# Applied Statistics using S-PLUS: Short course 

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## Introduction

What is S-PLUS?
$S$ is a language and an interactive programming environment for data analysis and graphics. The $S$ language is a very high-level language for specifying computations. The language is part of an interactive environment: S encourages you to compute, look at the data, and program interactively, with quick feedback to enable you to learn and understand. Refer to Becker et al., 1988 for more details.

The best way to learn to use the S-PLUS language is to just using it! It is possible to use S-PLUS with the same techniques used in other programming language such as FORTRAN (though this may not be the most efficient way to use S-PLUS).

Newer version of S-PLUS for Windows (user friendly interface) was designed for easy ("click-and-see"), intuitive analysis and visualization of data. This allows you to import and export data from many sources including spreadsheets like Excel and Lotus, analytical software such as SAS and SPSS, and databases. The software is quite expensive but cheaper student versions are always available. In this note, we will discuss using S-PLUS in Windows that is available in Math department (we have the newest version, V6.0).

## Before you start

You are in several projects or studies and you may want to have separate S+ workspaces. It is very convenient to have different $S+$ shortcut incons on your desktop so that you can directly get on the project without further configuration. For this make another $S+$ shortcut icon on the desktop and right-click then property. On the Target window add the folder name you are working on (usually where data are at) as follows;
"C:\Program Files\Insightful\splus6\cmd\SPLUS.exe" S_PROJ=C:\Research\OzoneStudy
Than change the icon name (this might be done beforehand).
Once it has been done, double-click on the icon and do your work in S+ system. Your work will be saved on the folder you specified above and next time when you open the workspace everything you have done late time will be there, unless you delete them on purpose.

## Basics

## Getting Started

To begin S-PLUS under Windows, double click the S-plus icon on your desktop. The layout might have two windows (Object Explorer and Commands Windows). Object Explorer does the same work as the Windows Explorer and the Commands Window is where you type your commands. Many commands can be executed via user interface menus, but yet some functions run only in the Commands Window. To receive help while in S-PLUS on various commands, use

```
> help("command")
```

Note that S-PLUS is case-sensitive; that is, "s" and "S" are different in S-PLUS.

## Prompt

The S-PLUS Commands Window prompt is:

```
>
A
+
```

prompt means that S-PLUS is waiting for you to finish your command: for example, you may have forgotten to close a function with a right parenthesis. Type

$$
>3 *(2+4
$$

and see what happens.

## Saving and Script File

You can type your commands here one-by-one or you may execute a series of S-Plus commands from a file (with an extension .ssc) using source command:

```
> source("filename")
```

or choosing Run button for running commands in a Script Window. Confusing?? Well, here's how to do. First, open a Script Window by choosing New, Script File, and then OK. Now you have the Script Window. In upper pane type

```
x<-1:10 # this will create a vector }\textrm{x}\mathrm{ with the element 1,2,3,_.,10
mean(x) # this will return the mean value of the vector x
stdev(x) # this will return the standard deviation of the vector }\textrm{x
```

Now click on the Run button (the right triangular arrow). You will see the calculated result in the lower pane. If you want to save the codes into a file, choose File from main menu then Save As.
More examples for using a Script Window will be discussed in class. If you type commands one-by-one in the Commands Window, you may want to record the resulted output and/or the commands you just typed into a file. For this we use sink command:

```
> sink("filename")
>...... # all the commands you want to
>...... # save of the outputs here
> sink( )
```

The record function in place of sink will also save the commands into the specified file. The outputs and graphs will also appear in the Object Explorer (Reports and Graphs folders), so that you can display on the screen and save into a file (by choosing File-Save As).

## In-line Data Creation and Some Fun

Now, let's have some fun.

S-PLUS is primarily meant to be an interactive data analysis system. When you create data vectors and functions in an S-PLUS session, they stay in your .Data directory. For example, if you make the assignment

```
>x <- 1:10 # you may also type > x_1:10
```

[1] 12345678910
to create a vector $x$ with length 10 and the elements 1 through 10, and then leave S-PLUS, next time you start S-PLUS you could type
> X
[1] 12345678910
and $x$ will still be there!

You may either make a data frame objective (in vector or matrix) by typing within S-PLUS environment or reading from an external data file. Unless the data is very small, the second case is more common. Let's make a data vector $x$ (you can name the vector as you like) of size 9 with the element $1,2, \ldots, 9$.

```
> X<-c(1,2,3,4,5,6,7,8,9)
> X
[1]123456789
```

Then $x$ will return the data you typed. Let's now make a matrix $x x$ (again, any name) of dimension $5 x 3$

```
> xx<-matrix(nrow=5,ncol=3)
```

5 by 3 matrix format is assigned to $x x$. Since we didn't type in any data, if you type $x x$ you will see

```
> XX
    [,1] [,2] [,3]
[1,] NA NA NA
[2,] NA NA NA
[3,] NA NA NA
[4,] NA NA NA
[5,] NA NA NA
```

Let's type the data for each column. Note that $x x[, n]$ means the $n^{\text {th }}$ column of the matrix $x x$. Similarly, $\mathrm{xx}[\mathrm{k}$,$] means the \mathrm{k}^{\text {th }}$ row.

```
> xx[,1]<-c(1,2,3,4,5)
> xx[,2]<-c(6,7,8,9,10)
> xx[,3]<-c(11,12,13,14,15)
> Xx
    [,1] [,2] [,3]
[1,] 1 6 11
[2,] 2 
[3,] 3
[4,] 4
[5,] }
```

The same result can be obtained by:

```
>xx<-1:15
>xx<-matrix(xx, nrow=5, ncol=3, byrow=F)
> XX
```


## Reading Data from a Text File (Example)

More commonly, we import data from an external data file. Note in S-PLUS Windows version we can import data in other formats as mentioned in Introduction. The following ASCII file called Sta131.txt contains name of 28 students, two midterm scores, final, and total score of a graduate statistics course that I taught before.

| Name | HW | MT. I | MT.II | Final | Total |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Al-Mefleh, N | 93.75 | 51 | 38 | 27 | 41.6 |
| Bennett, T | 91.75 | 80 | 52 | 33 | 53.7 |
| Buyuktas, D | 98.25 | 79 | 84 | 49 | 68.6 |
| Cao, Zh | 69.75 | 93 | 82 | 55 | 71.1 |
| Chen, J | 99.375 | 89 | 91 | 83 | 87.8 |
| Choi, J | 98.75 | 90 | 78 | 41 | 66.1 |

The read.table command provides a method to bring this data into the current data frame as a data frame objective. An object has intrinsic which give its structure. The data will be read into the data frame objective grade.data. You may also easily import the data file by choosing File, Import Data, From File, then choosing ASCII Text File format. We will discuss more in class. I believe that, these days, many of data files have Formatted ASCII forms and so we will discuss these formats in details.

```
> grade.data<- read.table("C:/..../Sta131.txt",header=T)
> grade.data
```

$\left.\begin{array}{rrrrrr}\text { Name } & \text { HW } & \text { MT. I } & \text { MT. II } & \text { Final } & \text { Total } \\ \text { Al-Mefleh, } & \text { N } & 93.750 & 51 & 38 & 27 \\ \text { Bennett, } & \text { T } & 91.750 & 80 & 52 & 33\end{array}\right) 53.7$

More detailed discussions on Importing and Exporting data are in the following section.
We can examine some of the properties of grade.data. It is a list object, made up of other objects. Objects can be atomic (with mode "logical", "numerical", "complex", or "character") or non-atomic (comprising other objects). The object grade.data is a recursive; that is, it is a list made up of several component objects. Let see several ways of accessing the parts of grade.data.

```
> mode (grade.data)
[1] "list"
> length(grade.data)
[1] 6
> grade.data[5]
        Final
    1 27
2 33
27 66
28 63
> grade.data[1,]
\begin{tabular}{rrrrrr} 
& Name & HW MT.I MT. II Final & Total \\
1 & Al-Mefleh,N 93.75 & 51 & 38 & 27 & 41.6
\end{tabular}
```

```
> grade.data[,"Final"]
    [1] 27 33 49 55 83 41 14 86 39 57 67 12 17 82 95 88 94
[18] 53 55 90 50 99 80 99 57 68 66 63
> grade.data[1,1]
[1] Al-Mefleh,N
> grade.data[1,5]
[1] 27
> grade.data[grade.data[,"Final"]>80,]
            Name HW... MT.I MT.II Final Total....
    X5 Chen, J 99.375 89 91 83 87.8
    X8 Dubin, J 99.750 98 74 86 87.4
X14 Li, B 98.125 100 74 82 85.9
X15 Lin, D 99.250 90 98 95 95.0
X16 Love, B 99.750 96 98 88 93.2
X17 Peck, L 98.625 97 92 94 94.7
X20 Singh, R 99.750 100 98 90 95.0
X22 Su, X 97.250 95 100 99 98.2
X24 Wai, N 98.875 87 100 99 96.5
> summary(grade.data[,"Final"])
    Min. 1st Qu. Median Mean 3rd Qu. Max.
        12 47 60 61.39 83.75 99
```


## Simple Linear Regression

Suppose that we are interested in relating the first midterm (MT.I) to the final score (Final). We can use the $l m$ function to do the linear regression analysis. What returns from $l m$ is a recursive object from which information about the regression can be extracted. Those information will be included in the object grade.fit (you name it).

The summary function can be used to print out the contents of the object. In the formula, the response variable will be placed on the left of a $\sim$ operator and explanatory variable on the right. In case of multiple regression, the + sign will be placed between the explanatory variables. The constant term is in the model by default. na.action is a function to filter missing data. na.omit will delete observations that contain one or more missing values.

```
> grade.fit<-lm(formula = Final ~ MT.I, data = grade.data, na.action
+ = na.omit)
> summary(grade.fit)
Call: lm(formula = Final ~ MT.I, data = grade.data, na.a
ction
            = na.omit)
Residuals:
\begin{tabular}{rrrr} 
Min & 12 & Median & 32 \\
-30.58 & -12.51 & 0.8994 & 11.07 \\
40.67
\end{tabular}
Coefficients:
\begin{tabular}{rrccr} 
& Value & Std. Error & t value & \(\operatorname{Pr}(>|t|)\) \\
(Intercept) & -16.3021 & 15.9951 & -1.0192 & 0.3175 \\
MT.I & 0.9760 & 0.1958 & 4.9858 & 0.0000
\end{tabular}
Residual standard error: 19.09 on 26 degrees of freedom
Multiple R-Squared: 0.4888
F-statistic: 24.86 on 1 and 26 degrees of freedom, the p
-value is 0.00003488
```

```
Correlation of Coefficients:
    (Intercept)
MT.I -0.9742
```

Following is to obtain Analysis of Variance table. The input to anova are the objects resulting from modelfitting function $l m$.

```
> anova(grade.fit)
Analysis of Variance Table
Response: Final
Terms added sequentially (first to last)
    Df Sum of Sq Mean Sq F Value Pr(F)
    MT.I 1 9055.450 9055.450 24.85862 0.00003488384
Residuals 26 9471.229 364.278
```


## Plotting

```
> xval<-grade.data[,"MT.I"]
> yval<-grade.data[,"Final"]
> grade.res<-residuals(grade.fit)
> grade.pre<-fitted.values(grade.fit)
> plot(xval,yval,xlab="MT.I",ylab="Final")
> plot(xval,grade.res,xlab="MT.I",ylab="Residuals")
```



It is important to note that you may make a command file (a file with list of commands separated by line) and execute the file in the S-PLUS environment. For exam, for the above regression work suppose you made a file (named, say, "grade.ssc") with contents

```
grade.data<- read.table("Sta131.dat",header=T)
grade.fit<-lm(formula = Final ~ MT.I, data = grade.data, na.action
+ = na.omit)
summary(grade.fit)
anova(grade.fit)
xval<-grade.data[,"MT.I"]
yval<-grade.data[,"Final"]
grade.res<-residuals(grade.fit)
grade.pre<-fitted.values(grade.fit)
plot(xval,yval,xlab="MT.I",ylab="Final")
plot(xval,grade.res,xlab="MT.I",ylab="Residuals")
```

Then,

```
>source("grade.ssc")
```

will execute the external command file (grade.ssc). To save the results, simply type sink("filename") and sink() at the beginning and the end. For example,

```
> sink("grade.out")
> source("grade.s")
> sink( )
```

Of course, it also can be done via Script Windows as discussed earlier.

## References

Becker, R.A., Chambers, J.M., and Wilks, A.R. (1988). The New S Language. Wadsworth and Books.
Everitt, B.S. (1994). A Handbook of Statistical Analysis using S-PLUS. Champman and Hall.
Krause, A and Melvin Olson (2000) The Basics of S and S-PLUS, Second ed., Springer

## DATA STRUCTURE

```
VECTOR
```

```
> x_c(4,3,5,7,12) #"c" stands for "concatenate" command
```

> x_c(4,3,5,7,12) \#"c" stands for "concatenate" command
> x
> x
[1] 4 3 5 7 12
[1] 4 3 5 7 12
>mean(x)
>mean(x)
[1] 6.2
[1] 6.2
> stdev(x)
> stdev(x)
[1] 3.563706
[1] 3.563706
> y_c(12,13,11,10)
> y_c(12,13,11,10)
> x_c(x,y)
> x_c(x,y)
> x

```
> x
```

There are two useful commands for creating vectors (sequence, replication):

```
> a_seq(0,15,2) # seq(lower, upper, increment)
a
[1] }0
> b_rep(0,5) # rep(pattern, number of times)
> b
[1] 0 0 0 0 0
> rep (7,5)
[1] 7 7 7 7 7
> rep(c(1,2,3),4)
[1] 1 2 3 1 2 3 1 2 3 1 2 3
> rep(c(4,5,6),c(1,2,3))
[1] 4 5 5 6 6 6
> rep(c(4,5,6),length=7)
[1] 4 5 6 4 5 6 4
```


## MATRIX

Some basics for matrix have been discussed from the last handout. Here, we will discuss how to modify a matrix and some matrix calculations. We can easily add extra columns and rows by using: cbind(matrixl,matrix2) and rbind(matrixl,matrix2). Try the followings;

```
> x_matrix(1:15,nrow=3,ncol=5,byrow=T)
> x
l [,1] [,2] [,3] [,4] [,5]
[2,] 
[3,] 11 12 12 13 14 15
> x_cbind(x,c(6,11,16))
> x
    [,1] [,2] [,3] [,4] [,5] [,6]
[1,] 
[3,]
> x_rbind(x,17:22)
> x
\begin{tabular}{lrrrrrr} 
& {\([, 1]\)} & {\([, 2]\)} & {\([, 3]\)} & {\([, 4]\)} & {\([, 5]\)} & {\([, 6]\)} \\
{\([1]\),} & 1 & 2 & 3 & 4 & 5 & 6 \\
{\([2]\),} & 6 & 7 & 8 & 9 & 10 & 11 \\
{\([3]\),} & 11 & 12 & 13 & 14 & 15 & 16 \\
{\([4]\),} & 17 & 18 & 19 & 20 & 21 & 22
\end{tabular}
```

Of course, this also can be done easily using the data spreadsheet in S-Plus. Most of discussion using window interface will be discussed in class. If you have a numeric ASCII data file, using the scan function you can create a matrix. For example,
> x_matrix(scan("filename"), ncol=5,byrow=T)
will create a matrix $x$ out of the file with five columns.
For a cross product, $x^{\prime} x$, of the matrix $x$ we use either
$>$ crossprod $(\mathrm{x})$
or

$$
>\mathrm{t}(\mathrm{x}) \% * \% \mathrm{x} \quad \# \mathrm{t}(\mathrm{x}) \text { means the transpose of } \mathrm{x}
$$

Note that a function " $>t(x) * x$ " will return a element-by-element multiplication. If the matrix is a nonsingular square matrix, a function solve will return the inverse matrix. For the singular value decomposition $s v d$ function can be used.

For some more discussion in matrix modification, let's revisit our STA131.dat data. Suppose that before assigning the final grade Sung decided to modify the distribution of proportion to be $20 \% \mathrm{HW}, 25 \%$ MT.I, $25 \%$ MT.II, and $30 \%$ Final. Then, he wanted to recalculate the Total score using these new proportions (I don't know what proportions I used originally, but that might be different than above).

```
> attach(grade.data) #this function will allow you to use the simple variable names (without the
    #messy grade.data$Final or messier grade.data[, 'Final']
> grade.data$Total_HW*.2+MT.I*.25+MT.II*.25+Final
> detach( )
```

Above code will replace the Total score. You may want to record the new score as another name and keep the old one in the same data object. Try this out

```
> attach(grade.data)
> Total.New_HW*.2+MT.I*.25+MT.II*.25+Final
> grade.data_cbind(grade.data, Total.New)
> detach( )
```

Now, you will have another column named Total.New in grade.data. You may want to change some of values in the data. For example, suppose that I want to change the Final score of the student named Kang, S to 78 (was 67).
> grade.data[11,"Final"]_78

Note that this change will not automatically recalculate the Total.New score of the student (Excel does it!).
Now I'd like to calculate the mean and the standard deviation of each of the scores. For this we use the apply function.
> apply(grade.data[,2:6], 2, mean) \#the number 2 in the middle means apply the function mean to \#columns. You may use 1 to refer to the rows
> apply(grade.data[,2:6], 2, stdev)
You may also "> colMeans(grade.data[,2:6])" and "> colStdevs(grade.data[,2:6])". The functions colVars, colSums, rowMeans, rowStdevs, rowVars, and rowSums are also available.

## ARRAY

Array is the extension of the matrix in dimension. That is, if the dimension of data is 2 , we call it "matrix" and more than 2 then "array". Assume that in an opinion poll we obtained the following results from the two states, California and Ohio.

| California |  |  |  |
| :--- | :--- | :--- | :--- |
|  | Yes | No | Don't <br> know |
| Male | 100 | 70 | 10 |
| Female | 50 | 60 | 20 |


| Ohio | Yes | No | Don't <br> know |
| :--- | :--- | :--- | :--- |
| Male | 120 | 50 | 20 |
| Female | 40 | 30 | 30 |

Try this out
poll_array (c(100,50,70,60,10,20,120,40,50,30,20,30),c(2,3,2))
gender_c("Male","Female")
opinion_c("Yes","No","don't know")
state_c("California","Ohio")
dimnames(poll)_list(gender,opinion,state)
poll
$>$ poll

| , California |  |  |  |
| :---: | ---: | :---: | :---: |
|  | Yes | no | Don't know |
| Male | 100 | 70 | 10 |
| Female | 50 | 60 | 20 |


| , , Ohio |  |  |  |
| :---: | ---: | ---: | :---: |
|  | Yes | no | Don't know |
| Male | 120 | 50 | 20 |
| Female | 40 | 30 | 30 |

> poll[,,"California"]

|  | Yes | no |  |
| :---: | :---: | :---: | :---: |
| Don't know |  |  |  |
| Male | 100 | 70 | 10 |
| Female | 50 | 60 | 20 |

```
> poll["Male",,]
```

|  | California | Ohio |
| :---: | :---: | :---: |
| Yes | 100 | 120 |
| no | 70 | 50 |
| Don't know | 10 | 20 |

Note that each of poll[,""California"], poll["Male",,], and etc. is treated as matrices. Hence, all functions we used for matrix can be used. For example,

```
> apply(poll["Male",,],1,sum)
```

| Yes | no | Don't know |
| :--- | :--- | ---: |
| 220 | 120 | 30 |

> apply(poll["Female",,],1,sum)

| Yes | no | Don't know |
| :---: | :---: | ---: |
| 90 | 90 | 50 |

## DATA FRAME

Data Frame is a generalized version of the matrix in the sense that the data frames allow you to mix data of different types (numeric, character, etc) into a single data object. The data frame is the most common data structure in S-Plus.
Data frame can be created via several ways. To create a data frame from an external file, read.table command can be used as we discussed before. You may also import the data file directly from the File menu.

```
>your.frame.name_ read.table("filename",header=T) #use header=F if your data
    #doesn't contain a header row.
```

You may want to bind S-Plus data objects of various kinds into a data frame. In the case use data.frame command.

```
> your.frame.name_data.frame(object1,object2,....)
```

Consider the following simple example.

```
> rdm_rnorm(10) #this wiil generate random sample of size 10 from N(0,1)
> assgn <- rep(NA, 10)
> assgn[rdm > 0] <- "A"
> assgn[rdm <= 0] <- "B"
> assgn1 <- cbind(rdm, assgn)
> assgn1
    rdm assgn
    [1,] "0.049086461868886" "A"
    [2,] "0.918544752343534" "A"
    [3,] "-0.126559993056653" "В"
    [4,] "0.33915786263237" "A"
    [5,] "1.43901265660863" "A"
    [6,] "0.0279969566945071" "A"
    [7,] "-1.47322223095435" "B"
    [8,] "-0.668673135299956" "В"
    [9,] "-0.345348406178856" "B"
[10,] "0.0884835844457507" "A"
> max(assgn1[, 1])
Problem in max(assgn1[, 1]): Numeric summary undefined for mode "character"
```

This will create a matrix using cbind command. By binding numeric with character variable, the variable $r d m$ is no longer numeric. Hence, some numeric calculations, like max and min, are no longer possible. It is interesting to note that some numeric calculations, like mean and stdev, are still working.

```
> mean(assgn1[, 1])
[1] 0.02484785
```

Now, let create a data frame, which will keep the original mode of the variables.

```
> assgn2 <- data.frame(rdm, assgn)
> assgn2
    rdm assgn
1 -0.7615447 B
2 -0.4632235 B
1.8197463 A
4 -0.1927243 B
5-0.1923333 B
6-0.1962358 B
```

| 7 | -1.5823391 | $B$ |
| ---: | ---: | ---: |
| 8 | -0.6647673 | $B$ |
| 9 | -0.4132076 | $B$ |
| 10 | 2.0184172 | $A$ |
| $>$ | max (assgn2\$rdm) |  |

[1] 2.018417
Any functions we used for matrix, like apply, also works for data frames. To combine data frames, use data.frame, cbind, rbind. You can merge two or more data frames using merge function.

```
> merge(dataframe1,dataframe2,...)
```

It can be explained by the following example. Consider that we have two data frames: the first one is general information about students in a class (provided from the university) and the second is their test scores and the final grade (prepared by the professor). We want to merge the two data from different sources.

```
example.list
    Name Class College
    Chen Senior AS
    Choi Master AS
Jackson Master Eng
Johnson Master AS
Lu Senior Edu
Mueller Junior Eng
    Park Master Edu
    Xiao Senior AS
example.grade
    Name MT Final Grade
Jackson 85 79 A
Mueller 70 98 A
    Lu 92 91 A
    Choi 78 68 B
Johnson 69 66 B
    Park 62 80 B
    Xiao 75 78 B
    Chen 54 66 C
merge(example.list, example.grade, by=1) #by=1 means merging by the first col.
    Name Class College MT Final Grade
    Chen Senior AS 54 66 C
    Choi Master AS 78 68 B
Jackson Master Eng 85 79 A
Johnson Master AS 69 66 B
Lu Senior Edu 92 91 A
Mueller Junior Eng 70 98 A
    Park Master Edu 62 80 B
    Xiao Senior AS 75 78 B
```

More discussion on Data Frames will be given later.

## LIST

List is a collection of vectors or matrices of arbitrary structures. List is useful when you want to collect related data with different structures into a big list object. Note that while both data frame and matrix require rectangular, list allows different structures. Consider the following example:

```
> a_rnorm(5) #random sample of size 5 from N(0,1)
>b a>0
> a\overline{b}_data.frame(a,b)
```

```
> c_rt(10,29) #random sample of size 10 from t(df=20)
> d_rchisq(15,29) #random sample of size 10 from chisquare(df=20)
> x_list(ab,c,d)
> X
[[1]]:
" 0 5284931" b b
1 " 0.5284931" "T"
2 "-0.5783929" "F"
3 "-0.7104860" "F"
4 " 0.1749112" "T"
5 " 0.8443500" "T"
[[2]]:
    [1] 0.1661215 -0.2214252 0.8668092 -0.1193410 -0.6454605 0.5767275
    [7] 0.7018636 0.8049501 1.1132858
[[3]]:
    [1] 22.74985 32.81265 47.81313 23.51771 31.96326 17.26032 31.40059
```



```
[15] 35.17972
```

To call the data frame $a b$ use either $\mathrm{x}[1]$ or $\mathrm{x}[[1]]$. Either $x[[1]] \$ a$ or $x[[1]][[1]]$ will return the vector $a$ (random sample from $\mathrm{N}(0,1)$ ).

```
> x[[1]]$a
[1] 0.5284931 -0.5783929 -0.7104860 0.1749112 0.8443500
> x[[1]][[1]]
[1] 0.5284931 -0.5783929 -0.7104860 0.1749112 0.8443500
> mean(x[[1]]$a)
[1] 0.05177509
```


## WRITING FUNCTIONS

This note discusses the basic techniques for writing functions in S+ (like macro in SAS). S+ provides a number of built-in functions (over 3800) and writing your own functions can extend it. The basic syntax of a function declaration is as follows:

```
Your-function-name <- function (arguments)
{ function body
    return (output arguments) }
```

To call the function, type
$>$ your-function-name (arguments).
As a simple example consider writing a function to calculate the two-sided p-value of a t statistic (text p3).

```
t.test.p_function (x, mu=0, alpha=0.05)
{ n_length(x)
    t- sqrt(n) * (mean(x) - mu) /stdev(x)
    p_2 * (1-pt(abs(t), n-1))
    if (p<alpha) result_"Reject Ho" else result_"Do Not Reject Ho"
    return(t,p, result)-}
```

Here, $x$ is data, $m u$ is the mean under the null hypothesis, and alpha is the level of significance. To call this function for a t -test for Ho: $\mu=1$ at $\alpha=.01$,
t.test.p(data, 1, 0.01)

If you don't specify the last two arguments, $\mathrm{S}+$ will use the default values of $m u=0$ and $a l p h a=0.05$. Let's use the function to test if the mean Final score of STA131 class is 67 (the mean from last year) or not.

```
> z_grade.dat$Final
>t.test.p(z,67)
$t:
[1] -1.11745
$p:
[1] 0.2736473
$result:
[1] "Do Not Reject Ho"
```

The calculated $t$ statistic and the corresponding $p$-value and the test result are printed above. Since we didn't specify the level of significance, the test is performed with the default value of 0.05 . Since the pvalue of the test is not less than 0.05 , we do not reject the null hypothesis, Ho: $\mu=67$, at $\alpha=.05$. In deed, $\mathrm{S}+$ has a built-in function for a t -test, for both one and two sample.

```
> t.test(z, mu=67)
One-sample t-Test
data: z
t = -1.1174, df = 27, p-value = 0.2736
alternative hypothesis: true mean is not equal to 67
95 percent confidence interval:
51.29976 71.62881
sample estimates:
mean of x
61.46429
```

Functions also can be used to define your own function name of a built-in function. For example, suppose you use the logarithm function with a base 2 very often. The built-in function expression is $\log b(x, 2)$. You want to simplify the expression.

```
> log2 <- function(x) { return (logb(x, 2)) }
> log2(16)
[1] 4
```

To get the on-line help for the argument names and default values for $S$-function, type
$>\operatorname{args}(f u n c t i o n-n a m e)$.
For example,

```
> args(t.test)
function(x, y = NULL, alternative = "two.sided", mu = 0, paired = F,
var.equal = T, conf.level = 0.95)
```

If you want to perform one-sided (left) two-sample t-test for non-paired and unequal variances, type

```
> t.test(x,y, alternative="less", paired=F, var.equal=F)
```

Elementary Functions: See handout

## is and as functions

Before applying functions to our data, we may want to check if our data has the particular type that the function argument required. Doing so, you can protect against unexpected error message.

```
> is(x,"numeric")
```

Consider the following function, which returns mean for number variable.

```
Just.fun function(x)
    { if(!is(x,"numeric")) stop ("Oops! The variable must be numeric.")
    else return(mean(x)) {
```

is( $x$, "numeric") is a logical function that will return T if $x$ is numeric. The complementary expression is !is(x, "numeric") that will return T if $x$ is not numeric. Now the variable gender is a factor with elements "Male" and "Female".
> Just.fun (gender)
Problem in Just.fun(gender): Oops! The variable must be numeric.
You can use the function to test for "array", "character", "complex", "data.frame", "double", "factor", "integer", "list", "logical", "matrix", "numeric", "single", and "vector".
as function is used to coerce the variable to have the specified data type. For example,
> as (x, "character")
will coerce the variable $x$ to have a character data type. Consider the data with 12-hour pollutant volume at a certain day with code " 9999 " for a missing value.


Of course, you could use the NA for the missing value (replace "Missing" with NA) keeping the variable numeric. We just assigned the character "Missing" to explain the use of as function. Since the pollut variable converts to character we use the $a s$ function to covert the variable back to numeric.

```
> pollut_as(pollut,"numeric")
Warning messages:
1 missing values generated coercing from character to numeric
> pollut
[1] 8
```

Now, we want to calculate the mean omitting the missing values.
$>\operatorname{mean}($ pollut[!is.na(pollut)])
[1] 4.818182
We have used the is.na function to determine which values are missing and to exclude the missing values from the mean calculation.

## ITERATION

It is extremely important to note that S-Plus is vector or matrix oriented (Fortran and C are not!), and hence, we can mostly avoid complicated loops in iterative computations. For example we can simply use $x \% * \% x$ for uncorrected sum of squares for variable $x$ instead of using the for loop. We will briefly discuss for, while, and repeat. These loops can be used independently or in the body of a function.

The for loop
$>$ for( i in invalues) $\{$ commands $\}$
Consider the calculation of a uncorrected sum of square of a variable $x$

```
> x_c(2,1,3,4,2,3,1,5)
> y_0
> for (i in 1:length(x)) {y_x[i]^2+y; print(y)}
[1] 4
[1] 5
[1] 14
[1] }3
[1] 34
[1] 43
[1] 44
[1] 69
> y
[1] 69
```


## The while loop

The while loop is used when the total number of iteration is unknown.
> while(condition) $\{$ commands \}
For an example of the use of the while loop, we consider the maximum likelihood estimation for the parameter $\lambda$ of the zero-truncated Poisson distribution as in the text p 95 . The probability distribution and the iterative estimation via Newton's method is in the test.

```
    yp_rpois(100, 1) #random sample of size 100 from Poisson(1)
    y_yp[yp>0] #truncate the zeros
    ybar_mean(y) #mean of the zero truncated Poisson r.v.
    lam_ybar #initial value of lambda
    it_0 #iteration count
    de\overline{l}1 #tolerance
    while(abs(del) > . 000001 && (it_it+1)<10)
        {del_(lam-ybar*(1-exp (-lam)))/(1-ybar*exp (-lam))
    lam_Iam-del
    cat("The estimated lambda after", it, "th iteration is", lam, "\n")
    }
The estimated lambda after 1 th iteration is 1.148994930761
The estimated lambda after 2 th iteration is 1.06264898980154
The estimated lambda after 3 th iteration is 1.0581687548983
The estimated lambda after 4 th iteration is 1.05815588823481
The estimated lambda after 5 th iteration is 1.05815588812837
```

In the above example, the condition of the while loop states that the iteration continues until the tolerance limit of 0.00001 and the number of iteration of 10 . To print the variable's values we use cat function, which is analogy to the cat function from the C language.

## The repeat loop

> repeat \{commands

## stop criterion \}

The repeat function repeats the commands until the stop criterion meets. We may rewrite the above code using repeat loop as follows;

```
yp_rpois(100, 1)
y_yp[yp>0]
ybar_mean(y)
lam_ybar
it \overline{1}
del_1
repeat
    {del_(lam-ybar*(1-exp(-lam))) /(1-ybar*exp (-lam))
    lam_lam-del
    cat("The estimated lambda after", it, "th iteration is", lam, "\n")
    if(abs(del) < .00001 || (it_it+1)>10) break
    }
The estimated lambda after 1 th iteration is 1.148994930761
The estimated lambda after 2 th iteration is 1.06264898980154
The estimated lambda after 3 th iteration is 1.0581687548983
The estimated lambda after 4 th iteration is 1.05815588823481
The estimated lambda after 5 th iteration is 1.05815588812837
```


## GRAPHICS

## Getting Started: plot( ), hist( ) functions, and more.

## Scatter plot

Let's revisit our grade.data data.

```
> attach(grade.data)
> plot(MT.I,Final)
```



We can change the character for the point by using pch parameter. For example,
$>\operatorname{plot}(\mathrm{MT} . \mathrm{I}$, Final, pch="*")
will replace the points in the plot with *. S+ has a number of numeric assignments for special symbols. Of these, commonly used seven are;

| $\square$ | $\bigcirc$ | $\Delta$ | + | $\times$ | $\diamond$ | $\nabla$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 2 | 3 | 4 | 5 | 6 |

> plot (MT.I, Final, pch=2)
can be used to have triangular points, etc. Numbers 7 to 14 are composite symbols formed by overprinting these symbols, and 15 to 19 are solid-filled versions of $0,1,2,5$, and 6 .

We can also change the type of the plot. For example,

```
> plot (x, y, type="l")
```

will have line plot connecting the data. The default is type=" p ", the point plot. Other available types are " b ", "h", "o", "s", and "n". I will leave you to explore these types. For complete list of useful options for plotting functions type > help (par). Some of the most commonly used are:

```
axes=T T for with axes, F for without axes
main=" Title" Title string
sub="Subtitle" Subtitle string
xlab="x axis label" x axis label,
ylab= "y axis label" y axis label,
xlim}=\textrm{c}(xmin, xmax) range for x axis
ylim}=\textrm{c}(ymin,ymax) range for y axis
```

```
pch="*" point character (see above)
type="l" plot type (see above)
Ity=1 1 for default solid line, 2 for dashed line
lwd=1 1 for default line width, 2 for twice thick, etc
```

We can also simply change the layout of the plot via interface (right click on the plot).
The function abline( ) will superimpose a line on the scatter plot. For example, the least square line for regressing Final on MT.I has the intercept and slope estimates of -16.187 and 0.9754 , respectively.

$$
>\text { abline(-16.187,0.9754) \# abline (intercept, slope) }
$$



Fitting and plotting the least square line can be done easily by using $\operatorname{lm}$ (linear model) function. The following code will return the same plot as above.

```
> fit lm(Final~MT.I)
> ablīne(fit)
```

More detailed discussion on the $\operatorname{lm}()$ function will follow.
Let put them together.

```
> plot(MT.I,Final, main="Fitted Regression line for Grade data",
+ xlab="Midterm I", ylab="Final", xlim=c(0,100), ylim=c(0,100), pch=16)
> abline(fit, lty=2,lwd=2)
> text(50, 90, "Final = -16.187 + 0.9754 * MT.I", cex=2)
```

The text function will add a text at the specified location; text(xlocation, ylocation, " text"). The option $c e x=2$ draws characters twice as big. You can rotate the character using the option crt=counterclockwise degree. The text adjustment option is adj= 0 ( 0 for left justified, 1 for right justified and 0.5 for centered). If you forgot to add title option in the plot function, you can add the title in the existing plot.

```
> title ("title","subtitle")
```

Fitted Regression line for Grade data


Histogram
The hist( ) function plots a histogram.
$>$ hist(Final)


To change the number of class we use nclass option. For example,
>hist (Final, nclass=10)
will return


Check >help(hist) for more options.
Multiple Plots: par( ) function
You can display several small plots as a table or matrix format. Use the par (mfrow=c(nrow, ncol)) function. A $2 \times 3$ matrix of plot can be created by

```
> par (mfrow=c (2,3))
```

Try this out.

```
> par(mfrow=c(1,3))
> hist(MT.I, break=c(0, 20, 40,60, 80,100))
> hist(MT.II, break=c(0, 20,40,60, 80,100))
> hist(Final, break=c(0, 20,40,60, 80,100))
```



To restore the default setting type $>\operatorname{par}($ mfrow $=c(1,1))$.

We may want customize the display of the multiple plots. It can be done using

$$
>\operatorname{par}(\mathrm{fig}=c(x 1, x 2, y 1, y 2)
$$

where the parameter $\mathrm{x} 1, \mathrm{x} 2$ are the plot location of left corner and right corner of x axis. Similarly for y axis. Note that the coordinate of the plot are set to $(0,0)$ for the lower left corner and $(1,1)$ for the top right corner. Let's consider the following example.

```
frame() #opening new graph
par(fig=c(0,0.7,0,0.6))
plot(MT.I,Final, main="Fitted Regression line for Grade data", xlab="Midterm
    I", ylab="Final", xlim=c(0,100), ylim=c(0,100), pch=16)
fit_lm(Final~MT.I)
ablīne(fit, lty=2,lwd=4)
par(fig=c(0,0.7,0.55,1))
hist(Final,main="Histogram of Final")
par(fig=c(0.65,1,0.15,0.85))
boxplot(Final,main="Boxplot of Final")
```

Histogram of Final


## More example...

Following example demonstrates the approximate normality of the sum of continuous uniform r.v.'s.

```
par(mfrow=c (2,3))
x_runif(1000) # random number of size 1000 from Unif(0,1)
hīst(x,nclass=20,main="n=1")
x_runif(1000)+x
hist(x,nclass=20,main="n=2")
```

```
x runif(1000)+x
hist(x,nclass=20,main="n=3")
x_runif(1000)+x
hist (x,nclass=20,main="n=4")
x_runif(1000)+x
hist(x,nclass=20,main="n=5")
x_runif(1000)+x
hist(x,nclass=20,main="n=6")
```








## TRELLIS GRAPHICS

Once data is categorized by one or more factors, we might want to have separated graphs conditioned on one or more factors. Let's consider an example of drawing a Trellis histogram.

## Example.

An experiment is designed to study the effects of treatment duration (factor A) and weight gain between treatment (factor B) on the number of days hospitalized (response, named days) for kidney failure patients. The factor A has two levels (1.short, 2.long) and the factor B has three levels (1.Mild, 2.Moderate, 3.Severe). A random sample of 10 patients per each of the 6 groups is collected. You can download the data from the class web site (kidney.dat).

First, we would like to see the distribution of days conditioned on the duration.
> histogram(~days|duration, data=kidney)


This also can be easily done using the user interface. First, open the data object, then mark the first two columns (days and duration). Then, choose the Plots $2 D$ button on the menu bar then Set Conditioning Model button. You may see small yellow bars appeared on the Plots $2 D$ palette. Then choose 1 for the \# of conditioning columns. Then, choose Histogram on the Plots $2 D$ palette. Once you have the Trellis plot via the interface you can easily change the conditioning column by just interacting between the Data Window and the Graph Window. To change the conditioning columns mark the columns in the Data Window and drag to the top of the Graph Window. You may choose multiple columns. We will discuss more in class.

Trellis Histogram conditioning on factor B (weight gain) using the user interface.


To change the number of class right-click on any bar of the histogram, then Options, then type the number you want for the Number of Bars. Click OK.


Now, let choose both factors as conditioning factors. Choose both columns in the Data Window and press and hold the mouse and drag the cursor to the top of the graph.

Example Trellis Histogram conditioning on two factors


Note that the above Trellis graph has the order as

| $(1,3)$ | $(2,3)$ |
| :--- | :--- |
| $(1,2)$ | $(2,2)$ |
| $(1,1)$ | $(2,1)$ |

Here ( 1,2 ) means (factor A level 1, factor B level 2).
To reverse the order right-click on any white space in the graph then choose Multipanel then change the Panel Order (bottom of the menu) to Table Order. To add the title of the graph choose Insert then Title.

## Data Preparation to Use for Trellis

If data consists of several columns and if we want to generate a Trellis graph conditioning on the column variables, we can use make.groups to make a group data and to ready for a Trellis graph. For better understanding let's revisit our STA131 grade data. The data has five numeric columns (HW, MT.I, MT.II, Final, Total) and we would like to generate scatter plots of Final versus each of HW, MT.I and MT.II.

```
> grp_make.groups(HW,MT.I,MT.II)
> final_rep(Final,3)
> grp.trel_data.frame(final,grp)
> grp.trel
    final data which
    1 27 93.750 HW
    2 33 91.750 HW
29*
30 33 80.000 MT.I
```

```
57 27 38.000 MT.II
58 33 52.000 MT.II
84 63 100.000 MMT.II
> xyplot(final~data|which, pch=16, col=1, data=grp.trel)
```

Final vs. other Scores


We have generated a Trellis scatter plot using the user interface or
> xyplot $(\mathrm{y} \sim \mathrm{x} \mid \mathrm{z})$
where x and y are the two variable for the scatter plot and z is the conditioning variable.
We can obtain better layout using Interface.


## DESCRIPTIVE STATISTICS

The summary function provides some basic statistics of the data or variables. Consider the grade data.

```
> summary(grade.data)
    Name HW MT.I
        Zhang, Li: 1 Min.:32.50 Min.: 33.00
        Wong, Gildas: 1 1st Qu.:93.06 1st Qu.: 69.25
White, Jennifer: 1 Median:97.31 Median: 87.50
            Wai, Newton: 1 Mean:91.92 Mean: 79.61
Sundstrom, Kurt: 1 3rd Qu.:98.97 3rd Qu.: 93.50
    Su, Xiao-Gang: 1 Max.:99.75 Max.:100.00
                (Other):22
            MT.II Final Total
        Min.: 36.00
    Min.:12.00 Min.:31.80
1st Qu.: 64.25 1st Qu.:47.00 1st Qu.:62.53
    Median: 75.50 Median:60.00 Median:73.50
        Mean: 76.00 Mean:61.46 Mean:71.86
3rd Qu.: 93.25 3rd Qu.:83.75 3rd Qu.:87.50
    Max.:100.00 Max.:99.00 Max.:98.20
```

The stem function gives the stem-and-leaf display of a variable and the quantile function gives the quantiles of the variable at the specified values.

```
> attach(grade.data)
> stem(Total)
N = 28 Median = 76.4125
Quartiles = 65.7125, 89.2625
Decimal point is 1 place to the right of the colon
    3 : 5
    4:299
    5 :
    6 : 1456
    7:22344589
    8 : 12589
    9:0555668
    > quantile(Final, c(0.25, 0.5, 0.95))
    25% 50% 95%
    47 60 97.6
> grade.data[Total>=90,]
                                    Name HW MT.I MT.II Final Total
            Lin, Dongqing 99.250 90 98 95 95.0
                Love, Brad 99.750 96 98 88 93.2
        Peck, Laura 98.625 97 92 94 94.7
        Singh, Ramanpreet 99.750 100 98 90 95.0
            Su, Xiao-Gang 97.250 95 100 99 98.2
                Wai, Newton 98.875 87 100 99 96.5
> apply(grade.data,2,mean)
    Name HW MT.I MT.II Final Total
        NA 91.91518 79.60714 76 61.46429 71.86429
```

Now, consider the kidney data. The data is categorized by two factors and we can have the summary of the response variable conditioning on factors.

```
> attach(kidney)
> summary(days[duration==1])
    Min. 1st Qu. Median Mean 3rd Qu. Max.
    0.00 2.25 5.00 8.20 11.50 30.00
> summary(days[duration==1 & wtgain==2])
    Min. 1st Qu. Median Mean 3rd Qu. Max.
    1.00 3.25 4.50 7.30 10.75 20.00
> tapply(days,list(duration,wtgain),mean)
    1 2 3
1 2.7 7.3 14.6
2 2.2 3.7 7.5
```

The tapply ( $t$ stands for table) splits the data by the given factors and apply the function (mean this case) to each subgroup. Another useful function for a categorized data is by. The by function is very convenient to obtain numerical summaries of the categorized data.

```
> by(days, duration, summary)
INDICES:1
            X
        Min.: 0.00
    1st Qu.: 2.25
    Median: 5.00
        Mean: 8.20
    3rd Qu.:11.50
        Max.:30.00
INDICES:2
            x
        Min.: 0.000
    1st Qu.: 1.000
        Median: 3.500
        Mean: 4.467
    3rd Qu.: 7.000
        Max.:15.000
```

Similarly,

```
> by(days,wtgain, summary)
> by(days,list(duration,wtgain), summary)
:1
:1
        Min.:0.00
    1st Qu.:0.25
    Median:2.00
        Mean:2.70
    3rd Qu.:4.50
        Max.:8.00
:2
:1
            X
        Min.:0.00
    1st Qu.:0.25
        Median:1.50
            Mean:2.20
3rd Qu.:3.75
```

```
    Max.:7.00
:1
:2
    Min.: 1.00
    1st Qu.: 3.25
    Median: 4.50
        Mean: 7.30
    3rd Qu.:10.75
        Max.:20.00
----------------------------------------------------------
:2
:2
            X
        Min.:0.00
    1st Qu.:1.25
    Median:3.00
        Mean:3.70
3rd Qu.:5.75
        Max.:9.00
:1
:3
        Min.: }3.0
    1st Qu.: 7.25
    Median:12.50
        Mean:14.60
    3rd Qu.:22.75
        Max.:30.00
------------------------------------------------------------
:2
:3
        Min.: 1.00
    1st Qu.: 4.50
    Median: 7.50
        Mean: 7.50
    3rd Qu.: 9.75
        Max.:15.00
>
```


## DISTRIBUTION RELATED FUNCTIONS

Example:

```
> z_qnorm(.95) # 95% quantiles under N(0,1)
> z
[1] 1.644854
> pnorm(z) # cumulated density at the 95% quantile
[1] 0.95
> qnorm(c(.05,.95))
[1] -1.644854 1.644854
> qt(.95,10)
[1] 1.812461
> pt(2.0,10) # cumulated density
[1] 0.963306
```

Character Type
d : Distribution Function
p : Cumulated Density Function
q: Quantile
$\mathbf{r}$ : Random number generation
The distribution names suffix one of the character types to define the $\mathrm{S}+$ functions. For the list of names and necessary parameters see the handout in class.
Let's consider the following S+ code to compare the normal distribution and t with 5 df .

```
pts_seq(-5,5,length=1000)
pts.nor_dnorm(pts)
pts.t_dt}(pts,4
yrange_range(pts.nor,pts.t)
plot(0,0,type="n",xlim=c(-5,5), ylim=yrange,ylab="Density")
lines(pts,pts.nor, col=1,lty=1,lwd=2)
lines(pts,pts.t,col=2,lty=2,lwd=4)
key(lines=list(lty=1:2, col=1:2),text=list(paste(c("Standard Normal","t(4)"))))
title("Standard Normal vs t(4)",cex=1.5)
```

Standard Normal vs t(4)


For another example of using the distribution related functions, let's consider a graphical display of the normal approximation to the binomial distribution. Let X be binomial with $\mathrm{n}=50$ and $\mathrm{p}=.3$. The density of the Binomial distribution and the normal distribution with mean of $n * p=15$ and the sd of $\operatorname{sqrt}\left(n^{*} p *(1-\right.$ $p))=3.24$ are given in the following graph.

```
n_50; p_0.3; x_0:n
y_dbinom(x,n,p)
plot(x,y,type="h")
x_seq(0,n,length=100)
m=n*p;s=sqrt(n*p*(1-p))
f dnorm(x,m,s)
lines(x,f)
title("Normal Approximation to Binomial")
text(25,.12,"n=50, p=0.3",cex=1.5)
```

Normal Approximation to Binomial


To calculate $\mathrm{P}(\mathrm{X} \geq 20)$ we use either pbinom (exact prob.) or pnorm (normal approx.). First, the exact probability from the Binomial distribution is;

```
> - pbinom(19, n, p)
[1] 0.0848026
```

The exact probability can be compared with a Normal approximation;

```
> z <- (19.5 - n * p)/sqrt(n * p * (1 - p))
> 1 - pnorm(z)
[1] 0.08245741
```

A list of the distributions and their $\mathrm{S}+$ function names can be found in the text p114.

## HYPOTHESIS TESTING

We have discussed one sample t-test earlier. S+ provides many functions for hypothesis testing. The names of functions are self-explanatory. To see the necessary arguments, for example t-test, type

```
> args(t.test)
function(x, y = NULL, alternative = "two.sided", mu = 0, paired = F,
    var.equal = T, conf.level = 0.95)
```

We may also type >help(t.test) for more details.
Let's consider the two sample $t$-test comparing the two different durations in the kidney data. If the data is paired (not this case), we need to specified paired $=T$ and do the paired t test.

```
> my.ttest_t.test(days[duration==1], days[duration==2], conf.level = .90)
> my.ttest
    Standard Two-Sample t-Test
data: days[duration == 1] and days[duration == 2]
t = 2.2319, df = 58, p-value = 0.0295
alternative hypothesis: true difference in means is not equal to 0
90 percent confidence interval:
    0.9372859 6.5293808
sample estimates:
    mean of }x\mathrm{ mean of }
        8.24.466667
```

The resulted p-value of the test is .0295 , which is compared with the specified significance level of 0.1 . Since the p -value is less than the significance level, the test for equal means is rejected.

Note that the function t.test returns a list type of object with some statistics and information for the test. To see the available information;

```
> summary(my.ttest)
    Length Class Mode
        statistic 1 numeric
parameters 1 numeric
            p.value 1 numeric
            conf.int 2 numeric
            estimate 2 numeric
    null.value 1 numeric
alternative 1 character
            method 1 character
    data.name 1 character
```

We now try to access some specific information.

```
> my.ttest$statistic
    t
    2.231888
> my.ttest$p.value
[1] 0.02950016
> my.ttest$conf.int
[1] 0.9372859 6.5293808
attr(, "conf.level"):
[1] 0.9
> my.ttest$data.name
[1] "days[duration == 1] and days[duration == 2]"
```

```
> my.ttest$null.value
    difference in means
```

    0
    > ttest\$alternative
[1] "two.sided"

The testing procedure and the result are well demonstrated in the following graph. The S+ code generating the graph is copied from the recommended text by Krause and Olson. I found it very useful for writing report for non-statisticians. We will discuss the $\mathrm{S}+$ code in class.

attach (kidney)
x_days [duration==1]
y days[duration==2]
df_length (x) +length (y) -2
alpha_. 1
bound.left_-3
bound.right_3
xaxis_seq(bound.left, bound.right, length=1000)
yaxis_dt (xaxis,df)
plot(xaxis,yaxis,type="l", ylab="t density")
critical.left_qt(alpha/2,df)
critical.right_qt(1-alpha/2,df)
xaxis_seq(bound.left, critical.left,length=100)
yaxis_c(dt(xaxis,df),0,0)
xaxis c(xaxis,critical.left,bound.left)
polygon(xaxis,yaxis, density=25)

```
xaxis seq(critical.right, bound.right,length=100)
```

yaxis_c (dt (xaxis,df), 0,0)
xaxis_c(xaxis,bound.right, critical.right)
polygōn(xaxis,yaxis, density=25)
test.stat_t.test(x, y, conf.level = 1-alpha) \$statistic

```
points(test.stat,.01,cex=2,adj=0.5, pch=16)
arrows(test.stat-1,.05,test.stat-.1,.01,open=T,rel=T)
text(test.stat-1,.07,"test statistic",adj=.5,cex=1.5)
text(bound.left, 0.08, "rejection \n region", adj=0)
text(bound.right, 0.08, "rejection \n region", adj=1)
text((bound.left + bound.right)/2, 0.16, "acceptance region")
xaxis_c(rep(critical.left,2),rep(critical.right,2))
yaxis_c(0.12,0.14,0.14,0.12)
```

Other statistical test in S+: binom.test, chisq.gof, chisq.test, cor.test, var.test, wilcox.test, etc.

## REGRESSION

In this section we will discuss fitting a regression model using the $l m$ (linear model) function. As we have discussed earlier, the syntax of the model is

```
lm(response~predictor1+predictor2+..., options)
```

For a detailed discussion let's consider the Real Estate data that we used for MATH 532 class.

## Data

A real estate expert is interested in developing a regression model that relates the selling price of suburban residential properties to characteristics of properties. Her interest lies in new, large residential property development on the outskirts of a major city for which she has data on 30 properties that were sold recently.

| $\mathrm{X}_{1}$ | Property taxes (annual taxes, in dollars) |
| :--- | :--- |
| $\mathrm{X}_{2}$ | House size (floor area, in square feet) |
| $\mathrm{X}_{3}$ | Lot size (in acres) |
| $\mathrm{X}_{4}$ | Lot size squared |
| $\mathrm{X}_{5}$ | Attractiveness index |
| $\mathrm{X}_{6}$ | Style (E, S, or M$)$ |


| Data for the property selling prices |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Property | Property <br> Taxes | House <br> Size | Lot <br> Size | Lot Size <br> Squared | Attrac- <br> tiveness | Style | Selling Price <br> (in \$1000) |
| 1 | 6337 | 3000 | 3.6 | 12.96 | 64 | M | 350 |
| 2 | 3204 | 2300 | 1.2 | 1.44 | 69 | E | 261 |
| 3 | 4574 | 3300 | 1.3 | 1.69 | 72 | S | 301 |
| 4 | 4924 | 2100 | 3.2 | 10.24 | 71 | E | 255 |
| 5 | 4182 | 3900 | 1.1 | 1.21 | 40 | S | 303 |
| $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |
| $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |
| 27 | 3917 | 3100 | 1.8 | 3.24 | 54 | E | 244 |
| 28 | 4068 | 2200 | 2.1 | 4.41 | 75 | S | 294 |
| 29 | 4068 | 2500 | 3.9 | 15.21 | 61 | E | 279 |
| 30 | 3612 | 2900 | 1.1 | 1.21 | 74 | E | 277 |

For the full data click on realestate.dat

For multivariate data, it is good idea to start the analysis with the pairwise scatterplots.

```
> pairs(realestate[,2:8])
```



Using the cor function, we can calculate the correlation matrix among variables.

```
> cor(realestate[,c(2:6,8)],realestate[,c(2:6,8)])
\begin{tabular}{rrrrrrr} 
& tax & Hsize & Lsize & Lsize.sq & attrac & price \\
tax & 1.0000000 & 0.2812810 & 0.73968353 & 0.72108667 & 0.02879220 & 0.4693318 \\
Hsize & 0.2812810 & 1.0000000 & -0.28982630 & -0.26804966 & -0.12844139 & 0.6258176 \\
Lsize & 0.7396835 & -0.2898263 & 1.00000000 & 0.98477889 & -0.01889162 & 0.1206351 \\
Lsize.sq & 0.7210867 & -0.2680497 & 0.98477889 & 1.00000000 & -0.06571432 & 0.1181183 \\
attrac & 0.0287922 & -0.1284414 & -0.01889162 & -0.06571432 & 1.00000000 & 0.3610034 \\
price & 0.4693318 & 0.6258176 & 0.12063505 & 0.11811831 & \(\mathbf{0 . 3 6 1 0 0 3 3 6}\) & 1.0000000
\end{tabular}
```

Note that the predictor style is qualitative and omitted from the correlation calculation. The pairwise scatterplot and the correlation suggest that Hsize has the strongest linear association with price. The variables tax and attrac also show moderately high correlation with the response.

Before we go any further, we need to note that we have a qualitative predictor, style, in the data. Many different codings of indicator variables are available. Here, we use the simple dummy coding ( 0,1 coding);

| Style | Sty1 | Sty2 |
| :--- | :--- | :--- |
| E | 1 | 0 |
| M | 0 | 1 |
| S | 0 | 0 |

Let add the two indicator variables in the data frame.

```
> sty1_rep(NA,30)
> sty2_rep(NA,30)
> sty1[style=="E"]_1
> sty1[style!="E"]_0
> sty2[style=="M"]-1
> sty2[style!="M"]_0
> realestate_data.frame(realestate,sty1,sty2)
```

At this moment you may want to recalculate the correlation matrix.

## Simple Regression

First, consider a simple regression with the response variable, price, and the predictor, Hsize.

```
> fit1 lm(price~Hsize,data=realestate)
> summary(fit1)
Call: lm(formula = price ~ Hsize, data = realestate)
Residuals:
    Min 1Q Median 3Q Max
-81.44 -27.09 -2.379 30.81 114.7
Coefficients:
            Value Std. Error t value Pr(>|t|)
(Intercept) 115.7431 46.9759 2.4639 0.0201
    Hsize 0.0676 0.0159 4.2457 0.0002
Residual standard error: 44.86 on 28 degrees of freedom
Multiple R-Squared: 0.3916
F-statistic: 18.03 on 1 and 28 degrees of freedom, the p-value
is 0.0002167
Correlation of Coefficients:
    (Intercept)
Hsize -0.9847
```

Specific information contained in the modeling can be accessed as before; object\$values.

```
> fit1$coefficients
    (Intercept) Hsize
        115.7431 0.06764303
> resid_fit1$residuals
> fitted_fit1$fitted.values
```

For the full list of available values see the help file for lm.object.
We can also access the residuals and the fitted values by resid(fitl) and fitted(fit1). Let's plot the residuals versus the fitted values.

```
> plot(fitted(fit1),resid(fit1),pch=16)
> abline(h=0)
```

abline $(\mathrm{h}=0)$ will draw the horizontal line at 0 .

Residual vs. Fitted


As discussed earlier,

```
> attach(realestate); plot(Hsize,price); abline(fit1)
```

will draw a scatterplot with the fitted line superimposed on.
For a QQ plot

```
> qqnorm(resid(fit2),main="QQ Plot with Line")
> qqline(resid(fit2))
```


## QQ Plot with Line



Let's put them together.

```
attach(realestate)
fit1_lm(price~Hsize,data=realestate)
par(\overline{mfrow=c (2,2))}
plot(Hsize,price,pch=16,sub="Scatterplot with Fitted Line"); abline(fit1)
plot(fitted(fit1),resid(fit1),pch=16,sub="Residual vs Fitted"); abline(h=0)
hist(resid(fit1),sub="Histogram of Residual",nclass=10)
qqnorm(resid(fit1),sub="QQ Plot with Line",pch=16); qqline(resid(fit1))
```



We can also examine the S+ default plots:
> plot(fit1)


260280300320340360380
Fitted :Hsize




Fitted Values Residuals



You can specify your choice of the plots to display by using the ask option:

```
> plot(fit1, ask=T)
```


## Multiple Regression

Now, consider a multiple regression with two predictors. The predictor Hsize is in the model and we want to figure out which predictor should be considered for the second predictor in the model. From the pairwise scatterplot and the correlation matrix suggest tax or attrac. We may fit models with all possible multiple models of two predictors with Hsize already in the model. This can be done easily in S+:

```
> add1(fit1, .~. +tax+Lsize+Lsize.sq+attrac+sty1+sty2)
Single term additions
Model:
price ~ Hsize
    Df Sum of Sq RSS Cp
    <none> 56358.65 64409.88
        tax 1 8654.25 47704.39 59781.25
        Lsize 1 9224.91 47133.74 59210.59
Lsize.sq 1 8156.81 48201.84 60278.69
    attrac 1 18351.16 38007.49 50084.34
        sty1 1 20842.36 35516.29 47593.14
        sty2 1 32570.78 23787.87 35864.72
```

We see that the style variable (sty1 and sty2) has the largest sums of squares (and the lowest Cp ) and thus these predictors should be considered in the model.

```
> fit2_lm(price~Hsize+sty1+sty2)
> summary(fit2)
Call: lm(formula = price ~ Hsize + sty1 + sty2)
Residuals:
    Min 1Q Median 3Q Max
-42.12 -14.61 -0.7273 14.55 87.48
Coefficients:
\begin{tabular}{rrcrr} 
& Value & Std. Error & t value & Pr \((>|t|)\) \\
(Intercept) & 219.9120 & 34.2463 & 6.4215 & 0.0000 \\
Hsize & 0.0290 & 0.0112 & 2.5929 & 0.0154 \\
sty1 & -31.8181 & 12.9440 & -2.4581 & 0.0209 \\
sty2 & 62.1801 & 13.3051 & 4.6734 & 0.0001
\end{tabular}
Residual standard error: 27.25 on 26 degrees of freedom
Multiple R-Squared: 0.7916
F-statistic: 32.93 on 3 and 26 degrees of freedom, the p-value is 5.24e-009
Correlation of Coefficients:
            (Intercept) Hsize styl
Hsize -0.9596
    sty1 -0.4754 0.2773
    sty2 0.0243 -0.2375 0.4730
```

For the hypothesis testing for no style effect, we do the test for both coefficients of sty1 and sty2.

```
> by(price,style,mean)
INDICES:E
[1] 264
------------------------------------------------------------------------------------
INDICES:M
[1] 375.5
```

INDICES:S
[1] 305.125

The model syntax

$$
\text { response~predictor } 1+\text { predictor } 2
$$

will fit a multiple regression with the two main effects only and

```
response~predictor1 + predictor 2+predictor1:predictor 2
```

or
response~predictor $1 *$ predictor 2
will fit the model with two main effects and the interaction between the two predictors.
Note that for the qualitative variable with three levels, we may assign three indicator variables (one for each level) and drop the intercept in the regression model. This coding of indicator also has widely used in application. The model statement with -1 at the end will drop the intercept in the model

```
> lm(y~x1+x2+...-1)
```

More will come......

## REGRESSION (con't)

## CODING OF FACTORS

Last time we have discussed how to create dummy variables for the qualitative predictors in a regression model. We extend the discussion to the use of a convenient $\mathrm{S}+$ function to create our own coding of factors. Let's consider the style variable in the realestate data.

```
> levels(style)
[1] "E" "M" "S"
```

We generate a matrix for the two dummy variables.

```
> my.cotr_matrix(c(1,0,0,0,1,0),ncol=2)
> my.cotr
    [,1] [,2]
[1,] 1 0
[2,] 0 1
[3,] 0 0
```

Now, use the $C$ function in the model statement of the $l m$ function. Note that $C$ stands for "contrasts", a linear combination of the dummy variables.

```
> summary(lm(price~C(style,my.cotr)))
Call: lm(formula = price ~ C(style, my.cotr))
Residuals:
    Min 1Q Median 3Q Max
    -48.5 -13.87 -4.812 13.75 98.5
Coefficients:
\begin{tabular}{rrccr} 
& Value & Std. Error & t value & Pr \((>|t|)\) \\
(Intercept) & 305.1250 & 10.6052 & 28.7714 & 0.0000 \\
C(style, my.cotr) & -41.1250 & 13.6912 & -3.0038 & 0.0057 \\
C(style, my.cotr)2 & 70.3750 & 14.2283 & 4.9461 & 0.0000
\end{tabular}
```

```
Residual standard error: 30 on 27 degrees of freedom
Multiple R-Squared: 0.7378
F-statistic: 37.98 on 2 and 27 degrees of freedom, the p-value is 1.42e-008
Correlation of Coefficients:
    (Intercept) C(style, my.cotr)1
C(style, my.cotr)1 -0.7746
C(style, my.cotr)2 -0.7454 0.5774
```

S+ provide four different built-in contrast functions; Helmert (default), Orthogonal polynomial, Sum, and Treatment. To see the matrix form for these function, for example, for a factor with three levels

```
> contr.helmert(3)
    [,1] [,2]
        -1 -1
        1 -1
3 0
> contr.treatment(3)
    2 3
10}
2 1 0
3 0 1
```

If you want to use one of the built-in contrasts, use the name of the contrast in the second argument of the C function. For example
lm(price~C(style,treatment))
will use the treatment contrast for the variable style. Note that the default contrast is the Helmert. So if you call
lm(price~style)
it will return the result with the Helmert contrast.
Another possibility is the use of $I$ (indicator) function. For example,

```
> lm(price~I(style=="E")+I(style=="M"),data=realestate)
```

The I function is very useful to assign indicator variables for a quantitative predictor. For example, if you are looking at the effect of "high" (attrac>75) attractiveness index versus "lower" (attrac<=75) instead of the effect of the attractiveness on a continuous scale,
> $\operatorname{lm}($ price~I (attrac>75), data=realestate).

## Model Selection: Stepwise Regression

Model selection procedure via Stepwise regression can be easily done using the user interface. We will discuss the procedure in details during the class and will not be illustrated in this note.

In the procedure we need to specify the full model (upper). We look at the correlation matrix to guess which interaction terms we need to consider for the full model.

|  | tax | Hsize | Lsize | Lsize.sq | attrac | sty1 | sty2 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| tax | 1.0000000 | 0.2812810 | 0.73968353 | 0.72108667 | 0.02879220 | -0.37758018 | 0.4872225 |
| Hsize | 0.2812810 | 1.0000000 | -0.28982630 | -0.26804966 | -0.12844139 | -0.45526549 | 0.4355324 |
| Lsize | 0.7396835 | -0.2898263 | 1.00000000 | 0.98477889 | -0.01889162 | -0.07395935 | 0.3030090 |
| Lsize.sq | 0.7210867 | -0.2680497 | 0.98477889 | 1.00000000 | -0.06571432 | -0.07975938 | 0.3186872 |
| attrac | 0.0287922 | -0.1284414 | -0.01889162 | -0.06571432 | 1.00000000 | -0.13282487 | 0.3093021 |

```
sty1 -0.3775802 -0.4552655 -0.07395935 -0.07975938-0.13282487 1.00000000-0.5773503
sty2 0.4872225 0.4355324 0.30300898 0.31868722 0.30930212 -0.57735027 1.0000000
```

The highlighted correlations seem to be high and important. We use all the main effects and the five interactions (we only considered two way interactions) for the upper model. Be sure to save the output object. For this example, the object was saved as step.real.

The resulted model from the stepwise procedure is

```
> summary(step.real)
Call: lm(formula = price ~ Hsize + attrac + sty1 + sty2 + Hsize:sty2, da
ta =
    realestate, na.action = na.exclude)
Residuals:
            Min 1Q Median 3Q Max
    -36.67-13.77 3.668 11.33 48.82
Coefficients:
\begin{tabular}{rrcrr} 
& Value & Std. Error & t value & Pr \((>|t|)\) \\
(Intercept) & 140.5705 & 52.0276 & 2.7018 & 0.0125 \\
Hsize & 0.0272 & 0.0102 & 2.6562 & 0.0138 \\
attrac & 1.2488 & 0.4854 & 2.5728 & 0.0167 \\
sty1 & -34.0227 & 10.4913 & -3.2429 & 0.0035 \\
sty2 & -180.8893 & 87.0854 & -2.0771 & 0.0487 \\
Hsize:sty2 & 0.0730 & 0.0273 & 2.6740 & 0.0133
\end{tabular}
Residual standard error: 21.94 on 24 degrees of freedom
Multiple R-Squared: 0.8753
F-statistic: 33.69 on 5 and 24 degrees of freedom, the p-value is 4.266e
-010
Correlation of Coefficients:
            (Intercept) Hsize attrac sty1 sty2
        Hsize -0.7882
        attrac -0.8254 0.3328
            sty1 -0.3074 0.2929 0.0443
            sty2 -0.2706 0.3391 0.0972 0.1661
Hsize:sty2 0.3119 -0.3813 -0.1449 -0.1106 -0.9913
```

You need to make interpretations of the parameter estimates. I will leave it to you. For the summary of the ANOVA is

```
> summary(aov(step.real))
            Df Sum of Sq Mean Sq F Value Pr(F)
        Hsize 1 36282.82 36282.82 75.37984 0.00000001
        attrac 1 18351.16 18351.16 38.12569 0.00000222
            sty1 1 13881.09 13881.09 28.83884 0.00001633
            sty2 1 9132.76 9132.76 18.97388 0.00021368
Hsize:sty2 1 3441.64 3441.64 7.15023 0.01327372
    Residuals 24 11552.00 481.33
```


## Estimating Mean Response

To estimate the mean response with the final model

```
> prd1_predict.lm(step.real,data.frame(Hsize=2000,attrac=70,sty1=1,sty2=0),
        se.fit=T,ci.fit=T,pi.fit=T)
> prdl
$fit:
    1
248.2893
```

```
$se.fit:
    8.851564
$residual.scale:
[1] 21.93931
$df:
[1] 24
$ci.fit:
    lower upper
1 230.0205 266.558
attr(, "conf.level"):
[1] 0.95
$pi.fit:
    lower upper
1 199.4623 297.1162
attr(, "conf.level"):
[1] 0.95
```

It is important to note that the option ci.fit $=T$ is used to obtain the interval estimation of the mean response at the values of predictors occurred in the data and pi.fit $=T$ will give us the prediction interval of new observation. The prediction interval is always wider than the confidence interval because the variation in prediction has an extra source of variation due to fact that the response at the new point will not equal to its expectation. For more detailed discussion see your note for MATH 532 or Chapter 2 of the text by Neter et.al. Both intervals are pointwise and based on $t$ distribution.

## Graphical Summary

For the graphical summary of the final model

```
> par(mfrow=c (2,3))
> plot(step.real)
```




Fitted Values Residuals



## Simultaneous Confidence Band: Working-Hotelling

For simultaneous 1- $\alpha$ confidence intervals for entire responses in the data, we use the Working-Hetelling confidence band based on F distribution (see p234, Neter et.al.).

The code below can be used to create a simultaneous confidence interval for the mean response.

```
"confint.lm"_function(object,alpha=.05,plot.it=T,...)
    {
    f_predict(object,se.fit=T)
    p_length(coef(object))
    fit_f$fit
    adjust_(p*qf(1-alpha,p,length(fit)-p))^0.5*f$se.fit
    lower \overline{fit-adjust}
    upper_fit+adjust
    if(plot.it){
        y_fit+resid(object)
        plot(fit,y)
        abline(0,1,lty=2)
        ord order(fit)
        lines(fit[ord],lower[ord])
        lines(fit[ord],upper[ord])
        invisible(list(lower=lower,upper=upper))
        }
    else list(lower=lower,upper=upper)
}
```

We use the function confint.lm to plot the simultaneous confidence intervals for the mean response from the simple regression model relating the price with Hsize.

```
> fit.Hsize_lm(price~Hsize)
> confint.lm(fit.Hsize)
```



## Identifying Outliers in predictors

The hat matrix, $X\left(X^{\prime} X\right)^{-1} X^{\prime}$, has been used to identify the outliers. The elements of the hat matrix, leverages, have the mean of $p / n$ where $p$ is the number of the parameters in the model and $n$ is the sample size. The leverages larger than $2 p / n$ are considered as an evidence of outliers. Bonferroni test may be used for formal test for outliers in response (see Neter et.al. p374), but most of the cases they can be well identified via residual plot.

We can identify the outliers in predictors via leverage as follows;

```
> rule_2*length(coef(step.real))/length(fitted(step.real))
> rule
[1] 0.4
> influ.real_lm.influence(step.real)
> cbind(realestate,lev=influ.real$hat)[influ.real$hat>rule,]
    property tax Hsize Lsize Lsize.sq attrac style price lev
5 [lllllllllll
```

If we exam the fifth property, we can see that the property has the largest Hsize and the lowest attractiveness.

We may want fit the model without the outlier.

```
> step.new <- lm(price ~ Hsize + attrac + sty1 + sty2 + Hsize:sty2, data =
    realestate[-5, ], na.action = na.exclude)
> summary(step.new)
Call: lm(formula = price ~ Hsize + attrac + sty1 + sty2 + Hsize:sty2, data =
```

```
    realestate[-5, ], na.action = na.exclude)
Residuals:
    Min 1Q Median 3Q Max
    -36.53-12.56 1.683 12.18 47.57
Coefficients:
\begin{tabular}{rrcrr} 
& Value & Std. Error & t value & \(\operatorname{Pr}(>|t|)\) \\
(Intercept) & 133.8143 & 55.2885 & 2.4203 & 0.0238 \\
Hsize & 0.0256 & 0.0110 & 2.3213 & 0.0295 \\
attrac & 1.3903 & 0.5962 & 2.3318 & 0.0288 \\
sty1 & -32.9926 & 10.9486 & -3.0134 & 0.0062 \\
sty2 & -184.1886 & 88.9544 & -2.0706 & 0.0498 \\
Hsize:sty2 & 0.0744 & 0.0280 & 2.6595 & 0.0140
\end{tabular}
Residual standard error: 22.32 on 23 degrees of freedom
Multiple R-Squared: 0.8762
F-statistic: 32.54 on 5 and 23 degrees of freedom, the p-value is 1.056e-009
Correlation of Coefficients:
            (Intercept) Hsize attrac sty1 sty2
    Hsize -0.6161
    attrac -0.8162 0.0739
        sty1 -0.3510 0.1956 0.1602
        sty2 -0.2329 0.3477 0.0312 0.1419
Hsize:sty2 0.2628 -0.3962 -0.0534 -0.0810 -0.9909
```

The Cock's distance provided in the graph above can be used to identify influential observations.

## Correlated error terms

Durbin-Watson statistic (DW) can be employed to test for first-order correlation (autocorrelation) in error terms. The test is useful when the data is observed over a systematic manner, like time or space. S+ provide the function, durbinWatson $(x)$. The argument $x$ can be either data vector or a object from fitting $l m$. The statistic is bounded between 0 and 4 , and for independent residuals we expect the value around 2 . If the value is close to 0 , it indicates positive correlation in error terms and if close to 4 , it means possible negative correlation. Neter et.al provides the critical values of the statistic (see Table B.7).

Let's check the DW statistics for the residuals from the final model of realestate data. Note that since the data was not collected over time or space, we expect the value close to 2 .

```
> durbinWatson(step.real)
Durbin-Watson Statistic: 1.960674
```

It is interesting to calculate the DW statistic for our Ozone data, since the data is collected over time. Note the variable volume is a column vector of ozone volume stacked over time.

```
> durbinWatson(volume[!is.na(volume)])
Durbin-Watson Statistic: 0.1490061
Number of observations: 1455
```

As we expected the DW value is very close to 0 , which indicates strong positive correlation in the raw volume data.

## Multicollinearity: Variance Inflation Factor (VIF)

Variance Inflation Factor has been widely used to measure the presence of multicollinearity in the model. Muticollinearity and its effect have been discussed in MATH 532 class. We will briefly discuss the concept of the VIF in class.

Following code will calculate the VIF.

```
        vif_function(y,x) {
            n=length(y);p=ncol (x)
            x.std_matrix(nrow=n,ncol=p)
            y.std_(y-mean(y))/(stdev(y)*sqrt(n-1))
            for (i}\mathrm{ in 1:p){
            x.std[,i]_(x[,i]-mean(x[,i]))/(stdev(x[,i])*sqrt(n-1))
            }
            VIF_ginverse(crossprod(x.std))
            varīf_matrix(nrow=p,ncol=1)
            for (i}\mathrm{ in 1:p){
            varif[i,]_VIF[i,i]
        }
varif
}
>attach(realestate)
> y_price
> x_data.frame(Hsize,attrac,sty1,sty2,Hsize*sty2)
> vif(y,x)
            [,1]
[1,] 1.723070
[2,] 1.248420
[3,] 1.646438
[4,] 105.039685
[5,] 108.206302
```

The VIF values considerably larger than 1 indicate muticollinearity problems.

## ANALYSIS OF VARIANCE

## Looking at the data: Kidney data revisited

Trellis boxplot conditioning on duration and on wtgain, respectively.


Other useful plots by plot.design and interaction.plot.
> plot.design(kidney[,1:3])


Main factor effects are evident.

```
    > interaction.plot(wtgain,duration,days,data=kidney)
```



Interaction effect does not seem to significant.

Before applying the aov function, be sure that the data types of two factors, duration and wtgain, are "factor". If they are recorded as "factor", use as function or Data $\rightarrow$ Change Data Type on the menu bar.

## One factor fixed effect ANOVA

```
Using aov function
> duration.anova_aov(days~duration,data=kidney)
> summary(duration.anova)
    Df Sum of Sq Mean Sq F Value Pr(F)
duration 1 209.067 209.0667 4.981322 0.02950016
Residuals 58 2434.267 41.9701
> dummy.coef(duration.anova)
$"(Intercept)":
    (Intercept)
        6.333333
$duration:
    1.866667 -1.866667
> contr.helmert(2)
    [,1]
1 -1
2 1
> duration.lm_lm(days~duration,data=kidney)
> summary(duration.lm)
Call: lm(formula = days ~ duration, data = kidney)
Residuals:
    Min 1Q Median 3Q Max
    -8.2 -4.267-1.467 2.533 21.8
Coefficients:
            Value Std. Error t value Pr (>|t|)
(Intercept) 6.3333 0.8364 7.5725 0.0000
    duration -1.8667 0.8364 -2.2319 0.0295
Residual standard error: 6.478 on 58 degrees of freedom
Multiple R-Squared: 0.07909
F-statistic: 4.981 on 1 and 58 degrees of freedom, the p-value is 0.0295
Correlation of Coefficients:
                (Intercept)
duration 0
> model.tables(duration.anova)
Tables of effects
    duration
        1 rra
> model.tables(duration.anova,"means")
```

```
Tables of means
Grand mean
    6.3333
    duration
            1 2
    8.2000 4.4667
Using my cotrast
> my.cotr.l2 matrix(c(1,0),ncol=1)
> my.cotr.l2
            [,1]
[1,] 1
[2,] 0
> duration.anova.new_aov(days~C(duration,my.cotr.l2),data=kidney)
> summary(duration.anova.new)
                            Df Sum of Sq Mean Sq F Value Pr(F)
C(duration, my.cotr.l2) 1 209.067 209.0667 4.981322 0.02950016
                Residuals 58 2434.267 41.9701
> dummy.coef(duration.anova.new)
$"(Intercept)":
    (Intercept)
                4.466667
$"C(duration, my.cotr.l2)":
            12
    3.733333 0
> wtgain.anova_aov(days~wtgain,data=kidney)
> summary(wtgaín.anova)
                    Df Sum of Sq Mean Sq F Value Pr(F)
        wtgain 2 760.433 380.2167 11.51009 0.00006327712
Residuals 57 1882.900 33.0333
> summary(wtgain.anova,split=list(wtgain=list(L=1,Q=2)))
                    Df Sum of Sq Mean Sq F Value Pr(F)
            wtgain 2 760.433 380.2167 11.51009 0.00006328
    wtgain: L 1 93.025 93.0250 2.81609 0.09879855
    wtgain: Q 1 667.408 667.4083 20.20409 0.00003460
    Residuals 57 1882.900 33.0333
```


## Two-factor fixed effects ANOVA

```
> kidney.anova_aov(days~duration*wtgain,data=kidney)
> summary(kidney.anova)
    Df Sum of Sq Mean Sq F Value Pr(F)
    duration 1 209.067 209.0667 7.21472 0.0095871
        wtgain 2 760.433 380.2167 13.12097 0.0000227
duration:wtgain 2 109.033 54.5167 1.88133 0.1622404
    Residuals 54 1564.800 28.9778
    > model.tables(kidney.anova,"means")
```

```
            Tables of means
            Grand mean
            6.3333
            duration
            1}r(2
            wtgain
            1 2 3
            2.45 5.50 11.05
            duration:wtgain
            Dim 1 : duration
            Dim 2 : wtgain
            1 2 3
            1 2.7 7.3 14.6
                    2 2.2 3.7 7.5
> par(mfrow=c (2,3))
> plot(kidney.anova)
> par(mfrow=c(1,1))
```



Fitted Values Residuals




The residual plot shows a strong evidence of non-constant variance. As the fitted values increase the residuals increase. From the QQ plot we also suspect a skewness of the error distribution. This recommends a proper transformation of the response.

## Transformation

A variance stabilizing transformation also corrects a non-normality in the error distribution. To suggest a appropriate transformation of the response we look at the relation between the treatment mean and the variance. Suggested transformations are

| Relation | Transformation |
| :--- | :--- |
| $\sigma_{i}^{2}=k \mu_{i}$ | $Y^{\prime}=\sqrt{Y}$ |
| $\sigma_{i}^{2}=k \mu_{i}^{2}$ | $Y^{\prime}=\log (Y)$ |
| $\sigma_{i}=k \mu_{i}^{2}$ | $Y^{\prime}=1 / Y$ |
| $\sigma_{i}^{2}=\pi_{i}\left(1-\pi_{i}\right) / n_{i}, \pi_{i}=p r$ (ithleve) | $Y^{\prime}=\arcsin (\sqrt{Y})$ |

Let's check which relation is most suitable for our kidney data.

```
> std.kidney_tapply(days,list(duration,wtgain),stdev)
> std.kidney
lrrrr
2 2.299758 2.945807 4.249183
> mean.kidney_tapply(days,list(duration,wtgain),mean)
> mean.kidney
    1 2 3
1 2.7 7.3 14.6
2 2.2 3.7 7.5
> sd.to.m_std.kidney/mean.kidney
> sd.to.m
    1 2 3
1 1.033651 0.8616718 0.6657904
2 1.045345 0.7961640 0.5665577
> sdsq.to.m_std.kidney^2/mean.kidney
> sdsq.to.m
lrrr
2 2.404040 2.345345 2.407407
> sd.to.msq_std.kidney/mean.kidney^2
> sd.to.msq
1
1 0.3828338 0.1180372 0.04560208
2 0.4751567 0.2151795 0.07554103
```

The ration $\sigma_{i} / \mu_{i}$ is the most stable, and this suggests a log transformation. Note that the response, days, is a count with some zero counts. The square root transformation also looks OK and thus we try the square root transformation below.
For more details, we may also consider a power transformation of the form (Box-Cox transformation):

$$
Y^{\prime}=Y^{\lambda}
$$

To find the power, $\lambda$, we regress $\log \sigma_{i}$ on $\log \mu_{i}$, that is we fit

$$
E\left(\log \sigma_{i}\right)=\hat{\beta}_{0}+\hat{\beta}_{1} \log \mu_{i}
$$

We estimate $\lambda$ by $\hat{\lambda}=1-\hat{\beta}_{1}$. The basic concept will be discussed in class.

```
> std.kidney_as(std.kidney,"vector")
> mean.kidne\overline{y_as(mean.kidney,"vector")}
> std.kidney
[1] 2.790858 2.299758 6.290204 2.945807 9.720540 4.249183
> plot(log(mean.kidney),log(std.kidney))
> log.fit_lsfit(log(mean.kidney),log(std.kidney))
> par(mfrow=c(1,1))
> plot(log(mean.kidney),log(std.kidney))
> abline(log.fit)
> log.fit$coef
    Intercept X
    0.2176716 0.7359919
```

From above we estimate $\hat{\lambda}=.264$. The value is about in the middle of 0 and 0.5 and this suggests that we may use either square root or log transformation. Note the $\lambda=0$ means $\log$ transformation by definition. For the same reason mentioned above, we take a square root transformation of the response, days. You may also consider $Y^{\prime}=\log (Y+1)$.

```
> sqrt.kidney.anova_aov(sqrt(days) ~duration*wtgain)
> summary(sqrt.kidney.anova)
    Df Sum of Sq Mean Sq F Value Pr(F)
    duration 1 5 5.95727 5.95727 5.48996 0.0228395
    wtgain 2 35.12196 17.56098 16.18343 0.0000031
duration:wtgain 2 2.02990 1.01495 0.93533 0.3987204
    Residuals 54 58.59654 1.08512
```



The interaction effect is not significant and thus we may fit the model without the interaction. Next time we will discuss Multiple comparison procedure and random and mix effect model.

## Multiple Comparisons: all pairwise comparison

```
> multicomp(sqrt.fit,focus="duration",plot=T)
95 % non-simultaneous confidence intervals for specified
linear combinations, by the Fisher LSD method
critical point: 2.0049
response variable: sqrt(days)
intervals excluding 0 are flagged by '****'
#-2 Estimate Std.Error Lower Bound Upper Bound
```

1-2

$\begin{array}{lllllllllllll}0.0 & 0.1 & 0.2 & 0.3 & 0.4 & 0.5 & 0.6 & 0.7 & 0.8 & 0.9 & 1.0 & 1.1 & 1.2\end{array}$ individual 95 \% confidence limits, LSD method response variable: sqrt(days)

```
> multicomp(sqrt.fit,focus="wtgain",plot=T)
95 % simultaneous confidence intervals for specified
linear combinations, by the Tukey method
critical point: 2.41
response variable: sqrt(days)
intervals excluding 0 are flagged by '****'
    Estimate Std.Error Lower Bound Upper Bound
\begin{tabular}{llllll}
\(1-2\) & -0.780 & 0.314 & -1.54 & -0.0228 & \(* * * *\) \\
\(1-3\) & -1.780 & 0.314 & -2.53 & -1.0200 & \(* * *\) \\
\(2-3\) & -0.997 & 0.314 & -1.75 & -0.2400 & ****
\end{tabular}
```


> multicomp(sqrt.fit,focus="duration", adjust=list(wtgain=seq(3)), plot=T)
95 \% simultaneous confidence intervals for specified
linear combinations, by the Tukey method
critical point: 2.41
response variable: sqrt(days)

```
intervals excluding O are flagged by '****'
\begin{tabular}{lrrrr} 
& Estimate & Std.Error & Lower Bound Upper Bound \\
1.adj1-2.adj1 & 0.128 & 0.444 & -0.9430 & 1.20 \\
1.adj2-2.adj2 & 0.731 & 0.444 & -0.3400 & 1.80 \\
1.adj3-2.adj3 & 1.000 & 0.444 & -0.0712 & 2.07
\end{tabular}
```

1.adj1-2.adj1
1.adj2-2.adj2
1.adj3-2.adj3


```
> multicomp(sqrt.fit,focus="wtgain",adjust=list(duration=seq(2)),plot=T)
95 % simultaneous confidence intervals for specified
linear combinations, by the Tukey method
critical point: 2.6509
response variable: sqrt(days)
intervals excluding 0 are flagged by '****'
\begin{tabular}{lrrrrr} 
& Estimate & Std.Error & Lower & Bound Upper Bound & \\
1.adj1-2.adj1 & -1.080 & 0.444 & -2.26 & 0.0964 & \\
1.adj1-3.adj1 & -2.210 & 0.444 & -3.39 & -1.0300 & \(* * * *\) \\
2.adj1-3.adj1 & -1.130 & 0.444 & -2.31 & 0.0464 & \\
1.adj2-2.adj2 & -0.479 & 0.444 & -1.66 & 0.6990 & \\
1.adj2-3.adj2 & -1.340 & 0.444 & -2.52 & -0.1640 & \(* * * *\) \\
2.adj2-3.adj2 & -0.863 & 0.444 & -2.04 & 0.3150
\end{tabular}
```

```
1.adj1-2.adj1
1.adj1-3.adj1
2.adj1-3.adj1
1.adj2-2.adj2
1.adj2-3.adj2
2.adj2-3.adj2
```



S+ uses the Tukey's pairwise comparison as default. If you want to specify other methods (like Scheffe, Bonferroni, etc) use the option method="scheffe" for Scheffe method and method="bon" for Bonferroni method, etc.

```
> multicomp(sqrt.fit,focus="wtgain",method="scheffe",plot=T)
```


## Inference for Linear Combinations of factor levels

We might want to construct a confidence interval for a linear combination of factor levels. Here, we will consider the interval for wtgain2-(wtgain1+wtgain 3 ) $/ 2$. We have seen that the interaction is not significant and thus we fit the model with the two main effects only. Note that with the full model the linear combination is not estimable.

```
> main.fit_aov(sqrt(days)~duration+wtgain)
> summary(main.fit)
    Df Sum of Sq Mean Sq F Value Pr(F)
    duration 1 5.75965 5.75965 5.83347 0.01901321
    wtgain 2 31.73837 15.86919 16.07258 0.00000305
Residuals 56 55.29134 0.98735
> lmat_matrix(c(0,0,0,-.5,1,-.5),ncol=1,dimnames=list(NULL,"wt2-(wt1+wt3)/2"))
> lmat
        wt2-(wt1+wt3)/2
[1,] 0.0
[2,] 0.0
[3,] 0.0
[4,] -0.5
[5,] 1.0
[6,] -0.5
> multicomp(main.fit,lmat=lmat,method="bon")
95 % non-simultaneous confidence intervals for specified
linear combinations, by the Fisher LSD method
critical point: 2.0032
response variable: sqrt(days)
intervals excluding 0 are flagged by '****'
    Estimate Std.Error Lower Bound Upper Bound
wt2-(wt1+wt3)/2 -0.109 0.272 0.437
```


## One case per treatment (no interaction model)

```
> premium_c(140,100,210,180,220,200)
> city_c("Small","Small","Med","Med","Large", "Large")
> regiōn_c("East","West","East","West","East","West")
> insur_data.frame(premium,city,region)
> insur
    premium city region
1 140 Small East
2 100 Small West
3 210 Med East
4 180 Med West
5 220 Large East
6 200 Large West
> attach(insur)
> insur.anova_aov(premium~city+region)
> summary(insur.anova)
                Df Sum of Sq Mean Sq F Value Pr(F)
        city 2 9300 4650 93 0.01063830
    region 1 1350 1350 27 0.03509872
Residuals 2 100 50
> model.tables(insur.anova,"means")
Tables of means
Grand mean
```

```
1 7 5
city
Large Med Small
210 195 120
region
East West
190 160
```

Test for Interaction effect

```
> interaction.plot(city,region,premium,lwd=2)
```



Tukey's 1df Test for no-interaction

## Random and Mixed effects Models

## Single-factor Random effect model

Model: $\quad Y_{i j}=\mu+\tau_{i}+\varepsilon_{i j}, i=1, \ldots, r, j=1, \ldots, n$
$\mu$ is a constant, $\tau_{i}$ are iid $N\left(0, \sigma_{\mu}^{2}\right), \varepsilon_{i j}$ are iid $N\left(0, \sigma^{2}\right), \tau_{i}$ and $\varepsilon_{i j}$ are independent.
As an example, we adopt the Apex Enterprises Example in Neter, et.al., chapter 24 on the evaluating ratings of potential employees by its personnel officers. Five personnel officers were randomly selected and four prospective employees were assigned at random to each officer.

```
> apex$officer_as.factor(apex$officer)
```

```
> apex$employee_as.factor(apex$employee)
> attach(apex)
> dotplot(officer~rating,pch=16,col=1)
```



## Test for the factor effect

For the random effect to test for the main effect we formulate the hypothesis in terms of the variance, $\sigma_{\mu}^{2}$;

$$
H_{0}: \sigma_{\mu}^{2}=0 \text { vs } H_{1}: \sigma_{\mu}^{2}>0
$$

For this single-factor random effect ANOVA model, testing procedure for the main effect is identical to that for the fixed effect. The different between the random and fixed effect appears in the expected mean square. The traditional ANOVA model is

| Source | df | Sum of Squares | Mean Squares | $\mathrm{E}(\mathrm{MS})$ |
| :---: | :---: | :---: | :---: | :---: |
| Treatment | $r-1$ | $S S T R$ | $M S T R$ | $\sigma^{2}+n \sigma_{\mu}^{2}$ |
| Residuals | $r(n-1)$ | $S S E$ | $M S E$ | $\sigma^{2}$ |
| Total | $r n-1$ | $S S T O$ |  |  |

We use the function raov, instead of aov, for the random effect model. From the ANOVA table below we have the estimated variances ( $\mathrm{E}(\mathrm{MS}$ ) in the table above). Note that to use the raov function the design must be balance. For unbalance design we may use varcomp function that will be discussed later in this section.

```
> random.fit_raov(rating~officer)
> summary(random.fit)
    Df Sum of Sq Mean Sq Est. Var.
    officer 4 1579.70 394.9250 80.41042
Residuals 15 1099.25 73.2833 73.28333
```

The calculated value of the test statistic is : $F^{*}=\frac{M S T R}{M S E}=\frac{394925}{73.2833}=5.39$. Under the null hypothesis this statistic follows an $\mathrm{F}(\mathrm{r}-1, \mathrm{n}(\mathrm{r}-1))$.

```
> qf(.95,4,15)
[1] 3.055568
```

Since $F^{*}$ is larger than the critical value we reject the null hypothesis and conclude that at 0.05 level of significance the mean ratings of the personnel officers are different. The p-value of the test is 0.0068 .

```
> 1-pf(5.39,4,15)
[1] 0.006797778
```


## Inference for $\mu$.

We may want to construct a confidence interval for the overall mean, $\mu$. The $95 \%$ CI is

```
Y.. }\pmt(.975r-1)*\frac{MSTF}{rn
> model.tables(random.fit,"means")
Tables of means
Grand mean
71.45
officer
    1 
75.00 70.50 54.75 79.75 77.25
```

For this example, the $95 \%$ CI for the overall mean is: $71.45 \pm 2.1324 .44)=(62,81)$.

CI for $\frac{\sigma_{\mu}^{2}}{\sigma_{\mu}^{2}+\sigma^{2}}$
For the random effect model the above ratio is in interest as it measures the proportion of the total variability of the response that is accounted for by the variability of the level means. The lower and upper bound of the CI based on F distribution is;

$$
L^{*}=\frac{L}{1+L} \text { and } U^{*}=\frac{U}{1+U}
$$

where

$$
L=\frac{1}{n}\left[\frac{M S T R}{M S E}(F(1-\alpha / 2 ; r-1, r(n-1)))^{-1}-1\right]
$$

and

$$
U=\frac{1}{n}\left[\frac{M S T R}{M S E}(F(\alpha / 2 ; r-1, r(n-1)))^{-1}-1\right]
$$

For the above example, $\operatorname{MSTR}=394.925$, $\mathrm{MSE}=73.2833, \mathrm{r}=5, \mathrm{n}=4, \mathrm{~F}(.025,4,15)=3.804, \mathrm{~F}(.975,4,15)=0.116$, then $\mathrm{L}=0.104$ and $\mathrm{U}=11.36$. The calculated $95 \% \mathrm{CI}$ is $(0.104 / 1.104,11.36 / 12.36)=(0.09,0.92)$.

You may want to construct CI's for $\sigma^{2}$ and $\sigma_{\mu}^{2}$. Both intervals base on chi-square distribution and I will leave it to you (see Chapter 24, Neter, et.al.).

Two-factor Model : Model II(both random) and Model III (mixed)
Model II (balanced design)
Model: $\quad Y_{i j k}=\mu_{. .}+\alpha_{i}+\beta_{j}+(\alpha \beta)_{i j}+\varepsilon_{i j k}, i=1, \ldots, a, j=1, \ldots, b, k=1, \ldots, n$
$\mu$ is a constant, $\alpha_{i}$ are iid $N\left(0, \sigma_{\alpha}^{2}\right), \beta_{j}$ are iid $N\left(0, \sigma_{\beta}^{2}\right),(\alpha \beta)_{i j}$ are iid $N\left(0, \sigma_{\alpha \beta}^{2}\right)$, $\varepsilon_{i j k}$ are iid $N\left(0, \sigma^{2}\right), \alpha_{i}, \beta_{j},(\alpha \beta)_{i j}$ and $\varepsilon_{i j}$ are pairwise independent.

## Model III (balanced design, factor $A$ fixed, factor $B$ random)

Model: $\quad Y_{i j k}=\mu_{. .}+\alpha_{i}+\beta_{j}+(\alpha \beta)_{i j}+\varepsilon_{i j k}, i=1, \ldots, a, j=1, \ldots, b, k=1, \ldots, n$
$\mu$ is a constant, $\alpha_{i}$ are constant with $\sum \alpha_{i}=0, \beta_{j}$ are iid $N\left(0, \sigma_{\beta}^{2}\right),(\alpha \beta)_{i j}$ are iid $N\left(0, \frac{a-1}{a} \sigma_{\alpha \beta}^{2}\right)$ with $\sum_{i}(\alpha \beta)_{i j}=0, \varepsilon_{i j k}$ are iid $N\left(0, \sigma^{2}\right), \alpha_{i}, \beta_{j},(\alpha \beta)_{i j}$ and $\varepsilon_{i j}$ are pairwise independent.

The expected mean squares and the test statistics are given in the following table.

| Source | df | MS | E(MS)( M II) | E(MS)( M III) | $\mathrm{F}^{*}$ (M II) | $\mathrm{F}^{*}$ (M III) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| A | a-1 | MSA | $\sigma^{2}+n b \sigma_{\alpha}^{2}+n \sigma_{\alpha \beta}^{2}$ | $\sigma^{2}+n b \frac{\sum \alpha_{i}^{2}}{a-1}+n \sigma_{\alpha \beta}^{2}$ | $\frac{M S A}{M S A 1}$ | $\frac{M S A}{M S A 1}$ |
| B | b-1 | MSB | $\sigma^{2}+n a \sigma_{\beta}^{2}+n \sigma_{\alpha \beta}^{2}$ | $\sigma^{2}+n a \sigma_{\beta}^{2}$ | $\frac{M S B}{M S A Z}$ | $\frac{M S B}{M S E}$ |
| AB | (a-1)(b-1) | MSAB | $\sigma^{2}+n \sigma_{\alpha \beta}^{2}$ | $\sigma^{2}+n \sigma_{\alpha \beta}^{2}$ | $\frac{M S A 1}{M S E}$ | $\frac{M S A 1}{M S E}$ |
| Residual Total | $\begin{gathered} \mathrm{ab}(\mathrm{n}-1) \\ \mathrm{abn}-1 \end{gathered}$ | MSE | $\sigma^{2}$ | $\sigma^{2}$ |  |  |

For the balanced Model II we can use raov function as before.

## Mixed effects

For mixed effects ANOVA we use varcomp function. The varcomp function is also used for unbalanced designs. Note that for the balanced mixed effects designs the estimated mean squares and corresponding degrees of freedom are identical to that of the fixed effects. However, the testing procedures vary as in the table above. Hence, for testing hypothesis for factor effects we can simply use aov function and recalculate the test statistics. For the mixed effects we also interested in the variance structures for further analyses. We use varcomp function for this purpose. We discuss the use of varcomp function using an unbalanced mixed effects example. Note that for the unbalanced design (either fixed, random, or mixed) the ANOVA modeling is difficult. We used the general linear test approach based on the maximum likelihood method. Example: (Unbalanced Mixed effect)

We used the data in Table 24.11 of Neter, et.al. The milkfat contents of a company's yogurt product are measured using two different measurement methods $(a=1)$ and randomly selected four laboratories $(b=4)$. This is unbalanced mixed effect model; the factor Method is fixed and the factor Laboratory is random.

```
> fat.data$method_as.factor(fat.data$method)
> fat.data$lab_as.factor(fat.data$lab)
> fat.data$method[fat.data$method==1]_"Goverment"
> fat.data$method[fat.data$method==2]_"Sheffield"
> dotplot(lab~fat|method,ylab="Laboratory",xlab="Fat",main="method1 vs
method2",pch=16,col=1,data=fat.data)
```



The following procedure is necessary to define which factor is random and which is fixed.

```
> is.random(fat.data$lab)_T
> is.random(fat.data$methōd)_F
> is.random(fat.data)
    method lab
        F T
> summary(varcomp(fat~method*lab,method="ml",data=fat.data))
Call:
varcomp(formula = fat ~ method * lab, data = fat.data, method = "ml")
Variance Estimates:
            Variance
    lab 0.05443933
method:lab 0.08570636
    Residuals 0.02325424
Method: ml
Approximate Covariance Matrix of Variance Estimates:
                                    lab method:lab Residuals (Intercept) method
            lab 0.00595752-0.00194176-0.00000400 0.00000255-0.00000171
    method:lab -0.00194176 0.00420470 -0.00001463-0.00000070-0.00000515
    Residuals -0.00000400 -0.00001463 0.00003545 -0.00000015 0.00000618
(Intercept) 0.00000255 -0.00000070 -0.00000015 0.00058123-0.00000445
            method -0.00000171 -0.00000515 0.00000618-0.00000445 0.01138762
Coefficients:
    (Intercept) method
                3.694149 -0.632899
Approximate Covariance Matrix of Coefficients:
                (Intercept) method
```

```
(Intercept) 0.0000135161 -0.0000001028
    method -0.0000001028 0.0002647853
```

Note that other possible methods in the estimation option of varcomp function are "reml", "minque0", and "winsor". Refer the text for the description of each method. From the output we can summary the results as

| Parameter | MLE | SE | $\mathrm{z}^{*}$ | p -value |
| :--- | :--- | :--- | :--- | :--- |
| $\mu$ | 3.694 | 0.024 | large | 0.00 |
| $\alpha_{1}$ | 0.633 | 0.107 | 5.916 | 0.00 |
| $\sigma_{\beta}^{2}$ | 0.054 | 0.077 | 0.701 | 0.483 |
| $\sigma_{\alpha \beta}^{2}$ | 0.086 | 0.065 | 1.32 | 0.187 |
| $\sigma^{2}$ | 0.023 | 0.006 | 3.83 | 0.00 |

From the table, we see that the method effect is significant and the interaction effect between the factors is not quite significant.

Now let's consider the subset of the fat.data to study the balanced mixed effects. We used the data with the count 1 and 2 so that each treatment has two observarions.

```
> summary(varcomp(fat~method*lab,method="ml",subset=(count<3), data=fat.data))
Call:
varcomp(formula = fat ~ method * lab, data = fat.data, method = "ml", subset =
(count < 3))
Variance Estimates:
            Variance
            lab 0.06845940
method:lab 0.06776157
    Residuals 0.01849374
Method: ml
Approximate Covariance Matrix of Variance Estimates:
                    lab method:lab Residuals (Intercept) method
            lab 0.006461886-0.001482569 0.000000000 0.000000000 0.000000000
method:lab -0.001482569 0.002986884 -0.000043493 0.000000000 0.000000000
    Residuals 0.000000000 -0.000043493 0.000086986 0.000000000 0.000000000
(Intercept) 0.000000000 0.000000000 0.000000000 0.000494539 0.000000000
            method 0.000000000 0.000000000 0.000000000 0.000000000 0.009626054
Coefficients:
    (Intercept) method
        3.740625 -0.618125
Approximate Covariance Matrix of Coefficients:
            (Intercept) method
(Intercept) 9.1459e-006 0.0000000000
        method 0.0000e+000 0.0001780217
```

Using the output we may make inferences on the variances.

## Analysis of Covariance (ANCOVA)

Covariance Model (Single factor) : $Y_{i j}=\mu+\tau_{i}+\gamma x_{i j}+\varepsilon_{i j}, i=1, \ldots, r, j=1, \ldots, n_{i}$,
where $\mu$ is a constant (overall mean), $\tau_{i}$ is a fixed treatment effect, $\gamma$ is a regression coefficient relating Y with x, $x_{i j}$ is a mean-adjusted continuous predictor variable (concomitant variable), and $\varepsilon_{i j}$ are iid $N\left(0, \sigma^{2}\right)$.

Example(Neter, et.al. Table 25.1): To study the effects of three types of promotions (treatments, $\mathrm{r}=3$ )) on sales (response) of crackers. The concomitant variable is sales from preceding period.

First to verify the model assumption of the equal regression coefficient, $\gamma$, over treatment, we need to plot Y versus X for each treatment level. Before further analysis it is convenient to make a groupedData data frame.

```
> cracker$period_cracker$period-mean(cracker$period)
> period.adj_cra\overline{cker$period-mean (cracker$period)}
> cracker_data.frame(cracker,period.adj)
> cracker.group_groupedData(sales~period.adj|treatment,data=cracker)
```

Now the object cracker.group is a groupedData object. The groupedData object can be summarized by using gsummary function.

```
> gsummary(cracker.group)
    sales period treatment count period.adj
3 27.2 25.4 
2 36.0 26.4 1.0
1 38.2 23.2 
```

To make a scatterplot by group (treatment) simply type

```
> plot(cracker.group)
```

From the plot we see that there is a clear linear relation between $Y$ and $x$ and we don't see any evidence of changing slopes over treatment. For a formal test of parallel slopes we fit a regression model with interactions and test for the zero interaction coefficients.


Before the model fitting we assign a contrast variable (dummy) for the treatment.

```
> my.cotr_matrix(c(1,0,-1,0,1,-1),ncol=2)
>my.cotr
    [,1] [,2]
[1,] 1 0
[2,] 0
[3,] -1 -1
```

```
> anova(lm(sales~C(treatment,my.cotr)*period.adj,data=cracker.group))
```

> anova(lm(sales~C(treatment,my.cotr)*period.adj,data=cracker.group))
Analysis of Variance Table
Analysis of Variance Table
Response: sales
Response: sales
Terms added sequentially (first to last)
Terms added sequentially (first to last)
Df Sum of Sq Mean Sq F Value Pr(F)
Df Sum of Sq Mean Sq F Value Pr(F)
C(treatment, my.cotr) 2 338.8000 169.4000 48.36801 0.0000153
C(treatment, my.cotr) 2 338.8000 169.4000 48.36801 0.0000153
period.adj 1 269.0287 269.0287 76.81453 0.0000106
period.adj 1 269.0287 269.0287 76.81453 0.0000106
C(treatment, my.cotr):period.adj }\begin{array}{rlrrrrrrl}{\mathrm{ Residuals }}\&{2}\&{7.0505}\&{3.5252}\&{1.00654.5208}\&{0.4031810}

```
C(treatment, my.cotr):period.adj }\begin{array}{rlrrrrrrl}{\mathrm{ Residuals }}&{2}&{7.0505}&{3.5252}&{1.00654.5208}&{0.4031810}
```

The p-value for the no interactions test is very high (.4), and this implies that the parallel slopes are evident.
Now ANCOVA can be done using regression approach. Indeed, the ANCOVA model is a special case of regression model.

```
> cracker.lm_lm(sales~C(treatment,my.cotr) +period.adj,data=cracker.group)
> summary(crācker.lm)
Call: lm(formula = sales ~ C(treatment, my.cotr) + period.adj, data =
cracker.group)
Residuals:
    Min 1Q Median 3Q Max
    -2.435 -1.274 -0.3363 1.671 2.487
```

```
Coefficients:
\begin{tabular}{rrcrr} 
& Value & Std. Error & t value Pr \((>|t|)\) \\
(Intercept) & 33.8000 & 0.4835 & 69.9079 & 0.0000 \\
C(treatment, my.cotr) & -6.9594 & 0.6850 & -10.1599 & 0.0000 \\
(treatment, my.cotr)2 & 0.9420 & 0.6987 & 1.3483 & 0.2047 \\
period.adj & 0.8986 & 0.1026 & 8.7592 & 0.0000
\end{tabular}
Residual standard error: 1.873 on 11 degrees of freedom
Multiple R-Squared: 0.9403
F-statistic: 57.78 on 3 and 11 degrees of freedom, the p-value is 5.082e-007
Correlation of Coefficients:
                            (Intercept) C(treatment, my.cotr)1 C(treatment, my.cotr)2
C(treatment, my.cotr)1 0.0000
C(treatment, my.cotr)2 0.0000 -0.4761
    period.adj 0.0000 -0.0599 -0.2056
> anova(cracker.lm)
Analysis of Variance Table
Response: sales
Terms added sequentially (first to last)
    Df Sum of Sq Mean Sq F Value Pr(F)
C(treatment, my.cotr) 2 338.8000 169.4000 48.31052 3.566360e-006
    period.adj 1 269.0287 269.0287 76.72324 2.731033e-006
        Residuals 11 38.5713 3.5065
```

The result will be discussed in class.
We may fit a reduced model without the treatment effect and do a generalized F-test (reduced vs. full) to test for the treatment effect.

## SIMPLE LOGISTIC REGRESSION

In many studies, the response variable may be a binary r.v. taking on the value 0 (failure) and 1 (success).
Example: In a longitudinal study of coronary heart disease as a function of age, gender, cholesterol level, etc. The response (Y) can be coded as 0 (no disease) and 1 (disease)

## Simple Regression?

$$
\begin{aligned}
& Y_{i}=\beta_{0}+\beta_{1} x_{i}+\varepsilon_{i} \\
& \text { Let } Y_{i}= \begin{cases}1 & \text { for"succes's } \\
0 & \text { for' }{ }^{\prime \prime} \text { failure }\end{cases}
\end{aligned}
$$

Assumption $\quad \varepsilon_{i} \sim N\left(0, \sigma^{2}\right) ? ? ?$

Note that for the binary response $\varepsilon_{i}$ can take only two values

$$
\begin{array}{ll}
\varepsilon_{i}=1-\beta_{0}-\beta_{1} x_{i} & \text { if } Y_{i}=1 \\
\varepsilon_{i}=-\beta_{0}-\beta_{1} x_{i} & \text { if } Y_{i}=0 .
\end{array}
$$

Therefore $\mathcal{E}_{i}$ can NOT be normally distributed!! The simple regression model can NOT be used for the binary response.

## Logistic Response Function

Let's denote $\pi_{i}$ to be the probability of success for the ith observation, that is $P\left(Y_{i}=1\right)=\pi_{i}$, and $P\left(Y_{i}=0\right)=1-\pi_{i}$. We want to relate $\pi_{i}$ to a linear combination of the independent variables, $x_{i}$. Note that generally for extremely large (or small) value of $x_{i}$ the probability $\pi_{i}$ is expected to be either 1 or 0 .

Example $: x_{i}=$ age $y_{i}=\left\{\begin{array}{l}1 \text { for'aliv"e } \\ 0 \text { for'death }\end{array}\right.$
For extremely large value of age, we expect the probability of survival to be 0 .
What about the relationship between $\pi_{i}$ and $x_{i}$ for intermediate value of $x_{i}$ ? Can we expect a linear relationship? Pretty close

General relation: S-shape configuration


These shapes are very common in application.
Logistic Response Function :

$$
\pi_{i}=\frac{\exp \left(\beta_{0}+\beta_{1} x_{i}\right)}{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)}
$$

formulates the S-shape relationship.

## Logistic Transformation

Logistic Regression Model:

$$
\log \left(\frac{\pi_{i}}{1-\pi_{i}}\right)=\beta_{0}+\beta_{1} x_{i}
$$

We use the logistic transformation $\log \left(\frac{\pi_{i}}{1-\pi_{i}}\right)$ as a response in simple regression.
Note that since $\pi_{i}$ is unknown, the response is unobservable. The parameters can be estimated via maximum likelihood method. We use glm (generalized linear model) function to fit the model with binomial family option.

The fitted response function is: $\hat{\pi}_{i}=\frac{\exp \left(b_{0}+b_{1} x_{i}\right)}{1+\exp \left(b_{0}+b_{1} x_{i}\right)}$.

Example (Neter, Table 14.1) We are interested in the effect of the experience on the ability to a complex programming task. For each of 25 individuals months of experience and the task result ( 1 for success, 0 for failure)


```
> fit.log_glm(task~exp,family=binomial,data=logist.data)
> summary(fit.log)
Call: glm(formula = task ~ exp, family = binomial, data = logist.data)
Deviance Residuals:
        Min 1Q Median 3Q Max
    -1.89916-0.7508921 -0.4140038 0.7992195 1.962354
Coefficients:
\begin{tabular}{rrrr} 
& Value & Std. Error & t value \\
(Intercept) & -3.0596954 & 1.2589852 & -2.430287 \\
\(\exp\) & 0.1614859 & 0.0649625 & 2.485833
\end{tabular}
(Dispersion Parameter for Binomial family taken to be 1 )
    Null Deviance: 34.29649 on 24 degrees of freedom
Residual Deviance: 25.42457 on 23 degrees of freedom
Number of Fisher Scoring Iterations: 4
```

```
Correlation of Coefficients:
    (Intercept)
exp -0.9214001
> 2*(1-pt(2.4858,23))
[1] 0.02062955
```

The p-value of 0.02 from a partial t-test testing the effect of the experience effect indicates that the effect is significant

We may do a chi-square test using the deviances (known as Person test) in the output. Again the null hypothesis is $H o: \beta_{1}=0$. The null deviance is the value of the test statistic under the null hypothesis, reduced model with intercept only, and the residual deviance is the value of the test statistic under the full model, with intercept and slope. The subtraction of the two statistics will follow a chi-square distribution with one degree of freedom. For this example

$$
\mathrm{G}^{2}=34.29649-25.42457=8.872
$$

The corresponding p -value of the test is 0.003 , which is much less than the p -value for the t -test. The chisquare test is preferred to the $t$-test. More example will be discuss later.

```
> 1-pchisq(8.872,1)
[1] 0.002895777
> par(mfrow=c (2,2))
> plot(fit.log)
```



Note that unlike usual regression models, for the binary response the residuals are not normally distributed and the usual residual analyses are not applicable. The diagnostic plots above are not quite informative for
the logistic regression. To detect outliers or/and influential observations we can use leverages as before.
Refer the example in the next section.
The fitted response function is $\hat{\pi}_{i}=\frac{\exp \left(-3.06+.1615 x_{i}\right)}{1+\exp \left(-3.06+.1615 x_{i}\right)}$.
We use the fitted response function to estimate the mean response at a given value of x . For example substituting 14 into x can obtain the estimated probability of successful performance for a person with 14 months experience. The estimated probability is 0.31 .

The estimated odd ratio $O R=\exp \left(b_{1}\right)=\exp (.1615)=1.175$. So, with each additional month of experience increases the odds of completing the task by $17.5 \%$.

## Multiple Logistic Regression

In this section we will discuss the logistic regression with two or more predictors.
Example (Christensen 1997, Example 4.1.1)
200 men are taken from the LA Heart Study to study the relations between the Coronary incident (CNT, 1 if an incident occurred, 0 otherwise) and six explanatory variables: age, Systolic blood pressure, Diastolic blood pressure, Cholesterol, Height, and Weight. The data can be downloaded from the class web (chapman.dat). We consider the logistic regression model:

```
    log}(\frac{\mp@subsup{\pi}{i}{}}{1-\mp@subsup{\pi}{i}{}})=\mp@subsup{\beta}{0}{}+\mp@subsup{\beta}{1}{}\operatorname{agq}+\mp@subsup{\beta}{2}{}\mp@subsup{S}{i}{}+\mp@subsup{\beta}{2}{}\mp@subsup{D}{i}{}+\mp@subsup{\beta}{3}{}C\mp@subsup{h}{i}{}+\mp@subsup{\beta}{4}{}\mp@subsup{H}{i}{}+\mp@subsup{\beta}{5}{}\mp@subsup{W}{i}{
> summary(chapman.logist)
Call: glm(formula = CNT ~ age + S + D + Ch + H + W, family = binomial, d
ata
    = chapman)
Deviance Residuals:
```



```
Coefficients:
            Value Std. Error t value
(Intercept) -4.517319021 7.479489249 -0.6039609
            age 0.045899976 0.023529058 1.9507783
            S 0.006855721 0.020194525 0.3394842
            D -0.006936751 0.038343820 -0.1809092
        Ch 0.006306448 0.003631292 1.7366953
                H -0.074001542 0.106189623 -0.6968811
                W 0.020141537 0.009868974 2.0408948
(Dispersion Parameter for Binomial family taken to be 1 )
    Null Deviance: 154.5547 on 199 degrees of freedom
Residual Deviance: 134.8515 on 193 degrees of freedom
Number of Fisher Scoring Iterations: 5
```

```
Correlation of Coefficients:
    (Intercept) age S
                            D D
                                Ch
                                H
age -0.2071983
    S 0.0130841 -0.2675552
    D -0.2094813 0.0126957 -0.7730439
    Ch -0.1406628 -0.1641129 0.0292113 -0.1133042
    H -0.9534236 0.1719066 -0.0194712 0.1426191 0.0203800
    W 0.2837116 -0.0023497 0.1522709 -0.3637363 0.1463836-0.4411074
```

Based on the t-value, age, cholesterol, and weight effects seem to exist. The multiple scatterplot below also supports the result.


We want to fit the model with the three variables only.

```
> chapman.logist.reduced_glm(CNT~age+Ch+W, family=binomial,data=chapman)
> summary(chapman.logist.reduced)
Call: glm(formula = CNT ~ age + Ch + W, family = binomial, data = chapma
n)
Deviance Residuals:
\begin{tabular}{rrrrr} 
Min & \(1 Q\) & Median & \(3 Q\) & Max \\
-1.104901 & -0.5541154 & -0.3776944 & -0.2510398 & 2.700912
\end{tabular}
Coefficients:
\begin{tabular}{rrrr} 
& Value & Std. Error & t value \\
(Intercept) & -9.255888319 & 2.070916857 & -4.469464 \\
age & 0.053003641 & 0.020821917 & 2.545570
\end{tabular}
```

```
        Ch 0.006517925 0.003587892 1.816645
        W 0.017538629 0.008270296 2.120677
(Dispersion Parameter for Binomial family taken to be 1 )
    Null Deviance: 154.5547 on 199 degrees of freedom
Residual Deviance: 135.5233 on 196 degrees of freedom
Number of Fisher Scoring Iterations: 5
Correlation of Coefficients:
    (Intercept) age Ch
age -0.3660495
    Ch -0.5167738 -0.2383809
    W -0.7669655 0.0100841 0.1319159
```

We may compare the model with the full model. For the test statistic, we use the difference between the residual deviances of the full model and the reduced model.

$$
\mathrm{G}^{2}=135.5233-134.8515=0.6718 \text { with the degrees of freedom of } 196-193=3
$$

The p-valued of the test is 0.88 and we conclude that the reduced model with three predictors only is an adequate substitute of for the full model. From the above output the variable Ch does not seem significant. We can repeat the above testing procedure for the Ch effect. A measure analogy to $\mathrm{R}^{2}$ can be obtained by

$$
R^{2}=\frac{\text { nulldeviance residuadlevianc }}{\text { nulldeviance }}
$$

For the above model with age, Ch , and $\mathrm{W}, \mathrm{R}^{2}=(154.55-135.52) / 154.55=0.12$. Only about $12 \%$ of variability can be explained by the model. This is not surprising for the binary data. Unless the probability $\pi_{i}$ is very close to 1 or 0 , the $\mathrm{R}^{2}$ will be much lower than you expected. The low $\mathrm{R}^{2}$ does not necessary mean a poor fit. So, the direct interpretation of the $R^{2}$ value should not be suggested. We can use the $R^{2}$ value for a tool of model comparisons.

Formal model selection procedure using AIC or Cp can be conveyed, but will not be discussed in this class. S+ does not provide the automatic search procedure, but SAS does via Proc Logistic.

Fitted response function: $\hat{\pi}_{i}=\frac{\exp \left(-9.26+.053 \text { age }_{i}+.0065 C h_{i}+.0175 W_{i}\right)}{1+\exp \left(-9.26+.053 \text { age }_{i}+.0065 C h_{i}+.0175 W_{i}\right)}$
For example, for 60 years old man with cholesterol reading of 300 and the weights 200 pounds, the estimated probability of a coronary incident is

$$
\hat{\pi}=\frac{\exp (-9.26+.053(60)+.0065(300)+.0175(200))}{1+\exp (-9.26+.053(60)+.0065(300)+.0175(200))}=0.35 .
$$

We can identify the outliers and/or influential observations using leverages as follows;

```
>rule_2*length(coef(chapman.logist.reduced))/length(fitted(chapman.logis
t.reduced))
> rule
[1] 0.04
```

```
> influ.chapman_lm.influence(chapman.logist.reduced)
> cbind(age,Ch,\overline{W},leverage=influ.chapman$hat)[influ.chapman$hat>rule,]
    age Ch W leverage
    18 40 302 225 0.04554945
    19 51 302 247 0.10435819
38 52 474 145 0.08053879
41 40 520 169 0.14885485
44 56 428 171 0.04979886
48 64 243 171 0.04341317
51 65 370 153 0.04235409
55 67 365 190 0.05636015
60 68 268 138 0.05473981
61 64 261 108 0.04480911
64 58 416 188 0.05418758
81 47 341 218 0.04645482
84 41 259 245 0.07883004
96 67 320 134 0.04994716
108 51 269 262 0.14683385
111 69 370 185 0.06171088
113 64 244 187 0.05093838
114 70 353 163 0.05816883
116 53 453 170 0.06694622
121 53 420 141 0.04030119
123 63 420 160 0.05607527
126 28 386 189 0.04183048
153 58 187 224 0.08980256
157 49273 245 0.09279471
193 60 317 206 0.04371181
>
```

Observations with high leverages are highlighted. We need to exam those observations closely. For example, the 41th observation (the highest leverage) has an extremely high cholesterol value, etc.

## BOOTSTRAPING, the basic

The bootstrap is a powerful computer-based tool for statistical inference in case standard approximations are not applicable. Suppose for example, we want to compare two groups by their medians. Unfortunately we do not have an explicit formula to calculate the standard errors of the median estimates (we do have it for means). For another example, for the inference about population means, the standard inferences rely on the large sample central limit theorem. Then, we may simply ask, "What if the sample size is very small with an unknown underline sampling distribution?" Theses questions can be answered by computer-based techniques, like bootstrap.

To illustrate the basic concept of the bootstrap, let's consider a simple example (I will do my best to avoid mathematical notations). Suppose we observed data with size eight: $x=(23,34,12,9,42,17,8,29)$. We are interested in the reciprocal of mean, $\theta=1 / \mu$. We can simply estimate it by $\hat{\theta}=1 / \bar{x}$, where $\bar{X}$ is the sample mean. Now, our question is how to calculate the standard error of the estimate. Intuitively thinking, if we have many estimates of the parameter, $\hat{\theta}_{1}, \hat{\theta}_{2}, \ldots, \hat{\theta}_{B}$, with B large enough positive integer, we could approximate it by the sample standard deviation of the B estimates; ie,

$$
\begin{equation*}
s e=\left[\sum_{i}^{B}\left(\hat{\theta}_{i}-\overline{\hat{\theta}}\right)^{2} /(B-1)\right]^{1 / 2}, \text { where } \overline{\hat{\theta}} \text { is the sample mean of the } \hat{\theta}_{i}^{\prime} s \tag{1}
\end{equation*}
$$

To have the B estimates we need B samples of size eight each. Since we don't have any other data source we generate each sample by randomly sampling eight times with replacement from the original data point and name it $x^{*}$. We do the sampling B times to generate $x^{* 1}, x^{* 2}, \ldots, x^{* B}$ (this is called bootstrap samples). From each of the B samples we estimate the parameter and using the B estimates we calculate the sample standard deviation in (1). The following bootstrap algorithm for estimating standard errors is adopted from An Introduction to the Bootstrap, by E. Efron and R. Tibshirani, Chapman \& Hall.

## Bootstrap standard error estimation

Consider a random sample $\boldsymbol{x}=\left(x_{1}, x_{2}, \ldots, x_{n}\right)$ from an unknown probability distribution. We are interested in a parameter $\theta$. We calculate an estimate $\hat{\boldsymbol{\theta}}$ from $\boldsymbol{x}$.

1. Select B independent bootstrap sample $x^{* 1}, x^{* 2}, \ldots, x^{* B}$ each consisting of $n$ data points randomly selected for the original data with replacement. S+ recommend at least 250 to estimate standard errors and 1000 to estimate percentiles.
2. From each bootstrap sample calculate the parameter estimates, $\hat{\theta}_{1}, \hat{\theta}_{2}, \ldots, \hat{\theta}_{B}$, called bootstrap replication
3. Evaluate the standard error by the sample standard deviation of the B replications as in (1).

In S+ we use the function bootstrap for the calculation. For the example we used $\mathrm{B}=100$.

```
> x_c(23, 34, 12, 9, 42, 17, 8, 29)
> bōot1_bootstrap(x,1/mean(x),B=100)
Forming replications 1 to 100
> summary(boot1)
Call:
bootstrap(data = x, statistic = 1/mean(x), B = 100)
Number of Replications: 100
Summary Statistics:
            Observed Bias Mean SE
Param 0.04598 0.0007052 0.04668 0.008573
Empirical Percentiles:
            2.5% 5% 95% 97.5%
Param 0.03455 0.03568 0.0646 0.06787
BCa Confidence Limits:
    2.5% 5% 95% 97.5%
Param 0.03463 0.03625 0.06615 0.06878
```

The estimated parameter is 0.04598 with the bootstrap standard error of 0.008573 . The empirical percentiles from 100 bootstrap estimates are given. A better confidence interval, named BCa (biascorrected and accelerated), is given. The BCa CI is better in terms of accuracy of the interval estimates and accurate coverage probability. Other possible CIs are bootstrap-t interval, ABC interval, and parametric approach via normal theory. For more detailed discussion on the bootstrap CI, consult An Introduction to the Bootstrap, by E. Efron and R. Tibshirani.

We will close this section with an interesting example. Note that the following example is just to give you the basic idea of the use of bootstrap. This is not a complete analysis and should not refer to other purpose.

## Example: Bootstrap Bioequivalence

A drug company has separately applied each of three hormone supplement medicinal patches, 'Approved (by FDA)', 'Placebo', and 'New', to eight patients who suffer from a hormone deficiency. Measurements
are blood pressure level after each patch wearing. The FDA requires proof of bioequivalence before it will approve for sale a previously approved product manufactured at a new facility. Data is give below;

| patient | placebo | approved | new |
| :--- | :--- | :--- | :--- |
| 1 | 9243 | 17649 | 16449 |
| 2 | 9671 | 12013 | 14614 |
| 3 | 11792 | 19979 | 17274 |
| 4 | 13357 | 21816 | 23798 |
| 5 | 9055 | 13850 | 12560 |
| 6 | 6290 | 9806 | 10157 |
| 7 | 12412 | 17208 | 16570 |
| 8 | 18806 | 29044 | 26325 |

Let $\mathrm{x}=$ approved - placebo, $\mathrm{y}=$ new-approved. Define $\gamma=\nu / \mu$, where $\mu=E(x)$ and $\nu=E(Y)$. The FDA bioequivalence requirement is that a $90 \% \mathrm{CI}$ for $\gamma$ lie within $[-0.2,0.2]$. Here the parameter estimate for $r$ is -0.0713 .

```
>mean(y)/mean(x)
```

[1] -0.0713061
Following plot shows the data. The wedge in the plot indicates the FDA requirement region and we see that four of them are outside of the region.

```
> plot(x,y,xlab="New-Approved",ylab="Approved-Placebo")
> plot(x,y,xlab="New-Approved",ylab="Approved-Placebo",xlim=c(0,12000),ylim=c(-6000,6000))
> xx_seq(0,12000,100)
> yy_0.2*xx
> lines(xx,yy,type="l")
> lines(xx,-yy,type="1")
> abline(h=0)
```



Are the FDA bioequivalence criteria satisfied by the data? To answer this question we use the bootstrap CIs.
> bot_bootstrap(data,mean(data[,"y"])/mean(data[,"x"]), 2000)
$>$ summary(bot)

Call:
bootstrap $($ data $=$ data, statistic $=\operatorname{mean}(\operatorname{data}[, " y "]) / \operatorname{mean}(\operatorname{data}[, " x "]), B=2000)$
Number of Replications: 2000
Summary Statistics:
Observed Bias Mean SE
Param -0.07131 0.008381-0.06292 0.1037

Empirical Percentiles:
$2.5 \% \quad 5 \% \quad 95 \% ~ 97.5 \%$
Param -0.2321-0.2135 0.1245 0.1709
BCa Confidence Limits:
2.5\% 5\% 95\% 97.5\%

Param -0.2257-0.2046 0.1382 0.1906

The estimated parameter is -0.07131 with a bootstrap standard error of 0.1037 . Neither of the lower bounds of the CIs do not quite satisfy the FDA criteria.

Then, the next question would be how many patients should be measured in a future experiments so that the FDA requirement will have a good chance of being satisfied. This question related to power or sample size question and we will not discuss in this class.

Following is the histogram of the 2000 bootstrap estimates.
$>\operatorname{plot}(\mathrm{bot})$


Next time we will discuss the use of bootstrap in regression analysis.

## BOOTSTRAP REGEESION

Bootstrap regression is very useful when the regression function is non-linear in the parameters. In this section we will discuss how the bootstrap regression works in a simple regression model.

There are two different ways of bootstrap regression

1. Bootstrapping pairs: Random sample pairs ( $\mathrm{x}, \mathrm{y}$ ) with replacement. For each bootstrap sample, we fit regression model and the based on the B estimates we make inferences.
2. Bootstrapping residuals: We replace the response using the fitted and resampled residuals. That is, we create a new data set by

$$
y_{i}^{*}=b_{0}+b_{1} x_{i}+e_{i}^{*}
$$

where $e_{i}^{*}$ are resampled with replacement from the residuals $e_{i}$.

## Example

Hormone data: $n=27$
Response: amount (amount of milligrams of anti-inflammatory hormone remaining in 27 devices) Predictor: hour (Number of hours of wear)
Group : lot ( 3 different manufacturing lots)
\# Regression model fit

```
> fit.lm_lm(amount~hour,data=hormone)
> summary(fit.lm)
Call: lm(formula = amount ~ hour, data = hormone)
Residuals:
    Min 1Q Median 3Q Max
    -4.936 -1.728 -0.02287 1.739 3.732
Coefficients:
            Value Std. Error t value Pr(>|t|)
(Intercept) 34.1675 0.8672 39.3999 0.0000
            hour -0.0574 0.0045 -12.8683 0.0000
Residual standard error: 2.378 on 25 degrees of freedom
Multiple R-Squared: 0.8688
F-statistic: 165.6 on 1 and 25 degrees of freedom, the p-value is 1.584e
-012
Correlation of Coefficients:
            (Intercept)
hour -0.8494
#Bootstrap regression by bootstrapping paris
> hor.boot_bootstrap(hormone,coef(eval(lm.fit$call)),B=200)
Forming rep}lications 1 to 100
Forming replications 101 to 200
> hor.boot
Call:
bootstrap(data = hormone, statistic = coef(eval(lm.fit$call)), B = 200)
Number of Replications: 200
Summary Statistics:
    Observed Bias Mean SE
```

```
(Intercept) 34.16753 0.0057033 34.17323 0.770618
    hour -0.05745 -0.0003323 -0.05778 0.004131
```

> plot (hor.boot)
(Intercept)



```
# Bootstrap regression by bootstrapping residuals
> library(boot)
> hormone2 data.frame(hormone,resid=resid(lm.fit),fitted=fitted(lm.fit))
> hormone.\overline{fun function(data,i) {}
+ d_data
+ d$amount d$fitted+d$resid[i]
+ coef(updāte(fit.lm,data=d))
+ }
> hor.lm.boot_boot(hormone2,hormone.fun,R=200)
> hor.lm
Problem: Object "hor.lm" not found
Use traceback() to see the call stack
> hor.lm.boot
ORDINARY NONPARAMETRIC BOOTSTRAP
```

Call:
boot (data $=$ hormone2, statistic $=$ hormone.fun, $R=200$ )
Bootstrap Statistics :

```
        original bias std. error
t1* 34.1675282 0.0414358271 0.782883776
t2* -0.0574463 -0.0002944581 0.004160554
> plot(hor.lm.boot)
```



COMPARING TWO SAMPLE: BOOTSTRAP CI for the mean difference
We use our grade.data to compare the means of MT.I and MT.II.

```
> attach(grade.data)
> t.test(MT.I-MT.II)
    One-sample t-Test
data: MT.I - MT.II
t = 1.3713, df = 27, p-value = 0.1816
alternative hypothesis: true mean is not equal to 0
95 percent confidence interval:
    -1.789946 9.004232
sample estimates:
    mean of }
    3.607143
> grade.boot_boot(MT.I-MT.II,function(x,i) mean(x[i]), R=200)
> boot.ci(grade.boot,type=c("norm","basic","perc","bca"))
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 200 bootstrap replicates
CALL :
```

```
boot.ci(boot.out = grade.boot, type = c("norm", "basic", "perc", "bca")
Intervals :
Level Normal Basic
95% (-1.609, 8.347 ) ( -2.061, 8.436)
Level Percentile BCa
95% ( -1.222, 9.275 ) ( -1.641, 8.870 )
Calculations and Intervals on Original Scale
Some basic intervals may be unstable
Some percentile intervals may be unstable
Some BCa intervals may be unstable
> plot(grade.boot)
```



Another possible CI is the studentized CI which based on the studentized statistics. This CI is known as the most reliable. To calculate the studentized CI we need a variance estimate of the parameter estimate from each bootstrap sample.

```
> mean.fun_function(d,i){n_length(i);c(mean(d[i]),(n-1)*var(d[i])/n^2) }
> grade.boot.stud_boot(MT.I-MT.II,mean.fun,R=200)
> boot.ci(grade.boot.stud,type="stud")
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 200 bootstrap replicates
CALL :
boot.ci(boot.out = grade.boot.stud, type = "stud")
Intervals :
Level Studentized
95% (-2.157, 8.808 )
Calculations and Intervals on Original Scale
Some studentized intervals may be unstable
> plot(grade.boot.stud)
```



## Comparing medians

```
> grade.boot_boot(MT.I-MT.II,function(x,i) median(x[i]), R=200)
> boot.ci(grade.boot,type=c("norm","basic","perc","bca"))
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 200 bootstrap replicates
CALL :
boot.ci(boot.out = grade.boot, type = c("norm", "basic", "perc", "bca")
    )
Intervals :
Level Normal Basic
95% (-3.606, 7.966) (-3.000, 8.000)
Level Percentile BCa
95% ( -3.00, 8.00 ) ( -4.50, 6.38 )
Calculations and Intervals on Original Scale
Some basic intervals may be unstable
Some percentile intervals may be unstable
Some BCa intervals may be unstable
> truehist(grade.boot$t,h=1)
```



The Studentized CI can be obtained as follows;

```
> median.fun_function(d,i){n_length(i);c(median(d[i]),(n-1)*var(d[i])/n^2)}
> grade.boot.stud_boot(MT.I-\overline{MT.II,median.fun, R=200)}
> boot.ci(grade.boot.stud,type="stud")
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 200 bootstrap replicates
CALL :
boot.ci(boot.out = grade.boot.stud, type = "stud")
Intervals :
Level Studentized
95% ( -1.785, 8.520 )
Calculations and Intervals on Original Scale
Some studentized intervals may be unstable
> truehist(grade.boot.stud$t,h=1)
```



## SMOOTH REGRESSION (Brief note)

Data: Random sample of size 100 to predict Life Span by the length of one's lifeline (left hand). Source: Newrick et.al. (1990) Journal of the Royal Society of Medicine and Modern Regression Methods, T.P. Ryan, Wiley Interscience.

## Kernel Regression

```
> plot(lifeline,lifespan,pch=16)
> lines(ksmooth(lifeline,lifespan,kernel="normal",bandwidth=10),lty=3)
> lines(ksmooth(lifeline,lifespan,kernel="normal",bandwidth=3),lty=4)
> legend(65,65,c("kernel bw=10","kernel bw=3"),lty=c(3,4))
```

The larger the bandwidth, the smoother the fit. For the more option of the kernel functions, refer the S+ help note.


```
> yhat approx(kernel.fit,xout=lifeline)$y
> resid <- lifespan-yhat
> plot(yhat,resid)
> lines(lowess(yhat,resid))
```



Locally weighted regression (Cleveland 1979)

```
> plot(lifeline,lifespan,pch=16)
> abline(lm(lifespan~lifeline))
> lines(lowess(lifeline,lifespan),lty=3)
> lines(lowess(lifeline,lifespan,0.1),lty=4)
> legend(60,65,c("simple regression","lowess f=default (.67)","lowess
f=0.1"),lty=c(1, 3,4))
```



Using interface,
Statistics $\rightarrow$ Smoothing $\rightarrow$ Loess $\rightarrow$ specify the data, x, and y $\rightarrow$ change the options for symbols and lines as you wish $\rightarrow$ Smooth/Sort option $\rightarrow$ Span: type in the smoothing parameter f (default is 0.75 ). The larger the value, the smoother the fit $\rightarrow$ Degree: 1 for linear 2 for quadratic fit $\rightarrow$ Family: Gauss for default, Symmetric for robust fitting

```
> yhat_approx(Lowess.fit,xout=lifeline)$y
> resi\overline{d}<- lifespan-yhat
> plot(yhat,resid)
> lines(lowess(yhat,resid))
```



Using the Interface: Statistics $\rightarrow$ Regression $\rightarrow$ Local (loess) $\rightarrow$ etc

## Natural Spline

```
> plot(lifeline,lifespan,pch=16)
> lines(lifeline, fitted(lm(lifespan~ns(lifeline,df=20))),lty=3)
> lines(lifeline, fitted(lm(lifespan~ns(lifeline,df=5))),lty=4)
> legend(65,65,c("Natural Spline df=20","Natural Spline df=5"),lty=c(3,4))
```



