## Data Wrangling I

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July 11, 2024

### Lesson Objectives

### At the end of this lecture you should be able to:

- 1. Generate random data
- 2. Derive new variables and subset data frames based on your existing data
- 3. Move between long and wide formatted data
- 4. Produce basic boxplots and scatter plots using ggpubr
- 5. Perform basic manipulation of character strings

#### Resources

Overview of ggpubr: https://rpkgs.datanovia.com/ggpubr/

Examples of reshape2 package: https://seananderson.ca/2013/10/19/reshape/

Wide vs long data frames: https://www.youtube.com/watch?v=pHPgMNXyzqc

### Generating Random Data

For this lecture, we will start by generating a new data set. To generate random variables, we can use the *rnorm* and *rbinom* functions.

```
# Define a variable of random systolic blood pressure
rnorm(n = 10,mean = 128.4,sd = 19.6)
```

```
## [1] 153.0027 122.0408 156.0632 100.7644 143.7820 112.4153 106.1646 151.1675 ## [9] 126.9746 102.2304
```

Did you get the same values as me? Why or why not?

```
set.seed(103)
rnorm(n = 10,mean = 128.4,sd = 19.6)
```

```
## [1] 112.99493 129.47288 105.41782 125.12067 91.84538 126.03937 144.58918
## [8] 151.72713 107.00754 121.04780
```

```
rnorm(n = 10, mean = 128.4, sd = 19.6)
```

```
## [1] 110.1285 129.0511 130.7935 178.9627 123.1178 110.9893 137.4007 130.6614
## [9] 123.8652 143.9297
```

```
set.seed(103)
rnorm(n = 10,mean = 128.4,sd = 19.6)
```

```
## [1] 112.99493 129.47288 105.41782 125.12067 91.84538 126.03937 144.58918
## [8] 151.72713 107.00754 121.04780
```

What do you think the set seed function does?

Many functions in R incorporate some level of randomziation such as sampling, some clustering algorithms, and some plotting functions. Always be aware of if you are using randomization, and always ensure that your code and results are reproducible by using the *set.seed()* function.

Now let's generate a random binary variable

```
set.seed(103)
rbinom(n = 10,size = 1,prob = 0.5)
```

```
## [1] 0 0 1 1 0 0 0 0 0 0
```

```
rbinom(n = 10, size = 10, prob = 0.5)
```

```
## [1] 5 4 6 6 7 3 3 4 4 4
```

What does the "size" parameter change? If we were creating a binary variable like biological sex, what would you set it as?

```
set.seed(103)
mean(rbinom(n = 100, size = 10, prob = 0.5))
```

```
## [1] 5.01
```

```
mean(rbinom(n = 100, size = 10, prob = 0.7))
```

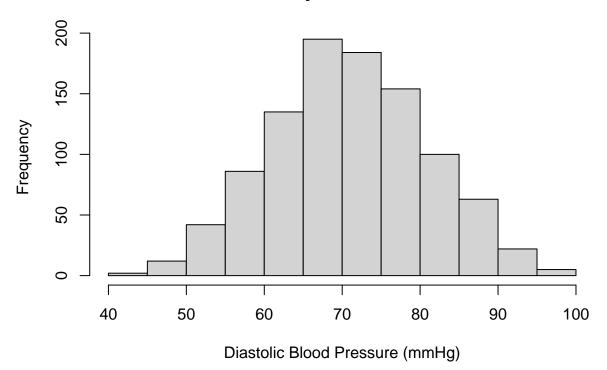
```
## [1] 6.93
```

What does the "prob" parameter change? When might you use different values here?

Okay now lets build a toy data set

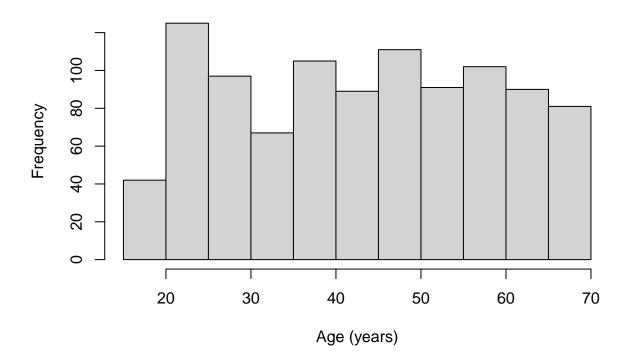
```
# Set a random seed
set.seed(103)
# Define a data frame with our randomly generated data
randomData <- data.frame('SubjectID' = seq(1:1000),</pre>
                         'systolicBP' = rnorm(n = 1000, mean = 128, sd = 20),
                         'diastolicBP' = rnorm(n = 1000, mean = 71, sd = 10),
                         'Age' = trunc(runif(n = 1000,min = 18,max = 70)),
                         'Male' = rbinom(n = 1000, size = 1, prob = 0.5))
# Take a peak at the top entries for our dataset
head(randomData)
    SubjectID systolicBP diastolicBP Age Male
                             75.52894 52
## 1
            1 112.28054
            2 129.09478
## 2
                             59.95778 56
## 3
            3 104.54879 74.51568 25
                                             1
## 4
            4 124.65374
                             52.99577 41
                                             0
## 5
            5 90.69937
                             71.17388 41
                                             0
            6 125.59120
                             69.50961 31
## 6
                                             0
# Assess the mean and standard deviation for systolic blood pressure
mean(randomData$systolicBP)
## [1] 128.4313
sd(randomData$systolicBP)
## [1] 19.37998
# Visualize the distribution of diastolic blood pressure
hist(randomData$diastolicBP,main = 'Randomly Generated Data',xlab = 'Diastolic Blood Pressure (mmHg)')
```

# **Randomly Generated Data**



# Visualize the distribution of age
hist(randomData\$Age,main = 'Randomly Generated Data',xlab = 'Age (years)')

### **Randomly Generated Data**



What differences do you notice in the distribution of these two variables?

# # Check the distribution of our variables summary(randomData)

```
##
      SubjectID
                        systolicBP
                                         diastolicBP
                                                               Age
##
                1.0
                      Min.
                              : 67.48
                                        Min.
                                                :43.07
                                                          Min.
                                                                 :18.00
##
    1st Qu.: 250.8
                      1st Qu.:115.12
                                         1st Qu.:64.15
                                                          1st Qu.:29.75
    Median : 500.5
                      Median :127.77
                                        Median :70.67
                                                          Median :44.00
##
           : 500.5
                              :128.43
                                                :70.99
##
    Mean
                      Mean
                                        Mean
                                                          Mean
                                                                 :43.54
    3rd Qu.: 750.2
                      3rd Qu.:141.24
                                         3rd Qu.:78.02
                                                          3rd Qu.:56.00
##
##
    Max.
            :1000.0
                      Max.
                              :207.49
                                        Max.
                                                :98.99
                                                          Max.
                                                                 :69.00
##
         Male
##
    Min.
            :0.000
##
    1st Qu.:0.000
    Median :1.000
##
##
    Mean
            :0.525
##
    3rd Qu.:1.000
    Max.
            :1.000
```

Is it summarizing the factor variable the way we want? Why or why not?

#### **Deriving New Variables**

Lets try converting the binary variable to a more logical format

```
# Define a new factor variable from an old binary
randomData$BiologicalSex <- factor(ifelse(randomData$Male == 1,'Male','Female'))
# Re-check the distribution of our variables
summary(randomData)</pre>
```

```
##
      SubjectID
                       systolicBP
                                       diastolicBP
                                                            Age
##
   Min.
          :
               1.0
                     Min. : 67.48
                                      Min.
                                              :43.07
                                                       Min.
                                                              :18.00
                     1st Qu.:115.12
##
   1st Qu.: 250.8
                                      1st Qu.:64.15
                                                       1st Qu.:29.75
  Median : 500.5
                     Median :127.77
                                      Median :70.67
                                                       Median :44.00
          : 500.5
                            :128.43
                                              :70.99
##
  Mean
                     Mean
                                      Mean
                                                       Mean
                                                              :43.54
   3rd Qu.: 750.2
                     3rd Qu.:141.24
                                       3rd Qu.:78.02
                                                       3rd Qu.:56.00
##
                            :207.49
                                             :98.99
##
  Max.
           :1000.0
                     {\tt Max.}
                                      Max.
                                                       Max.
                                                              :69.00
##
        Male
                    BiologicalSex
           :0.000
                    Female:475
##
  {	t Min.}
##
   1st Qu.:0.000
                    Male :525
## Median :1.000
## Mean
           :0.525
## 3rd Qu.:1.000
## Max.
           :1.000
```

We can also generate a new binary variable from a continuous variable

```
# Define variable specifying age above 65 (medicare eligible)
randomData$MedicareAge <- ifelse(randomData$Age < 65,F,T)
# Re-check the distribution of our variables
summary(randomData)</pre>
```

```
##
                       systolicBP
                                       diastolicBP
      SubjectID
                                                           Age
##
          :
                     Min. : 67.48
                                      Min.
                                             :43.07
                                                             :18.00
   Min.
               1.0
                                                      Min.
   1st Qu.: 250.8
                     1st Qu.:115.12
##
                                      1st Qu.:64.15
                                                      1st Qu.:29.75
  Median : 500.5
                     Median :127.77
                                      Median :70.67
                                                      Median :44.00
##
   Mean
          : 500.5
                     Mean
                            :128.43
                                      Mean
                                             :70.99
                                                      Mean
                                                              :43.54
##
   3rd Qu.: 750.2
                     3rd Qu.:141.24
                                      3rd Qu.:78.02
                                                      3rd Qu.:56.00
##
   Max.
           :1000.0
                     Max.
                            :207.49
                                      Max.
                                             :98.99
                                                      Max.
                                                              :69.00
##
                    BiologicalSex MedicareAge
         Male
##
           :0.000
                    Female:475
                                  Mode :logical
   Min.
                                  FALSE:903
##
   1st Qu.:0.000
                    Male :525
  Median :1.000
                                  TRUE :97
## Mean
           :0.525
   3rd Qu.:1.000
##
## Max.
           :1.000
```

#### **Subsetting Data**

As we learned in a previous lecture, we can subset a data frame in a few ways

```
# Subset to only those at medicare age
medicareData1 <- randomData[which(randomData$MedicareAge == T),]
medicareData2 <- randomData[which(randomData$Age >= 65),]

# We can use the following statement to ensure both methods produced the same result
all(medicareData1 == medicareData2)

## [1] TRUE

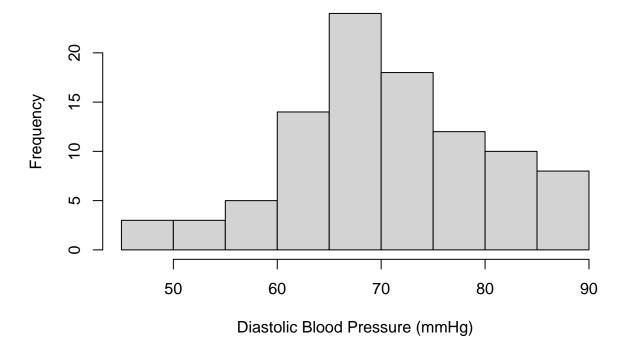
table(medicareData1 == medicareData2)

## ## TRUE
## 679
```

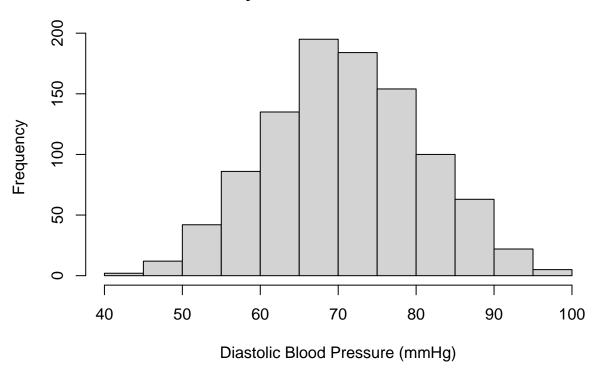
Now we can look at the distribution in diastolic blood pressure just among individuals meeting a given age cutoff

```
# Visualize the distribution of diastolic blood pressure in Medicare Only
hist(medicareData1$diastolicBP,main = 'Randomly Generated Data: Medicare Eligible Only',xlab = 'Diastol
```

### Randomly Generated Data: Medicare Eligible Only



### **Randomly Generated Data: Full Cohort**

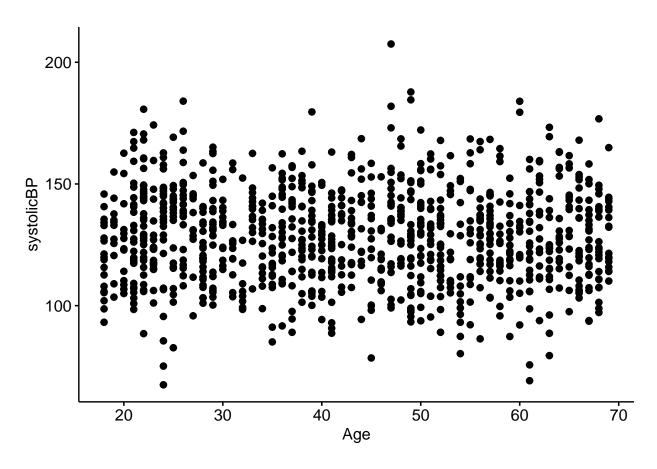


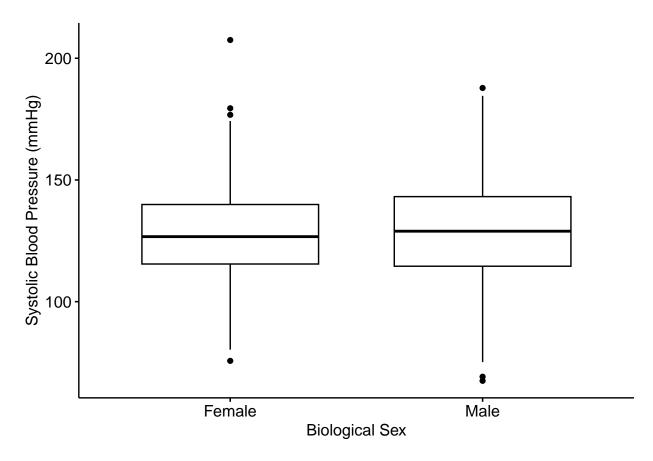
Does the distribution in the subsetted data look any different than in the full data set? Should it?

### Basic Plotting Using ggpubr

```
# Run the following line of code one time to install the package if you haven't already
# install.packages('ggpubr')

# Generate a scatter plot of age by systolic blood pressure
ggpubr::ggscatter(randomData,x = 'Age',y = 'systolicBP')
```





Was there any visual association between age or sex and blood pressure?

Would we expect there to be based on how we generated the data?

What if we want to look at systolic and diastolic blood pressure in the same plot? To do this, we need to convert out data to a long format.

### Wide vs Long Dataframes

Wide format data will have each subject in a single row and then multiple measures related to that subject in a unique column.

```
## PatientID Age Height.in
## 1 P001 24 67
## 2 P002 35 70
## 3 P003 27 64
```

Long format data will have each measurement in a new row.

```
##
     PatientID
                  Measure Value
## 1
          P001
                      Age
## 2
          P001 Height.in
                              67
## 3
          P002
                              35
                      Age
## 4
          P002 Height.in
                              70
## 5
                              27
          P003
                      Age
          P003 Height.in
## 6
                              64
```

While this might seem odd for this type of use case, it is a very useful tool for datasets with **repeated** measures, i.e. measurements taken over time like this:

```
##
     PatientID Age.yrs Height.in
## 1
          P001
                                 40
                       5
## 2
          P001
                      10
                                 53
## 3
          P002
                       5
                                 43
## 4
                      10
          P002
                                 58
## 5
          P003
                       5
                                 39
## 6
          P003
                      10
                                 51
```

### Long Format Data

Currently, our data is in a **wide** format because each subject is only in a single row and all measures from that subject are in columns. There are a few different ways to convert between wide an long format data.

To achieve this today, we will use the *melt* function from the package *reshape2*. Next class, we will discuss how to achieve this in *tidyverse*.

```
# Run the following line of code one time to install the package if you haven't already
# install.packages('reshape2')
# Melt the data frame into a long form
```

```
longData <- reshape2::melt(randomData[,c('SubjectID','systolicBP','diastolicBP','Age','BiologicalSex')]</pre>
                            id.vars = c('SubjectID', 'Age', 'BiologicalSex'), value.name = 'BP',
                           variable.name = 'BP.Type')
# Check enteries for our first subject
longData[longData$SubjectID == 1,]
##
        SubjectID Age BiologicalSex
                                         BP.Type
                                                        BP
## 1
                1 52
                             Female systolicBP 112.28054
## 1001
                1 52
                             Female diastolicBP 75.52894
# How it would look if we forgot one of our ID variables
longData2 <- reshape2::melt(randomData[,c('SubjectID','systolicBP','diastolicBP','Age','BiologicalSex')</pre>
                           id.vars = c('SubjectID', 'Age'), value.name = 'BP',
                           variable.name = 'BP.Type')
## Warning: attributes are not identical across measure variables; they will be
## dropped
typeof(longData2$BP)
## [1] "character"
longData2[longData2$SubjectID == 1,]
##
        SubjectID Age
                            BP.Type
## 1
                1 52
                         systolicBP 112.280536472035
                1 52
                        diastolicBP 75.5289415224527
## 1001
## 2001
                1 52 BiologicalSex
                                               Female
We can also use the order function to ensure that all our subjects values are listed in sequence in the table
or to look at subjects who have the oldest age easily
# Print first 20 values
longData$Age[1:20]
  [1] 52 56 25 41 41 31 69 67 46 60 36 56 40 39 38 52 52 60 20 61
order(longData$Age)[1:20]
## [1]
             121 158 214 237
                                  337 342 350 594 616 653 656 717 736 739
## [16]
         846 976 991 1035 1121
What does the order function return?
longData$Age[14]
```

## [1] 39

```
# Order by subject ID
head(longData[order(longData$SubjectID,decreasing = F),])
```

```
##
       SubjectID Age BiologicalSex
                                      BP.Type
                                                     BP
## 1
               1 52
                            Female systolicBP 112.28054
## 1001
               1 52
                            Female diastolicBP 75.52894
## 2
               2 56
                            Female systolicBP 129.09478
## 1002
               2 56
                            Female diastolicBP 59.95778
## 3
               3 25
                              Male systolicBP 104.54879
## 1003
               3 25
                              Male diastolicBP 74.51568
```

```
# Order by decreasing age
head(longData[order(longData$Age,decreasing = T),])
```

```
##
       SubjectID Age BiologicalSex
                                     BP.Type
## 7
              7 69
                           Female systolicBP 144.5196
            114 69
## 114
                             Male systolicBP 119.9431
## 124
            124 69
                           Female systolicBP 140.5145
## 336
            336 69
                            Male systolicBP 115.8081
## 363
            363
                 69
                           Female systolicBP 139.2851
## 391
            391 69
                             Male systolicBP 119.4529
```

The order function can be particularly helpful when trying to merge two data frames and want to first ensure that subjects or samples are in the same order in each data frame.

### **Manipulating Character Strings**

If we don't like the end of systolic and diastolic labels having "BP" we can remove it using the sub function.

```
# Look for cases of "BP" and replace with ""
longData$BP.Type <- sub(pattern = 'BP',replacement = '',x = longData$BP.Type)

# Now lets see what values we have for this variable
table(longData$BP.Type)

##
## diastolic systolic
## 1000 1000

# We could also just replace the values using indexing as follows
longData[which(longData$BP.Type == 'systolic'),'BP.Type'] <- 'Systolic'
longData[which(longData$BP.Type == 'diastolic'),'BP.Type'] <- 'Diastolic'

# Now lets check again what values we have for this variable
table(longData$BP.Type)</pre>
```

```
## ## Diastolic Systolic ## 1000 1000
```

sub and gsub can both be used to search and replace in character strings. Can you identify the difference between what each one does?

```
# Define a list of character strings
charStrings <- c('QBS Graduate Program at Dartmouth College','QBS 103','QBS! QBS!')

# sub function
sub(pattern = 'QBS',replacement = 'Dartmouth',x = charStrings)

## [1] "Dartmouth Graduate Program at Dartmouth College"
## [2] "Dartmouth 103"
## [3] "Dartmouth! QBS! QBS!"

# gsub function
gsub(pattern = 'QBS',replacement = 'Dartmouth',x = charStrings)

## [1] "Dartmouth Graduate Program at Dartmouth College"
## [2] "Dartmouth 103"
## [3] "Dartmouth! Dartmouth! Dartmouth!"</pre>
```

This may seem easy enough to do on your own, but sometimes you will have large lists of character strings between two dataframes that have been entered in different formats.

Here, I have 2 lists of sample IDs that I need to make sure are in the same order in both lists but you can see, they are formatted differently across both lists.

```
# Define two lists of sample names
d1 <- c('20210323_PB4_01_09.RCC','20210323_PB4_01_11.RCC','20210323_PB4_01_12.RCC','20210401_ch5-040121
d2 <- c('20210323-PB4 01 11.RCC','20210323-PB4 01 12.RCC','20210323-PB4 01 09.RCC','20210401-ch5-040121
# Check if same samples are in both lists
table(d1 %in% d2)
##
## FALSE
##
      7
# Compare formatting
head(d1)
## [1] "20210323_PB4_01_09.RCC"
                                       "20210323_PB4_01_11.RCC"
## [3] "20210323_PB4_01_12.RCC"
                                       "20210401_ch5-040121_01_01.RCC"
## [5] "20210401_ch5-040121_01_02.RCC" "20210401_ch5-040121_01_02.RCC"
```

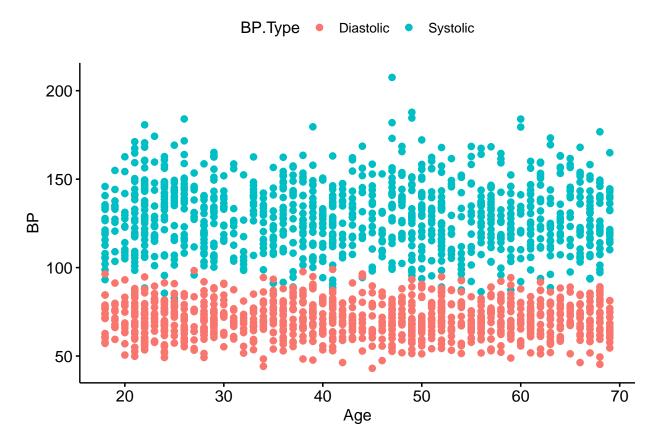
```
## [1] "20210323-PB4_01_11.RCC"
                                         "20210323-PB4_01_12.RCC"
## [3] "20210323-PB4_01_09.RCC"
                                         "20210401-ch5-040121-01-01.RCC"
## [5] "20210401-ch5-040121-01-02.RCC" "20210401-ch5-040121-01-02.RCC"
 We can change the formatting using qsub
# Replace all "_" with "-" in list of sample names
d1 <- gsub(d1,pattern = '_',replacement = '-')</pre>
d2 <- gsub(d2,pattern = '_',replacement = '-')
# Verify all names in d1 are now also in d2
table(d1 %in% d2)
##
## TRUE
##
      7
\# Check if D1 and D2 are in the same order
table(d1 == d2)
##
## FALSE TRUE
       3
# Reorder both vectors
d1 <- d1[order(d1)]</pre>
d2 <- d2[order(d2)]</pre>
# Check if D1 and D2 are in the same order
table(d1 == d2)
##
## TRUE
##
     7
```

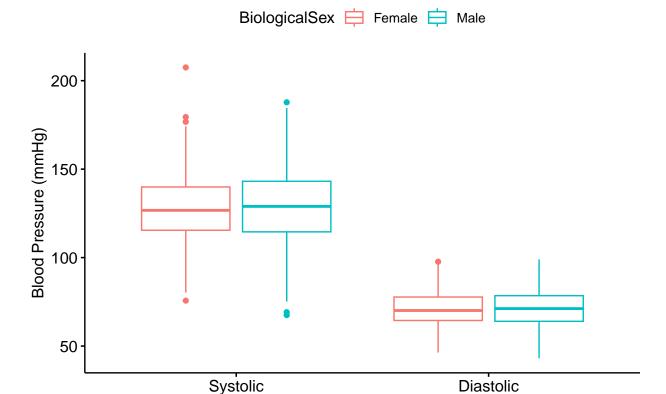
### Adding Color to Our ggpubr Plots

head(d2)

Now we can go back and generate out plots with both measures of blood pressure in one plot.

```
# Generate a scatter plot of age by systolic blood pressure
ggpubr::ggscatter(longData,x = 'Age',y = 'BP',color = 'BP.Type')
```





### Converting Back to Wide Format Data

We can also change our data back into a wide format using the *cast* function as follows:

```
# Cast into a data frame
wideData <- reshape2::dcast(longData,formula = SubjectID + Age + BiologicalSex ~ BP.Type,value.var = "
# Note: using dcast because we want a dataframe as output.
# If we want a vector or matrix as output, we use acast
# Lets see if our data look the same as when we started
head(wideData)
##
     SubjectID Age BiologicalSex Diastolic Systolic
## 1
             1
               52
                          Female 75.52894 112.28054
## 2
             2
               56
                          Female
                                 59.95778 129.09478
               25
## 3
             3
                            Male 74.51568 104.54879
               41
                          Female 52.99577 124.65374
## 4
               41
## 5
                          Female 71.17388 90.69937
               31
                          Female 69.50961 125.59120
## 6
# Our original data set
head(randomData)
```

## SubjectID systolicBP diastolicBP Age Male BiologicalSex MedicareAge

```
## 1
             1 112.28054
                             75.52894
                                             0
                                                      Female
                                                                    FALSE
## 2
            2 129.09478
                                             0
                                                      Female
                                                                    FALSE.
                             59.95778 56
## 3
            3 104.54879
                             74.51568 25
                                             1
                                                        Male
                                                                    FALSE
## 4
             4 124.65374
                             52.99577 41
                                             0
                                                      Female
                                                                    FALSE
## 5
             5
                 90.69937
                             71.17388 41
                                             0
                                                      Female
                                                                    FALSE
## 6
             6 125.59120
                             69.50961 31
                                             Ω
                                                      Female
                                                                    FALSE
```

We can also use the dcast function to make summary values. For example, what if we wanted to known the average BP for males and females based on their age group.

## [1] 104 4

```
# Look at the top enteries
head(summaryTable)
```

```
##
     Age BiologicalSex Diastolic Systolic
## 1 18
               Female 76.03626 119.5091
## 2 18
                 Male 68.47743 118.7080
## 3 19
               Female 74.30795 135.8965
## 4
     19
                 Male 71.88793 124.2671
                       71.04246 123.8012
## 5
      20
               Female
## 6
     20
                 Male 71.27133 127.4093
```

We can also use this to tabulate how many observations there are for each category

## [1] 104 4

```
# Look at the top enteries
head(summaryTable)
```

```
##
     Age BiologicalSex Diastolic Systolic
## 1 18
                Female
                              10
                                        10
                  Male
                               8
## 2 18
                                        8
## 3 19
                Female
                               5
                                        5
                               6
                                        6
## 4 19
                  Male
## 5 20
                Female
                               5
                                        5
## 6 20
                  Male
                               8
                                        8
```

### In Class Activity

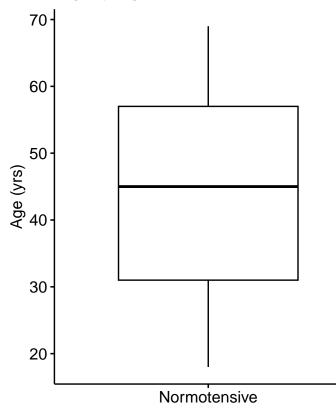
Working in groups, define a new variable for hypertension in our original dataset (randomData). Here we will define hypertension as systolic blood pressure over 130 or a diastolic blood pressure over 80. Plot the distribution in age for individuals with and without hypertension using boxplots.

Use the *melt* function to generate boxplots of the distribution of systolic and diastolic blood pressure in hypertensive vs. normotensive individuals (color should be based on hypertension status).

Use the *dcast* function to generate a table summarizing the mean age, systolic, and diastolic BP for males and females, seperately, with and without hypertension. Your table should have 4 rows. Order your table output such that it lists values for normotensive individuals first and hypertensive individuals second.

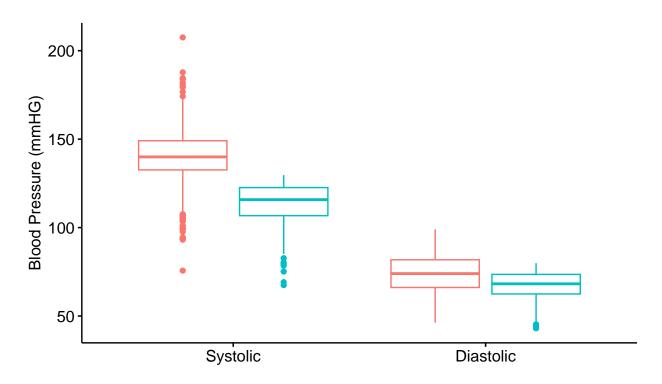
### Sample Solution

Remember: There are many ways to solve any problem in R. As long as you get the same end



product, what you did is likely just as valid as what I did.





```
##
     BiologicalSex Hypertension systolicBP diastolicBP
## 2
           Female Normotensive
                                  114.7668
                                              67.23993 43.64706
## 4
              Male Normotensive
                                  112.6688
                                              67.64147 44.62162
            Female Hypertensive
## 1
                                  138.8948
                                              73.64332 43.98425
                                  141.1750
              Male Hypertensive
                                              73.96578 42.28713
## 3
```