Class 6: R Functions

The Spanish Inquisition

April 18, 2019

About

This is my **class 6** R functions *code* that I wrote for today (April 18th)

```r
read.table("test1.txt",
           header = T,
           sep = ",")
```

```
##   Col1 Col2 Col3
## 1    1    2    3
## 2    4    5    6
## 3    7    8    9
## 4    a    b    c
```

```r
read.table("test3.txt"
)
```

```
##   V1 V2 V3
## 1  1  6  a
## 2  2  7  b
## 3  3  8  c
## 4  4  9  d
## 5  5 10  e
```

```r
read.table("test2.txt",
           sep = "$",
           header = T)
```

```
##   Col1 Col2 Col3
## 1    1    2    3
## 2    4    5    6
## 3    7    8    9
## 4    a    b    c
```

Can you improve this analysis code?

```r
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

```
##   Note: Accessing on-line PDB file
```

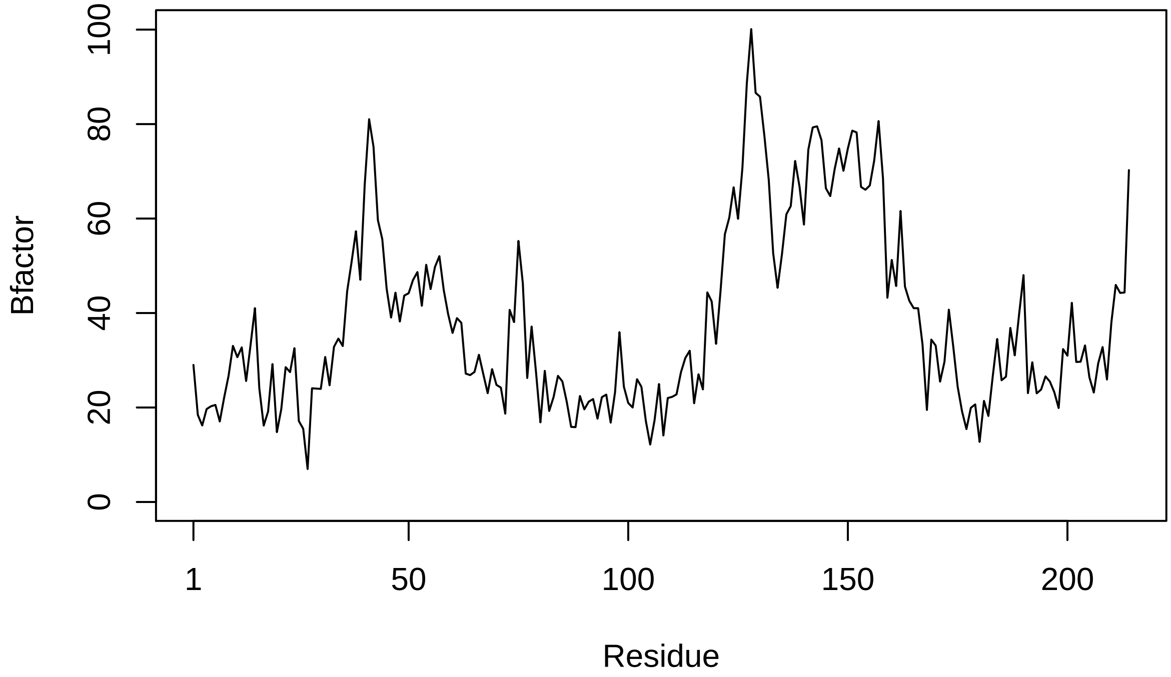
```r
s2 <- read.pdb("1AKE") # kinase no drug
```

```
##   Note: Accessing on-line PDB file
##    PDB has ALT records, taking A only, rm.alt=TRUE
```

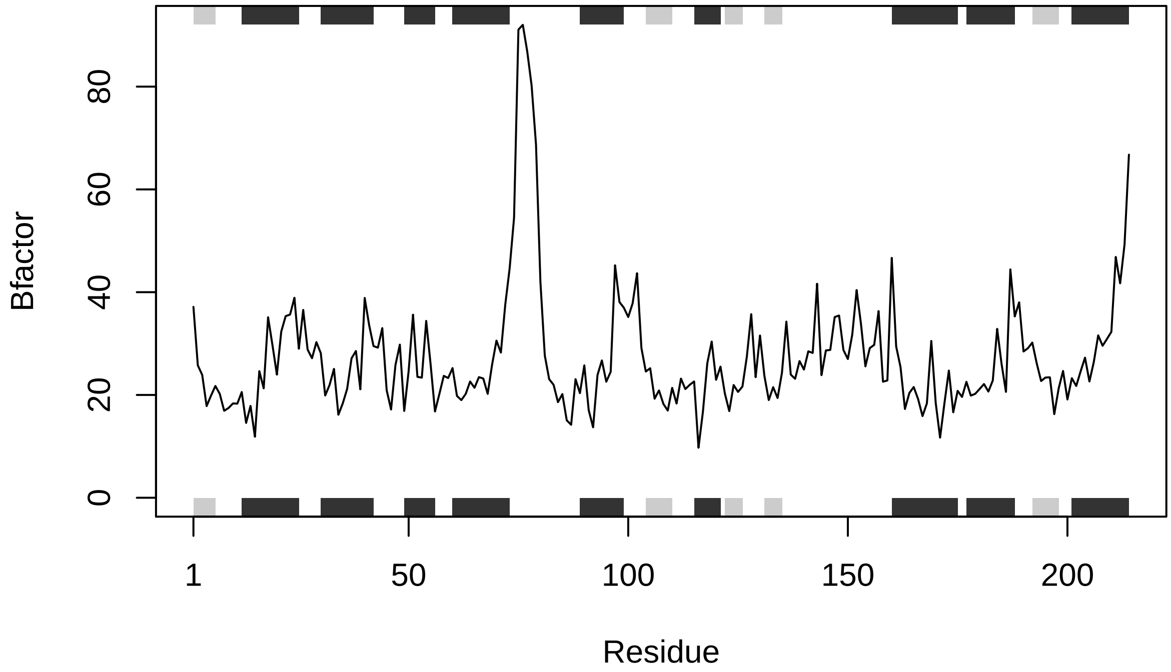
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

```
##   Note: Accessing on-line PDB file
```

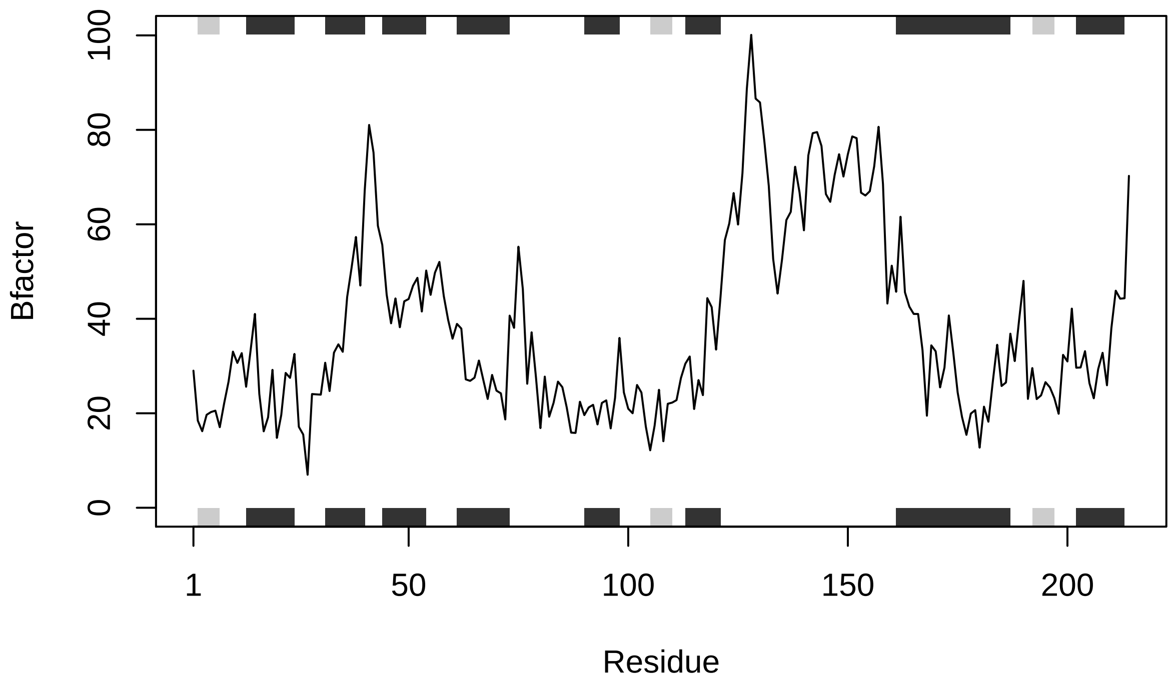
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, typ="l", ylab="Bfactor")
```



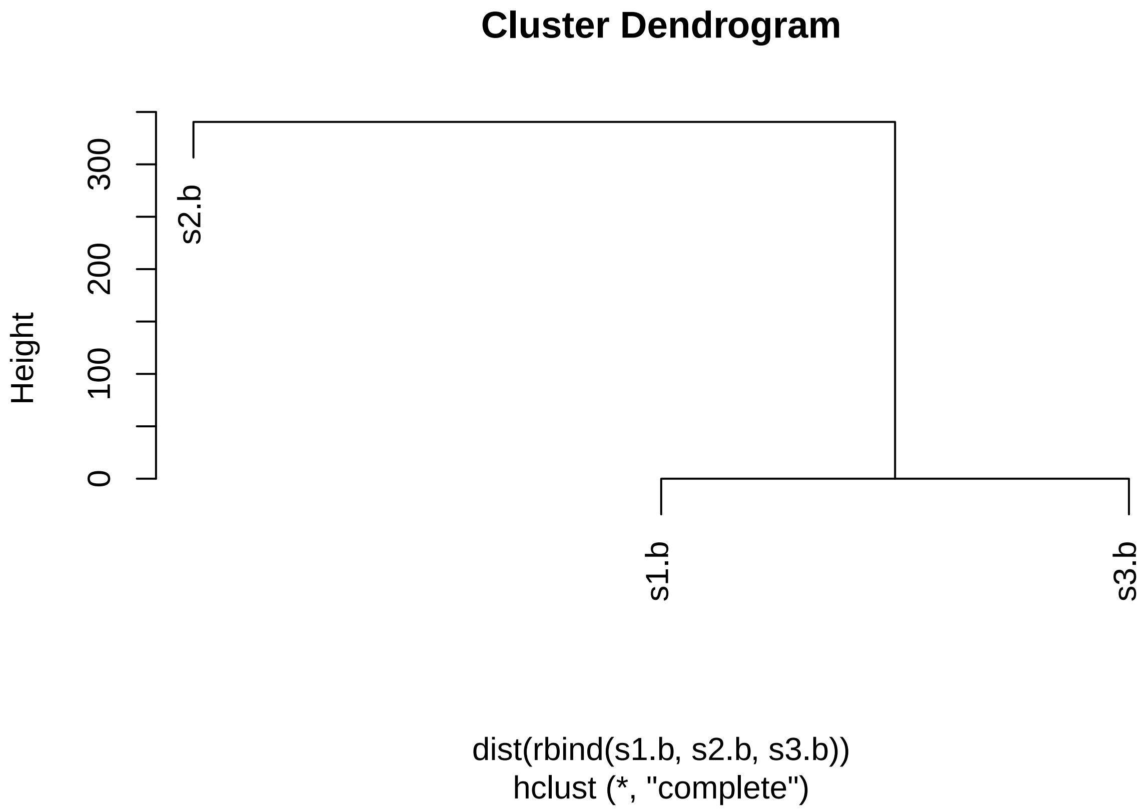
```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```



```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



```
hc <- hclust(dist(rbind(s1.b, s2.b, s3.b)))
plot(hc)
```



This is my simplified function to run bio3d. The simplePDBfunc takes three inputs into consideration. This function is a simplified version of the code above, which takes in protein codes as input, looks them up in Protein Data Bank, and gives data about that protein. The inputs should be a four character PDB (protein data bank) ID, such as 4HHB, or used in Barry's example, 4AKE, 1AKE, 1E4Y. Note that the function assumes that 3 proteins will be compared at once.

```r
simplePDBfunc <- function (x, y, z){
readx <- read.pdb(x)
x1.chain <- trim.pdb(readx, chain = "A", elety = "CA")
x1.b <- x1.chain$atom$b

ready <- read.pdb(y)
y1.chain <- trim.pdb(ready, chain = "A", elety = "CA")
y1.b <- y1.chain$atom$b

readz <- read.pdb(z)
z1.chain <- trim.pdb(readz, chain = "A", elety = "CA")
z1.b <- z1.chain$atom$b

par(mar = c(2,7,1,1))
par(mfrow = c(3,1))
plotb3(x1.b, x1.chain, sse = x1.chain, type = "l", col = "black", ylab = "Bfactor")
plotb3(y1.b, y1.chain, sse = y1.chain, type = "l", col = "red3", ylab = "Bfactor")
plotb3(z1.b, z1.chain, sse = z1.chain, type = "l", col = "blue3", ylab = "Bfactor")
}
```