BART::wbart: BART for Numeric Outcomes

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1 BART

BART is Bayesian Additive Regression Trees (see Chipman, George, and McCulloch). We fit the basic model:

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

We use Markov Chain Monte Carlo to get draws from the posterior distribution of the parameter (f, σ) . In this vignette we look at BART::wbart which is the basic function in the R package **BART**.

1.1 Boston Housing Data

Let's just use the good old Boston housing data.

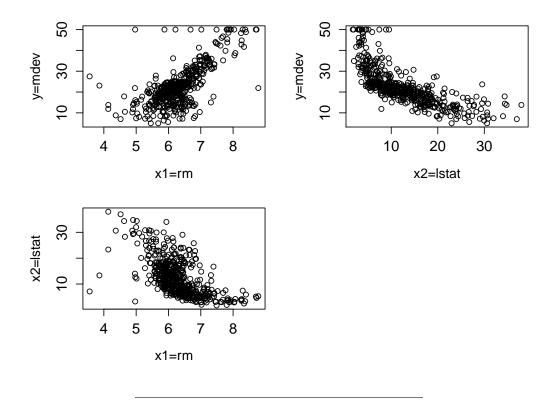
We'll predict the median house value, y=mdev, from x1=rm (number of rooms) and x2=lsat (% lower status).

```
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 stored the results of running wbart in the list bf.

```
names(bf)
   [1] "sigma"
                          "yhat.train.mean" "yhat.train"
    [4] "yhat.test.mean"
                          "yhat.test"
                                             "varcount"
##
  [7] "varprob"
                          "treedraws"
                                             "proc.time"
                          "varcount.mean"
                                            "varprob.mean"
## [10] "mu"
## [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 burn-in draws and nd=200 kept draws.

Let's look at a couple key list components:

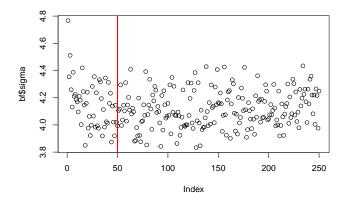
- **sigma**: burnin + kept (burn+nd) draws of σ .
- yhat.train.mean: j^{th} value is posterior mean of $f(x_j)$, f evaluated at the j^{th} training observation.
- yhat.train: i, j value is the i^{th} kept MCMC draw of $f(x_i)$.

1.5 Assess Convegence with σ Draws

As with any high-dimensional MCMC, assessing convergence may be tricky.

A nice simple thing to look at is 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")
```



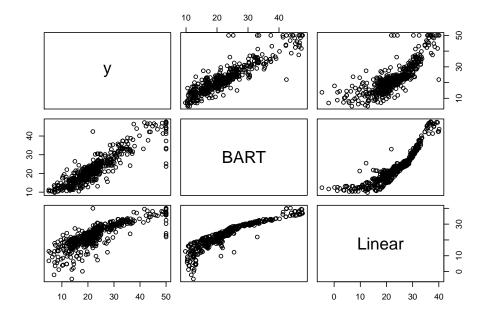
Look's like it burned in almost right away.

Just one initial draw looking a bit bigger than the rest. Hopefully, subsequent variation is legitimate posterior variation.

In a more difficult problem you may see the σ draws initially declining as the MCMC search for 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 and the fits from a multiple linear regression.

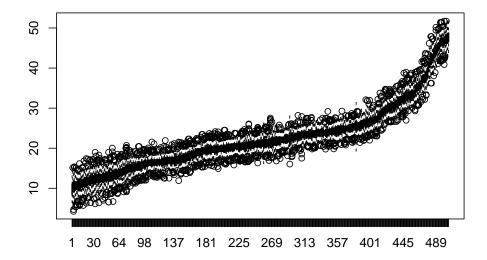


The BART fit is noticeably different from the linear fit.

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 are still pretty sure some houses should cost more that others!!

2 Using predict.wbart

We can get out of sample predictions two ways.

First, we can can just ask for them when we call wbart by supply a matrix of test x value.

Second, we can call a predict method.

2.1 Train and Test Data Sets

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 train to learn and predict at xtest.

First, we'll just give xtest to the wbart call.

```
set.seed(99)
bfp1 = wbart(xtrain,ytrain,xtest) #predict.wbart wants a matrix
```

```
dim(bfp1$yhat.test)
## [1] 1000 127
length(bfp1$yhat.test.mean)
## [1] 127
```

Now

- yhat.test: 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: j^{th} value is posterior mean of $f(x_i)$, 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)
yhat = predict(bfp2,as.matrix(xtest)) #predict wants a matrix
```

Then 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 -1.186e-09 2.484e-11 2.288e-12 1.188e-09 6.790e-09
```

3 Thining

[1] 200 127

In our simple 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.

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

3.1 The thinning arguments:

• **nkeeptrain**: number of f(x) draws to save for training x.

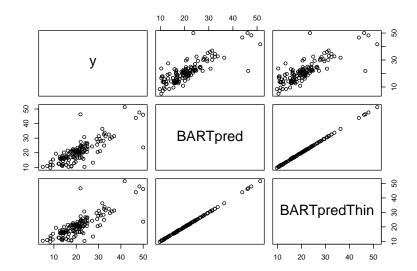
- **nkeeptest**: number of f(x) draws to save for test x.
- **nkeeptestmeam** : number of draws to use in computing yhat.test.mean.
- nkeeptreedraws: number of tree ensembles to keep.

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.

3.2 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 BARTpred predictions are from a run are from a BART run with seed=99 and all default values.

The **BARTpredThin** are from 200 kept trees out of a long run with 1,000 burn-in and 10,000 kept draws and seed=4.

Interesting how similar they are !!!!