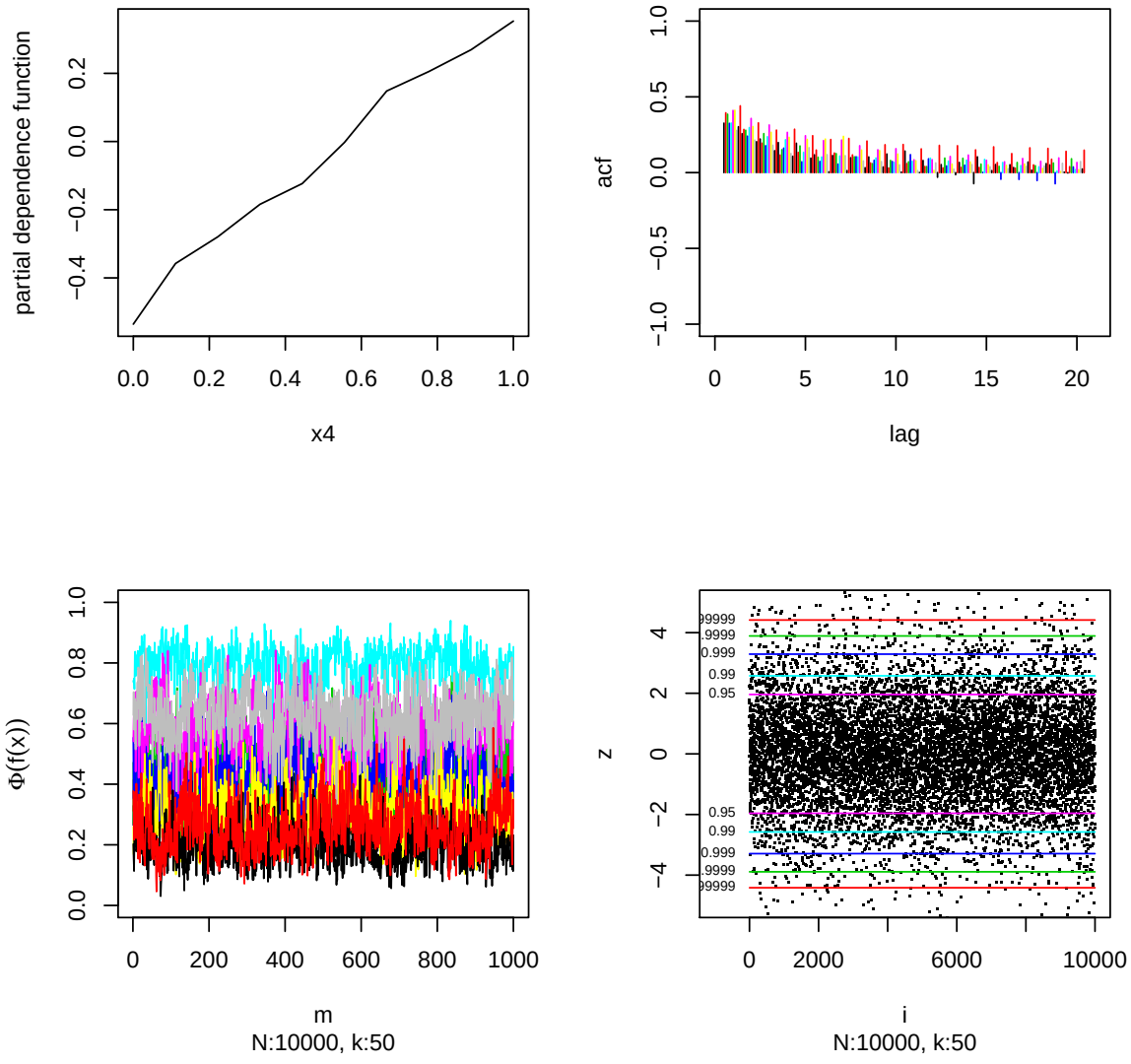




Geweke convergence diagnostics for binary BART: $N = 1000$



Geweke convergence diagnostics for binary BART: $N = 10000$

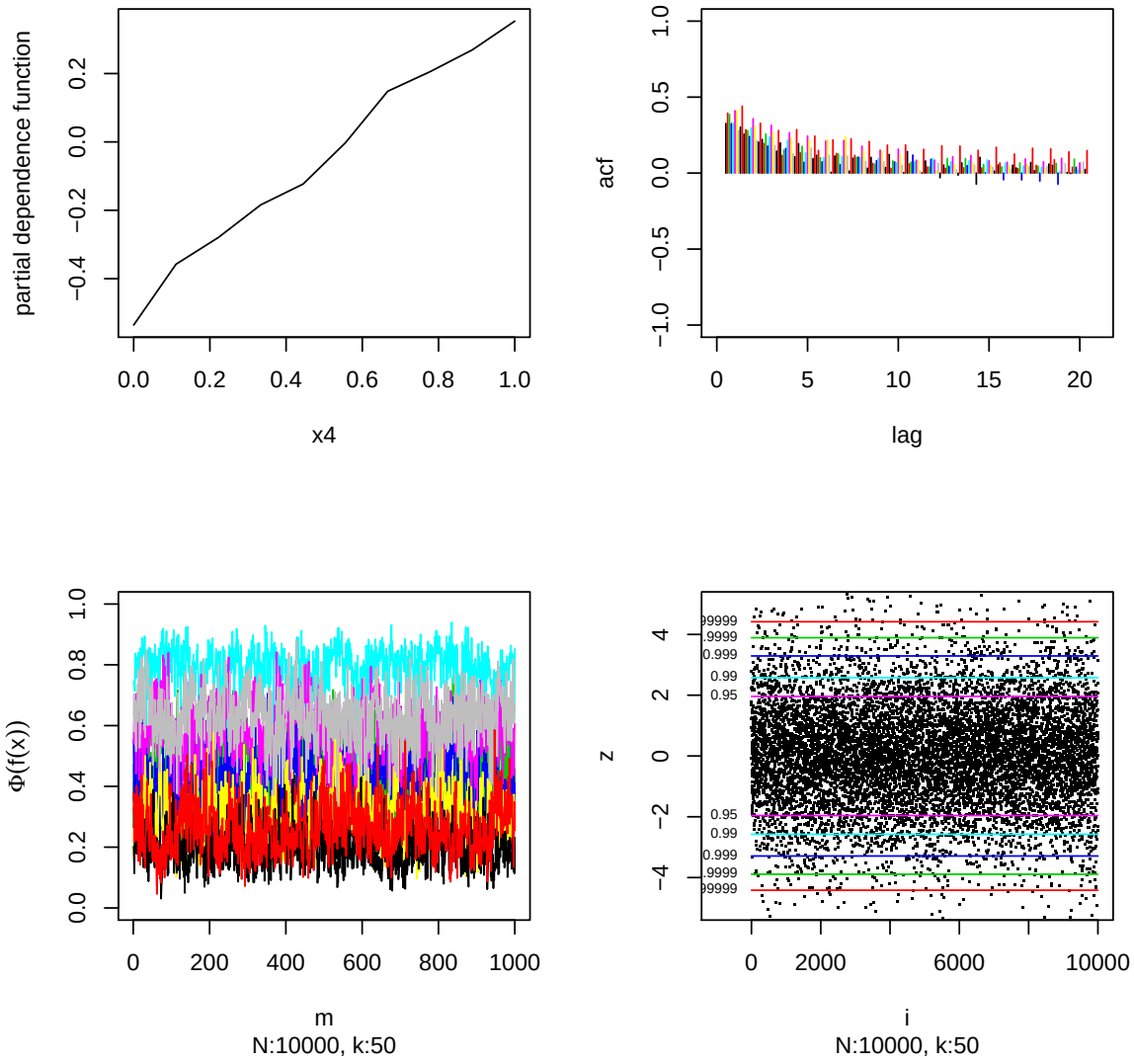


Geweke convergence diagnostics for binary BART: convergence countermeasures for $N = 10000$

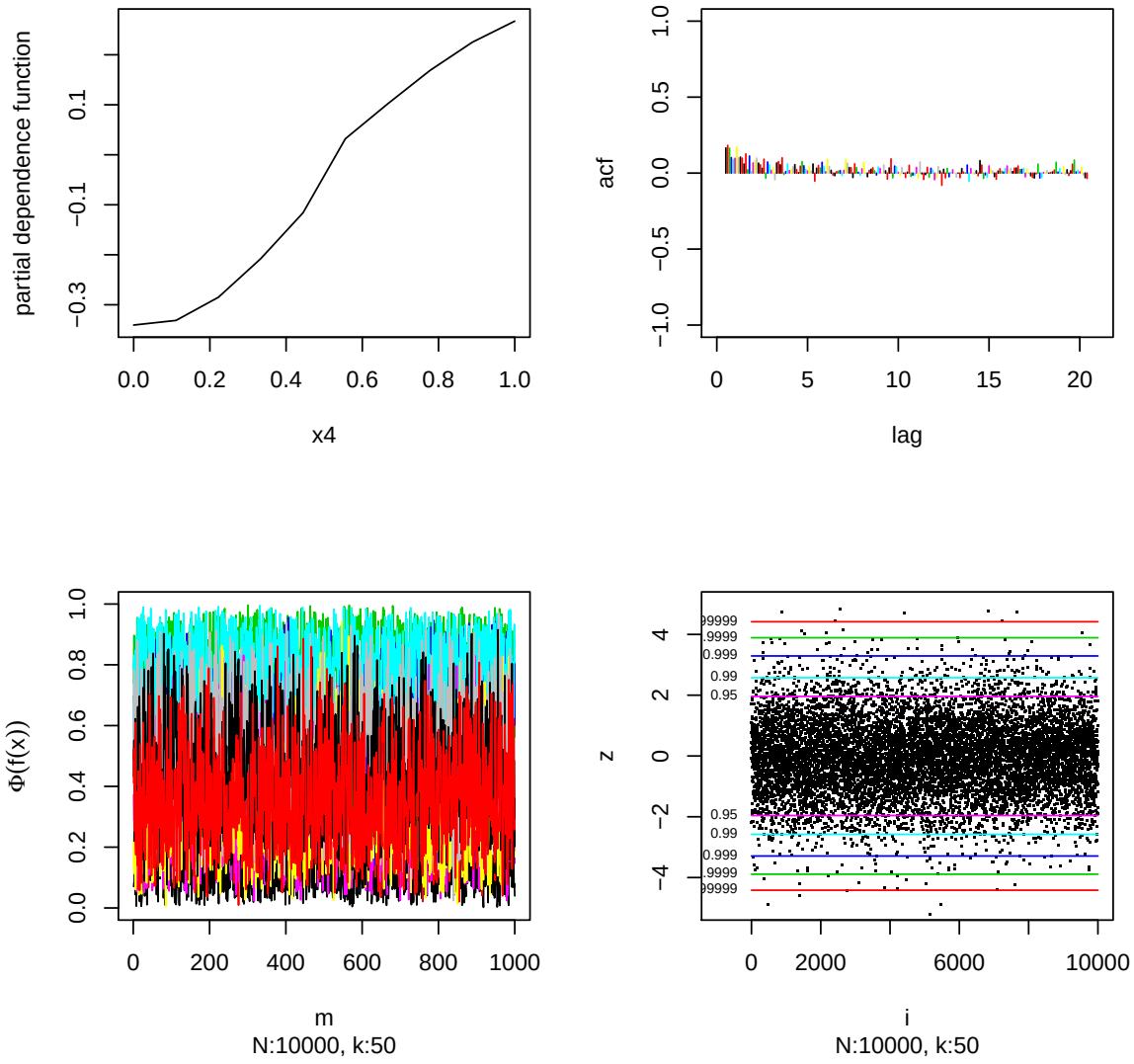
```
system.file('demo/geweke.pbart3.R', package='BART')
```

- Validation set is a 10% random sample of the training set
- Randomly partition the training set into 10 sets of $N = 1000$
- Analyze the 10 training sets independently with BART
- Combine/stack the 10 validation set MCMC chains
- Perform convergence diagnostics and inference on the combined validation chains

Geweke convergence diagnostics for binary BART: $N = 10000$ without countermeasures



Geweke convergence diagnostics for binary BART: $N = 10000$ with countermeasures



Geweke convergence diagnostics for binary BART: $N = 1000$ without countermeasures