# Introduction to BART: BART::wbart

Brent, Rob, Rodney, Prakash

4/23/2023

Basic BART Ideas

Simulated Examples

More on BART: Model and Prior

wbart Prior Options

Using Predict and Controlling What Is Saved

The Diabetes Example

# Basic BART Ideas

The original BART model is:

$$Y_i = f(x_i) + \epsilon_i, \ \epsilon_i \sim N(0, \sigma^2), \ iid.$$

### where

the function f is represented as the sum of many regression trees.

How can we find a complex nonlinear function f with little (human) work ???!!!

BART was inspired by the Boosting literature, in particular the work of Jerry Friedman.

The connection to boosting is obvious in that the model is based on a sum of trees.

However, BART is a fundamentally different algorithm with some consequent pros and cons.

### BART is a Bayesian MCMC procedure.

We:

- put a prior on the model parameters  $(f, \sigma)$ .
- run a Markov chain with state (f, σ) such that the stationary distribution is the posterior

$$(f,\sigma) \mid D = \{x_i, y_i\}_{i=1}^n.$$

Examine the draws as a representation of the full posterior.

The respresentation of f is complex with changing dimension so it is difficult to look directly of draws of f.

*However*, we can look at marginals of  $\sigma$  and f(x) at any given x.

Pick of set of  $\{x_j\}$ ,  $j = 1, 2, ..., n_p$  and evaluate f at these x values.

So, if  $f_d$  is the  $d^{th}$  kept MCMC draw, then at every draw we have the fixed dimensional results

 $(f_d(x_1), f_d(x_2), \ldots, f_d(x_{n_p}))$ 

Simulated Examples

# A Simple One Dimensional Simulated Example

Let's simulate some simple data to try BART on.

```
##simulate training data
sigma = .1
f = function(x) {x^3}
set.seed(17)
n = 200
x = sort(2*runif(n)-1)
y = f(x) + sigma*rnorm(n)
#xtest: values we want to estimate f(x) at
# this is also our prediction for y.
xtest = seq(-1,1,by=.2)
```

We have just one x so we can see the results with simple plots.

### Let's have a look at our data:

```
##plot simulated data
plot(x,y,cex=.5)
points(xtest,rep(0,length(xtest)),col="red",pch=16,cex=.8)
```



Now we run BART on the simulated data using the function BART::wbart.
##run wbart
library(BART)
set.seed(14) #it is MCMC, set the seed!!
rb = wbart(x.v.xtest.nskip=500.ndpost=2000)

- nskip: the number of draws (MCMC iterations) that will be treated as burn-in, default is 500.
- ndpost: results will be kept after burn-in. Default is 1,000.

As usual, rb is a list containing results from the BART run.

*wbart* is for *weighted BART*, you can supply weights for each observation, but we won't be using this.

So, rb is the list containing the results of the call to wbart.

WI	hat i	s in rb ?????!!!	!!			
nam	es(ri	o)				
##	[1]	"sigma"	"yhat.train.mean"	"yhat.train"	"yhat.test.mean"	
##	[5]	"yhat.test"	"varcount"	"varprob"	"treedraws"	
##	[9]	"proc.time"	"mu"	"varcount.mean"	"varprob.mean"	
##	[13]	"rm.const"				
dim	(rb\$y	/hat.test)				
##	[1] 2	2000 11				

\$yhat.test:

The (d, j) element of yhat.test is the  $d^{th}$  draw of f evaluated at the  $j^{th}$  value of xtest. 2,000 draws of f, each of which is evaluated at 11 xtest values.

Let's have a look at the fit and uncertainty.



```
names(rb)
## [1] "sigma"
                        "yhat.train.mean" "yhat.train"
                                                          "yhat.test.mean"
                                         "varprob"
## [5] "yhat.test"
                        "varcount"
                                                          "treedraws"
## [9] "proc.time"
                        "m11"
                                         "varcount.mean"
                                                          "varprob.mean"
## [13] "rm.const"
dim(rb$yhat.train)
## [1] 2000 200
summary(rb$yhat.train.mean-apply(rb$yhat.train,2,mean))
        Min. 1st Qu. Median
                                       Mean
##
                                               3rd Qu.
                                                            Max.
## -1.166e-15 -8.327e-17 -3.469e-18 3.388e-17 5.551e-17 1.665e-15
summary(rb$yhat.test.mean-apply(rb$yhat.test,2,mean))
        Min. 1st Qu. Median
                                       Mean
##
                                               3rd Qu.
                                                            Max.
## -4.441e-16 -9.368e-17 1.041e-17 1.501e-16 1.353e-16 1.665e-15
```

\$yhat.train:

The (d, j) element of yhat.train is the  $d^{th}$  draw of f evaluated at the  $j^{th}$  value of x.

\$yhat.train(test).mean:

Average the draws to get the estimate of the posterior mean of f(x) (remember, f is the random variable !!).

What should happen when we bump up n (the sample size)?





We nail f and the uncertainty goes down.

# The Friedman Simulated Example

```
Let's try a tougher simulated problem.
## f and sigma
f = function(x)
   10*sin(pi*x[,1]*x[,2]) + 20*(x[,3]-.5)^2+10*x[,4]+5*x[,5]
}
sigma = 1.0 \#y = f(x) + sigma * z, z \sim N(0, 1)
## simulate
n = 100
             #number of observations
set.seed(99)
x=matrix(runif(n*10), n, 10) #10 variables, only first 5 matter
Ey = f(x)
y=Ey+sigma*rnorm(n)
## run BART
burn=500:nd=5000
rbf = wbart(x,y,nskip=burn,ndpost=nd)
dim(rbf$yhat.train); dim(rbf$yhat.test); length(rbf$sigma)
## [1] 5000 100
## [1] 5000 0
## [1] 5500
$sigma:
```

MCMC draws of  $\sigma$  including burn-in. So, the length is nskip + ndpost.

### Let's look at the draws of $\sigma$ including burn-in: plot(rbf\$sigma) abline(y=burn,col="blue",lty=2)



You can see the initial burn-in.

Burns in pretty fast, but after that there is substantial autocorrelation!

```
par(mfrow=c(2,1))
acf(rbf$sigma)
ii = burn + (1:1000)*(nd/1000)
acf(rbf$sigm[ii])
```

Series rbf\$sigma



### Did it work??!!



```
        cor(fmat)
        y
        Ey
        BART-fit
        Im-fit

        ##
        y
        1.000000
        0.9847984
        0.9973980
        0.8841787

        ##
        y
        0.9847984
        1.0000000
        0.9892571
        0.9009389

        ##
        BART-fit
        0.9973980
        0.9892571
        1.0000000
        0.9008033

        ##
        Im-fit
        0.8841787
        0.9009389
        0.9008033
        1.000000
```

- BART was able to fit the data very well.
- looks like it overfit a bit.
- burned in fast.
- draws may be autocorrelated, but not so much that you can't thin them out and get something nice.

# How about our simple simulated data? dim(rb\$yhat.train) ## [1] 2000 200 plot(rb\$sigma)



Burns in right away with no autocorrelation.

Our course, whether it and converged and how autocorrelated the draws are can depend on what you look at.

For example, you might really care about f(x) at particular set of x and the draws  $f_d(x)$  might exhibit more autocorrelation than  $\sigma$ .

Nevertheless, looking at draws of  $\sigma$  gives you a quick feel for how BART is finding fit.

# More on BART: Model and Prior

So far we have been using wbart with only an understanding of the abstract model  $% \left[ {{\left[ {{{\left[ {{{\left[ {{{\left[ {{{\left[ {{{c_{{}}}}} \right]}}} \right.}$ 

$$Y_i = f(x_i) + \epsilon_i, \ \epsilon_i \sim N(0, \sigma^2).$$

To use more of the wbart options we need to have deeper understanding of how the BART model works.

In particular, we need to understand something about the BART prior on the function f.

First, we review regression trees to set the notation for BART.

Note however that even in the simple regression tree case, our Bayesian approach is very different from the usual CART type approach.

The model will have *parameters* and corresponding *priors*.

### Model with a Single Tree

Let T denote the tree structure including the decision rules.

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

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

A single tree model:

$$y = g(x; \theta) + \epsilon.$$



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



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

# The BART Model

In BART, the function f is expresses as a sum of regression trees:

 $\mathsf{Y} = \mathsf{g}(\mathsf{x};\mathsf{T}_1,\mathsf{M}_1) + \mathsf{g}(\mathsf{x};\mathsf{T}_2,\mathsf{M}_2) + \ldots + \mathsf{g}(\mathsf{x};\mathsf{T}_\mathsf{m},\mathsf{M}_\mathsf{m}) + \sigma z, \ z \sim \mathsf{N}(0,1)$ 



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

 $f(x \mid \cdot)$  is the sum of all the corresponding  $\mu$ 's at each bottom node. Such a model combines additive and interaction effects.

All parameters but  $\sigma$  are unidentified !!!!

... the connection to Boosting is obvious...

But, ....

Rather than simply adding in fit in an iterative scheme, we will explicitly specify a prior on the model which directly impacts the performance.

In wbart we have the parameter:

**ntree**: the parameter *m*, the number of trees in the sum.

# Complete the Model with a Regularization Prior

$$\pi(\theta) = \pi((T_1, M_1), (T_2, M_2), \dots, (T_m, M_m), \sigma)$$
  
=  $\pi(\sigma) \prod_{i=1}^m \pi(T_i, M_i)$   
=  $\pi(\sigma) \prod_{i=1}^m \pi(T_i) \pi(M_i | T_i)$ 

 $\pi$  wants:

- ▶ each *T* small.
- $\blacktriangleright$  each  $\mu$  small.
- "nice' '  $\sigma$  (e.g. smaller than the least squares estimate).

We refer to  $\pi$  as a regularization prior because it restrains the overall fit. In addition, it keeps the contribution of each  $g(x; T_i, M_i)$  model component small.

# $\pi(T)$ , prior on T

Since the  $T_i$  are iid, we must choose a single  $\pi(T)$ .

We specify a process we can use to draw a tree from the prior. The probability a current bottom node, at depth d, gives birth to a left and right child is

# $\frac{\alpha}{(1+d)^{\beta}}$

In wbart we have the parameters: **base**: the parameter  $\alpha$  with default value .95. **power**: the parameter  $\beta$  with default value 2.0.

This makes non-null but small trees likely.

Prior distribution on the number of bottom nodes:

Number of Bottom Nodes	Probability
1	.05
2	.55
3	.28
4	.09
5	.03

*But note*, *if the data demands it*, you can build deeper trees than this prior would suggest.

This would be needed to model complex interactions.

## $\pi(M \mid T)$ , prior on bottom node $\mu$

Let *b* be the number of bottom nodes in the tree *T*. Then  $M = \{\mu_1, \mu_2, \dots, \mu_b\}$ . We let,

$$\pi(M \mid T) = \prod_{i=1}^{b} \pi(\mu_i)$$

That is

$$\mu_i \sim \pi(\mu), \quad iid$$

Now we only have to choose  $\pi(\mu)$ .

First of all we *center the data* so that we can assume we want to think f, and hence each  $\mu$  towards 0.

So, essentially, we fit the model:

$$Y_i = \mu + f(x_i) + \epsilon_i$$

but pick a value  $\hat{\mu}$  for  $\mu$ .

The code just subtracts  $\hat{\mu}$  from each  $y_i$  and then adds it back to the draws of f(x).

In wbart:

**fmean** : the value  $\hat{\mu}$ , with default value  $\bar{y}$ .

**\$mu**: the  $\hat{\mu}$  that was used (so default will just be  $\bar{y}$ ).

We let

$$\mu_i \sim N(0, \tau^2)$$

where the zero mean is justified by the centering.

How do we choose the key parameter  $\tau$  ??

The key observation is that:

$$f(x \mid T, M) = \mu_1 + \mu_2 + \cdots + \mu_m.$$

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



$$\mu_i \sim N(0, \tau^2)$$

$$f(x \mid T, M) = \mu_1 + \mu_2 + \cdots + \mu_m.$$

Which gives us,

$$f(x) \mid T \sim N(0, m \tau^2)$$

which does not depend on T or x !!!!!

$$f(x) \mid T \sim N(0, m \tau^2)$$

In wbart we use the parameter k to specify the  $\mu$  prior via

$$\tau = \frac{\max(y) - \min(y)}{2 \, k \, \sqrt{m}}$$

that way

$$k\sqrt{m}\,\tau=\frac{\max(y)-\min(y)}{2}$$

so that from the "middle" of f to the extreme is k standard deviations. In wbart, k is called k:

k:

number of standard deviations of f(x) that equal half the range of y, the default value is 2.

You can also just directly set the standard deviation of f(x).

$$f(x) \sim N(0, \sigma_f^2)$$

which is the same as just setting

$$\tau^2 = \frac{\sigma_f^2}{m}$$

In wbart:

**sigmaf** : prior standard deviation of f(x).

# $\pi(\sigma)$ , prior on $\sigma$ .

$$\sigma^2 \sim \frac{\nu \,\lambda}{\chi_{\nu}^2}$$

The wbart strategy is to choose  $\nu$  and a rough estimate of  $\sigma$ ,  $\hat{\sigma}$ .

If p < n,  $\hat{\sigma}$  is the usual least squares estimate, else sd(y).

We then choose  $\lambda$  so that  $\hat{\sigma}$  is at a chosen quantile q of the prior.

Solid blue line at  $\hat{\sigma}$ .

 $p(\sigma < \hat{\sigma}) = q.$ 



In wbart:

**sigdf**:  $\nu$ , default is 3.

sigest:  $\hat{\sigma}$ , default is least squares estimate if p < n and sd(y) otherwise. sigquant: q, default is .9.

You can also just set  $\lambda$  directly:

lambda:  $\lambda$ .

wbart Prior Options

### In summary:

wbart has the following BART prior related parameters:

T: power, base.

- M: k, sigmaf.
- $\sigma$ : sigest, sigdf, sigquant, lambda

In addition, you must choose ntree and numcut.

**numcut** is the number of cutpoints c used for the decision rules  $x_i < c$ .

Let's just look at a few examples to get some intuition for the effect of these prior choices on the BART inference.

### Back to our 1-D example so we can see what happens.

```
sigma = .1
f = function(x) \{x^3\}
set_seed(17)
n = 100
x = sort(2*runif(n)-1)
v = f(x) + sigma * rnorm(n)
lmf = lm(y~x,data.frame(x,y))
sigest = summary(lmf)$sigma
cat("least squares estimate of sigma is: ", sigest ,"\n")
## least squares estimate of sigma is: 0.1742962
#density of sigma for sigma^2 ~ nu*lam/chisg nu
sden=function(sv,nu,lam) {
   dchisq(nu*lam/sv<sup>2</sup>,df=nu)*(2*nu*lam)/sv<sup>3</sup>
ŀ
#lam val which puts sigest and sigquant quantile
lamval = function(sigest, sigquant, nu) {
   qchi = qchisq(1.0-sigguant,nu)
   lambda = (sigest*sigest*qchi)/nu #lambda parameter for sigma prior
```

}

lambda

```
#vary quantile and nu
qv=c(.5,.9,.99); nuv = c(3,200)
pg = expand.grid(qv,nuv)
names(pg) = c("quantile","nu")
pg
##
    quantile nu
## 1 0.50 3
## 2 0.90 3
## 3 0.99 3
## 4 0.50 200
## 5 0.90 200
## 6 0.99 200
#evaluate prior density of sigma for our 6 priors
sv = seq(from=.05*sigest,to=2*sigest,length.out=100)
pmat = matrix(0.0,length(sv),nrow(pg))
for(i in 1:nrow(pg)) {
  pmat[,i] = sden(sv,pg[i,2],lamval(sigest,pg[i,1],pg[i,2]))
}
```

```
plot(range(sv),range(pmat),type="n")
lwv = rep(1,nrow(pg)); lwv[2]=3; ltyv = 1+floor(0:5/3)
for(i in 1:nrow(pg)) lines(sv,pmat[,i],col=i,lwd=lwv[i],lty=ltyv[i])
abline(v=sigma,col="blue",lty=4,lwd=3)
abline(v=sigma,col="blue",lty=4,lwd=3)
```



range(sv)

Run BART at our 6 prior settings and a seventh where we use ntree=5000 and k=5, this will give us a smoother function.

```
fmat = matrix(0.0,n,nrow(pg))
for(i in 1:nrow(pg)) {
    bf = wbart(x,y,sigquant=pg[i,1],sigdf=pg[i,2])
    fmat[,i] = bf$yhat.train.mean
}
#more trees and more shrinkage => smoother f
bf2 = wbart(x,y,ntree=5000,k=5)
```

```
plot(x,y)
for(i in 1:nrow(pg)) lines(x,fmat[,i],col=i,lwd=lwv[i],lty=ltyv[i])
lines(x,bf2$yhat.train.mean,lty=1,lwd=3)
```



The fit with a lot of trees is indeed smoother, but the other fits are remarkably similar.

Ok, let's mess it up!!

We'll put in  $\sigma$  too small prior, a  $\sigma$  too big prior, and a  $\sigma$  just right prior.

```
bfb1 = wbart(x,y,sigest=.01,sigdf=500) #sigma small => overfit
bfb2 = wbart(x,y,sigest=3,sigdf=500) #sigma big => underfit
bfg = wbart(x,y,sigest=sigma,sigdf=5000) #got sigma right!
```

```
plot(x,y)
lines(x,bfb1$yhat.train.mean,col="red")
lines(x,bfb2$yhat.train.mean,col="green")
lines(x,bfg$yhat.train.mean,col="blue")
```



That worked.

Using Predict and Controlling What Is Saved

Up to now we have given wbart  $(X, y, X_p)$ .

At every iteration of the MCMC,  $(f, \sigma)$  is updated.

Updating f means all the  $(T_j, M_j), j = 1, 2, ..., m$  are updated.

In addition, we evaluate f at each x in X and each x in  $X_p$ .

We can simplify things and speed things up by thinning these evaluations for both  $x \in X$  and  $x \in X_p$ .

In addition, we can save draws of f and evaluate them at x after we have run the MCMC as you would with a "predict" function.

wbart has the parameters:

### nkeeptrain:

number of draws of f to evaluate the training data at. The draws are evenly spaced so that if ndpost=1,000 and nkeeptran=100, then we would evaluate every 10th draw of f at the  $x \in X$ .

**nkeeptest**: same thing for the test data.

**nkeeptestmean**: number of draws of *f* to evaluate the test data in order to compute **\$yhat.test.mean**.

**nkeeptreedraws**: number of draws of f (the set of  $(T_i, M_i)$ ) to return.

The tree draws are not terribly interpretable, but by saving them we can evaluate f draws at a new set of x vectors without rerunning the MCMC.

### Let's try it.

```
##simulate data
set.seed(99)
n=5000
p=10
beta = 3*(1:p)/p
sigma=1.0
X = matrix(rnorm(n*p),ncol=p)
y = 10+X %*% matrix(beta,ncol=1) + sigma*rnorm(n)
y=as.double(y)
np=100000
Xp = matrix(rnorm(np*p),ncol=p)
```

The trees are stored in one long character string which is not too useful to look at but we can see that there are 100 draws each consisting of 200 trees.

For example, it might be fast to just keep 100 trees:

```
dim(pred2)
## [1] 100 100000
t1
## user system elapsed
## 114.877 0.272 115.147
t2
## user system elapsed
## 23.322 0.000 23.321
t3
## user system elapsed
## 70.681 0.048 8.922
```

pred2 has row dimension equal to the number of kept tree draws (100) and column dimension equal to the number of row in  $X_p$  (100,000).

33+18 seconds to get predictions on 100,000 observations using 100 stored trees. while it took 188 seconds to do it the old way.



Could be perfectly good as a practical matter.

```
Let's compare the BART fit to a linear fit (we simulated from the linear model).
```



The Diabetes Example

Let's look at an example with real data.

We'll try the diabetes data which is available at Hastie, Tibshirani, Wainright website.

### Diabetes data

These data consists of observations on 442 patients, with the response of interest being a quantitative measure of disease progression one year after baseline. There are ten baseline variables—age, sex, body-mass index, average blood pressure, and six blood serum measurements—plus quadratic terms, giving a total of 64 features.

First used in LARS paper

Tab-delimited diabetes data (text file)

Note that these data are first standardized to have zero mean and unit L2 norm before they are used in the examples.

```
Let's read in the data.
```

```
db = read.csv("http://www.rob-mcculloch.org/data/diabetes.csv")
#first col is y, 2-11 are x, 12-65 are xi^2, x_i * x_j (except sex dummy)
xB = as.matrix(db[,2:11]) #x for BART
xL = as.matrix(db[,2:ncol(db)]) #x for lasso, includes transformations
yBL = db$y #y for BART and lasso
dim(db)
## [1] 442 65
names(db[,1:15])
## [1] "y" "age" "sex" "bmi" "map" "tc" "ldl" "hdl" "tch"
## [10] "ltg" "glu" "age.2" "bmi.2" "map.2" "tc.2"
```

So there are 442 observations. The first column is our response and the next 10 columns are the x's.

The rest of the columns are the squares and products of the original 10 x's giving 64 "variables".

For BART we just want a matrix of the 10 x's.

We will compare BART with just the 10 original vars to glmnet with all 64 predictors.

Note that all the predictors have been standardized. This is crucial for glmnet and does not matter for BART. We'll just do some random train/test splits and to compare the out of sample performance of BART to that of the lasso.

```
rmsef = function(y,yhat) {return(sqrt(mean((y-yhat)^2)))}
nd=30 #number of train/test splits
n = length(yBL)
ntrain=floor(.75*n) #75% in train each time
rmseB = rep(0,nd) #BART rmse
rmseL = rep(0,nd) #BART rmse
fmatL=matrix(0.0,n-ntrain,nd) #out-of-sample lasso predictions
fmatB=matrix(0.0,n-ntrain,nd) #out-of-sample BART predictions
```

So, 30 times we will randomly pick 75% of the data to be train and predict on the remaining 25%.

We'll just do some random train/test splits and to compare the out of sample performance of BART to that of the lasso.

```
library(glmnet)
for(i in 1:nd) {
   set.seed(i)
   # train/test split
   ii=sample(1:n,ntrain)
   #y
   yTrain = yBL[ii]; yTest = yBL[-ii]
   #x for BART
   xBTrain = xB[ii,]; xBTest = xB[-ii,]
   #x for lasso
   xLTrain = xL[ii,]; xLTest = xL[-ii,]
```

#### #BART

}

bfTrain = mc.wbart(xBTrain,yTrain,xBTest,mc.cores=8,keeptrainfits=FALSE)

```
#get predictions on test
```

```
yBhat = bfTrain$yhat.test.mean
yLhat = predict(fLTrain,xLTest,s=bestlam,type="response")[,1]
#store results
rmseB[i] = rmsef(yTest,yBhat); rmseL[i] = rmsef(yTest,yLhat)
fmatL[,i]=yLhat; fmatB[,i]=yBhat
```

Just using default BART!!

Using parallel version of wbart.

The basic arguments for mc.wbart are the same as in wbart.

Data is already standardized so don't have standardize=FALSE in glmnet.

# Let's compare the out of sample RMSEs. qqplot(rmseB,rmseL) abline(0,1,col="red",lwd=2)



Very comparable !!!.

# Let's compare the out of sample predictions. plot(as.double(fmatB),as.double(fmatL),xlab="preds from BART",ylab="preds from LASSO") abline(0,1,col="red",lwd=2) lmtemp = lm(B-L,data.frame(B=as.double(fmatB),L=as.double(fmatL))) abline(lmtemp\$coef,col="blue",lty=2,lwd=3)



Now that we know the default prior *may* be giving reasonable results let's look at a longer run.

bfd = wbart(xB,yBL,nskip=1000,ndpost=5000) #keep it simple

plot(bfd\$sigma)



Index

# plot(bfd\$yhat.train.mean,yBL) abline(0,1,col="red",lty=2)



bfd\$yhat.train.mean

 $\sigma$  is about 50 !!

# ii = order(bfd\$yhat.train.mean) boxplot(bfd\$yhat.train[,ii],ylim=range(yBL))



### A lot of uncertainty !!!!

Very automatically, BART gaves us good out of sample results, did not have to choose transformations to include !!

BART gave us the uncertainty!!!