Class 6

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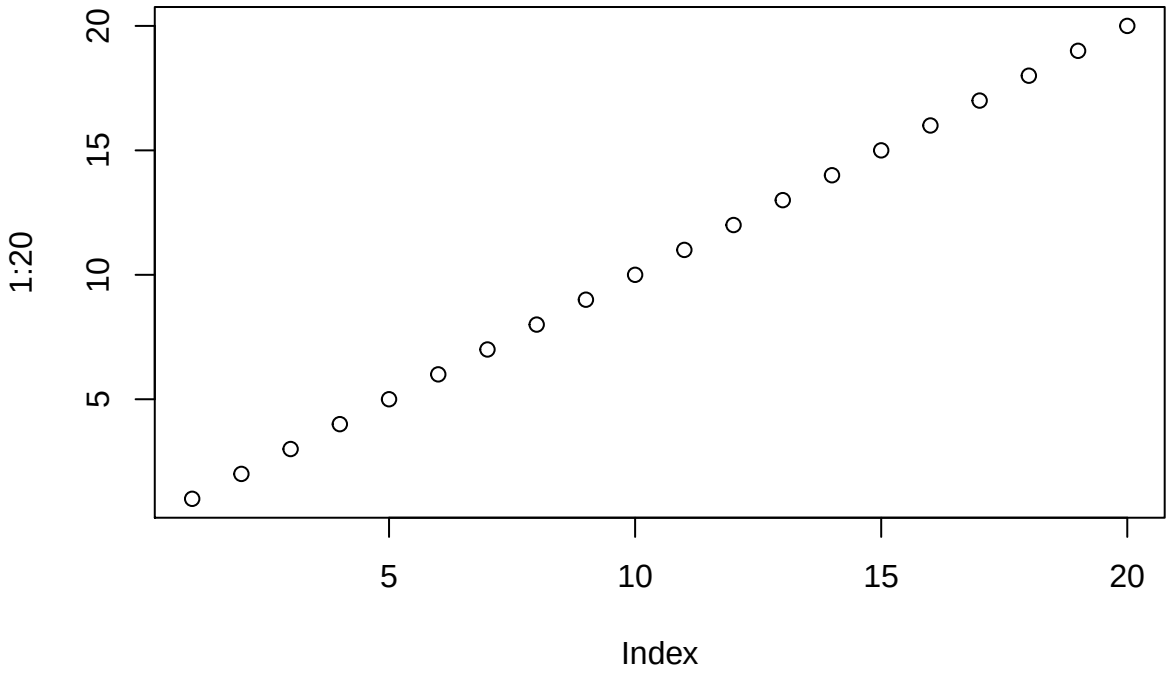
Section 1: Reading Files again :)

Going to use the **read.table()** function and friends to read example flat files

First, we add a simple plot:

```
plot(1:20)
```



Back to file reading...

```
read.table("https://bioboot.github.io/bimm143_W19/class-material/test1.txt", header = TRUE, sep = ",")
```

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

For this common CSV format we can use “”read.csv()**

```
data1 <- "https://bioboot.github.io/bimm143_W19/class-material/test1.txt"
data1 <- read.csv(data1)
data1
```

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

```
data2 <- "https://bioboot.github.io/bimm143_W19/class-material/test2.txt"
data2 <- read.csv(data2, sep = "$")
data2
```

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

```
data3 <- "https://bioboot.github.io/bimm143_W19/class-material/test3.txt"
data3 <- read.table(data3, sep = "")
data3
```

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

Section 2: R Functions

My first function:

```
add <- function(x, y=1) {
 # Sum the input x and y
 x + y
}
```

Using this function

```
add(1)
```

```
## [1] 2
```

```
add(1,100)
```

```
## [1] 101
```

```
add( c(1, 2, 3) )
```

```
## [1] 2 3 4
```

```
add( c(1, 2, 3), 4 )
```

```
## [1] 5 6 7
```

some improper add() use:

```
#add(1, 2, 2)
```

```
#add(x=1, y="b")
```

When would you write a function? . . . when you find yourself doing the same thing 3+ times

My second function:

```
rescale <- function(x) {
 rng <- range(x)
```

```
 (x - rng[1]) / (rng[2] - rng[1])
}
```

testing this function on a small sample, where we know what answer SHOULD be:

```
rescale(1:10)
```

```
##  [1] 0.0000000 0.1111111 0.2222222 0.3333333 0.4444444 0.5555556 0.6666667
##  [8] 0.7777778 0.8888889 1.0000000
```

Test, **Fail**, Change, Test again,...

```
# How would you get your function to work here...
rescale( c(1,2,NA,3,10) )
```

```
## [1] NA NA NA NA NA
```

```
# What should your function do here?
#rescale( c(1,10,"string") )
```

```
rescale2 <- function(x) {
 rng <- range(x, na.rm = TRUE)
 (x - rng[1]) / (rng[2] - rng[1])
}

x <- (c(1,2,NA,3,10) )
rng <- range(x)
#rng
```

```
rescale2( c(1,2,NA,3,10))
```

```
## [1] 0.0000000 0.1111111        NA 0.2222222 1.0000000
```

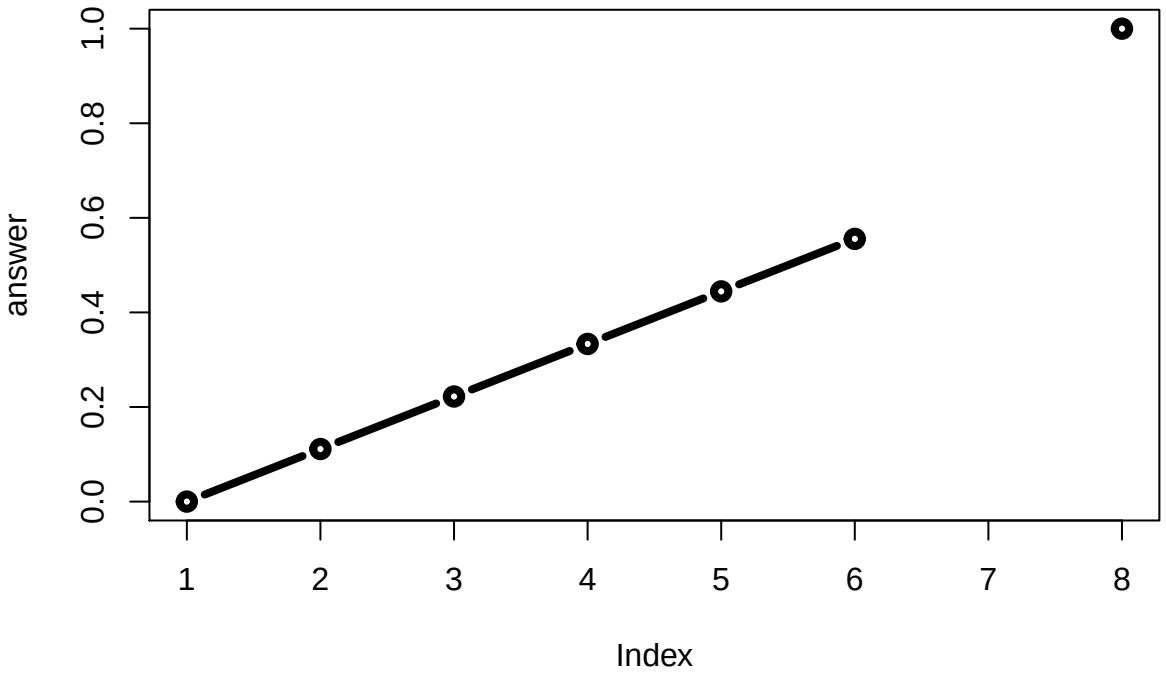
Trying another function...

```
rescale3 <- function(x, na.rm=TRUE, plot=FALSE) {
 rng <-range(x, na.rm=na.rm)
 print("Hello")
 answer <- (x - rng[1]) / (rng[2] - rng[1])
 print("is it me you are looking for?")
 if(plot) {
 plot(answer, typ="b", lwd=4)
   print("please don't ever sing again ;)")
 }
 print("I can see it in ...")
 return(answer)
}
```

using it

```
rescale3( c(1:6, NA, 10), plot = TRUE)
```

```
## [1] "Hello"
## [1] "is it me you are looking for?"
```




```
## [1] "please don't ever sing again ;)"
## [1] "I can see it in ..."
```

```
## [1] 0.0000000 0.1111111 0.2222222 0.3333333 0.4444444 0.5555556        NA
## [8] 1.0000000
```

Working with the bio3d package

To install this package I used the command **install.packages("bio3d")**

Time to use it! :)

need to call library function to use the functions within the package...

```
library(bio3d)
```

```
# Read a PDB file from the database

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

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

```
s1
```

```
##
##  Call:  read.pdb(file = "4AKE")
##
##    Total Models#: 1
##      Total Atoms#: 3459,  XYZs#: 10377  Chains#: 2  (values: A B)
##
##      Protein Atoms#: 3312  (residues/Calpha atoms#: 428)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 147  (residues: 147)
##      Non-protein/nucleic resid values: [ HOH (147) ]
```

```
##
##    Protein sequence:
##       MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##       DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##       VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##       YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILGMRIILLGAPGA...<cut>...KILG
##
## + attr: atom, xyz, seqres, helix, sheet,
##         calpha, remark, call
```

Let's improve this code!

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

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/
## fr/y7xylnkn785fn1z6g_690nhm0000gn/T//RtmpCYaCmG/4AKE.pdb exists. Skipping
## download
```

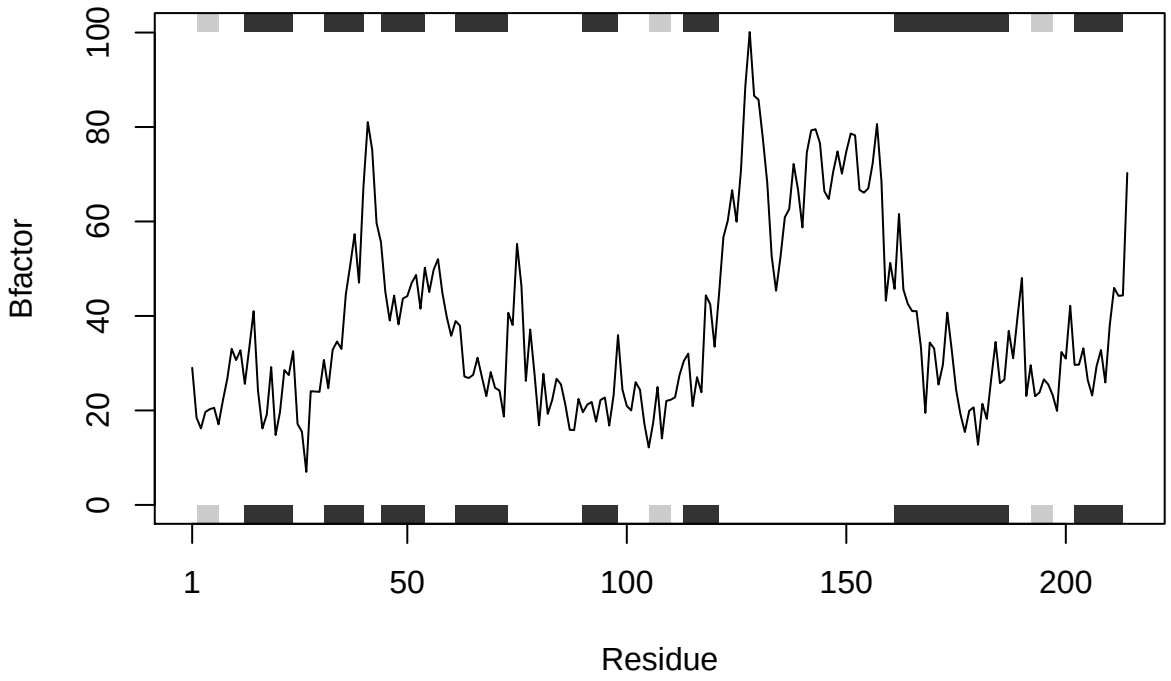
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

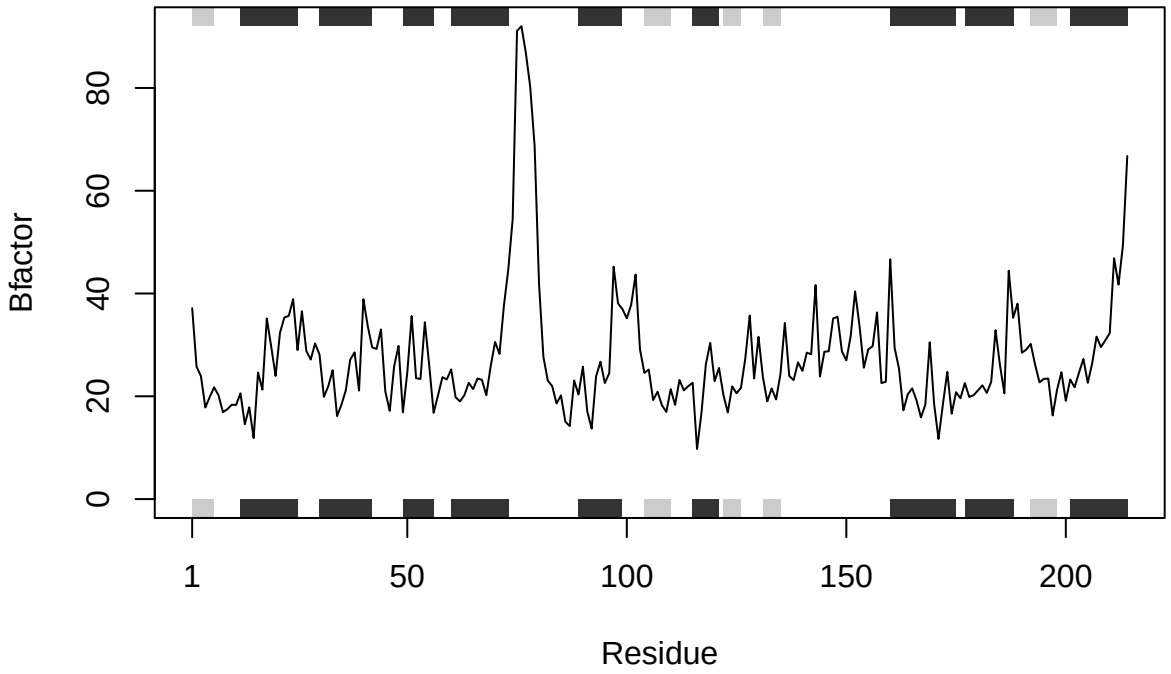
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

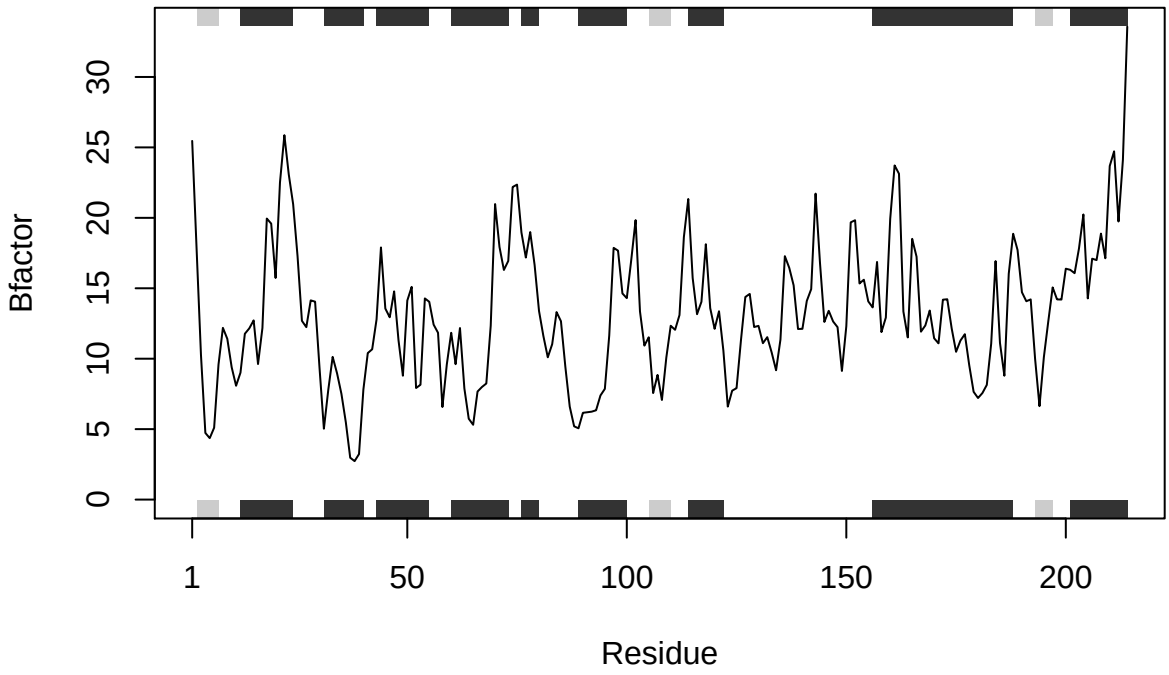
```
s1.chainA <- trim.pdb(s1, chain = "A", elety = "CA")
s2.chainA <- trim.pdb(s2, chain = "A", elety = "CA")
s3.chainA <- trim.pdb(s3, chain = "A", elety = "CA")

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")
```



HOMEWORK: find the smallest working snipet of code, make it as simple as possible wrap it into a function . . . see if it works! Then, you'd be able to run it on any protein structure!