BART:
Bayesian additive regression trees

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Most of the notes were kindly provided by Rob McCulloch (Arizona State University), which are based on Chipman, George and McCulloch (2010) BART: Bayesian additive regression trees, *The Annals of Applied Statistics*, 4(1), 266-298.

Outline

Nonlinear multiple regression

- Example of nonlinear function
- `R` package `BayesTree`
- Comparing 42 datasets
- Ensemble methods

A regression tree model

- A coordinate view of $g(x;\theta)$
- The BART model
- BART MCMC
- Connections to other modeling ideas
- Some Distinguishing Feastures of BART
- Example: Friedman simulated exercise
- Example: Drug Discovery
- `motorcycle` dataset

Abstract of the BART paper

We develop a Bayesian "sum-of-trees" model where each tree is constrained by a regularization prior to be a weak learner, and fitting and inference are accomplished via an iterative Bayesian backfitting MCMC algorithm that generates samples from a posterior.

Effectively, BART is a nonparametric Bayesian regression approach which uses dimensionally adaptive random basis elements.

Motivated by ensemble methods in general, and boosting algorithms in particular, BART is defined by a statistical model: a prior and a likelihood.

By keeping track of predictor inclusion frequencies, BART can also be used for model-free variable selection.

Outline

Nonlinear regression

We want to "fit" the fundamental model:

$$y_i = g(x_i; \theta) + \epsilon_i$$

BART is a Markov Monte Carlo Method[1] that draws from

$$g(x; \theta) \mid (x, y)$$

We can then use the draws as our inference for $g(x; \theta)$.

[1] Monte Carlo tools were crucial to popularize Bayesian estimation/inference/tools over the last 30 or so years across a wide range of sciences and industry.

Turning the Bayesian crank

To get the draws, we will have to:

- Put a prior on $g(x;\theta)$.
- Specify a Markov chain whose stationary distribution is $p\left(g(x;\theta) \mid (x,y)\right)$.

Example of nonlinear function

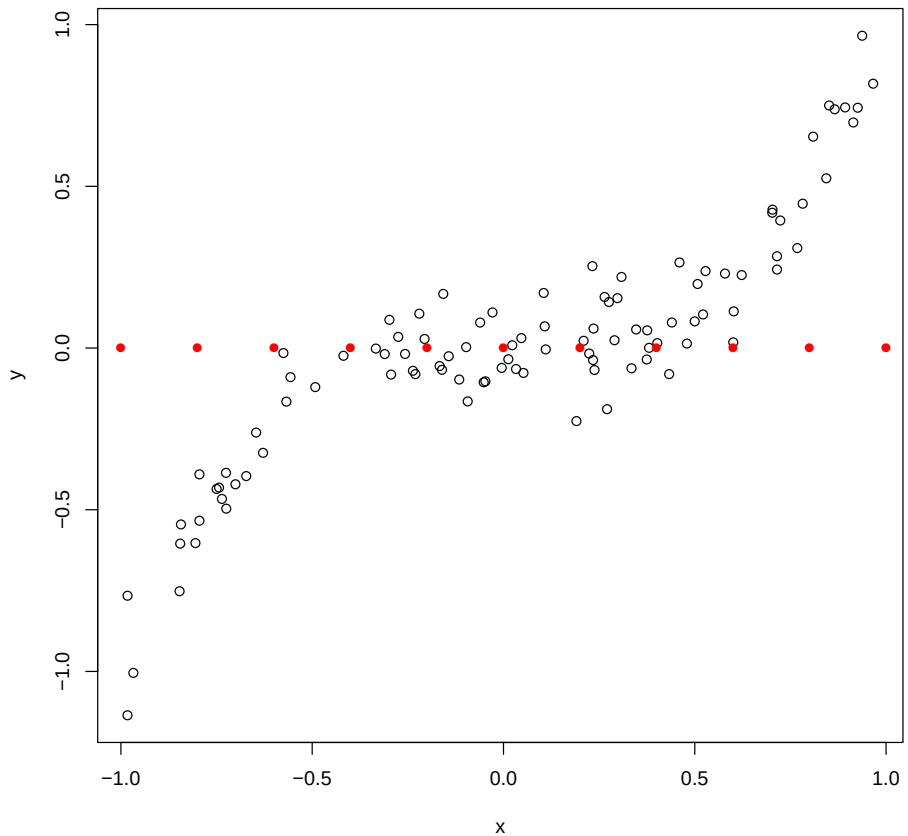
Simulate data from the model:

$$y_i = x_i^3 + \epsilon_i \quad \epsilon_i \sim N(0, \sigma^2) \ \ iid$$

```
-----------------------------------------
n = 100
sigma = 0.1
g = function(x) {x^3}
set.seed(14)
x = sort(2*runif(n)-1)
y = g(x) + sigma*rnorm(n)
xtest = seq(-1,1,by=0.2)
-----------------------------------------
```

`xtest` are *out of sample* x values at which we wish to infer g or make predictions.

```
plot(x,y)
points(xtest,rep(0,length(xtest)),col="red",pch=16)
```



Red is `xtest`

R package BayesTree

```
library(BayesTree)
rb = bart(x,y,xtest)
length(xtest)
[1] 11
dim(rb$yhat.test)
[1] 1000   11
```

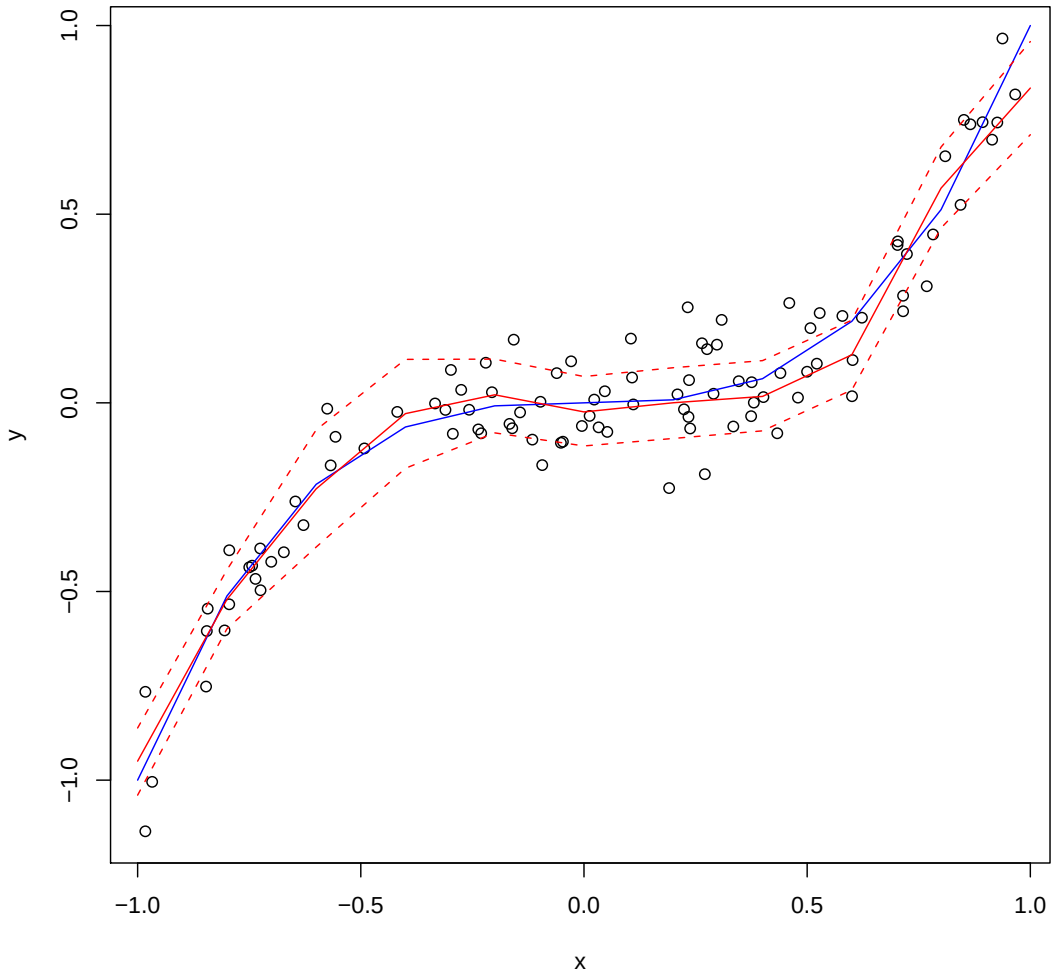
The (i, j) element of `yhat.test` is

the i^{th} draw of g evaluated at the j^{th} value of `xtest`.

1,000 draws of g, each of which is evaluated at 11 `xtest` values.

Fitted model

```
plot(x,y)
lines(xtest,xtest^3,col='blue')
lines(xtest,apply(rb$yhat.test,2,mean),col='red')
qm = apply(rb$yhat.test,2,quantile,probs=c(.05,.95))
lines(xtest,qm[1,],col='red',lty=2)
lines(xtest,qm[2,],col='red',lty=2)
```



Let us get serious: out of sample prediction

- Out of sample predictive comparisons on 42 data sets (thanks to Wei-Yin Loh!!)
- $p = 3 - 65$, $n = 100 - 7,000$.
- for each data set 20 random splits into 5/6 train and 1/6 test
- use 5-fold cross-validation on train to pick hyperparameters (except BART-default!)
- gives $20 \times 42 = 840$ out-of-sample predictions, for each prediction, divide rmse of different methods by the smallest

Competitors

- Linear regression with L1 regularization - Efron et al. (2004)
- Gradient boosting - Friedman (2001)
  Implemented as `gbm` in R by Ridgeway (2004)
- Random forests - Breiman (2001)
  Implemented as `randomforest` in R
- Neural networks with one layer of hidden units
  Implemented as `nnet` in R by Venables and Ripley (2002)

These competitors, like BART, are black box predictors.

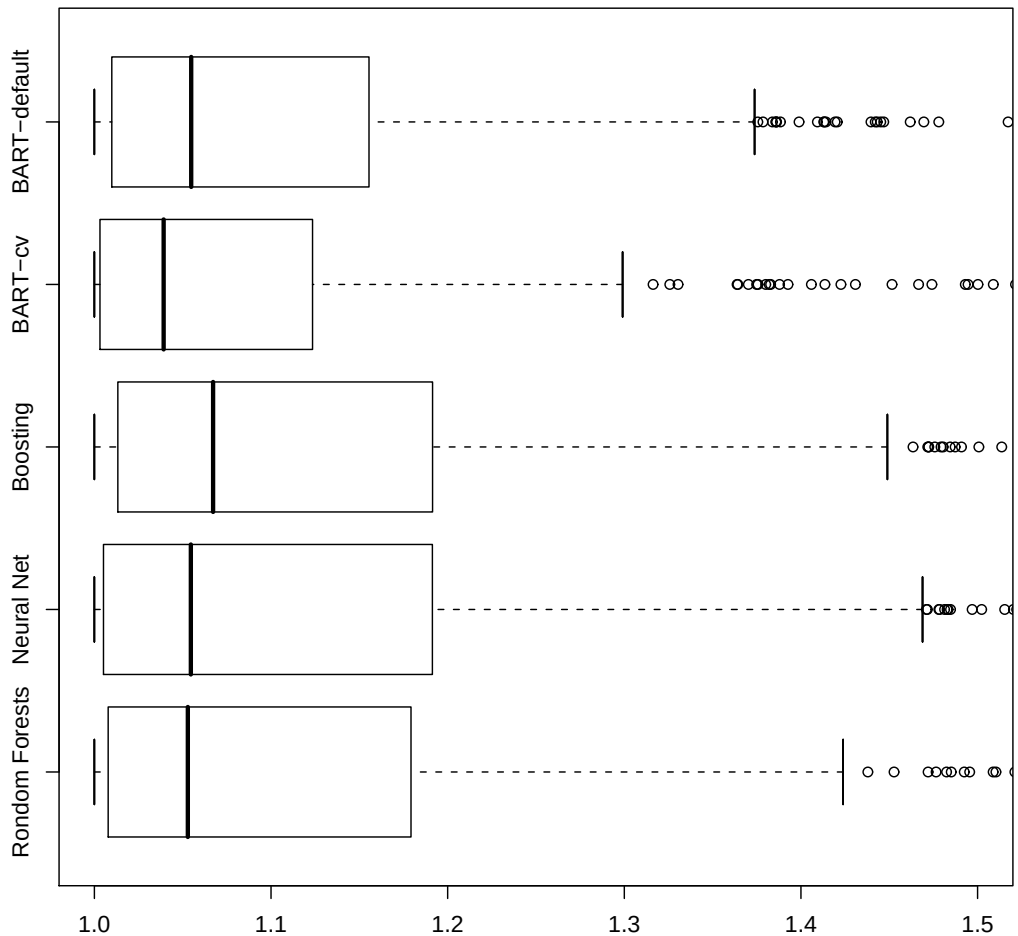
Trees, Bayesian CART[2] and Bayesian treed regression[3] models were not considered, since they tend to sacrifice predictive performance for interpretability.

With the exception of BART-default (which requires no tuning), the operational parameters of every method were chosen via 5-fold cross-validation within each training set.

[2] Chipman, George and McCulloch (1998)
[3] Chipman, George and McCulloch (2002)

Comparison

- Each boxplots represents 840 predictions for a method
- 1.2 means you are 20% worse than the best
- BART-cv best
- BART-default (use default prior) does amazingly well!!



Relative RMSE

TABLE 3
(50%, 75%) quantiles of relative RMSE values for each method across the 840 test/train splits

Method	**(50%, 75%)**
Lasso	(1.196, 1.762)
Boosting	(1.068, 1.189)
Neural net	(1.055, 1.195)
Random forest	(1.053, 1.181)
BART-default	(1.055, 1.164)
BART-cv	(1.037, 1.117)

Relative RMSE > 1.5

- Lasso: 29.5%
- Random forests: 16.2%
- Neural net: 9.0%
- Boosting: 13.6%
- BART-cv: 9.0%
- BART-default: 11.8%

Ensemble methods

Various methods which combine a set of tree models, so called ensemble methods, have attracted much attention, each of which use different techniques to fit a linear combination of trees.

- Bagging (Breiman, 1996)
- Random forests (Breiman, 2001)
- Boosting (Friedman, 2001)
- Bayesian model averaging (Chipman, George and McCulloch, 1998)

Bagging and random forests use randomization to create a large number of independent trees, and then reduce prediction variance by averaging predictions across the trees.

Boosting fits a sequence of single trees, using each tree to fit data variation not explained by earlier trees in the sequence.

Bayesian model averaging (BMA) applied to the posterior arising from a Bayesian single-tree model.

Key references

Breiman (1996) Bagging predictors
Machine Learning, 26, 123-140.

Hastie and Tibshirani (2000) Bayesian Backfitting
Statistical Science, 15(3), 196-223.

Friedman (2001) Greedy function approximation: A gradient boosting machine
Annals of Statistics, 29, 1189-1232.

Breiman (2001) Random forests
Machine Learning, 45, 5-32.

Chipman, George and McCulloch (1998) Bayesian CART model search
Journal of the American Statistical Association, 93, 935-960.

Efron, Hastie, Johnstone and Tibshirani (2004) Least angle regression
Annals of Statistics, 32, 407-499.

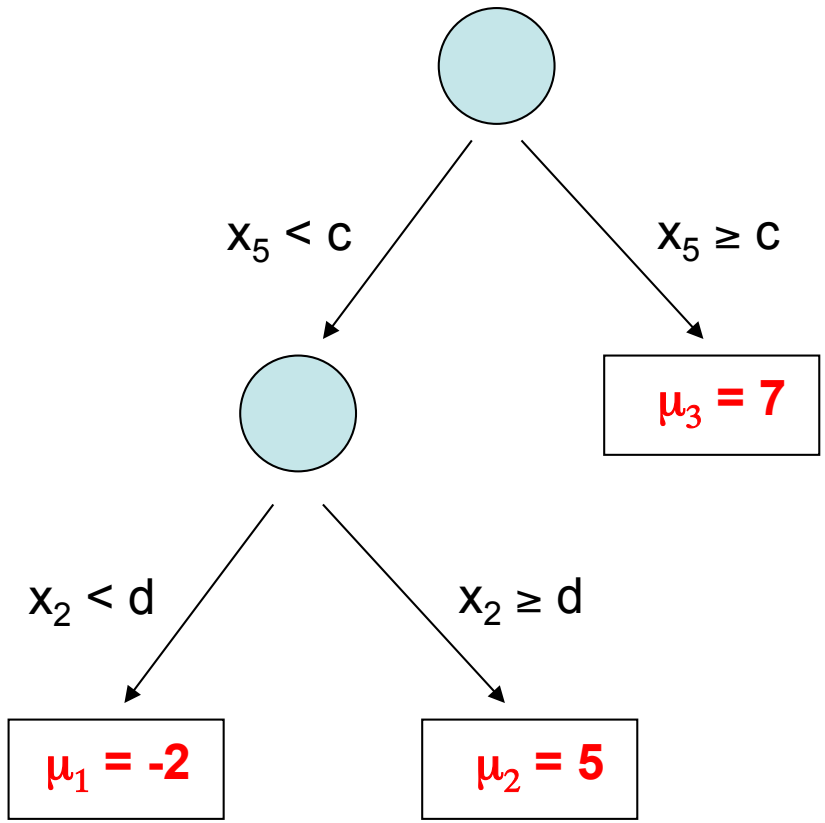
Outline

A regression tree model

Let T denote the tree structure including the decision rules.

Let $M = \{\mu_1, \mu_2, \ldots, \mu_b\}$ denote the set of bottom node μ's.

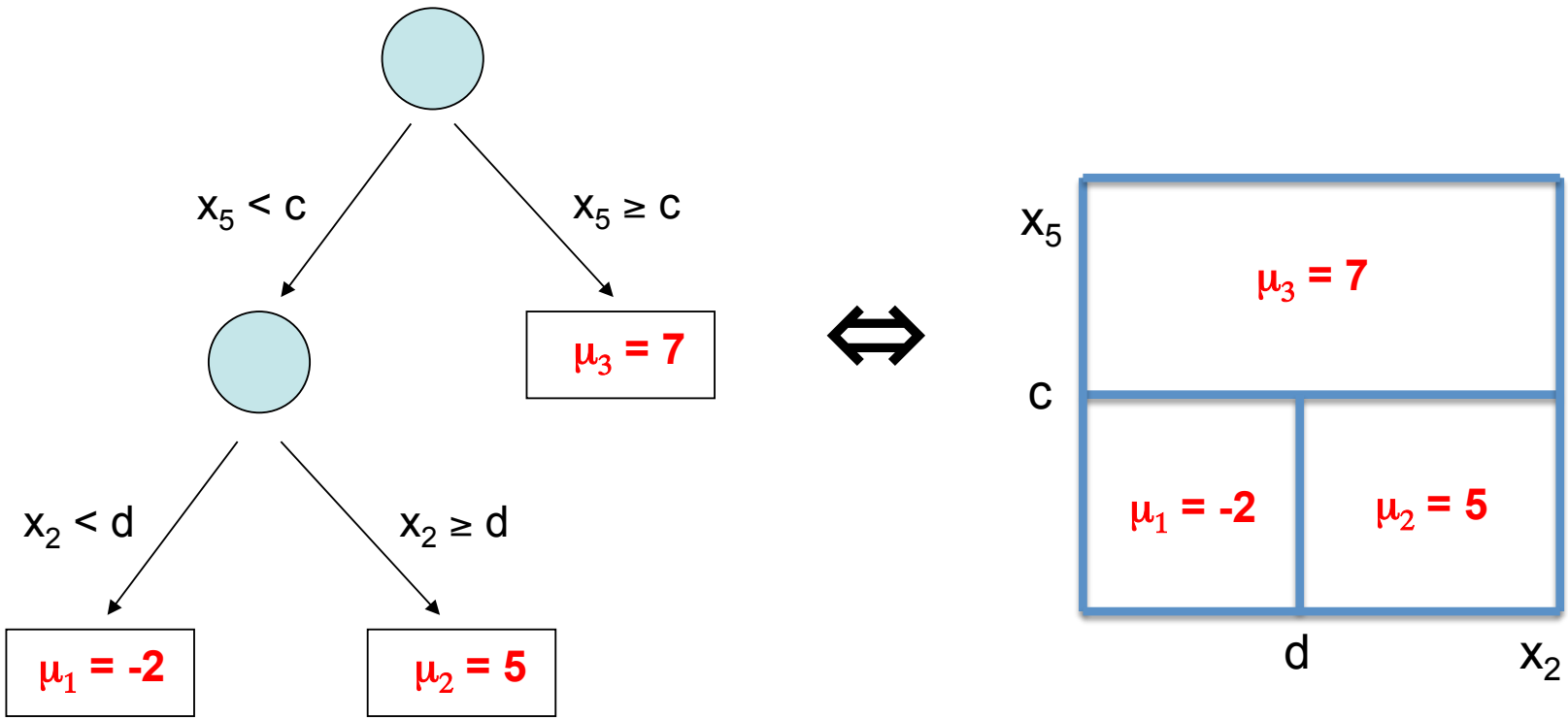
Let $g(x; \theta)$, $\theta = (T, M)$ be a regression tree function that assigns a μ value to x.



A single tree model:

$$y_i = g(x_i; \theta) + \epsilon_i.$$

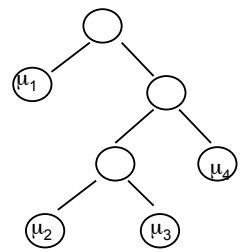
A coordinate view of $g(x;\theta)$



Easy to see that $g(x;\theta)$ is just a step function.

The BART model

$$Y = g(x;T_1,M_1) + g(x;T_2,M_2) + \ldots + g(x;T_m,M_m) + \sigma z, \quad z \sim N(0,1)$$



$m = 200, 1000, \ldots,$ big, $\ldots$

$f(x \mid \cdot)$ is the sum of all the corresponding μ's at each bottom node.

Such a model combines additive and interaction effects.

Complete the model with a regularization prior

The prior of the BART model can be written as

$$\pi(\theta) = \pi((T_1, M_1), (T_2, M_2), \ldots, (T_m, M_m), \sigma).$$

π wants:

- Each T small.
- Each μ small.
- "nice" σ (smaller than least squares estimate).

We refer to π as a regularization prior because it keeps the overall fit small.

In addition, it keeps the contribution of each $g(x; T_i, M_i)$ model component small.

Consider the prior on μ.
Let θ denote all the parameters.

$$f(x \mid \theta) = \mu_1 + \mu_2 + \cdots \mu_m.$$

Let $\mu_i \sim N(0, \sigma_\mu^2)$, iid.

$$f(x \mid \theta) \sim N(0, m\,\sigma_\mu^2).$$

In practice we often, unabashadly, use the data by first centering and then choosing σ_μ so that

$$f(x \mid \theta) \in (y_{min}, y_{max})$$

with high probability:

$$\sigma_\mu^2 \propto \frac{1}{m}.$$

BART MCMC

The model/prior is described by

$$Y = g(x;T_1,M_1) + ... + g(x;T_m,M_m) + \sigma z$$
plus
$$\pi((T_1,M_1),....(T_m,M_m),\sigma)$$

First, it is a "simple" Gibbs sampler:

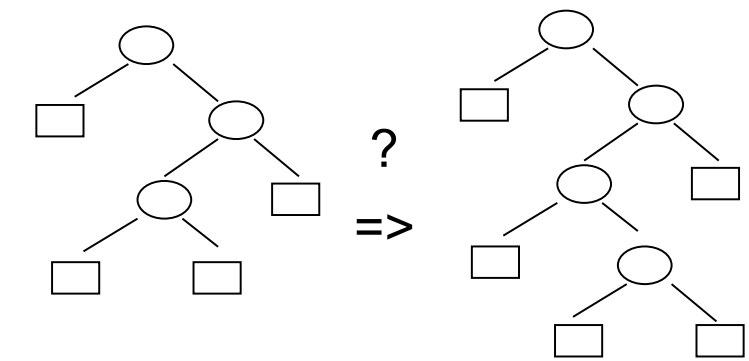
$$\begin{aligned} (T_i, M_i) \quad &| \quad (T_1, M_1, \ldots, T_{i-1}, M_{i-1}, T_{i+1}, M_{i+1}, \ldots, T_m, M_m, \sigma) \\ \sigma \quad &| \quad (T_1, M_1, \ldots, \ldots, T_m, M_m) \end{aligned}$$

To draw $(T_i, M_i) \,|\, \cdot$ we subract the contributions of the other trees from both sides to get a simple one-tree model.

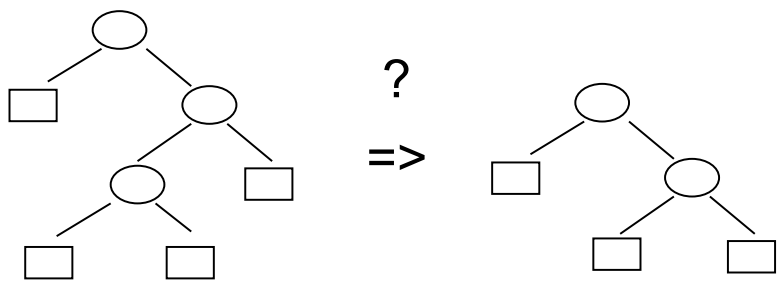
We integrate out M to draw T and then draw $M \,|\, T$.

Birth-death moves

To draw T we use a Metropolis-Hastings with Gibbs step.
We use various moves, but the key is a "birth-death" step.

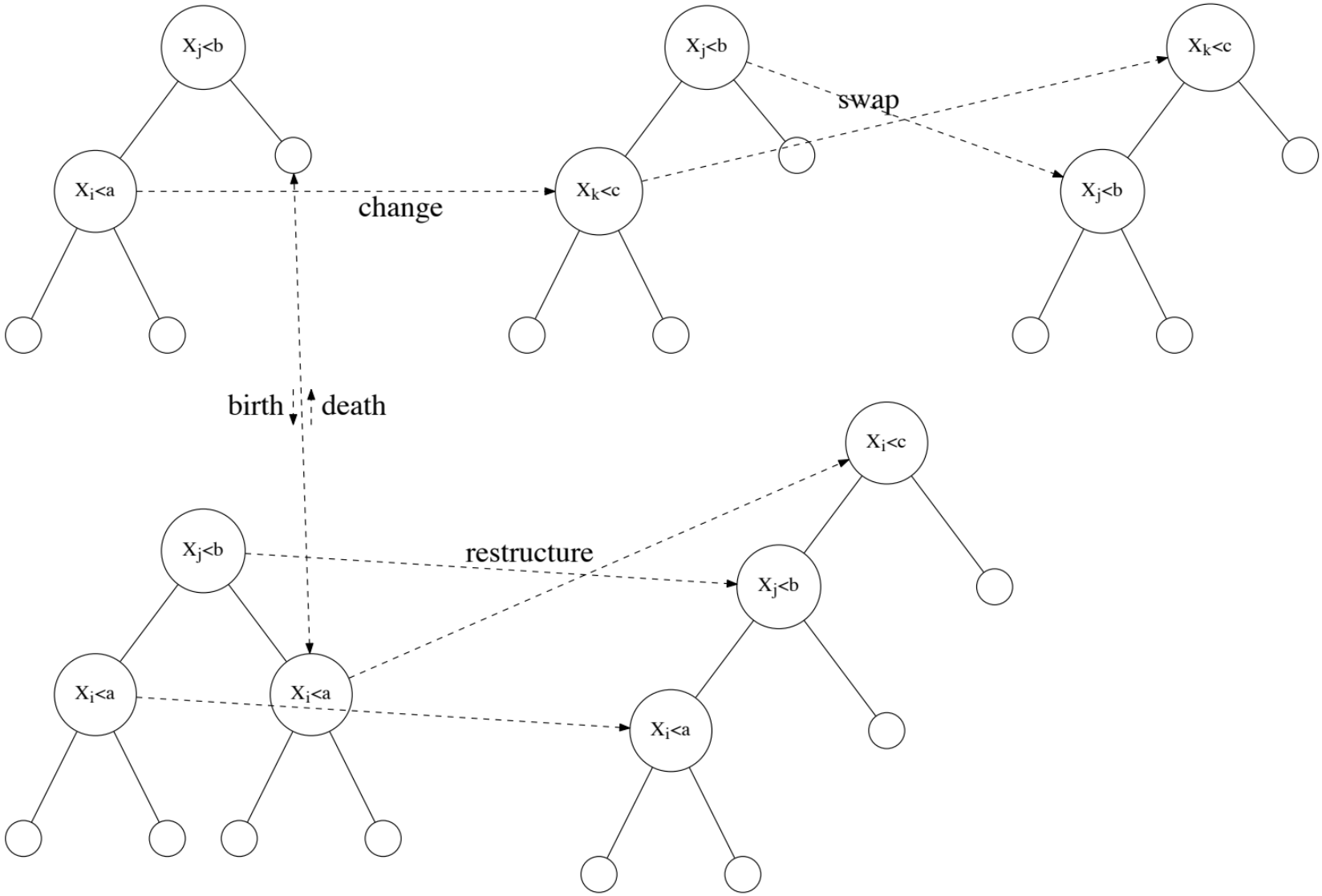


propose a more complex tree



propose a simpler tree

Tree moves[4]



[4] http://www.matthewpratola.com/wp-content/uploads/2017/11/stat8810-slides13.pdf

Connections to other modeling ideas

$$Y = g(x;T_1,M_1) + \ldots + g(x;T_m,M_m) + \sigma z$$
plus
$$\pi((T_1,M_1),\ldots.(T_m,M_m),\sigma)$$

Bayesian nonparametrics:

- Lots of parameters to make model flexible.
- A strong prior to shrink towards a simple structure.
- BART shrinks towards additive models with some interaction.

Dynamic random basis:

- $g(x; T_1, M_1), g(x; T_2, M_2), \ldots, g(x; T_m, M_m)$ are dimensionally adaptive.

Gradient boosting:

- Overall fit becomes the cumulative effort of many weak learners.

Some Distinguishing Feastures of BART

$$Y = g(x;T_1,M_1) + ... + g(x;T_m,M_m) + \sigma z$$
plus
$$\pi((T_1,M_1),....(T_m,M_m),\sigma)$$

- BART is NOT Bayesian model averaging of single tree model.
- Unlike boosting and random forests, BART updates a set of m trees over and over, *stochastic search*.
- Choose m large for flexible estimation and prediction.
- Choose m smaller for variable selection
  - fewer trees forces the x's to compete for entry.

Example: Friedman simulated exercise

For $i = 1, \ldots, n = 100$,

$$y_i = g(x_i) + \epsilon_i, \quad \epsilon_i \sim N(0, 1),$$

where

$$g(x_i) = 10 \sin(\pi x_{i1} x_{i2}) + 20(x_{i3} - 0.5)^2 + 10 x_{i4} + 5 x_{i5}$$

Add 5 irrelevant $x_{i6}, \ldots, x_{i,10}$ $(p = 10)$.

$x_{ij} \sim \text{uniform}(0, 1)$.

$\hat{g}(x)$ is the posterior mean.

Root MSE

Compute out of sample RMSE using 1,000 simulated $x \in R^{10}$.

$$\text{RMSE} = \sqrt{\frac{1}{1000}\sum_{i=1}^{1000}(g(x_i) - \hat{g}(x_i))^2}$$

Method	average RMSE	se(RMSE)
Random Forests	2.655	0.025
Linear Regression	2.618	0.016
Neural Nets	2.156	0.025
Boosting	2.013	0.024
MARS	2.003	0.060
BART-cv	1.787	0.021
BART-default	1.759	0.019

Details about competing schemes

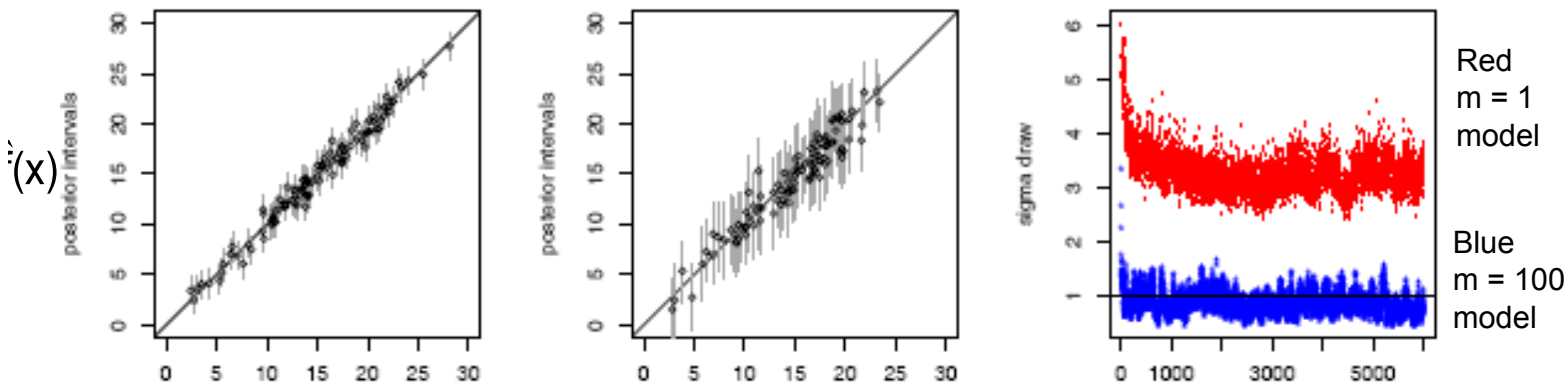
Method	Parameter	Values considered
Boosting	# boosting iterations	`n.trees`= $1, 2, \ldots, 2000$
	Shrinkage (multiplier of each tree added)	`shrinkage`= 0.01, 0.05, 0.10, 0.25
	Max depth permitted for each tree	`interaction.depth`= 1,2,3,4
Neural Nets	# hidden units	`size`= 10, 15, 20, 25, 30
	Decay (penalty coef on sum-squared weights)	`decay`= 0.50, 1, 1.5, 2, 2.5
	(Max # optimizer iterations, # restarts)	fixed at `maxit`= 1000 and 5
Random Forests	# of trees	`ntree`= 200, 500, 1000
	# variables sampled to grow each node	`mtry`= 3, 5, 7, 10
MARS	GCV penalty coefficient	`gcv`= 1, 2, ..., 8
BART -cv	Sigma prior: (ν, q) combinations	(3,0.90), (3,0.99), (10,0.75)
	μ Prior: k value for σ_μ	1, 1.5, 2, 2.5, 3
	(# trees m, iterations used, burn-in iterations)	fixed at (200, 1000,500)
BART -default	Sigma prior: (ν, q) combinations	fixed at (3,0.90)
	μ Prior: k value for σ_μ	fixed at 2
	(# trees m, iterations used, burn-in iterations)	fixed at (200, 1000,500)

Table 1: Operational parameters for the various competing models. `Names` in last column indicate parameter names in R.

Results for one draw

95% posterior intervals vs true f(x)

σ draws



in-sample f(x)

out-of-sample f(x)

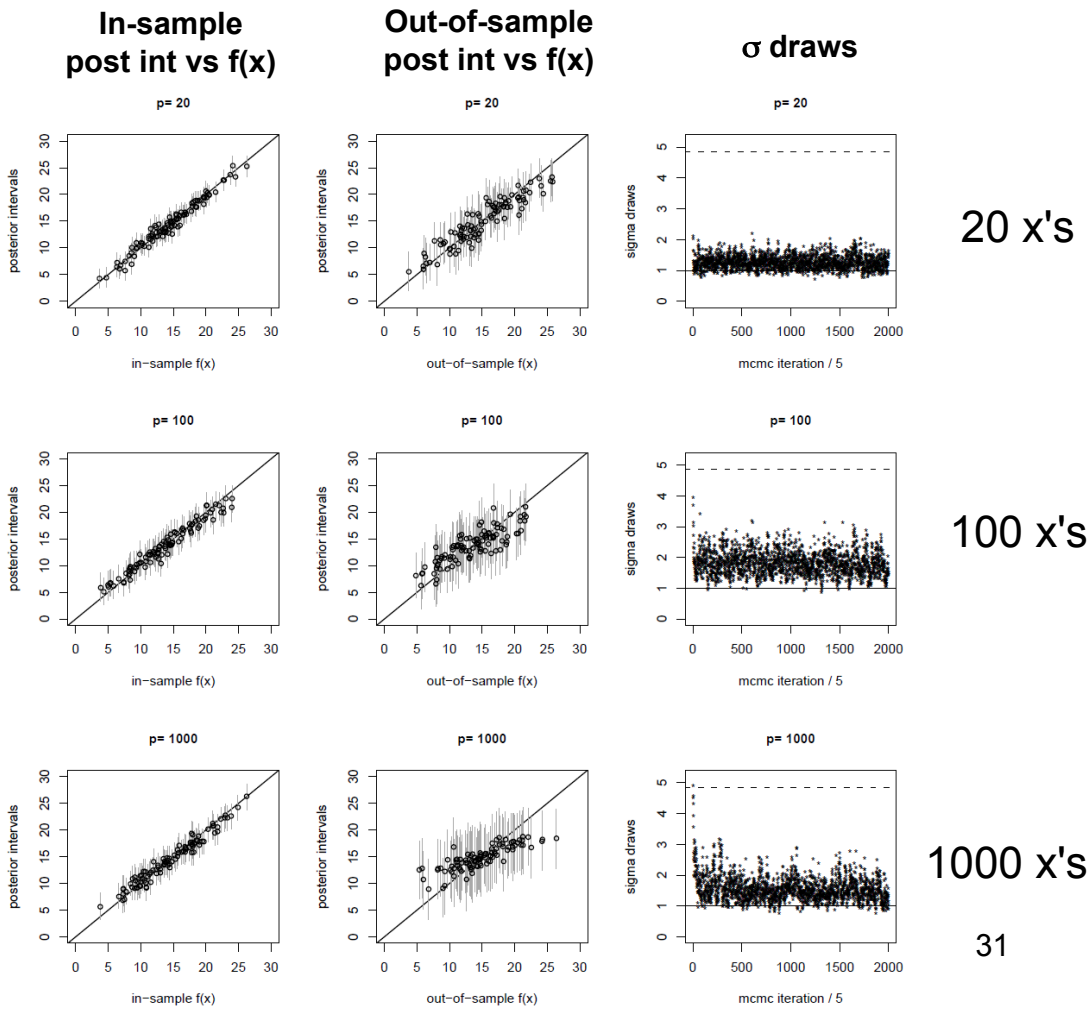
MCMC iteration

Frequentist coverage rates of 90% posterior intervals:
in sample: 87%
out of sample: 93 %.

Adding many useless predictors

Added many useless x's to Friedman's example

With only 100 observations on y and *1000 x's, BART yielded "reasonable" results !!!!*

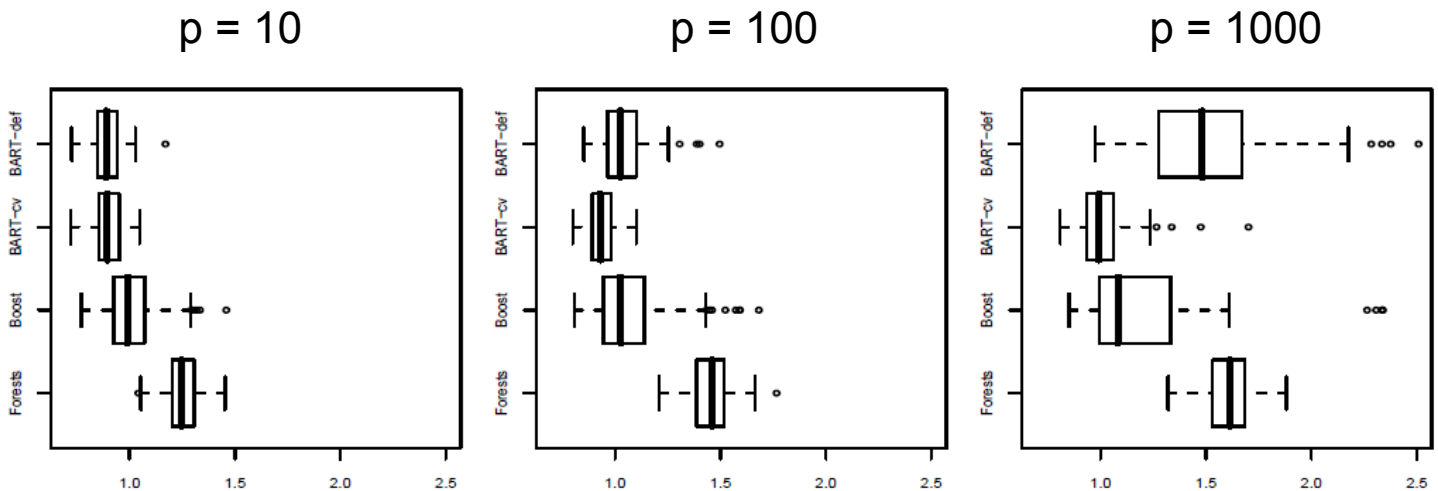


Big p, small n

$n = 100$.

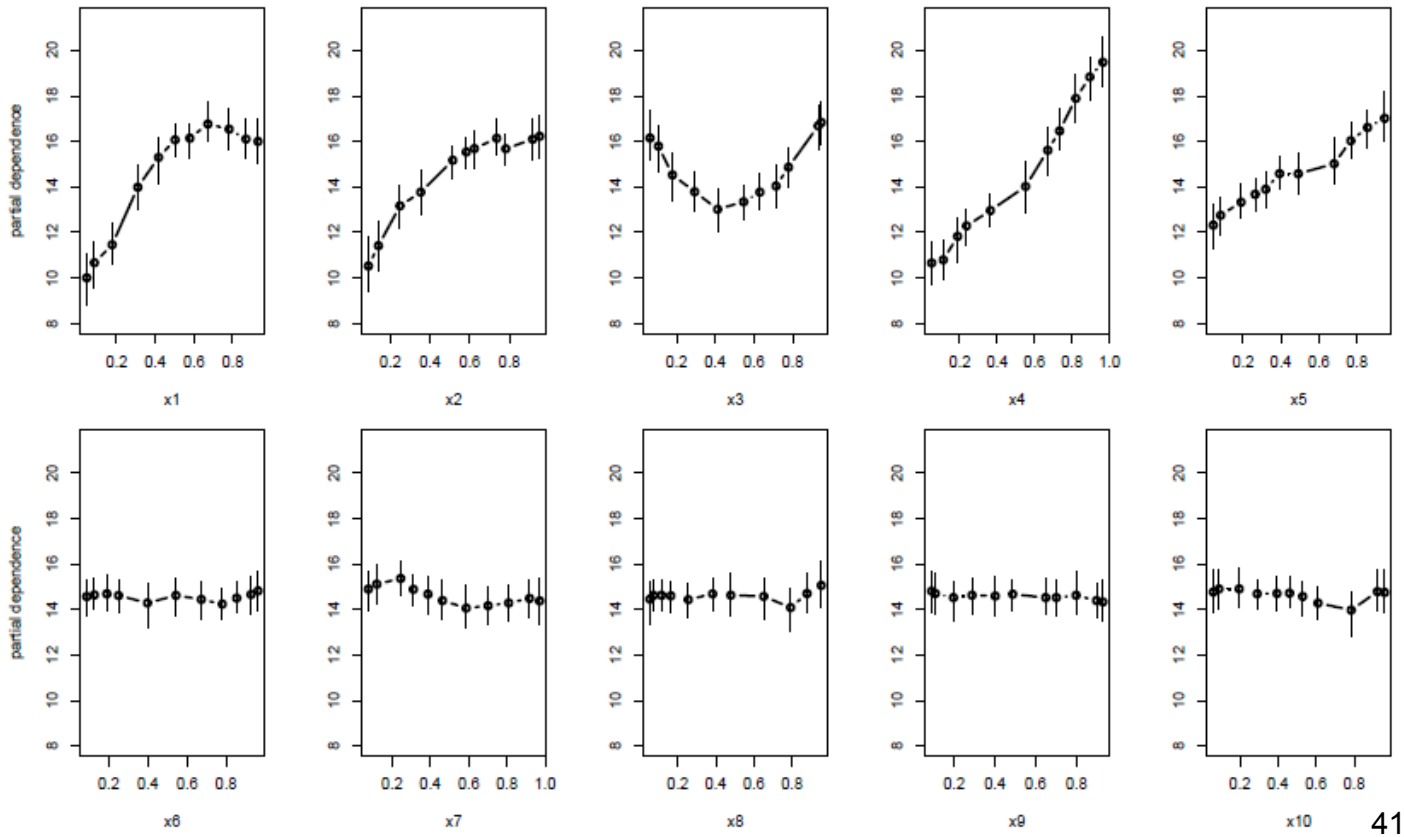
Compare BART-default,BART-cv,boosting, random forests.

Out of sample RMSE.



Partial Dependence plot

Vary one x and average out the others.



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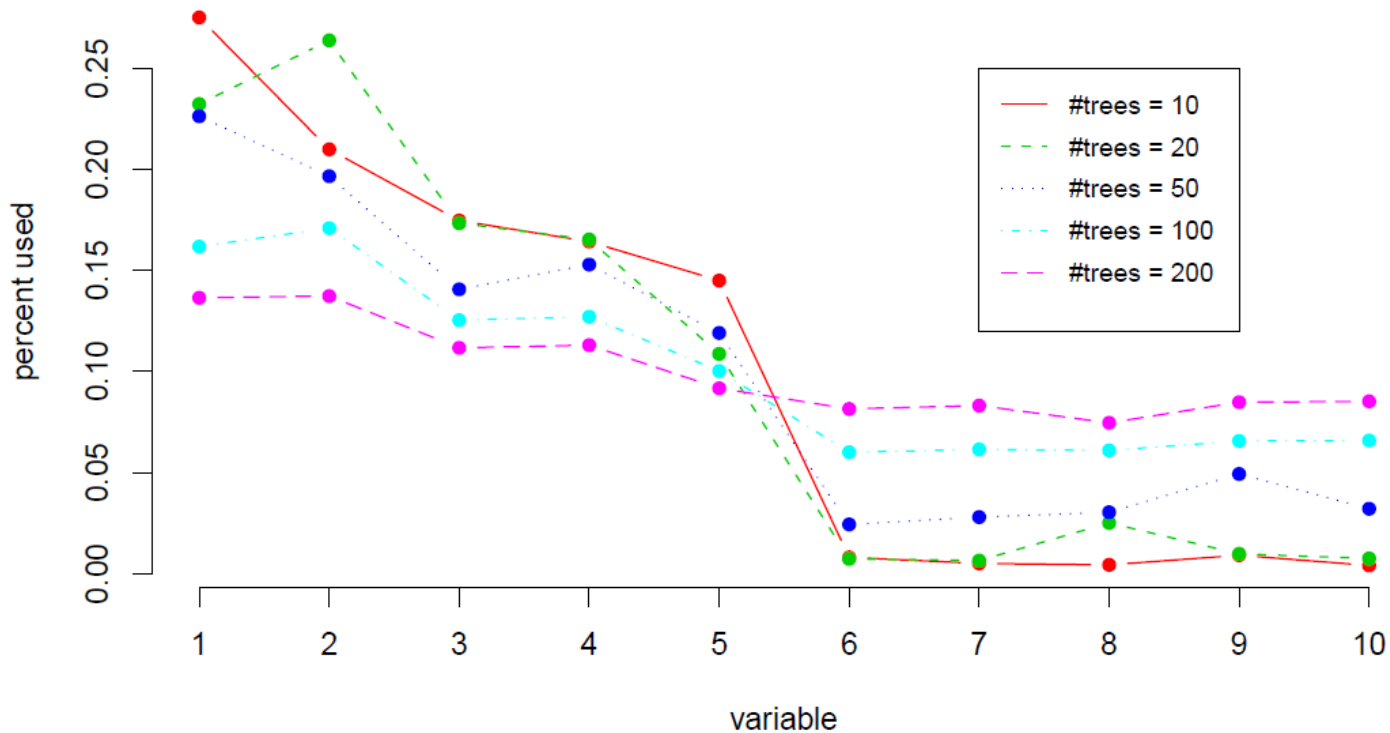
Variable selection

Frequency with which a variable is used.



Example: Drug Discovery

Goal: To predict the "activity" of a compound against a biological target.

That is: $y = 1$ means drug worked (compound active), 0 means it does not.

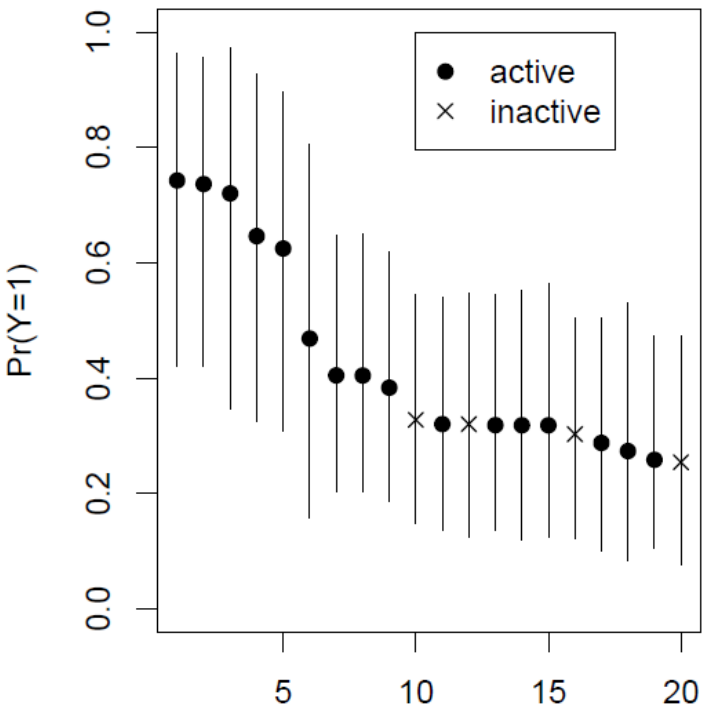
Easy to extend BART to binary y using Albert & Chib.

$n = 29,3744 \rightarrow$ 14,687 train, 14,687 test.
$p = 266$ characterizations of the compound's molecular structure.

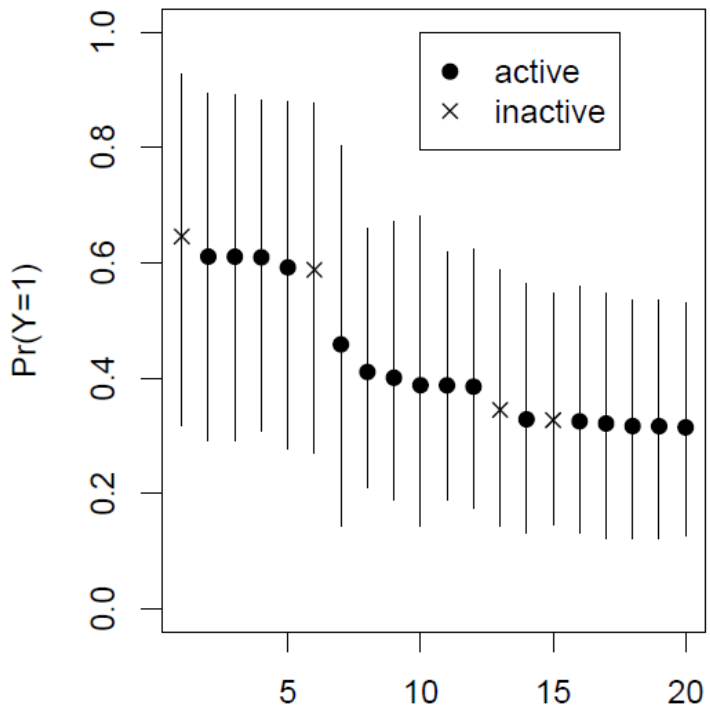
Again, out-of-sample prediction competitive with other methods, compared to neural-nets, boosting, random forests, support vector machines.

20 compounds with highest $Pr(Y = 1 \mid x)$ estimate.
90% posterior intervals for $Pr(Y = 1 \mid x)$.

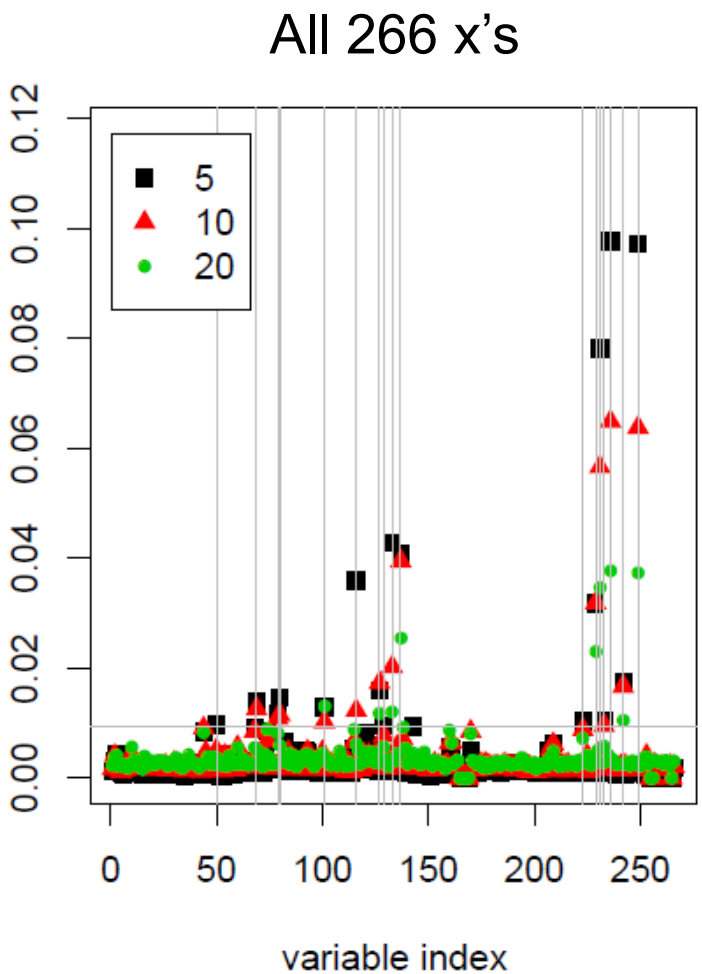
In-sample

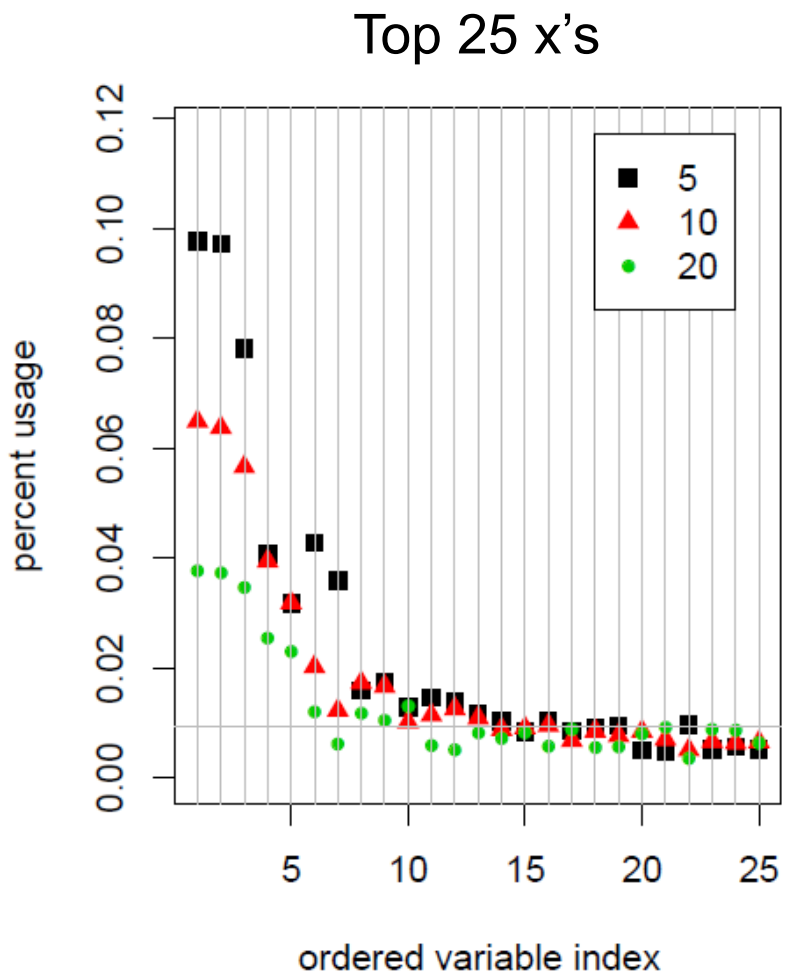


Out-of-Sample

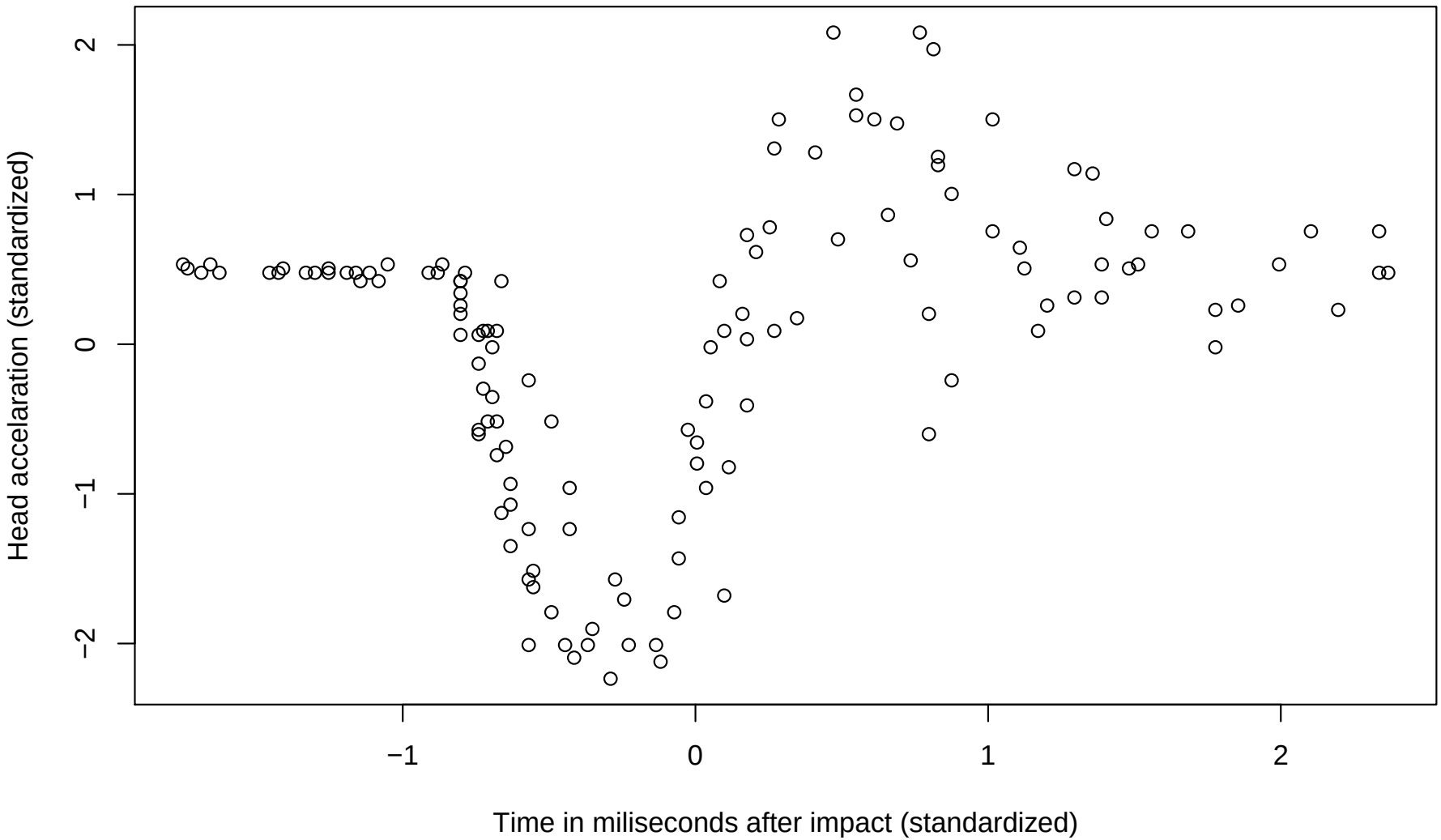


Variable selection





motorcycle dataset (revisited)



Smooth spline

The goal is to find $g(\cdot)$ that minimizes

$$\sum_{i=1}^{n}(y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

for tuning parameter $\lambda > 0$.

The basis functions for a global cubic polynomial are $B_i(x) = x^{i-1}$ for $i = 1, 2, 3, 4$, so

$$g(x) = \sum_{j=1}^{4} \beta_j B_j(x)$$

Splines are piecewise cubic polynomials: $B_1(x) = 1$, $B_2(x) = x$ and

$$B_{2+i}(x) = \frac{(x - x_i)_+^3 - (x - x_n)_+^3}{x_n - x_i} - \frac{(x - x_{n-1})_+^3 - (x - x_n)_+^3}{x_n - x_{n-1}}$$

R code

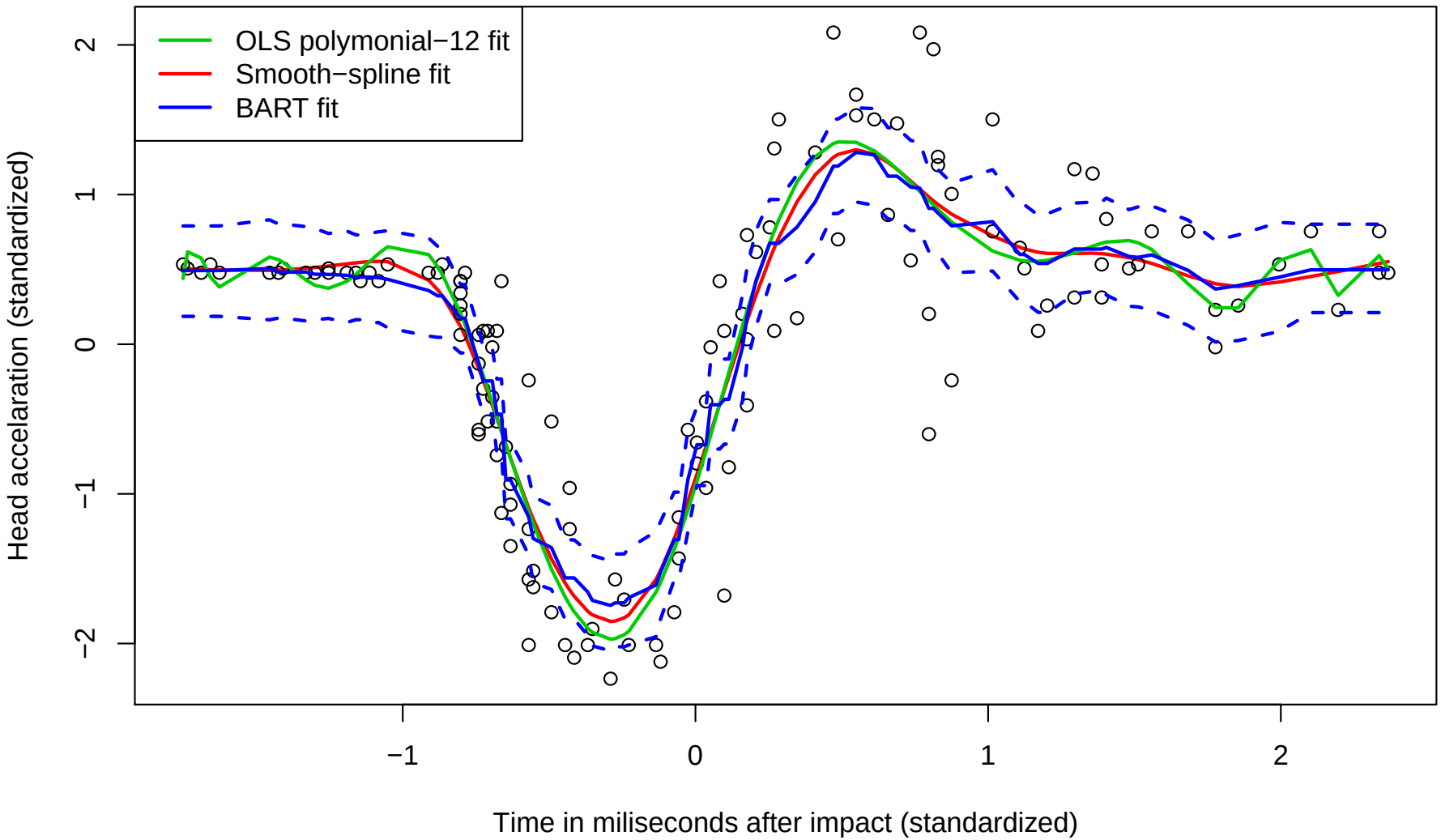
```
install.packages("BART")
library(MASS)
library(BART)
xt = mcycle$times[1:132]
yt = mcycle$accel[1:132]
xt = (xt-mean(xt))/sqrt(var(xt))
yt = (yt-mean(yt))/sqrt(var(yt))

d=12
xx = NULL
for (i in 1:d)
  xx = as.matrix(cbind(xx,xt^i))
xx = (xx - matrix(apply(xx,2,mean),n,d,byrow=TRUE))%*%diag(sqrt(1/apply(xx,2,var)))

# OLS, smooth spline and BART fits
linear.fit = lm(yt~xx-1)
fit = smooth.spline(xt,yt)
bart.fit   = wbart(xt,yt)
bart.q     = t(apply(bart.fit$yhat.train,2,quantile,c(0.05,0.5,0.95)))

plot(fit,xlab="Time in miliseconds after impact (standardized)",
     ylab="Head accelaration (standardized)",type="l",lwd=2,col=2,
     xlim=range(xt),ylim=range(yt))
points(xt,yt)
lines(xt,linear.fit$fit,col=3,lwd=2)
lines(xt,bart.q[,2],col=4,lwd=2)
lines(xt,bart.q[,1],col=4,lwd=2,lty=2)
lines(xt,bart.q[,3],col=4,lwd=2,lty=2)
legend("topleft",legend=c("OLS polymonial-12 fit","Smooth-spline fit","BART fit"),
      col=c(3,2,4),lwd=2,lty=1)
```

lm, smooth.spline and wbart in action

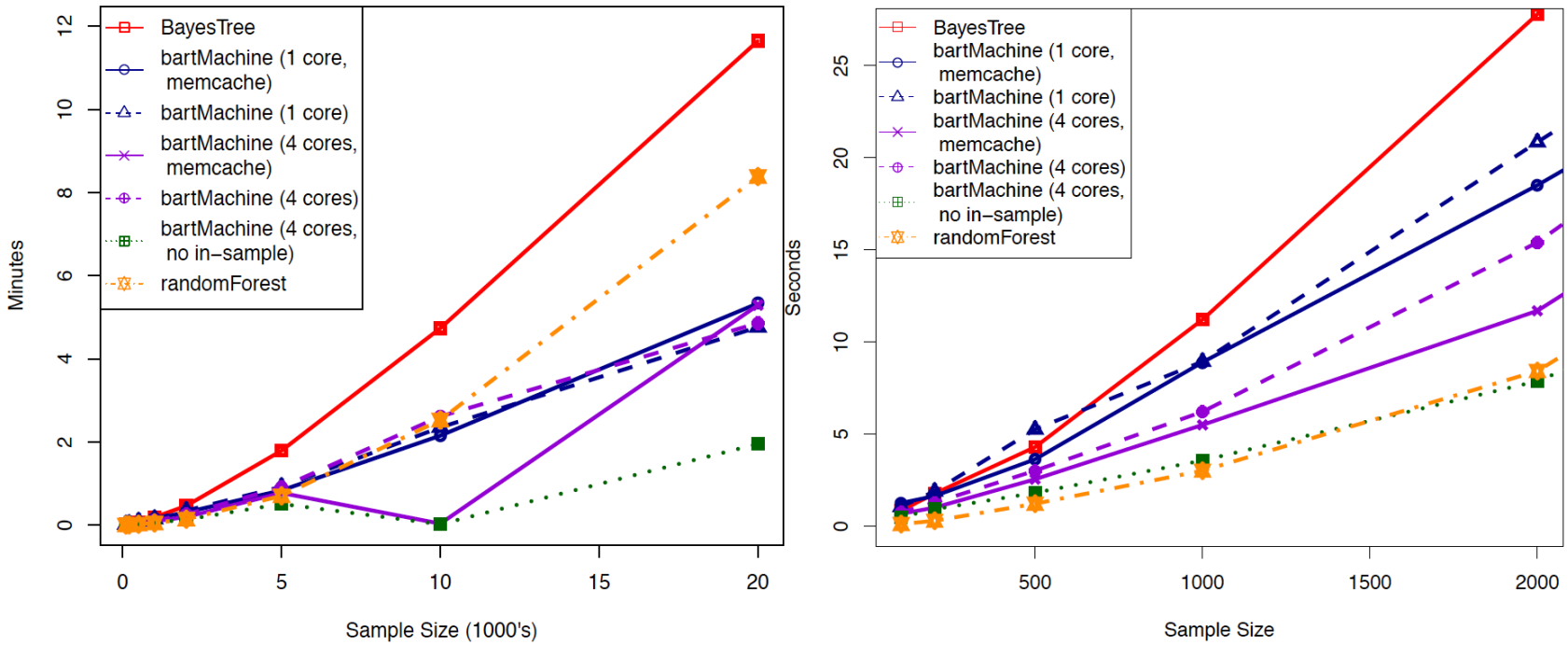


BayesTree versus bartMachine

Feature	**bartMachine**	**BayesTree**
Implementation language	Java	C++
External predict function	Yes	No
Model persistence across sessions	Yes	No
Parallelization	Yes	No
Native missing data mechanism	Yes	No
Built-in cross-validation	Yes	No
Variable importance	Statistical tests	Exploratory
Tree proposal types	3 types	4 types
Partial dependence plots	Yes	Yes
Convergence plots	Assess trees and σ^2	Assess σ^2
Model diagnostics	Yes	No
Incorporation into larger model	No	Through **dbarts**

Table 1: Comparison of features between **bartMachine** and **BayesTree**.

BayesTree versus bartMachine



(a) Large sample sizes

(b) Small sample sizes

Figure 1: Model creation times as a function of sample size for a number of settings of **bartMachine**, **BayesTree** and **randomForest**. Simulations were run on a quad-core 3.4GHz Intel i5 desktop with 24GB of RAM running the Windows 7 64bit operating system.

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