# chemistry

2023-06-25

### **Data**

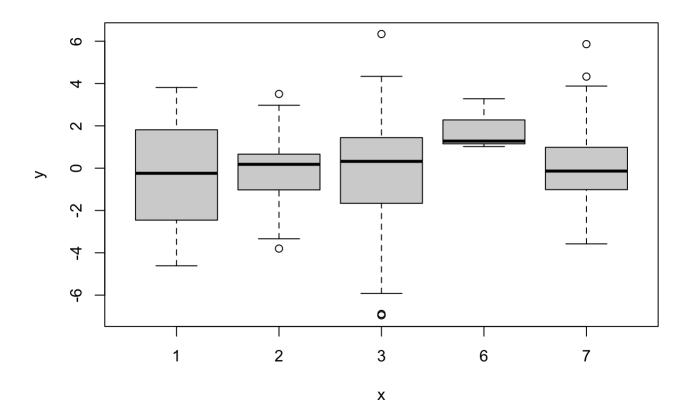
```
chem <- read.table("~/Downloads/momeg/a-level-chemistry.txt", dec = ".", sep = " ")
colnames(chem) <- c('Board','Ascore','Total','GNum','Gender','Age','InstType','LEAID','L
EAInst','StuID')
chem <- chem[1:500,]</pre>
```

## **Tree**

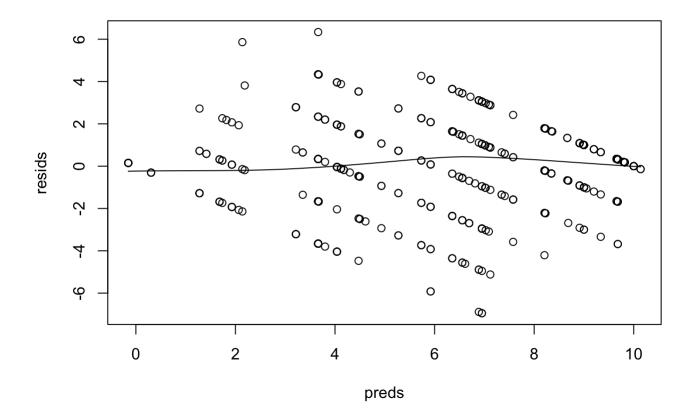
width(chemLM\$tree)

## [1] 26

```
resids <- residuals(chemLM)
preds <- predict(chemLM)
plot(factor(chem$Board), resids)</pre>
```



scatter.smooth(preds, resids)



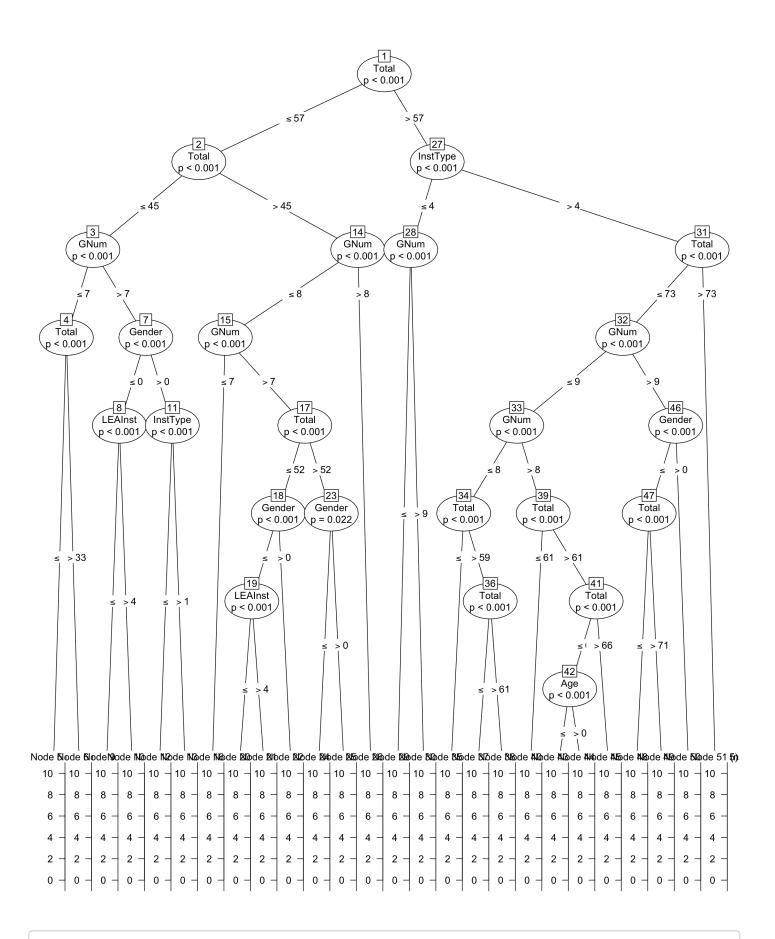
### fligner.test(resids ~ chem\$Board)

```
##
## Fligner-Killeen test of homogeneity of variances
##
## data: resids by chem$Board
## Fligner-Killeen:med chi-squared = 9.6607, df = 4, p-value = 0.04655
```

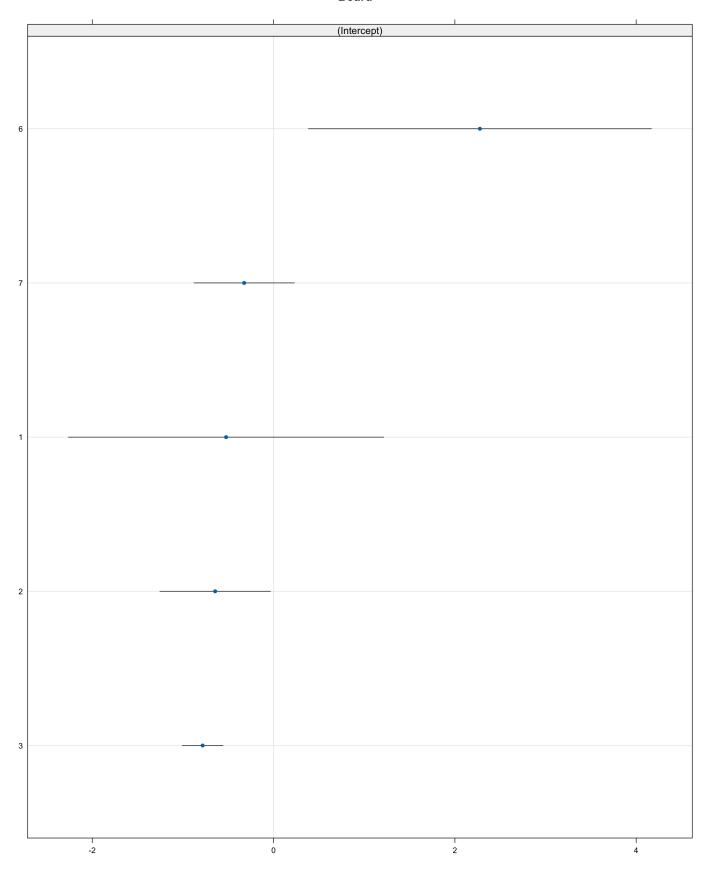
#### bartlett.test(resids ~ chem\$Board)

```
##
## Bartlett test of homogeneity of variances
##
## data: resids by chem$Board
## Bartlett's K-squared = 14.233, df = 4, p-value = 0.006588
```

```
Chem_Train <- chem[1:300,]</pre>
cp_{vals} = 10^{eq}(-5, 5, length = 100)
colnames(Chem_Train) <- make.names(colnames(Chem_Train))</pre>
control = trainControl("repeatedcv", number = 10, repeats=10)
set.seed(2022)
Chem_Tree <- train(data=Chem_Train, Ascore ~ Total + GNum + Gender + Age + LEAInst + Ins
tType + LEAID , method="rpart", trControl=control,tuneGrid=expand.grid(cp=cp_vals))
## Warning in nominalTrainWorkflow(x = x, y = y, wts = weights, info = trainInfo,
## : There were missing values in resampled performance measures.
Chem_Best_Tree <- rpart(Ascore ~ Total + GNum + Gender + Age + LEAInst + InstType + LEAI
D, data=Chem_Train, cp=Chem_Tree$bestTune)
data <- head(chem$Ascore,10)</pre>
pre <- predict(chemLM, newdata = chem[1:10,])</pre>
sum((pre-data)^2)
## [1] 12.14109
rmse(data, pre)
## [1] 1.101866
pre <- predict(Chem_Best_Tree, newdata = chem[1:10,])</pre>
sum((pre-data)^2)
## [1] 13.4973
rmse(data,pre)
## [1] 1.161779
plot(chemLM)
```







rpart.plot(Chem\_Best\_Tree, box.palette="RdBu", shadow.col="gray", nn=TRUE, cex=1, extra=
1)

