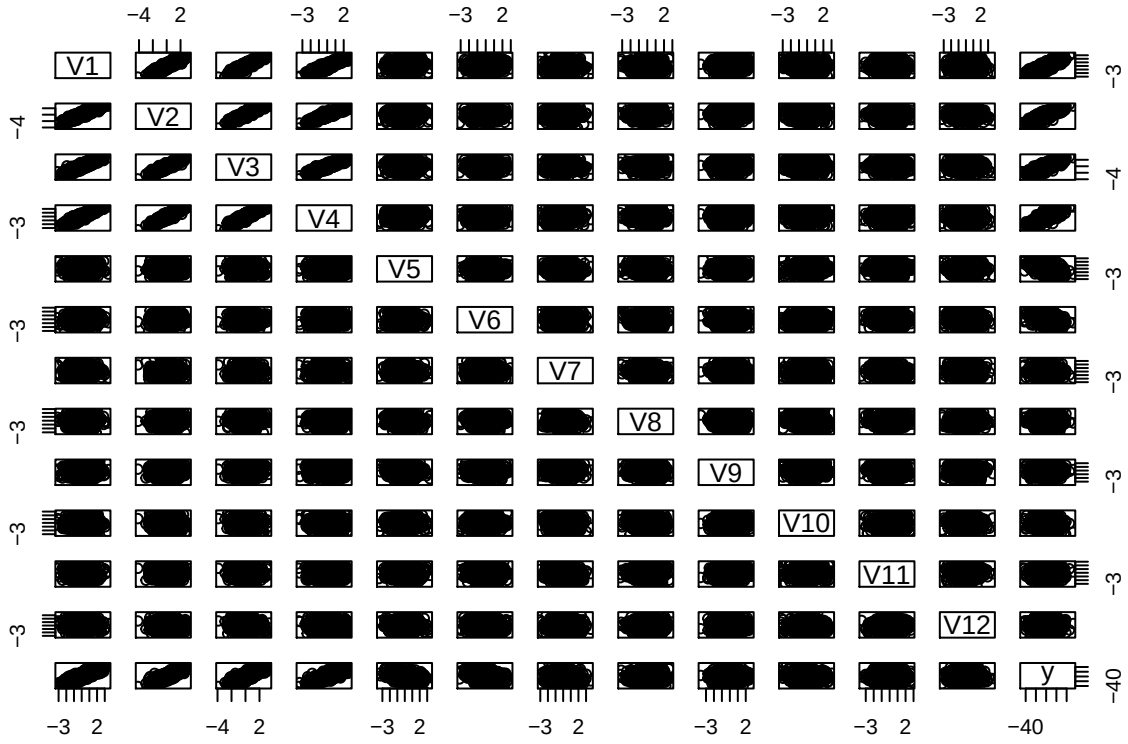
Simulations and Comparisons

Simulated Data

To aid in comparisons between the methods, one of the simulated datasets considered in this paper will be generated from the same method as used in (Strobl et al, 2008???). Under this method, the 13 x 1000 data set, D_1, has 12 predictors, $V_1, .., V_{12}$, where $V_j \sim N(0, 1)$. The first four are, however, block correlated to each other with $\rho = .9$. They are related to Y by the linear equation:

$$Y = 5 \cdot V_1 + 5 \cdot V_2 + 2 \cdot V_3 + 0 \cdot V_4 + -5 \cdot V_5 + -5 \cdot V_6 + 0 \cdot V_7 + 0 \cdot ..... + E, E \sim N(0, \frac{1}{2})$$

Note that the coefficents for $V_7, ..., V_{12}$ are all zero.




```
##                V1            V2           V3           V4           V5
## V1   1.000000000  0.9146541132  0.907895351  0.907066765 -0.034234292
## V2   0.914654113  1.0000000000  0.913780977  0.913731929 -0.020066937
## V3   0.907895351  0.9137809775  1.000000000  0.902766836 -0.016703104
## V4   0.907066765  0.9137319288  0.902766836  1.000000000 -0.002169185
## V5  -0.034234292 -0.0200669374 -0.016703104 -0.002169185  1.000000000
## V6   0.006059950 -0.0007016153 -0.006844401 -0.014814462  0.043610533
## V7   0.011864999 -0.0013307105  0.006951044  0.022724703  0.005306628
## V8   0.012429245  0.0180018750  0.021232744  0.020871464 -0.031895007
## V9   0.035378928  0.0383359616  0.036338439  0.037906433 -0.024882964
## V10 -0.027164872 -0.0205322792 -0.021277153 -0.021746391  0.005239249
## V11 -0.062839803 -0.0447873818 -0.029615955 -0.053826143 -0.018439527
## V12  0.001895378 -0.0040846930 -0.005222882 -0.017304444 -0.043550921
## y    0.828867870  0.8301277767  0.808338105  0.788791607 -0.388422174
##                V6           V7           V8           V9          V10
## V1   0.0060599505  0.011864999  0.01242924  0.035378928 -0.027164872
## V2  -0.0007016153 -0.001330711  0.01800187  0.038335962 -0.020532279
```

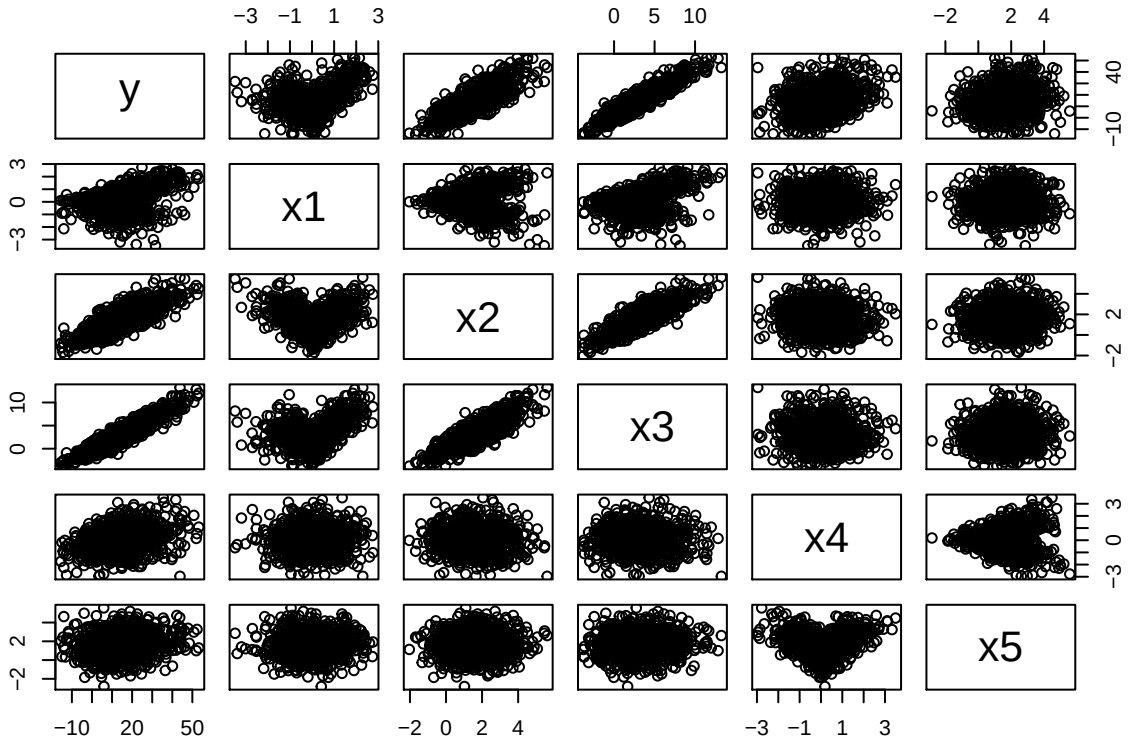
```
## V3  -0.0068444008  0.006951044  0.02123274  0.036338439 -0.021277153
## V4  -0.0148144624  0.022724703  0.02087146  0.037906433 -0.021746391
## V5   0.0436105331  0.005306628 -0.03189501 -0.024882964  0.005239249
## V6   1.0000000000 -0.004856916 -0.02539841 -0.013632377  0.036331634
## V7  -0.0048569164  1.000000000 -0.02367510  0.006567436  0.018156112
## V8  -0.0253984113 -0.023675099  1.00000000 -0.038840769 -0.089374372
## V9  -0.0136323768  0.006567436 -0.03884077  1.000000000  0.001732069
## V10  0.0363316342  0.018156112 -0.08937437  0.001732069  1.000000000
## V11 -0.0217988171 -0.033514884  0.02826398 -0.075004886  0.010676447
## V12 -0.0422332641  0.032644574  0.02539601  0.009560373  0.015536556
## y   -0.3637688830 -0.141169908  0.03665375  0.045997408 -0.037738613
##             V11          V12           y
## V1  -0.06283980  0.001895378  0.82886787
## V2  -0.04478738 -0.004084693  0.83012778
## V3  -0.02961595 -0.005222882  0.80833811
## V4  -0.05382614 -0.017304444  0.78879161
## V5  -0.01843953 -0.043550921 -0.38842217
## V6  -0.02179882 -0.042233264 -0.36376888
## V7  -0.03351488  0.032644574 -0.14116991
## V8   0.02826398  0.025396015  0.03665375
## V9  -0.07500489  0.009560373  0.04599741
## V10  0.01067645  0.015536556 -0.03773861
## V11  1.00000000  0.022521656 -0.02183787
## V12  0.02252166  1.000000000  0.02427605
## y   -0.02183787  0.024276053  1.00000000
```

Let's move on to a more difficult situation. The dataset $D2$ contains five predictors, $X_1, ...X_5$, that have an interesting structure- several of the predictors are correlated, but are not one -to -one. This violates an important assumtion of the linear model and means that these variables have low correlation. Note that this only makes sense in higher dimensions where we are estimating the value of X_j given $X_1, ..., X_n$.

```
x1 <- rnorm(1000)

x2 <- 2*sqrt(abs(x1)) + rnorm(1000)

x3 <- x1 + 2*x2 + rnorm(1000)

x4 <- rnorm(1000)

x5 <- 2*sqrt(abs(x4)) + rnorm(1000)

y <- x1 + 2*x2 + 3 * x3 + 4*x4 + 1*x5 + rnorm(1000)

d2 <- data.frame(y,x1,x2,x3,x4,x5)

cor(d2)
```

```
##            y         x1          x2          x3          x4         x5
## y  1.0000000 0.37370066  0.81852208  0.92926643  0.30615522 0.15357237
## x1 0.3737007 1.00000000  0.01253512  0.37828457  0.02553116 0.01196494
## x2 0.8185221 0.01253512  1.00000000  0.85944303 -0.04770287 0.04253338
## x3 0.9292664 0.37828457  0.85944303  1.00000000 -0.03116991 0.04579883
## x4 0.3061552 0.02553116 -0.04770287 -0.03116991  1.00000000 0.01984835
## x5 0.1535724 0.01196494  0.04253338  0.04579883  0.01984835 1.00000000
```

```
plot(d2)
```

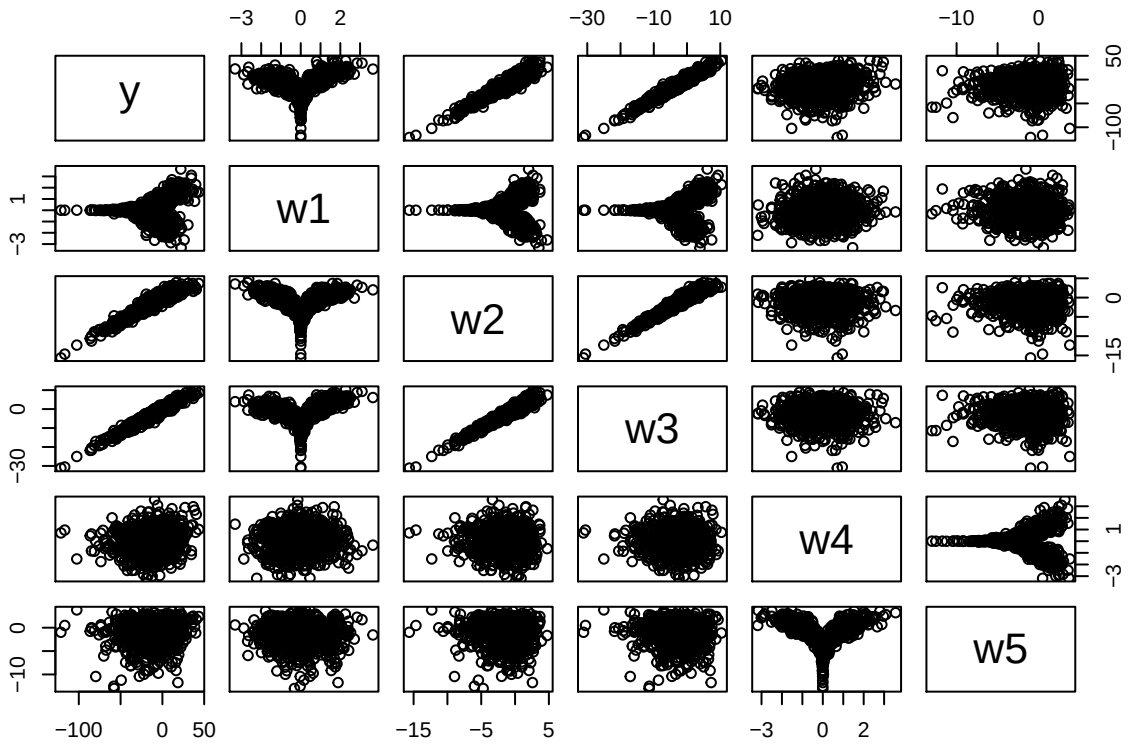


The tricker relationship between the variables in $D2$ was because they were generated using the square root of the absolute value of the other variable. Here, in $D3$ the process is repeated but with the log of the absolute value.

```
w1 <- rnorm(1000)

w2 <- 2*log(abs(w1)) + rnorm(1000)

w3 <- w1 + 2*w2 + rnorm(1000)

w4 <- rnorm(1000)

w5 <- 2*log(abs(w4)) + rnorm(1000)

y <- w1 + 2*w2 + 3 * w3 + 4*w4 + 1*w5 + rnorm(1000)

d3 <- data.frame(y,w1,w2,w3,w4,w5)

cor(d3)
```

```
##             y          w1          w2          w3          w4          w5
## y  1.00000000  0.15728407  0.94764704  0.97416878  0.17279746  0.05578763
## w1 0.15728407  1.00000000 -0.02714818  0.15752508  0.03050113 -0.05109218
## w2 0.94764704 -0.02714818  1.00000000  0.96531545 -0.01975103 -0.04414540
## w3 0.97416878  0.15752508  0.96531545  1.00000000 -0.01042494 -0.05419898
## w4 0.17279746  0.03050113 -0.01975103 -0.01042494  1.00000000 -0.03325170
## w5 0.05578763 -0.05109218 -0.04414540 -0.05419898 -0.03325170  1.00000000
```

```
plot(d3)
```



Models and Comparisons

Trees

CART: Regression Trees

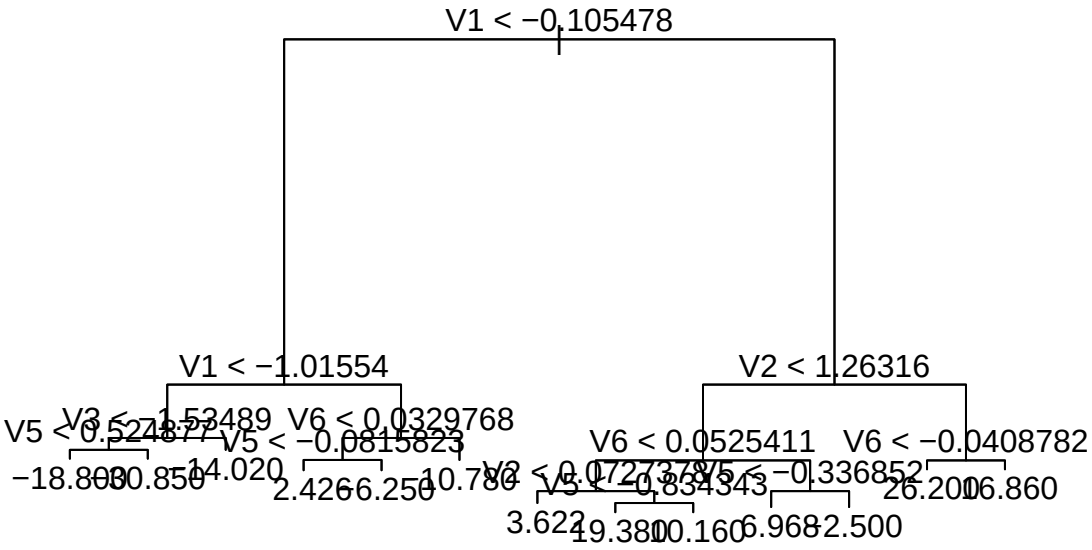
As outlined in the 1984 textbook, *Classification and Regression Trees*, _____ described their method for creating, pruning, and testing regression trees. What follows is their basic algorithm for fitting regression trees:

Algorithm 2: CART, Regression Trees

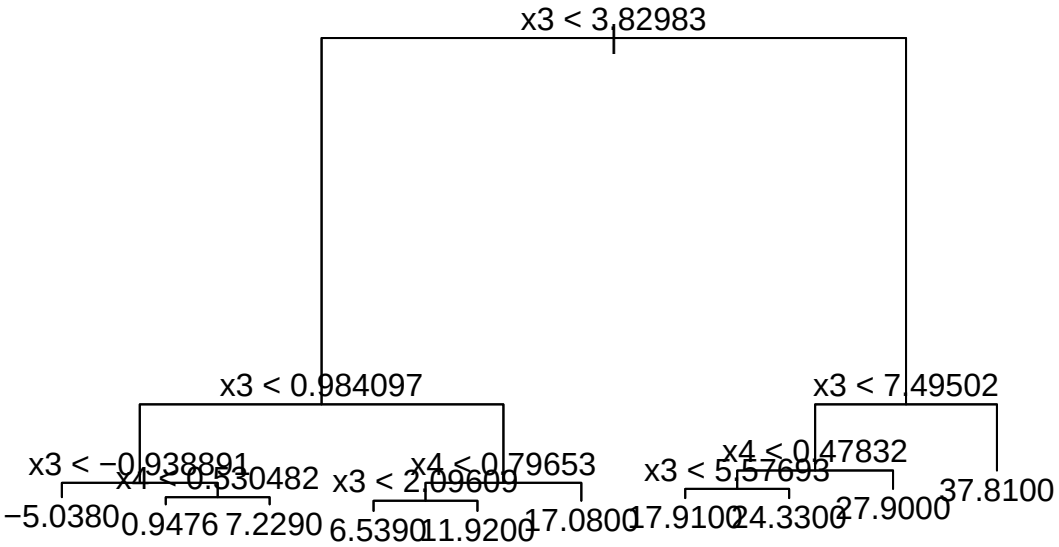
1.
2.
3.
4.

Let's return to our simulated datasets. Here is what trees grown for each dataset using the model $Y \sim X_1, ...X_n$.

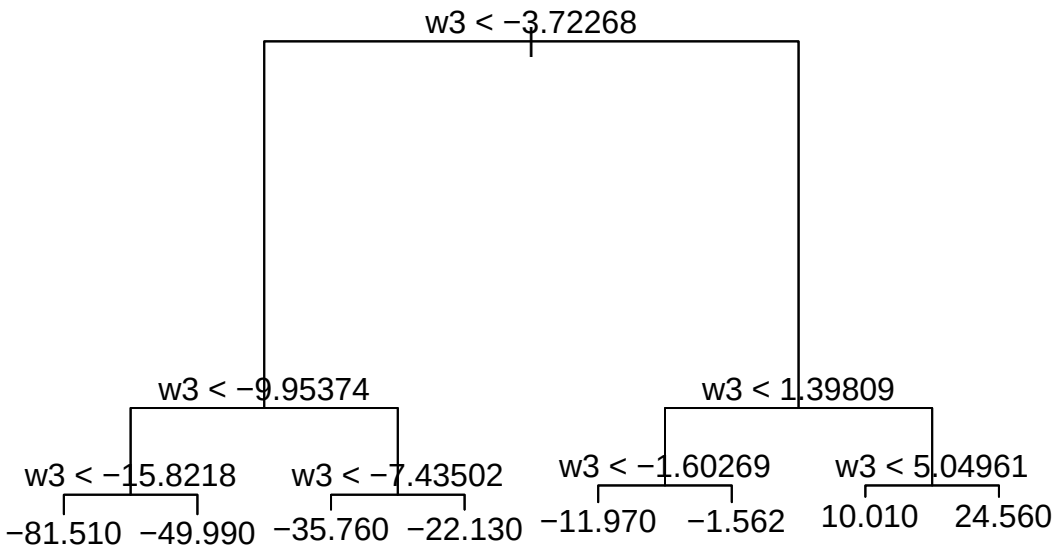
```
library(tree)
t1 <- tree(y~., d1)
t2 <- tree(y~., d2)
t3 <- tree(y~., d3)

plot(t1)
text(t1)
```




```
plot(t2)
text(t2)
```




```
plot(t3)
text(t3)
```



Conditional Inference Trees

Another popular method for creating regression tree models is Conditional Inference Trees.

CI trees

```
1. For case weights  $w$  test the global null hypothesis of independence between any of the m covariat

2. Choose a set  $A \subset X_{j}$  in order to split  $X_{j}$  into two disjoint sets  $A$  and  $X_{j

3. Recursively repeat steps 1 and 2 with modified case weights  $w_left$  and  $w_right$, respectively.
```

from https://eeecon.uibk.ac.at/~zeileis/papers/Hothorn+Hornik+Zeileis-2006.pdf

After step 1 is completed, any goodness of fit method can be used to generate the split and choose the set A.
Note that in this method the splitting is done separately from the variable selection.

Bagged Forests

As mentioned in the introduction, single trees can have some variablility that in practice, limits their use.
This simulation demonstrates this principle:

```
for 1000 trials:

1. separete D3 into a training set and a test set where the training set contains 2/3 of the observatio

2. fit a CART tree

3. Predict the response using the test set

4. Calculate the mean squared error
```

Here is a histogram of the MSE found using this method:

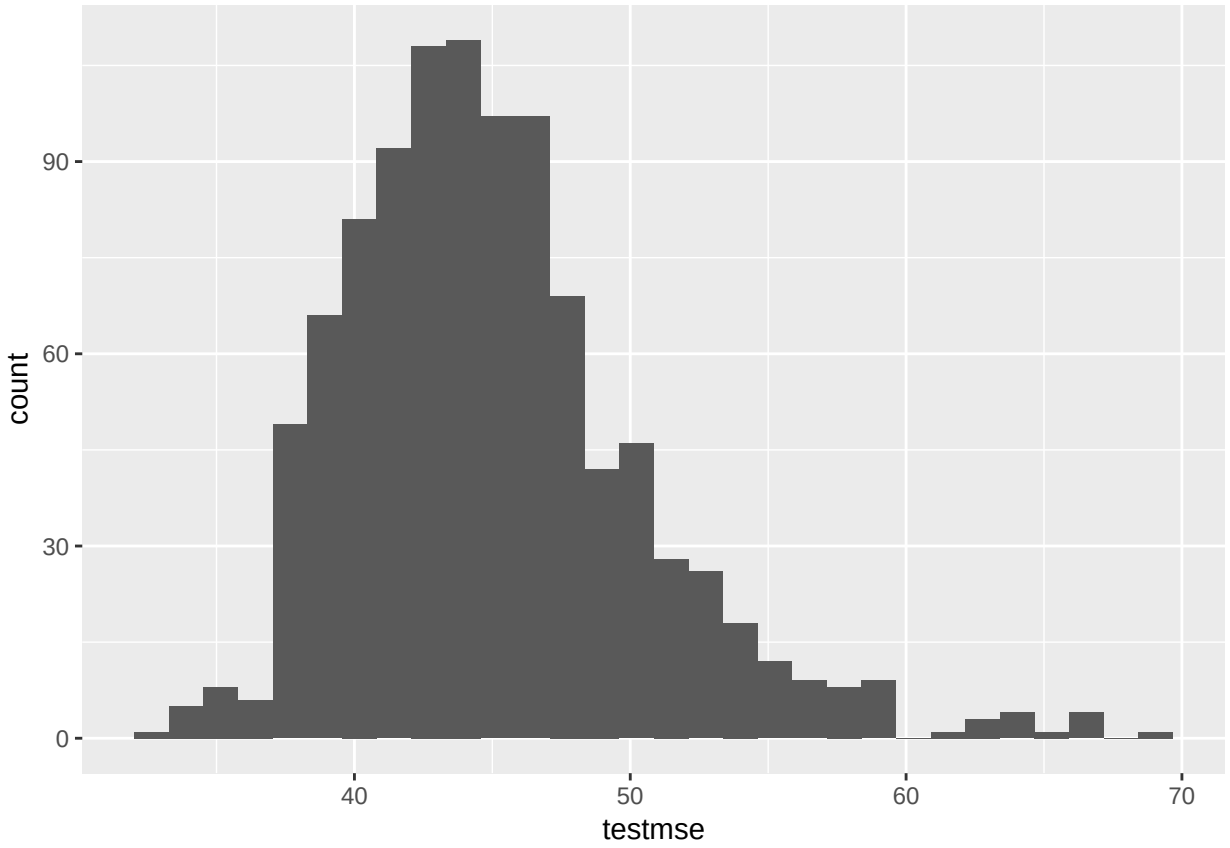
```
testmse <- rep(0,1000)

for(i in 1:1000){
  train <- sample(1000, 666)
```

```
  t <- tree(y~., d3[train,])
  testmse[i] <- mean((d3[-train,]$y - predict(t, d3[-train,]))^2)
}

testmse <- as.data.frame(testmse)

var(testmse)
```

```
##          testmse
## testmse 28.56955
```

```
ggplot(aes(x = testmse), data = testmse) + geom_histogram()
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



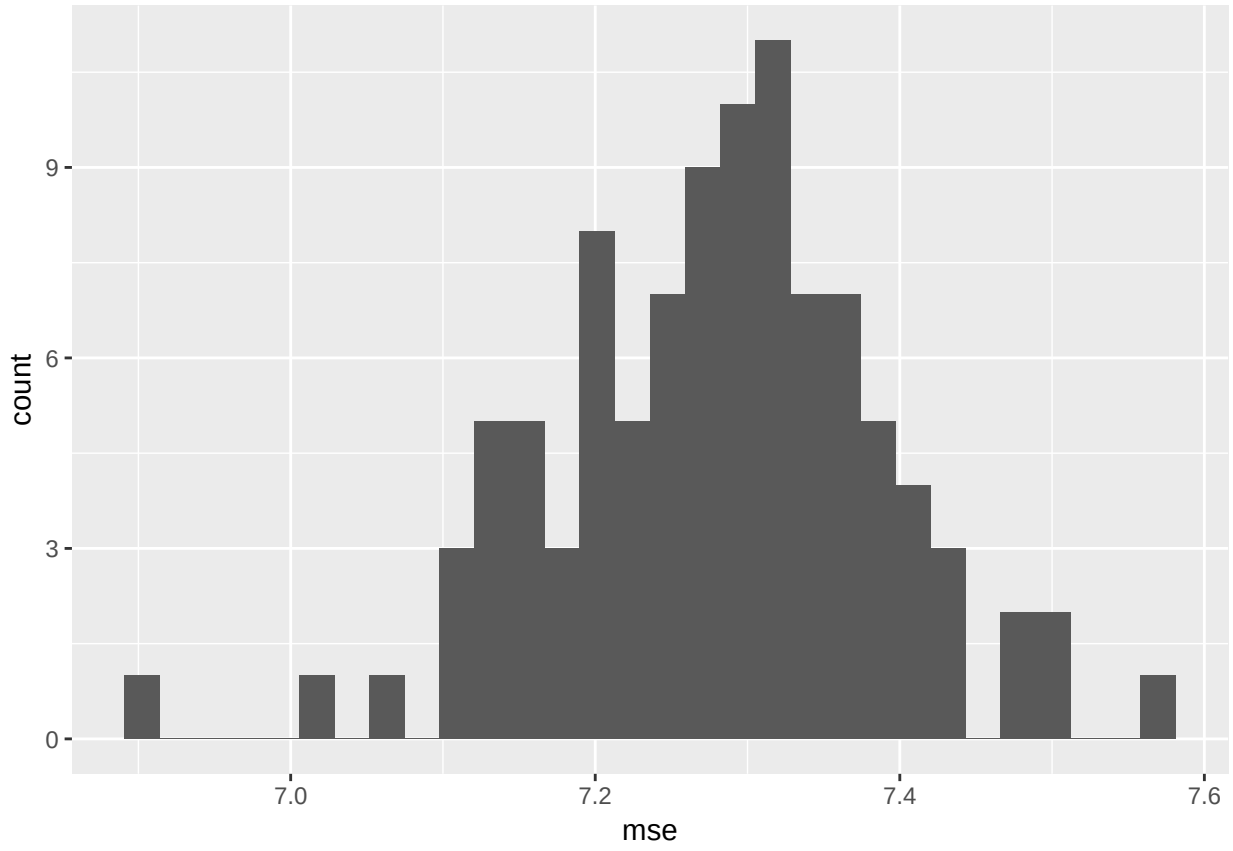
As one can see, there is a fair amount of variability in a single tree, they are heavily dependent on fluctuations in the starting data set. As mention briefly in the introduction, bagged forests present one solution to this problem. To create a bagged forest, as outlined in *An Introduction to Statistical Learning* by James, Witten, Hastie and Tibshirani, 2013, many bootsrtapped samples are taken from the itintial dataset and trees are fitted to them. The final predictions are, then, averaged over all of the trees. This ensures that while each tree has high variance, when they are aggregated the variance will decrease.

Let's put that to the test here using our dataset $D3$ again. We'll build 100 forests of 100 trees each and compare the variability of the MSE distributions.

```
library(bagRboostR)

mse <- rep(0,100)
train = sample(1000,666)
```

```
for (i in 1:100){
  b <- randomForest(y~., data = d3, subset = train, mtry = 5)
  mse[i] <- mean((d3$y[-train] - predict(b, d3[-train,]))^2)
}

mse <- as.data.frame(mse)

ggplot(aes(x = mse), data = mse) + geom_histogram()
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```




```
var(mse)
```

```
##             mse
## mse 0.01181591
```

As one can see, the values of MSE_{test} for the bagged forest were entirely below the MSE_test for the trees and the variance was much smaller.

Random Forests