Introduction to Machine Learning

Lab 3

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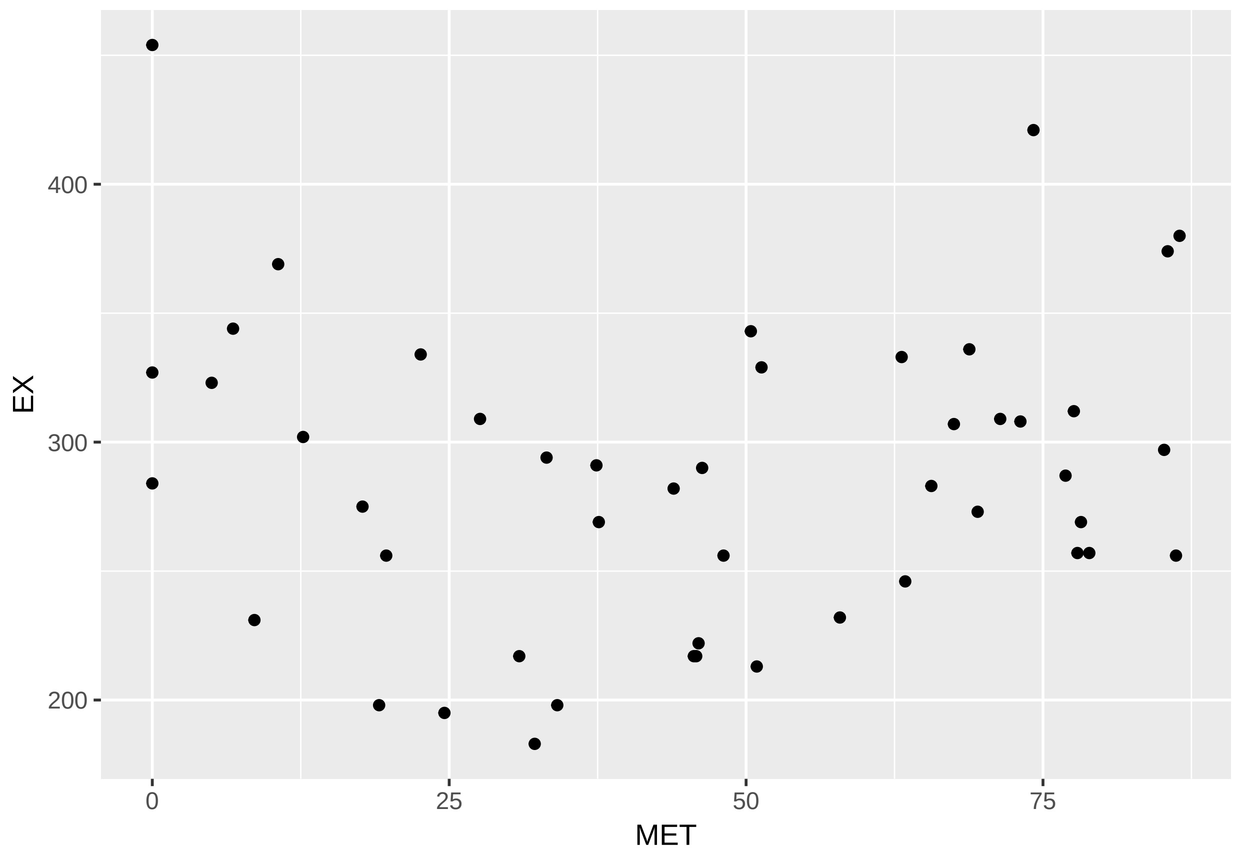
Contents

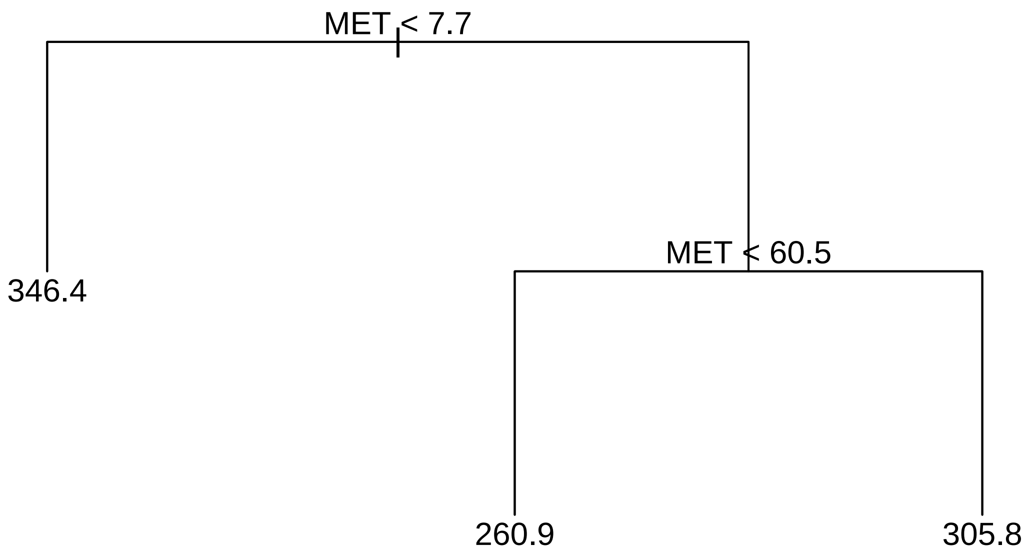
Assignment 1

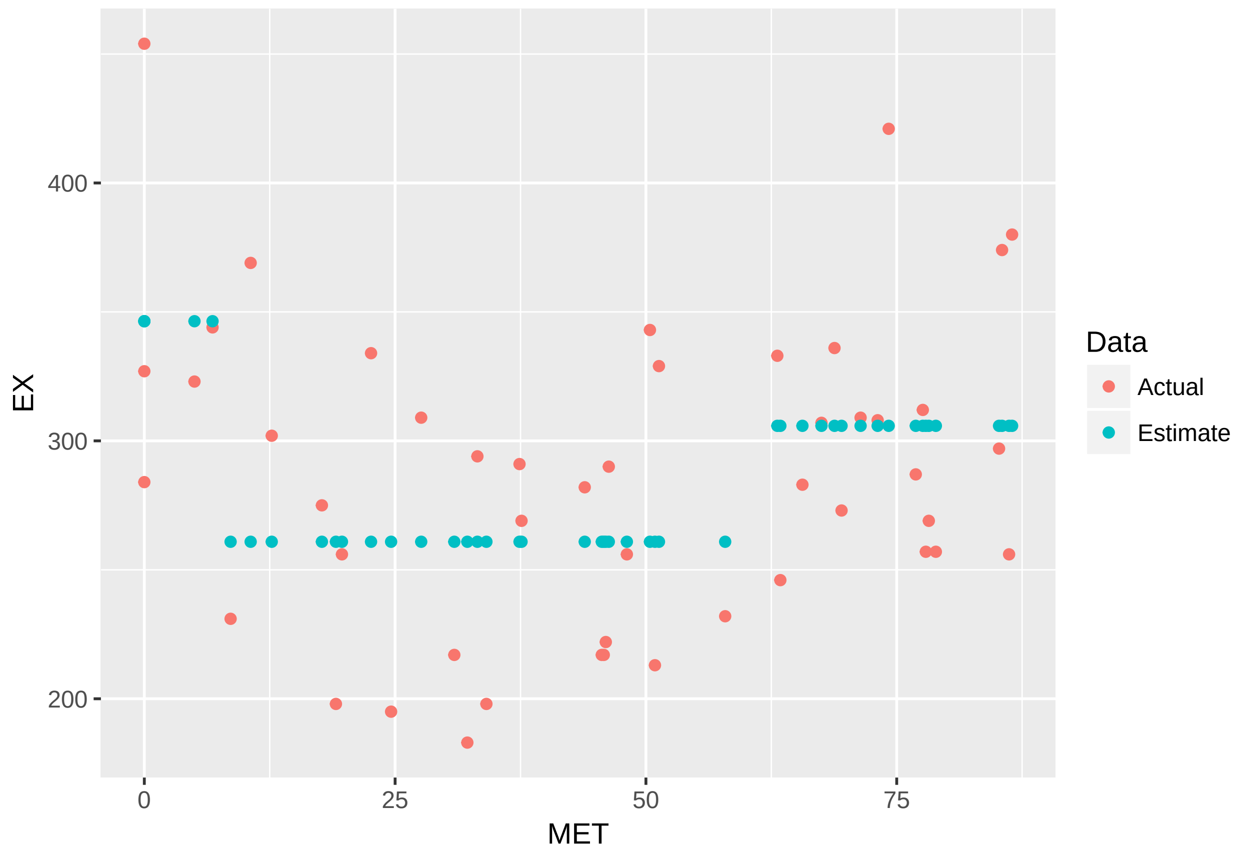
1

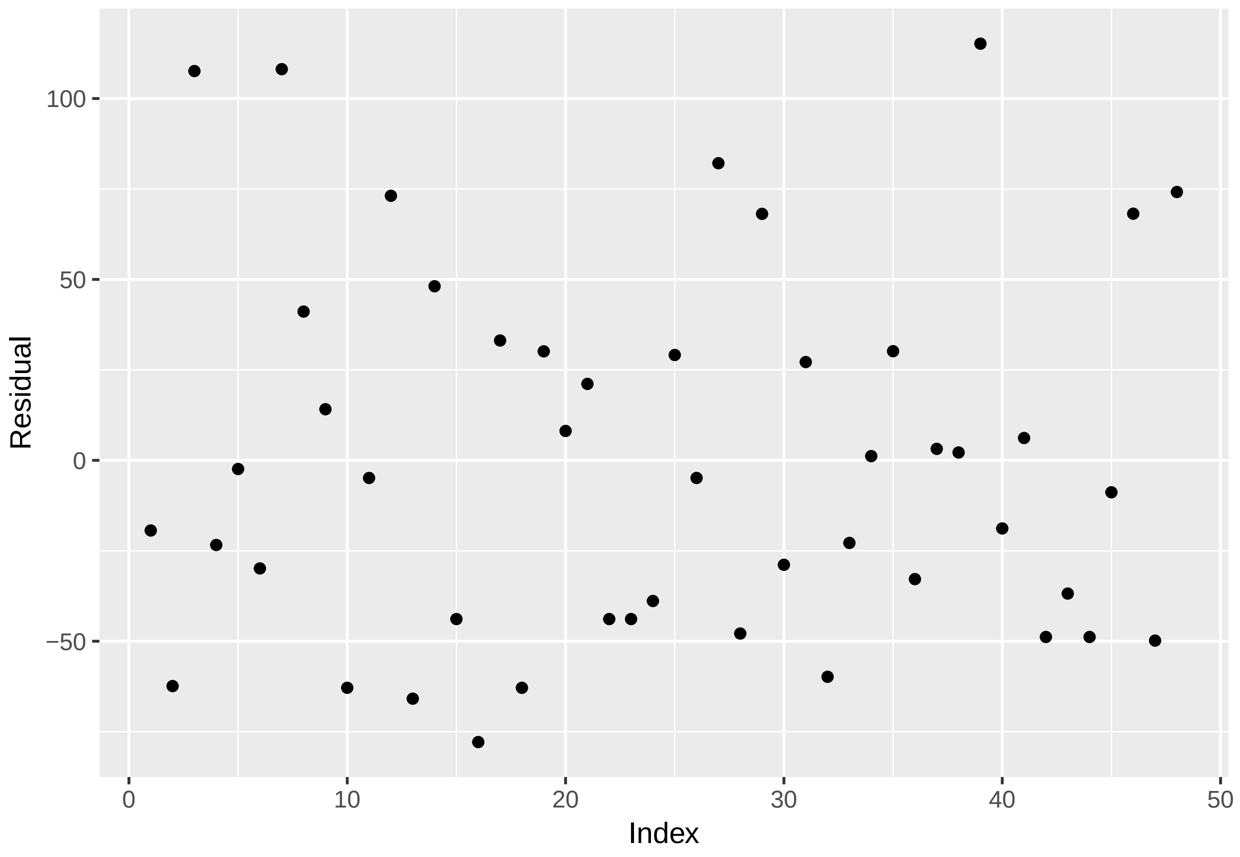


The data looks like it could be modelled by a cubic spline function.

2




EX
400
300
200
0
25
50
75
MET
Data
Actual
Estimate


Residual
100
50
0
−50
0
10
20
30
40
50
Index

3

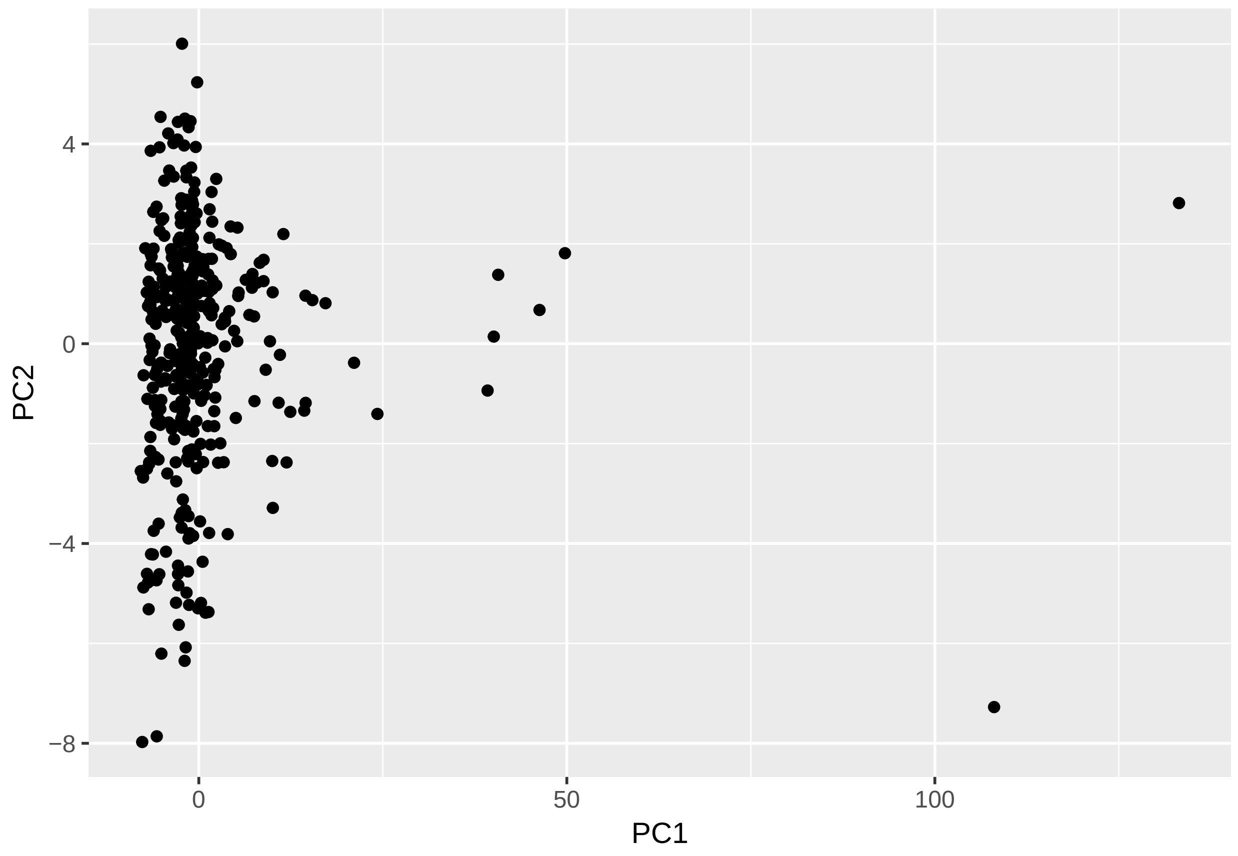
4

5

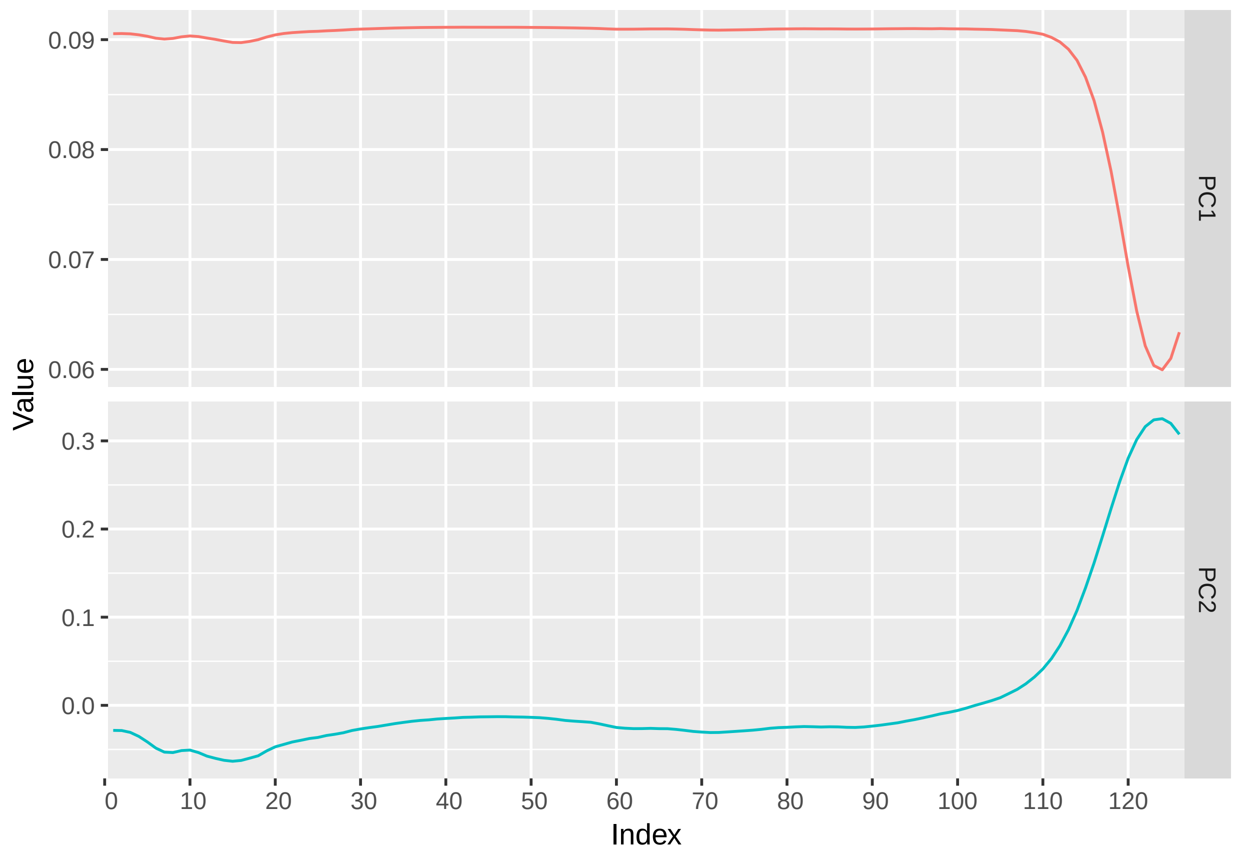
Assignment 2

1

```
#>   [1] "95.385" "4.229"  "0.186"  "0.084"  "0.072"  "0.021"  "0.007" 
#>   [8] "0.003"  "0.003"  "0.002"  "0.001"  "0.001"  "0.001"  "0.001" 
#>  [15] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [22] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [29] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [36] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [43] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [50] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [57] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [64] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [71] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [78] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [85] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [92] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>  [99] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#> [106] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#> [113] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#> [120] "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000"  "0.000" 
#>   [1] "0.954" "0.996" "0.998" "0.999" "1.000" "1.000" "1.000" "1.000"
#>   [9] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [17] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [25] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [33] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [41] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [49] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [57] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [65] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [73] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [81] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [89] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#>  [97] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#> [105] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#> [113] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
#> [121] "1.000" "1.000" "1.000" "1.000" "1.000" "1.000"
```

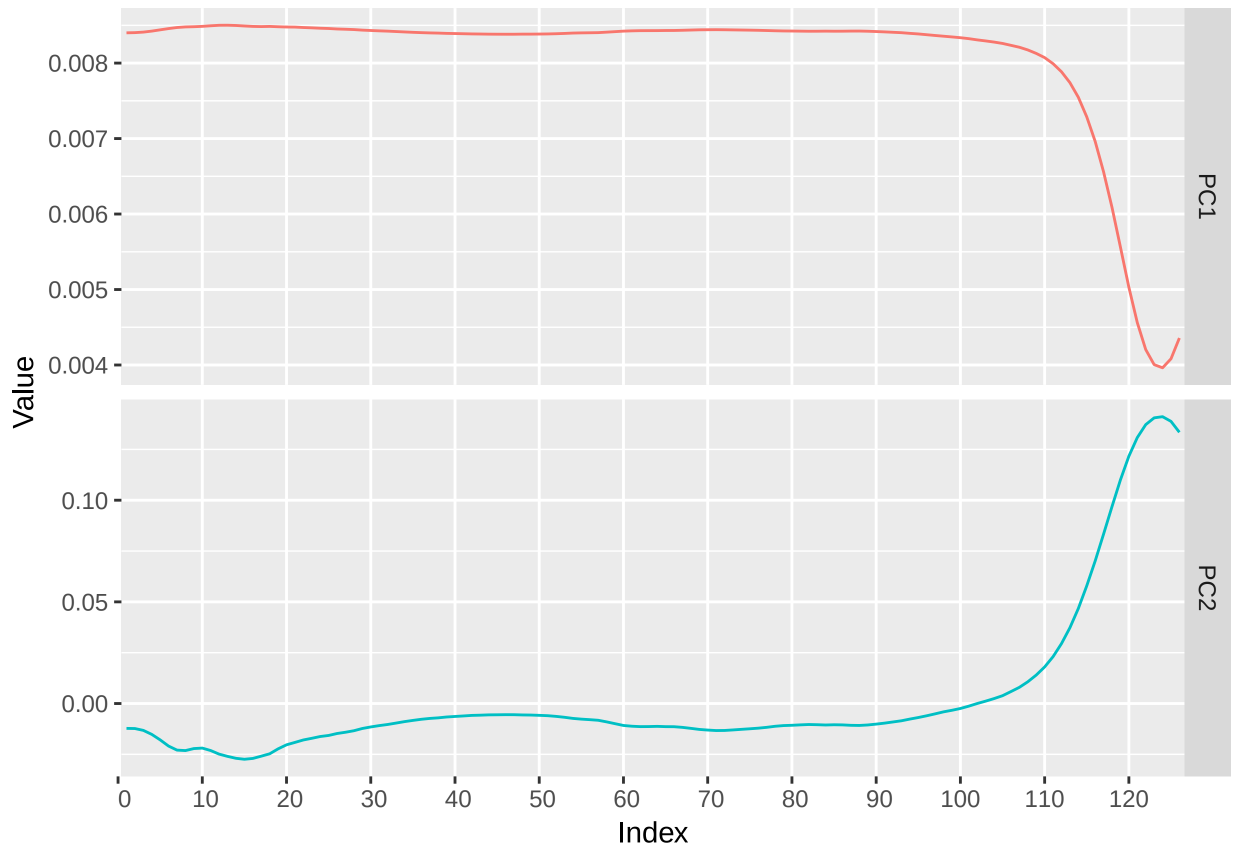

4
0
−4
−8
0
50
100
PC1
PC2

2

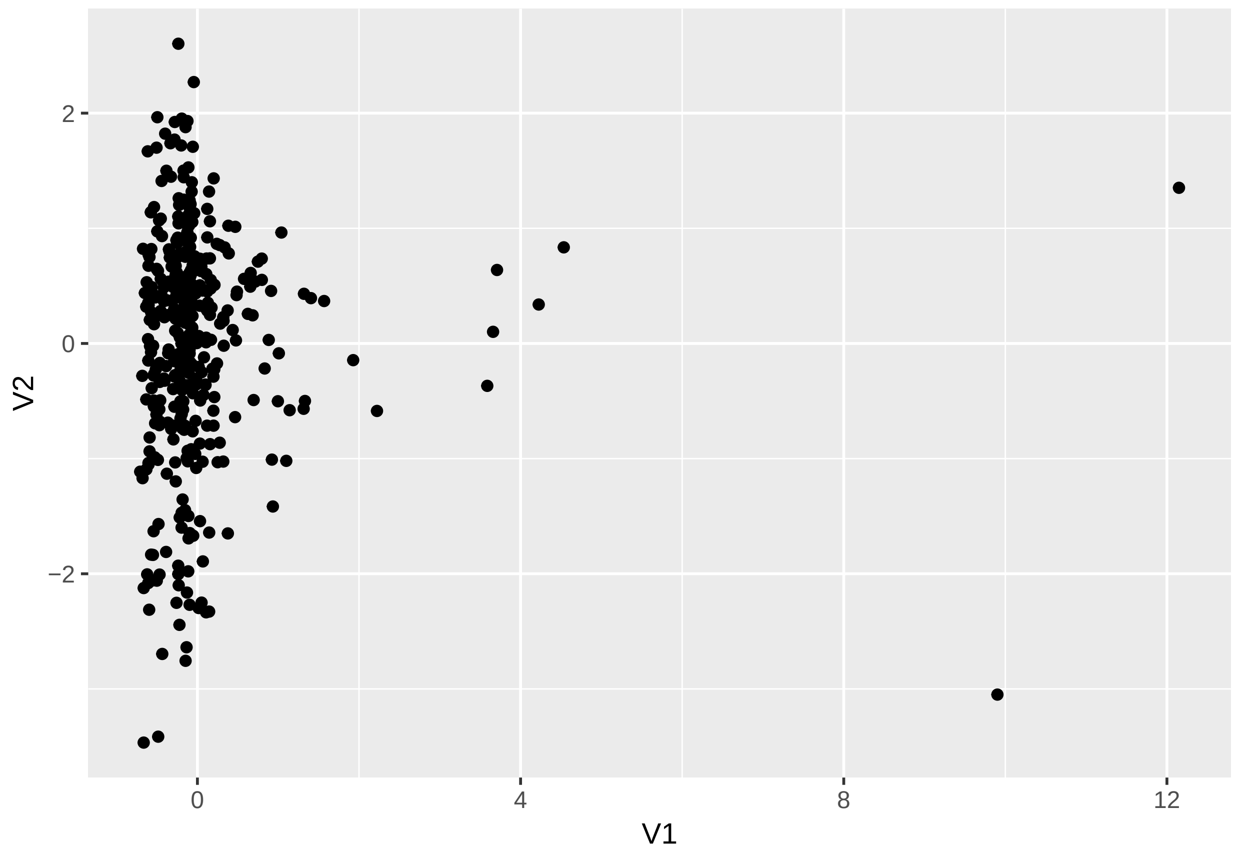


Value
0.09
0.08
0.07
0.06
PC1
0.3
0.2
0.1
0.0
PC2
0
10
20
30
40
50
60
70
80
90
100
110
120
Index

3

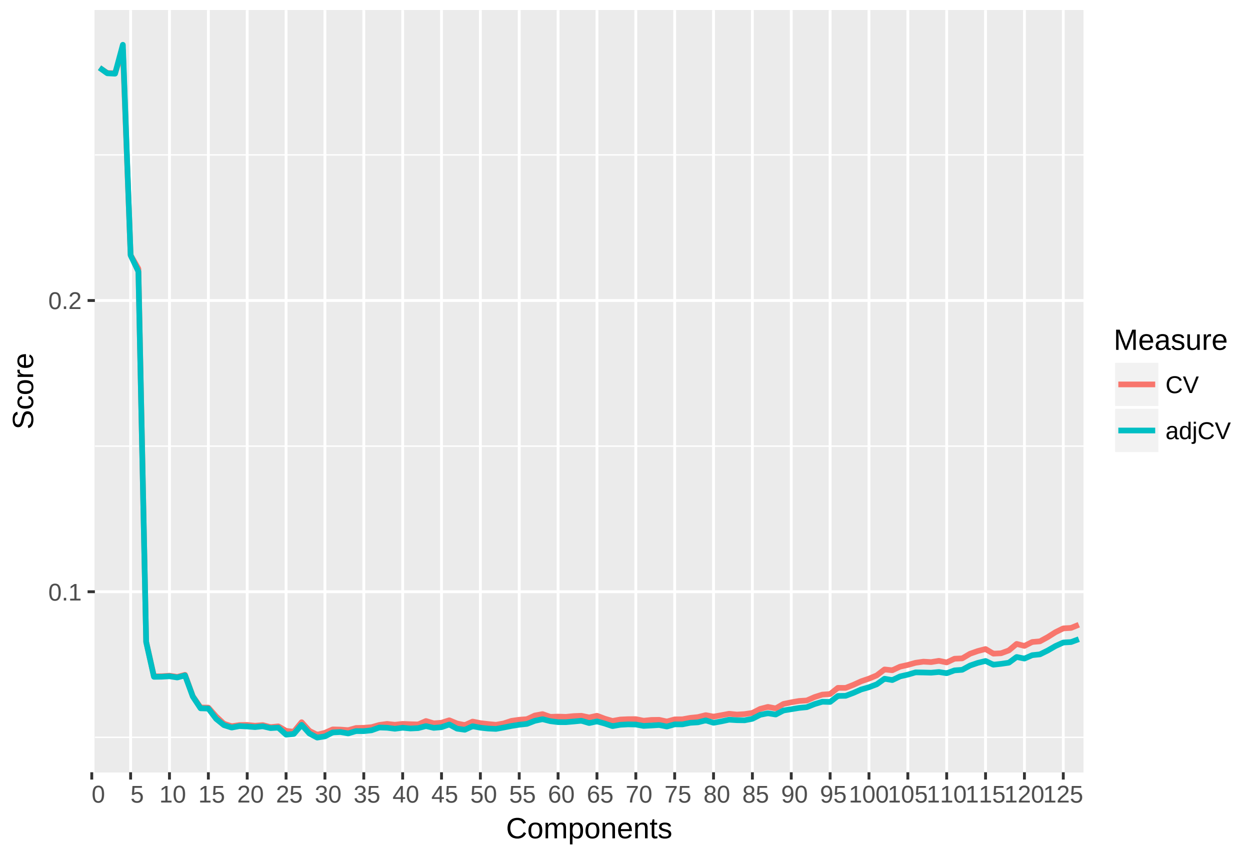


Value
0.008
0.007
0.006
0.005
0.004
0.10
0.05
0.00
PC1
PC2
0
10
20
30
40
50
60
70
80
90
100
110
120
Index



V2
2
0
−2
V1
0
4
8
12

4



Score
0.2
0.1
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100
105
110
115
120
125
Components
Measure
CV
adjCV

Appendix

Code for Assignment 1

```r
library(ggplot2)
library(tree)
library(reshape)

data <- read.csv2("../data/State.csv", header=TRUE, sep=";")
data <- data[order(data$MET),]
ggplot(data) +
    geom_point(aes(x=MET, y=EX))

tree.control(nobs=nrow(data), minsize=8)
treefit <- tree(EX ~ MET, data=data)

set.seed(12345)
treefit.cv <- cv.tree(treefit, FUN=prune.tree, K=10)
optimal_leaf_count<- treefit.cv$size[which.min(treefit.cv$dev)]

optimal_tree <- prune.tree(treefit, best=optimal_leaf_count)
plot(optimal_tree)
text(optimal_tree, pretty=0)
predicted <- predict(optimal_tree, data)
plot_data <- data.frame(MET=data$MET, Actual=data$EX, Estimate=predicted)
plot_data <- melt(plot_data, id.vars="MET")
names(plot_data) <- c("MET", "Data", "EX")

ggplot(plot_data) +
    geom_point(aes(x=MET, y=EX, color=Data))
residuals <- resid(optimal_tree)

plot_data <- data.frame(x=1:length(residuals), y=residuals)

ggplot(plot_data) +
    xlab("Index") +
    ylab("Residual") +
    geom_point(aes(x=x, y=y))
```

Code for Assignment 2

```r
library(ggplot2)
library(fastICA)
library(pls)
library(reshape2)

data <- read.csv2("../data/NIRSpectra.csv")

X <- scale(data[, -ncol(data)])
y <- data[, ncol(data)]
```

```r
traceplot <- function(n, pc1, pc2) {
    plot_data <- data.frame(x=1:n, PC1=pc1, PC2=pc2)
    plot_data <- melt(plot_data, id="x")
    names(plot_data) <- c("Index", "Component", "Value")
    xlimits <- seq(0, n, by=10)

    ggplot(plot_data) +
        geom_line(aes(x=Index, y=Value, color=Component), show.legend=FALSE) +
        scale_x_discrete(limits=xlimits) +
        facet_grid(Component ~ ., scales="free")
}

pca <- prcomp(X)

## Eigenvalues
lambda <- pca$sdev^2
variances <- lambda / sum(lambda)

var99_comp_count <- which.max(cumsum(variances * 100) > 99)
components <- as.data.frame(pca$x[, 1:var99_comp_count])




U <- pca$rotation
traceplot(nrow(U), U[, 1], U[, 2])

set.seed(12345)
ica <- fastICA(X, var99_comp_count, alg.typ = "parallel", fun = "logcosh", alpha = 1,
               method = "R", row.norm = FALSE, maxit = 200, tol = 1e-06, verbose = FALSE)

W_prime <- ica$K %*% ica$W
components <- as.data.frame(ica$S)
traceplot(nrow(W_prime), W_prime[, 1], W_prime[, 2])
ggplot(components) +
    geom_point(aes(x=V1, y=V2))

set.seed(12345)
pcrfit <- pcr(Viscosity ~ ., data=data, scale=TRUE)
cvcvpcrfit <- crossval(pcrfit, segments=10, segment.type="random")
cv_scores <- t(matrix(MSEP(cvpcrfit)$val, nrow=2))
plot_data <- data.frame(cbind(1:ncol(data), cv_scores))
colnames(plot_data) <- c("Components", "CV", "adjCV")
plot_data <- melt(plot_data, id="Components", variable_name="Measure")
names(plot_data)[ncol(plot_data)] <- "Score"
xlimits <- seq(0, ncol(data), by=5)

ggplot(plot_data) +
    geom_line(aes(x=Components, y=Score, color=Measure), size=1) +
    scale_x_discrete(limits=xlimits)
```