class06 hw

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A. Can you improve this analysis code?

```
df <- data.frame(a=1:10, b=seq(200,400,length=10),c=11:20,d=NA)
df$a <- (df$a - min(df$a)) / (max(df$a) - min(df$a))
df$b <- (df$b - min(df$a)) / (max(df$b) - min(df$b))
df$c <- (df$c - min(df$c)) / (max(df$c) - min(df$c))
df$d <- (df$d - min(df$d)) / (max(df$a) - min(df$d))
df
```

Answer

```
df <- data.frame(a=1:10, b=seq(200,400,length=10),c=11:20,d=NA)
HW6_Q1 <- function(input) {
  Q1_function <- function(x, na.rm = TRUE) { #Function that executes repetitive calculatio
  range <- range(x, na.rm=na.rm) #range(x) returns c(minimum of x, maximum of x)
  x <- (x - range[1]) / (range[2] - range[1]) #Overwrite x with result of given equation
  }

for(i in 1:length(input)){
  Q1_function(input[ ,i]) #Execute function above for all column of input
 }
 return(input) #Print result of function
}

HW6_Q1(df) #Run function
```

```
Warning in min(x, na.rm = na.rm): min             Inf
```

```
Warning in max(x, na.rm = na.rm): max             -Inf
```

```
    a        b  c  d
1   1 200.0000 11 NA
2   2 222.2222 12 NA
3   3 244.4444 13 NA
4   4 266.6667 14 NA
5   5 288.8889 15 NA
6   6 311.1111 16 NA
7   7 333.3333 17 NA
8   8 355.5556 18 NA
9   9 377.7778 19 NA
10 10 400.0000 20 NA
```

B. Can you improve this analysis code?

```
# Can you improve this analysis code?
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

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

```
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
```

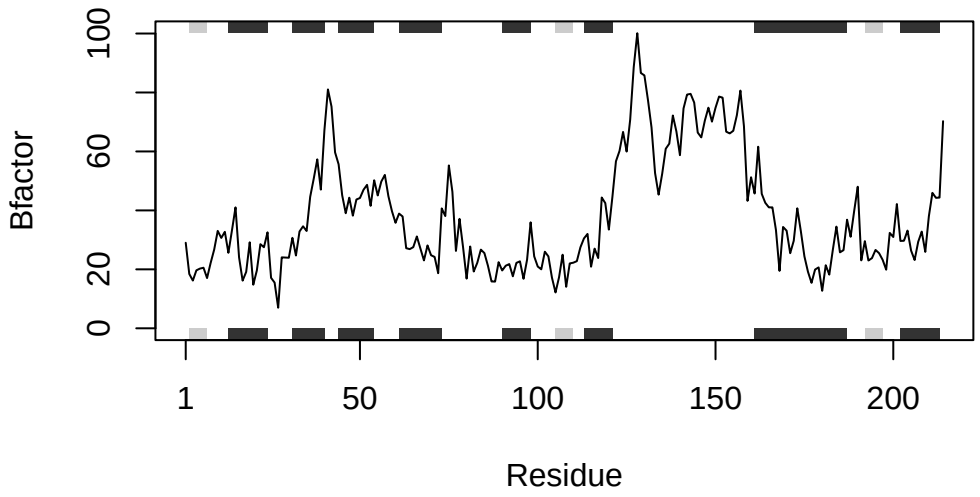
```
Note: Accessing on-line PDB file
```

```
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, sse=s1.chainA, typ="l", ylab="Bfactor")
#plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```

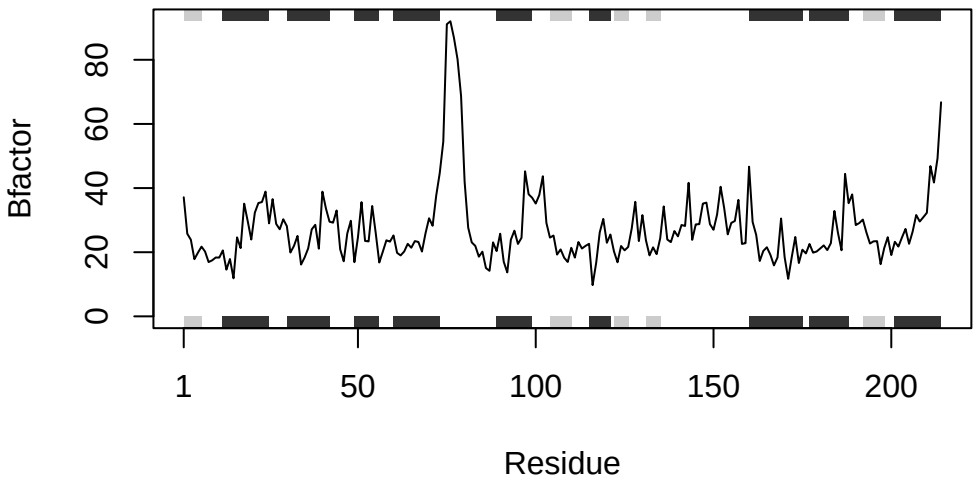
```
#plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```

Answer

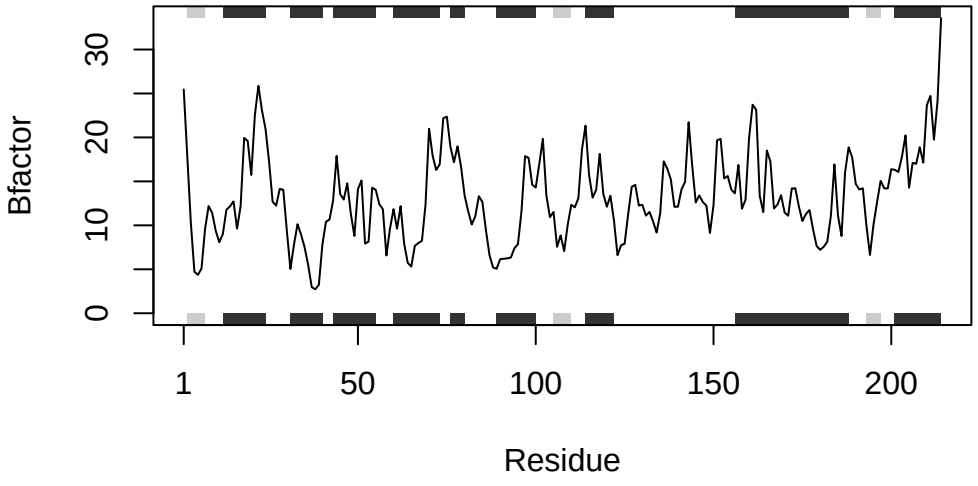
```
library(bio3d)
# First, Read s1~s3
#s1 <- read.pdb("4AKE") #s1 = kinase with drug
#s2 <- read.pdb("1AKE") #s2 = kinase no drug
#s3 <- read.pdb("1E4Y") #s3 = kinase with drug

HW6_Q2 <- function(x) {
    x.chainA <- trim.pdb(x, chain="A", elety="CA") #Extract aa with alpha carbon in A chai
    x.b <- x.chainA$atom$b # Assign temperature factor of x.chainA as x.b
    plotb3(x.b, sse=x.chainA, typ="l", ylab="Bfactor") #plot value b vs. residue
}

HW6_Q2(s1) #run functions
```




```
HW6_Q2(s2)
```


Bfactor
0
20
40
60
80
1
50
100
150
200
Residue

```
HW6_Q2(s3)
```


Bfactor
0
10
20
30
1
50
100
150
200
Residue

Q1. What type of object is returned from the read.pdb() function?

```
# read.pdb() returns pdb class in form of data frame.
```

Q2. What does the trim.pdb() function do?

```
# trim.pdb() extract desired component and returns smaller pdb object in form of data fram
# For instance, x.chainA <- trim.pdb(x, chain="A") create data frame containing only A cha
```

Q3. What input parameter would turn off the marginal black and grey rectangles in the plots and what do they represent in this case?

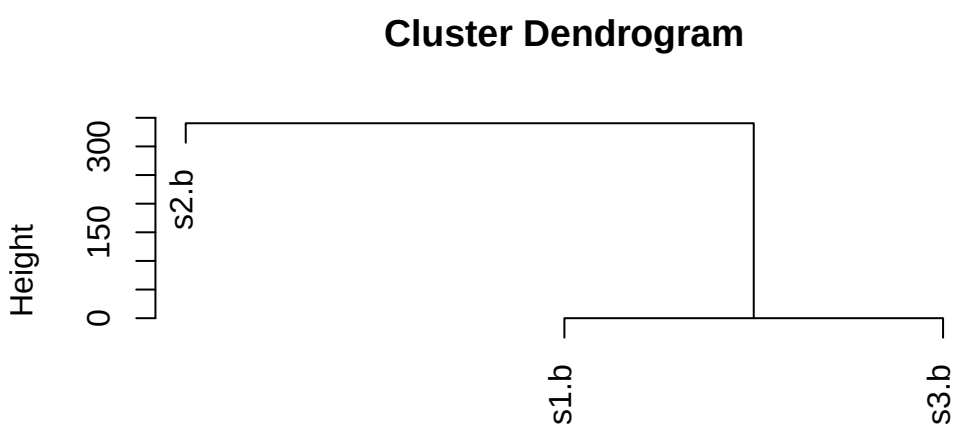
```
# In plotb3(x.b, sse=x.chainA, typ="l", ylab="Bfactor"), sse = x.chainA plots secondary st

# Hence, black and grey rectangles represents possible secondary structure of x.chainA, an
```

Q4. What would be a better plot to compare across the different proteins?

```
#For observing sequential difference across proteins, dot plot could be useful.
#For comparing different bfactors, either 1) plotting multiple line graphs with different
```

Q5. Which proteins are more similar to each other in their B-factor trends. How could you quantify this? HINT: try the rbind(), dist() and hclust() functions together with a resulting dendrogram plot. Look up the documentation to see what each of these functions does.

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




```
#rbind - combine s1.b~s3.b into one table, and dist() finds a difference between pairs of

# In the plot produced, s1 and s3 are more similar in bfactors, while s2 is quite differen
```

Q6. How would you generalize the original code above to work with any set of input protein structures?

```
# 1) Set loaded pdb file as global variable
# 2) Create sub pdb with aa of desired chain/element
# 3) Since $ cannot be used as input, filter aa with desired element
# 4) Replicate factor values in interest
# 5) Generate plot with plotb3(). Specify type of plot, along with enabling secondary stru
# 6) Add lines using lines(). To differentiate colors of each lines, take variable colors
# 7) create color vector 'plot_col' for colors input in lines()
# 8) Repeat HW6_Q6() for each proteins in vector 'files'
# 9) Execute factor_calc() for ith protein in 'files'
# 10) For first index of 'flies', execute draw_factor()
# 11) For ith (i>1), excute add_line() using color plot_col[i]
# 12) Generate legend for each lines
# 13) Create vector with protein names to be read in factor_calc()
# 14) Execute main function HW6_Q6()
```

```r
#Calculate factor values
#Takes pdb file as input, alone with specification of chain, element, and factor in intere
factor_calc <- function(file, chain, element, factor) {
 protein <<- read.pdb(file)                                          # 1)
 protein.chain <<- trim.pdb(protein, chain = chain, elety = element)  # 2)
 element_filtered <<- protein.chain$atom                             # 3)
 protein.factor <<- element_filtered[ ,factor]                       # 4)
}

#For first pdb file, create line plot. Takes protein.factor as input
draw_factor <- function(input_factor){
    plotb3(input_factor, sse = protein.chain, typ = "l", ylab = "factor") # 5)
}

# Per additional pdb file, add line on existing plot rather than generating new plot
add_line <- function(next_input, colors) {
  lines(next_input, col = colors)                                    # 6)
}

# Main function for executing all functions from reading pdb to drawing plot
HW6_Q6 <- function(file, chain, element, factor){
  plot_col <- rainbow(20)                                            # 7)

  for(i in 1:length(file)){                                          # 8)
    factor_calc(file[i], chain, element, factor)                     # 9)

    if(i==1){
      draw_factor(protein.factor)                                    # 10)
    }
    else{
      add_line(protein.factor, plot_col[i])                          # 11)
    }
  }
  legend("topright", title = "PDB File Name", file, fill = plot_col, horiz=TRUE, cex = 0.6
}

files <- c("4AKE", "1AKE", "1E4Y")                                   # 13)
HW6_Q6(files, "A", "CA", "b")                                        # 14)
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
```

```
C:\Users\louis\AppData\Local\Temp\RtmpwxeD9G/4AKE.pdb exists. Skipping download

  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\louis\AppData\Local\Temp\RtmpwxeD9G/1AKE.pdb exists. Skipping download

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

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\louis\AppData\Local\Temp\RtmpwxeD9G/1E4Y.pdb exists. Skipping download
```