Continuous outcomes with BART: Part 2

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Abstract

This short article illustrates examples of analyzing continuous outcomes with the **BART** R package.

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1. BART

In this section, we demonstrate the analysis of continuous outcomes with BART via the **BART** R package. For continuous outcomes, Bayesian Additive Regression Trees (BART) (Chipman, George, and McCulloch 2010) fit the basic model:

$$y_i = f(x_i) + \epsilon_i, \;\; \epsilon_i \sim N(0, w_i^2\sigma^2)$$

We use Markov Chain Monte Carlo (MCMC) to get draws from the posterior distribution of the parameter (f, σ). In this section, we describe the functionality of `BART::wbart` which is the basic function in the **BART** R package. But first, we delve into the details of the BART prior itself.

1.1. Boston Housing Data

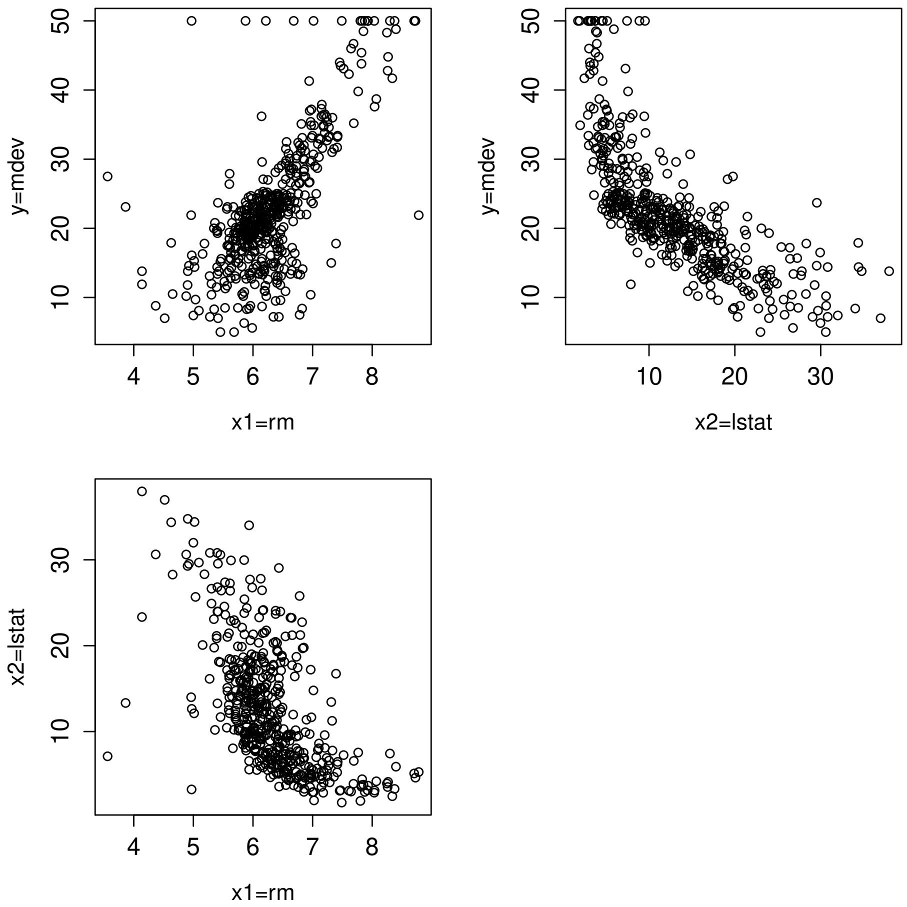
Let's examine the classic example of the Boston housing data. We'll predict the median house value, `y=mdev`, from `x1 = rm` (number of rooms) and `x2=lsat` (lower status).

```
library(MASS)
x = Boston[,c(6,13)] #rm=number of rooms and lstat= percent lower status
y = Boston$medv # median value
head(cbind(x,y))

##      rm lstat    y
## 1 6.575  4.98 24.0
## 2 6.421  9.14 21.6
## 3 7.185  4.03 34.7
## 4 6.998  2.94 33.4
## 5 7.147  5.33 36.2
## 6 6.430  5.21 28.7
```

1.2. A Quick Look at the Data

```
par(mfrow=c(2,2))
par(mai=c(.8,.8,.2,.2))
plot(x[,1],y,xlab="x1=rm",ylab="y=mdev",cex.axis=1.3,cex.lab=1.2)
plot(x[,2],y,xlab="x2=lstat",ylab="y=mdev",cex.axis=1.3,cex.lab=1.2)
plot(x[,1],x[,2],xlab="x1=rm",ylab="x2=lstat",cex.axis=1.3,cex.lab=1.2)
```



1.3. Run wbart

```
library(BART) #BART package
set.seed(99) #MCMC, so set the seed
nd=200 # number of kept draws
burn=50 # number of burn in draws
bf = wbart(x,y,nskip=burn,ndpost=nd)

## *****Into main of wbart
## *****Data:
```

```
## data:n,p,np: 506, 2, 0
## y1,yn: 1.467194, -10.632806
## x1,x[n*p]: 6.575000, 7.880000
## *****Number of Trees: 200
## *****Number of Cut Points: 100 ... 100
## *****burn and ndpost: 50, 200
## *****Prior:beta,alpha,tau,nu,lambda: 2.000000,0.950000,0.795495,3.000000,5.979017
## *****sigma: 5.540257
## *****w (weights): 1.000000 ... 1.000000
## *****Dirichlet:sparse,theta,omega,a,b,rho,augment: 0,0,1,0.5,1,2,0
## *****nkeeptrain,nkeeptest,nkeeptestme,nkeeptreedraws: 200,200,200,200
## *****printevery: 100
## *****skiptr,skipte,skipteme,skiptreedraws: 1,1,1,1
##
## MCMC
## done 0 (out of 250)
## done 100 (out of 250)
## done 200 (out of 250)
## time: 1s
## check counts
## trcnt,tecnt,temecnt,treedrawscnt: 200,0,0,200
```

1.4. Results returned with a list

We returned the results of running `wbart` in the object `bf` of type `wbart` which is essentially a list.

```
names(bf)

##  [1] "sigma"           "yhat.train.mean" "yhat.train"
##  [4] "yhat.test.mean"  "yhat.test"       "varcount"
##  [7] "varprob"         "treedraws"       "proc.time"
## [10] "mu"              "varcount.mean"   "varprob.mean"
## [13] "rm.const"

length(bf$sigma)

## [1] 250

length(bf$yhat.train.mean)

## [1] 506

dim(bf$yhat.train)

## [1] 200 506
```

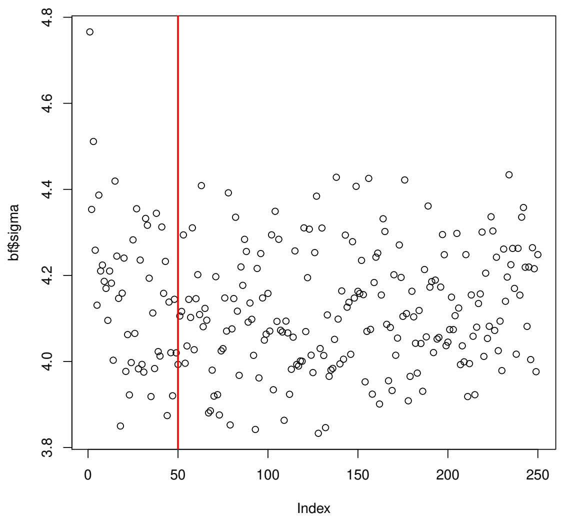
Remember, the training data has $n = 506$ observations, we had `burn=50` burnin discarded draws and `nd=200` draws kept.

Let's look at a couple of the key list components. `$sigma`: burnin + kept (250) draws of σ. `yhat.train.mean`: j^{th} value is posterior mean of $f(x_j)$, f evaluated at the j^{th} training observation. `yhat.train`: i, j value is the i^{th} kept MCMC draw of $f(x_j)$.

1.5. Assess Convegence

As with any high-dimensional MCMC, assessing convergence may be tricky. The simplest thing to look at are the draws of σ. The parameter σ is the only identified parameter in the model and it also gives us a sense of the size of the errors.

```
plot(bf$sigma)
abline(v=burn,lwd=2,col="red")
```



Look's like it burned in very quickly. Just one initial draw looking a bit bigger than the rest. Apparently, subsequent variation is legitimate posterior variation. In a more difficult problem you may see the σ draws initially declining as the MCMC searches for a good fit.

1.6. Look at in-sample Fit and Compare to a Linear Fit

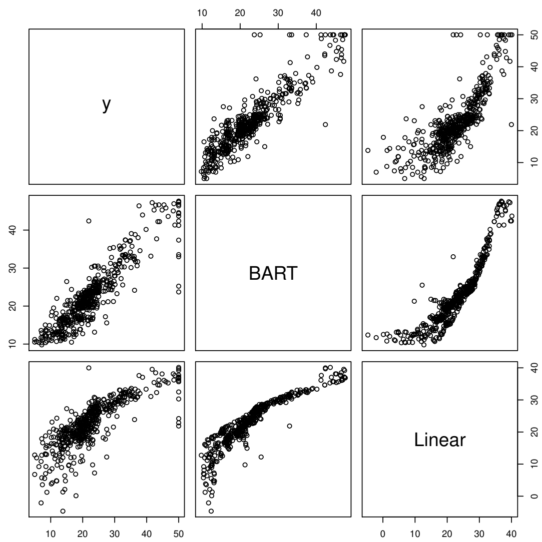
Let's look at the in-sample BART fit (`yhat.train.mean`) and compare it to `y=medv` fits from a multiple linear regression.

```
lmf = lm(y~.,data.frame(x,y))
fitmat = cbind(y,bf$yhat.train.mean,lmf$fitted.values)
colnames(fitmat)=c("y","BART","Linear")
cor(fitmat)

##                  y      BART    Linear
```

```
## y      1.0000000 0.9051200 0.7991005
## BART   0.9051200 1.0000000 0.8978003
## Linear 0.7991005 0.8978003 1.0000000

pairs(fitmat)
```

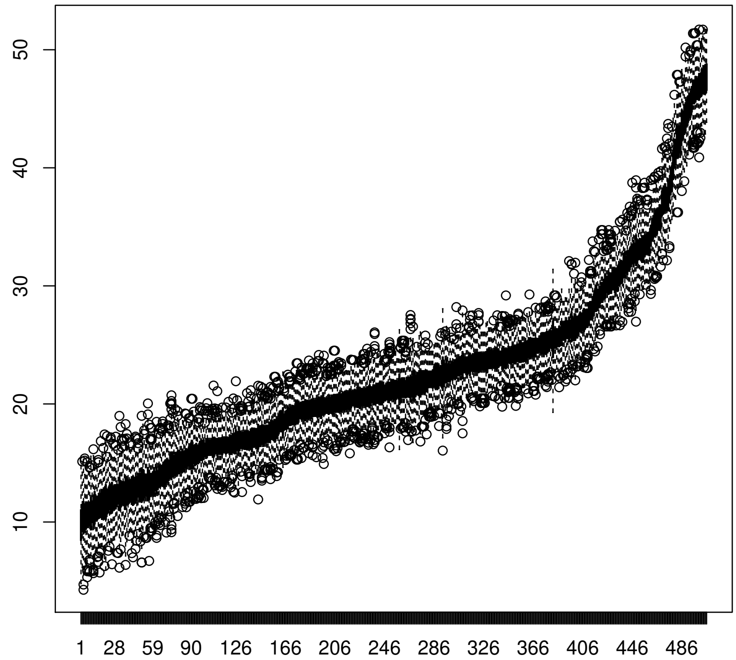


The BART fit is noticeably different from the linear fit.

1.7. A Quick Look at the Uncertainty

We order the observations by the fitted house value (`yhat.train.mean`) and then use boxplots to display the draws of $f(x)$ in each column of `yhat.train`.

```
ii = order(bf$yhat.train.mean) #order observations by predicted value
boxplot(bf$yhat.train[,ii]) #boxplots of f(x) draws
```



Substantial predictive uncertainty, but you can still be fairly certain that some houses should cost more than other.

1.8. Using predict.wbart

We can get out of sample predictions in two ways. First, we can can just ask for them when we call `wbart` by supplying a matrix or data frame of test x values. Second, we can call a `predict` method.

Let's split our data into train and test subsets.

```
n=length(y) #total sample size
set.seed(14)  # Dave Keon, greatest Leaf of all time!
ii = sample(1:n,floor(.75*n)) # indices for train data, 75% of data
xtrain=x[ii,]; ytrain=y[ii] # training data
xtest=x[-ii,]; ytest=y[-ii] # test data
cat("train sample size is ",length(ytrain)," and test sample size is ",length(ytest),"\n")

## train sample size is  379  and test sample size is  127
```

And now we can run `wbart` using the training data to learn and predict at `xtest`. First, we'll just pass `xtest` to the `wbart` call.

```
dim(bfp1$yhat.test)

## [1] 1000  127

length(bfp1$yhat.test.mean)

## [1] 127
```

Now, `yhat.test`: the i, j value is the i^{th} kept MCMC draw of $f(x_j)$ where x_j is the j^{th} row of `xtest`.
`yhat.test.mean`: the j^{th} value is the posterior mean of $f(x_j)$, i.e., f evaluated at the j^{th} row of `xtest`.

Alternatively, we could run `wbart` saving all the MCMC results and then call `predict.wbart`.

```
set.seed(99)
bfp2 = wbart(xtrain,ytrain)

## *****Into main of wbart
## *****Data:
## data:n,p,np: 379, 2, 0
## y1,yn: -4.903958, 1.596042
## x1,x[n*p]: 6.431000, 9.520000
## *****Number of Trees: 200
## *****Number of Cut Points: 100 ... 100
## *****burn and ndpost: 100, 1000
## *****Prior:beta,alpha,tau,nu,lambda: 2.000000,0.950000,0.795495,3.000000,5.669300
## *****sigma: 5.394855
## *****w (weights): 1.000000 ... 1.000000
## *****Dirichlet:sparse,theta,omega,a,b,rho,augment: 0,0,1,0.5,1,2,0
## *****nkeeptrain,nkeeptest,nkeeptestme,nkeeptreedraws: 1000,1000,1000,1000
## *****printevery: 100
## *****skiptr,skipte,skipteme,skiptreedraws: 1,1,1,1
##
## MCMC
## done 0 (out of 1100)
## done 100 (out of 1100)
## done 200 (out of 1100)
## done 300 (out of 1100)
## done 400 (out of 1100)
## done 500 (out of 1100)
## done 600 (out of 1100)
## done 700 (out of 1100)
## done 800 (out of 1100)
## done 900 (out of 1100)
## done 1000 (out of 1100)
```

```
## time: 3s
## check counts
## trcnt,tecnt,temecnt,treedrawscnt: 1000,0,0,1000

yhat = predict(bfp2,as.matrix(xtest)) #predict wants a matrix

## *****In main of C++ for bart prediction
## tc (threadcount): 1
## number of bart draws: 1000
## number of trees in bart sum: 200
## number of x columns: 2
## from x,np,p: 2, 127
## ***using serial code
```

So `yhat` and `bfp1$yhat.test` are the same.

```
dim(yhat)

## [1] 1000  127

summary(as.double(yhat-bfp1$yhat.test))

##       Min.    1st Qu.     Median       Mean    3rd Qu.       Max.
## -9.091e-09 -1.188e-09  2.455e-11  1.559e-12  1.186e-09  6.789e-09
```

1.9. Thinning

In our simple example of the Boston housing data set `wbart` runs pretty fast. But with more data and longer runs you may want to speed things up by saving less and then using `predict`. Let's just keep a thinned subset of 200 tree ensembles.

```
set.seed(4) #Bobby Orr's jersey number is the seed
bfthin = wbart(xtrain,ytrain,nskip=1000,ndpost=10000,
                     nkeeptrain=0,nkeeptest=0,nkeeptestmean=0,nkeeptreedraws=200)

## *****Into main of wbart
## *****Data:
## data:n,p,np: 379, 2, 0
## y1,yn: -4.903958, 1.596042
## x1,x[n*p]: 6.431000, 9.520000
## *****Number of Trees: 200
## *****Number of Cut Points: 100 ... 100
## *****burn and ndpost: 1000, 10000
## *****Prior:beta,alpha,tau,nu,lambda: 2.000000,0.950000,0.795495,3.000000,5.669300
## *****sigma: 5.394855
```

```
## *****w (weights): 1.000000 ... 1.000000
## *****Dirichlet:sparse,theta,omega,a,b,rho,augment: 0,0,1,0.5,1,2,0
## *****nkeeptrain,nkeeptest,nkeeptestme,nkeeptreedraws: 0,0,0,200
## *****printevery: 100
## *****skiptr,skipte,skipteme,skiptreedraws: 10001,10001,10001,50
##
## MCMC
## done 0 (out of 11000)
## done 100 (out of 11000)
## done 200 (out of 11000)
## done 300 (out of 11000)
## done 400 (out of 11000)
## done 500 (out of 11000)
## done 600 (out of 11000)
## done 700 (out of 11000)
## done 800 (out of 11000)
## done 900 (out of 11000)
## done 1000 (out of 11000)
## done 1100 (out of 11000)
## done 1200 (out of 11000)
## done 1300 (out of 11000)
## done 1400 (out of 11000)
## done 1500 (out of 11000)
## done 1600 (out of 11000)
## done 1700 (out of 11000)
## done 1800 (out of 11000)
## done 1900 (out of 11000)
## done 2000 (out of 11000)
## done 2100 (out of 11000)
## done 2200 (out of 11000)
## done 2300 (out of 11000)
## done 2400 (out of 11000)
## done 2500 (out of 11000)
## done 2600 (out of 11000)
## done 2700 (out of 11000)
## done 2800 (out of 11000)
## done 2900 (out of 11000)
## done 3000 (out of 11000)
## done 3100 (out of 11000)
## done 3200 (out of 11000)
## done 3300 (out of 11000)
## done 3400 (out of 11000)
## done 3500 (out of 11000)
## done 3600 (out of 11000)
## done 3700 (out of 11000)
## done 3800 (out of 11000)
```

```
## done 3900 (out of 11000)
## done 4000 (out of 11000)
## done 4100 (out of 11000)
## done 4200 (out of 11000)
## done 4300 (out of 11000)
## done 4400 (out of 11000)
## done 4500 (out of 11000)
## done 4600 (out of 11000)
## done 4700 (out of 11000)
## done 4800 (out of 11000)
## done 4900 (out of 11000)
## done 5000 (out of 11000)
## done 5100 (out of 11000)
## done 5200 (out of 11000)
## done 5300 (out of 11000)
## done 5400 (out of 11000)
## done 5500 (out of 11000)
## done 5600 (out of 11000)
## done 5700 (out of 11000)
## done 5800 (out of 11000)
## done 5900 (out of 11000)
## done 6000 (out of 11000)
## done 6100 (out of 11000)
## done 6200 (out of 11000)
## done 6300 (out of 11000)
## done 6400 (out of 11000)
## done 6500 (out of 11000)
## done 6600 (out of 11000)
## done 6700 (out of 11000)
## done 6800 (out of 11000)
## done 6900 (out of 11000)
## done 7000 (out of 11000)
## done 7100 (out of 11000)
## done 7200 (out of 11000)
## done 7300 (out of 11000)
## done 7400 (out of 11000)
## done 7500 (out of 11000)
## done 7600 (out of 11000)
## done 7700 (out of 11000)
## done 7800 (out of 11000)
## done 7900 (out of 11000)
## done 8000 (out of 11000)
## done 8100 (out of 11000)
## done 8200 (out of 11000)
## done 8300 (out of 11000)
## done 8400 (out of 11000)
```

```
## done 8500 (out of 11000)
## done 8600 (out of 11000)
## done 8700 (out of 11000)
## done 8800 (out of 11000)
## done 8900 (out of 11000)
## done 9000 (out of 11000)
## done 9100 (out of 11000)
## done 9200 (out of 11000)
## done 9300 (out of 11000)
## done 9400 (out of 11000)
## done 9500 (out of 11000)
## done 9600 (out of 11000)
## done 9700 (out of 11000)
## done 9800 (out of 11000)
## done 9900 (out of 11000)
## done 10000 (out of 11000)
## done 10100 (out of 11000)
## done 10200 (out of 11000)
## done 10300 (out of 11000)
## done 10400 (out of 11000)
## done 10500 (out of 11000)
## done 10600 (out of 11000)
## done 10700 (out of 11000)
## done 10800 (out of 11000)
## done 10900 (out of 11000)
## time: 26s
## check counts
## trcnt,tecnt,temecnt,treedrawscnt: 0,0,0,200

yhatthin = predict(bfthin,as.matrix(xtest)) #predict wants a matrix

## *****In main of C++ for bart prediction
## tc (threadcount): 1
## number of bart draws: 200
## number of trees in bart sum: 200
## number of x columns: 2
## from x,np,p: 2, 127
## ***using serial code
```

```
dim(bfthin$yhat.train)

## [1]   0 379

dim(yhatthin)

## [1] 200 127
```

Now, there are no kept draws of $f(x)$ for training x, and we have 200 tree ensembles to use with `predict.wbart`.

The thinning arguments.

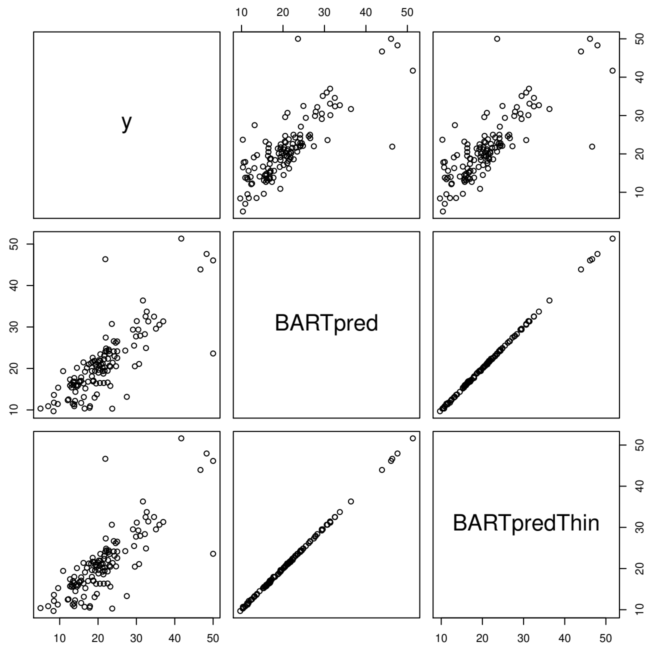
- `nkeeptrain` : number of $f(x)$ draws to save for training x.
- `nkeeptest` : number of $f(x)$ draws to save for test x.
- `nkeeptestmeam` : number of draws to use in computing `yhat.test.mean`.
- `nkeeptreedraws` : number of tree ensembles to keep.

The default values are to keep all the draws (e.g., `nkeeptrain=ndpost`).

Of course, if you keep 100 out of 100,000, you keep every 1,000th draw.

Now, let's have a look at the predictions.

```
fmat=cbind(ytest,bfp1$yhat.test.mean,apply(yhatthin,2,mean))
colnames(fmat) = c("y","BARTpred","BARTpredThin")
pairs(fmat)
```



Recall, the predictions labeled "BARTpred" are from a BART run with `seed=99` and all default values. The predictions labeled "BARTpredThin" are from 200 kept trees out of a long run with 1,000 burnins discarded and 10,000 draws kept with `seed=4`. It is interesting how similar they are !!!!

References

Chipman HA, George EI, McCulloch RE (2010). "BART: Bayesian Additive Regression Trees." *Annals of Applied Statistics*, **4**, 266–98.

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