HW06

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Code to improve (A)

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$b$)) / ($\max$(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$))

Create dataframe

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

create function to normalize values in columm a to range btw 0-1 (make different variables comparable)

```
normalize_formula <- function (x) {
  (x - min(x))/(max(x) - min(x))
  }
```

Apply function only to numeric columns

```
sapply(df[, sapply(df, is.numeric)], normalize_formula)
```

```
            a         b         c
 [1,] 0.0000000 0.0000000 0.0000000
 [2,] 0.1111111 0.1111111 0.1111111
 [3,] 0.2222222 0.2222222 0.2222222
 [4,] 0.3333333 0.3333333 0.3333333
 [5,] 0.4444444 0.4444444 0.4444444
 [6,] 0.5555556 0.5555556 0.5555556
 [7,] 0.6666667 0.6666667 0.6666667
 [8,] 0.7777778 0.7777778 0.7777778
 [9,] 0.8888889 0.8888889 0.8888889
[10,] 1.0000000 1.0000000 1.0000000
```

Code to improve (B)

library(bio3d) s1 <- read.pdb("4AKE") # kinase with drug s2 <- read.pdb("1AKE") # kinase no drug s3 <- read.pdb("1E4Y") # kinase with drug 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")

Create list to store kinases and function to read Protein Data Bank (PDB)

```
library(bio3d)
kinase_list <-c("4AKE","1AKE","1E4Y")
structure_list <- lapply(kinase_list, read.pdb)
```

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

Use trim function to create new, smaller PDB chain from kinases

```
trim_pdb_function <- function(x) trim.pdb(x, chain="A", elety="CA")
trimmed_chains <- lapply(structure_list, trim_pdb_function)
```

Extract B-factor values from atom data of trimmed chain

```
extract_function <- function(x) {
  x$atom$b
}
b_factor_values <- lapply(trimmed_chains, extract_function)
```

Plot B-factors vs Trimmed Chains

```
plot_bfactors_values <- function(b_factors_values, trimmed_chains) {
  for (i in seq_along(b_factors_values)) {
    plotb3(b_factors_values[[i]], sse=trimmed_chains[[i]], typ="l", ylab="Bfactor")
  }
}
plot_bfactors_values(b_factor_values, trimmed_chains)
```

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